Ternary and quaternary Lennard-Jones clusters: the effects of atomic sizes on the compositions, geometries and relative stability

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Supplementary data

Table S1. The potential energies of the global minima (E_N/ε) of the ternary Lennard-Jones clusters, the number of initial geometries (N_{ini}), the number of times that the global minimum was obtained (N_{hit}), the average number of local optimizations in the run (N_{ls}), and the numbers of the A, B, and C atoms (N_A, N_B, N_C) in the clusters. For the clusters with N = 5, the atom-type conversion operator yielded the putative global minimum many times and thus the interior and surface operators were not applied to them. For the clusters with N = 6 – 7, the maximum numbers of atoms moved by the interior and surface operators were set at N – 3 and N – 4, respectively.

Table S2. The potential energies of the global minima (E_N/ε) of the quaternary Lennard-Jones clusters, the number of initial geometries (N_{ini}), the number of times that the global minimum was obtained (N_{hit}), the average number of local optimizations in the run (N_{ls}), and the numbers of the A, B, C, and D atoms (N_A, N_B, N_C, N_D) in the clusters. For the clusters with N = 5, the atom-type conversion operator yielded the putative global minimum many times and thus the interior and surface operators were not applied to them. For the clusters with N = 6 – 7, the maximum numbers of atoms moved by the interior and surface operators were set at N – 3 and N – 4, respectively.

Table S3. The global-minimum geometries of the ternary Lennard-Jones clusters.

Table S4. The global-minimum geometries of the quaternary Lennard-Jones clusters.

Table S1. The potential energies of the global minima (E_N/ε) of the ternary Lennard-Jones clusters, the number of initial geometries (N_{ini}), the number of times that the global minimum was obtained (N_{hit}), the average number of local optimizations in the run (N_{ls}), and the numbers of the A, B, and C atoms (N_A, N_B, N_C) in the clusters.

	S_C = 1.1							S_C = 1.2						
N	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C
5	-9.119302	999	1000	21.0	3	0	2	-9.135241	999	1000	21.0	3	0	2
6	-12.715734	806	1000	54.1	2	0	4	-12.727718	821	1000	53.1	2	0	4
7	-16.557098	865	1000	53.5	3	0	4	-16.565375	113	1000	77.7	5	0	2
8	-19.948687	256	1000	72.7	2	0	6	-20.233378	879	1000	79.5	2	0	6
9	-24.300649	636	1000	83.5	4	0	5	-24.442494	414	1000	88.1	2	0	7
10	-28.771585	186	1000	87.7	1	0	9	-28.968925	812	1000	117.0	2	1	7
11	-33.371304	977	1000	110.4	1	0	10	-33.966602	1000	1000	102.0	2	0	9
12	-38.954245	990	1000	98.8	1	0	11	-39.067162	550	1000	121.4	4	1	7
13	-45.543272	1000	1000	100.3	1	0	12	-45.595012	760	1000	133.3	2	5	6
14	-49.049898	323	1000	102.3	1	2	11	-49.338750	956	1000	125.9	4	2	8
15	-53.606128	999	1000	147.0	2	2	11	-54.064278	969	1000	156.6	5	0	10
16	-58.279990	476	1000	130.5	4	0	12	-58.855874	989	1000	186.5	6	0	10
17	-63.059172	292	1000	142.0	4	0	13	-63.726293	16	1000	211.3	3	1	13
18	-68.792764	958	1000	189.9	2	0	16	-69.601233	951	1000	228.6	7	0	11
19	-75.433396	987	1000	184.0	2	0	17	-76.235787	124	1000	198.1	7	0	12
20	-80.143826	999	1000	187.5	4	0	16	-81.092028	612	1000	239.8	5	4	11
21	-85.005952	984	1000	219.1	3	2	16	-86.020468	64	1000	207.8	7	2	12
22	-90.741441	1000	1000	199.0	3	2	17	-91.918291	127	1000	221.7	7	2	13
23	-97.490709	1000	1000	210.8	3	2	18	-98.733192	125	1000	227.2	5	6	12
24	-102.264046	1000	1000	222.6	4	1	19	-103.715032	308	1000	233.0	5	6	13
25	-108.045220	1000	1000	223.8	4	0	21	-109.690856	239	1000	250.6	5	6	14
26	-114.892839	1000	1000	218.1	4	0	22	-116.671227	562	1000	233.9	5	6	15
27	-119.543605	997	1000	216.4	5	0	22	-121.665371	645	1000	243.8	5	6	16
28	-125.296607	1000	1000	219.0	5	0	23	-127.653748	814	1000	262.0	5	6	17
29	-132.108090	1000	1000	228.1	5	0	24	-134.647054	825	1000	257.7	5	6	18
30	-136.773271	854	1000	271.5	5	2	23	-139.619624	630	1000	289.8	6	7	17
31	-142.440277	997	1000	298.7	6	1	24	-145.630414	810	1000	286.7	6	6	19
32	-149.212031	989	1000	251.6	6	0	26	-152.637091	831	1000	302.7	6	7	19
33	-154.633546	868	1000	273.4	7	0	26	-158.568530	847	1000	345.5	7	5	21
34	-161.360048	433	1000	257.9	7	0	27	-165.595214	998	1000	359.8	7	5	22
35	-166.185706	304	1000	283.6	7	0	28	-170.625245	167	1000	340.7	7	7	21
36	-171.524014	392	1000	283.5	8	0	28	-176.661687	974	1000	335.7	8	4	24
37	-178.167061	876	1000	309.5	8	0	29	-183.593664	903	1000	346.9	8	4	25
38	-183.371989	208	1000	322.1	9	0	29	-189.594078	905	1000	354.6	9	4	25
39	-189.903875	670	1000	362.0	9	0	30	-196.583321	983	1000	371.8	9	4	26
40	-195.069803	581	1000	400.1	9	1	30	-203.169138	155	1000	335.9	13	0	27
41	-201.346753	182	1000	388.8	10	0	31	-210.149549	392	1000	363.9	13	0	28
42	-207.024045	560	1000	415.1	10	0	32	-217.116931	757	1000	410.6	13	0	29
43	-213.011525	424	1000	421.6	11	0	32	-224.072028	788	1000	396.7	13	0	30
44	-218.627890	225	1000	453.9	12	1	31	-231.099052	738	1000	403.4	13	0	31
45	-224.652192	68	1000	457.3	13	0	32	-238.202225	873	1000	456.5	13	0	32
46	-229.387288	34	1000	473.3	12	0	34	-242.531934	693	1000	480.5	13	0	33
47	-234.934267	15	1000	474.3	12	0	35	-248.218022	789	1000	482.2	14	0	33
48	-240.864301	67	1000	494.2	12	1	35	-255.212873	775	1000	510.9	14	0	34
49	-247.645882	149	1000	496.4	12	1	36	-260.339254	775	1000	529.3	15	0	34
50	-254.482500	183	1000	509.6	12	1	37	-267.329407	497	1000	515.6	15	0	35

Table S1 (continued)

	S_C = 1.3							S_C = 1.4						
N	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C
5	-9.151532	999	1000	21.0	3	0	2	-9.168058	999	1000	21.0	3	0	2
6	-12.751325	829	1000	50.9	2	0	4	-12.797426	1000	1000	39.5	2	0	4
7	-16.578938	438	1000	70.0	3	1	3	-16.590292	534	1000	72.4	3	1	3
8	-20.400814	979	1000	75.1	2	0	6	-20.491743	542	1000	72.4	3	0	5
9	-24.646775	913	1000	94.7	2	1	6	-25.532740	797	1000	86.4	1	0	8
10	-29.896713	938	1000	113.3	1	0	9	-30.595637	978	1000	84.0	2	0	8
11	-34.749685	1000	1000	93.6	3	0	8	-35.274878	774	1000	82.8	3	0	8
12	-39.203335	450	1000	115.5	4	0	8	-39.688603	664	1000	101.5	5	0	7
13	-45.620242	670	1000	129.3	5	4	4	-45.626548	580	1000	132.7	7	3	3
14	-49.451546	170	1000	139.0	4	6	4	-49.554107	386	1000	144.6	7	3	4
15	-54.248982	120	1000	151.7	5	3	7	-54.477032	86	1000	143.7	5	0	10
16	-59.470682	68	1000	154.7	4	0	12	-60.382227	238	1000	145.9	4	0	12
17	-64.831372	54	1000	168.8	3	5	9	-65.332397	21	5000	187.1	7	0	10
18	-70.151377	358	1000	188.5	7	0	11	-70.757536	48	1000	195.3	5	0	13
19	-76.859376	699	1000	203.3	7	0	12	-77.314533	200	1000	186.4	7	0	12
20	-81.847352	682	1000	205.7	8	1	11	-82.495693	146	1000	201.0	9	0	11
21	-86.806107	410	1000	237.5	8	0	13	-88.055752	456	1000	212.4	5	1	15
22	-92.815928	658	1000	236.9	9	2	11	-93.611361	175	1000	216.6	10	1	11
23	-99.738709	581	1000	235.7	9	2	12	-100.740941	133	1000	231.4	11	0	12
24	-104.737335	326	1000	236.2	9	3	12	-106.012643	30	1000	236.8	11	0	13
25	-110.727192	132	1000	267.9	10	2	13	-111.736937	64	1000	255.9	12	2	11
26	-117.787805	548	1000	272.6	10	4	12	-118.914648	112	1000	255.1	14	0	12
27	-122.790987	432	1000	310.4	10	3	14	-124.164812	338	1000	269.9	10	4	13
28	-128.704872	414	1000	321.9	10	5	13	-129.926891	138	1000	304.7	14	1	13
29	-135.666872	192	1000	287.4	10	7	12	-136.904799	154	1000	331.1	11	6	12
30	-140.749116	78	1000	296.3	10	6	14	-142.222695	177	1000	327.6	11	6	13
31	-146.716717	213	1000	334.9	10	7	14	-148.299963	206	1000	329.5	11	6	14
32	-153.689832	122	1000	311.3	9	9	14	-154.998180	170	1000	363.3	13	5	14
33	-159.852426	274	1000	330.2	10	8	15	-161.247490	111	1000	377.2	12	8	13
34	-167.004069	430	1000	317.0	9	10	15	-168.561841	251	1000	384.0	12	10	12
35	-172.171999	241	1000	350.9	10	9	16	-173.830523	260	1000	396.8	12	10	13
36	-178.095471	32	1000	358.2	10	9	17	-180.176688	20	5000	407.8	13	0	23
37	-185.149212	96	1000	369.7	11	9	17	-186.681359	37	5000	430.0	12	1	24
38	-191.367987	31	1000	394.1	12	8	18	-193.649484	23	5000	451.0	13	0	25
39	-198.598200	490	1000	387.0	9	12	18	-200.345070	34	5000	452.5	12	1	26
40	-205.265704	23	1000	409.4	13	6	21	-207.322597	33	5000	492.1	13	0	27
41	-212.399942	27	1000	428.9	13	7	21	-213.953616	331	1000	503.4	13	16	12
42	-219.510509	331	1000	474.0	13	6	23	-221.041456	55	1000	531.5	14	15	13
43	-226.660589	344	1000	460.9	13	6	24	-228.228786	132	1000	523.4	13	16	14
44	-233.881468	400	1000	512.9	13	6	25	-235.607582	719	1000	523.1	13	18	13
45	-241.118334	707	1000	515.3	13	5	27	-243.153322	879	1000	536.4	13	20	12
46	-246.140507	321	1000	498.0	13	5	28	-248.152248	806	1000	582.8	13	20	13
47	-252.089942	829	1000	535.1	14	5	28	-253.919902	635	1000	626.2	13	20	14
48	-259.193028	802	1000	535.0	14	5	29	-260.843948	712	1000	614.9	14	19	15
49	-264.959341	373	1000	566.4	15	6	28	-266.474802	182	1000	636.2	14	19	16
50	-272.160352	83	1000	558.0	15	6	29	-273.590250	374	1000	642.2	15	18	17

Table S1 (continued)

	S_C = 1.5							S_C = 1.6						
N	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C
5	-9.184718	999	1000	21.0	3	0	2	-9.201428	999	1000	21.0	3	0	2
6	-12.968869	1000	1000	39.7	2	0	4	-13.138655	1000	1000	39.8	2	0	4
7	-16.609636	238	1000	62.3	3	0	4	-16.634759	175	1000	47.2	3	0	4
8	-20.714043	624	1000	67.8	2	0	6	-20.902561	926	1000	71.3	2	0	6
9	-25.991730	943	1000	80.4	1	0	8	-26.148194	323	1000	68.1	3	0	6
10	-30.932271	1000	1000	90.4	3	1	6	-31.451692	1000	1000	83.9	4	0	6
11	-35.492339	625	1000	87.9	2	2	7	-35.754363	623	1000	106.5	2	4	5
12	-40.000211	551	1000	107.1	5	0	7	-40.300987	188	1000	126.2	4	1	7
13	-45.658104	460	1000	120.2	7	5	1	-45.640754	194	1000	119.1	7	5	1
14	-50.489724	463	1000	150.8	4	0	10	-51.095901	116	1000	139.8	6	0	8
15	-55.390724	137	1000	138.4	5	0	10	-56.181783	294	1000	143.1	4	0	11
16	-60.940375	285	1000	162.6	5	2	9	-61.799365	230	1000	152.5	5	0	11
17	-66.634088	344	1000	179.2	3	3	11	-67.488171	286	1000	184.2	3	3	11
18	-71.741405	265	1000	190.9	5	1	12	-73.165711	226	1000	188.0	6	0	12
19	-78.191386	96	1000	194.3	7	0	12	-79.045725	79	1000	188.2	5	0	14
20	-83.514565	79	1000	198.7	7	0	13	-84.683290	21	1000	202.9	6	0	14
21	-89.330178	117	1000	216.3	7	0	14	-90.592181	21	1000	213.4	7	2	12
22	-95.143253	26	1000	227.6	7	0	15	-96.825772	62	1000	215.2	6	4	12
23	-101.901346	28	1000	238.4	11	0	12	-103.276147	14	1000	222.5	11	0	12
24	-107.209036	253	1000	248.8	8	3	13	-108.932853	52	5000	234.5	11	0	13
25	-113.169927	118	1000	251.3	10	2	13	-115.066104	84	1000	245.8	10	2	13
26	-120.425633	55	1000	268.3	14	0	12	-122.006208	24	1000	264.1	14	0	12
27	-125.697620	54	1000	278.2	14	0	13	-127.430425	25	1000	273.1	14	0	13
28	-131.301741	52	1000	297.1	14	0	14	-133.150523	36	1000	280.6	14	1	13
29	-138.240894	86	1000	311.1	15	2	12	-139.776145	13	1000	291.4	16	1	12
30	-143.726427	67	1000	319.2	14	3	13	-145.483456	17	1000	309.3	14	2	14
31	-149.961720	66	1000	332.0	13	4	14	-152.530780	20	5000	319.7	13	0	18
32	-156.357354	13	5000	351.3	14	4	14	-158.700621	24	5000	338.0	13	0	19
33	-162.524534	51	5000	364.6	16	4	13	-165.783355	15	5000	354.0	13	0	20
34	-169.680088	23	5000	377.9	17	5	12	-171.512160	21	5000	366.2	19	3	12
35	-175.449420	3	15000	394.5	12	1	22	-177.660242	13	5000	383.4	13	0	22
36	-182.632268	10	5000	410.1	13	0	23	-184.203078	14	1000	398.3	15	6	15
37	-188.771096	11	15000	435.8	12	3	22	-190.836246	4	15000	415.7	17	2	18
38	-195.963276	16	5000	456.6	13	0	25	-197.652143	14	1000	431.0	18	4	16
39	-202.761172	223	1000	484.2	13	12	14	-204.510557	8	5000	450.3	17	2	20
40	-209.561505	271	1000	496.2	13	14	13	-211.271861	12	5000	467.3	17	3	20
41	-215.757815	138	1000	516.6	13	16	12	-217.502470	45	5000	483.6	15	12	14
42	-221.966034	9	15000	524.4	20	7	15	-224.031675	13	5000	491.8	17	8	17
43	-229.311691	10	5000	534.9	17	12	14	-230.912134	5	5000	507.5	21	8	14
44	-236.595757	137	1000	546.8	16	15	13	-237.799468	8	5000	522.2	19	12	13
45	-244.497736	10	5000	556.2	13	20	12	-244.859918	17	5000	538.7	18	15	12
46	-249.583005	187	1000	591.6	15	18	13	-251.048217	9	5000	553.8	22	0	24
47	-255.444596	134	1000	602.6	15	18	14	-258.543192	3	15000	566.4	20	6	21
48	-262.390731	14	5000	618.5	13	20	15	-264.768267	20	5000	584.6	22	0	26
49	-268.179401	20	5000	633.2	13	20	16	-270.956019	17	5000	601.7	22	0	27
50	-275.148772	22	5000	653.5	15	21	14	-278.361820	4	5000	617.4	24	0	26

Table S2. The potential energies of the global minima (E_N/ε) of the quaternary Lennard-Jones clusters, the number of initial geometries (N_{ini}), the number of times that the global minimum was obtained (N_{hit}), the average number of local optimizations in the run (N_{ls}), and the numbers of the A, B, C, and D atoms (N_A, N_B, N_C, N_D) in the clusters.

	S_D = 1.15								S_D = 1.3							
N	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C	N_D	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C	N_D
5	-9.127219	999	1000	31.0	3	0	0	2	-9.151532	999	1000	31.0	3	0	0	2
6	-12.720554	805	1000	68.5	2	0	0	4	-12.751325	859	1000	65.1	2	0	0	4
7	-16.562111	341	1000	90.0	4	0	0	3	-16.576938	473	1000	94.3	3	0	1	3
8	-20.102320	595	1000	108.0	2	0	0	6	-20.400814	988	1000	97.7	2	0	0	6
9	-24.364017	158	1000	115.5	5	0	0	4	-24.647772	913	1000	136.1	2	1	0	6
10	-28.863193	693	1000	155.5	1	1	0	8	-29.896713	999	1000	160.3	1	0	0	9
11	-33.571031	83	1000	139.5	1	0	0	10	-34.749685	1000	1000	125.1	3	0	0	8
12	-39.019558	666	1000	165.7	2	0	2	8	-39.203335	315	1000	164.5	4	0	0	8
13	-45.596007	1000	1000	185.4	1	0	6	6	-45.632956	521	1000	216.4	4	4	2	3
14	-49.252081	1000	1000	167.6	4	0	0	10	-49.455205	264	1000	209.9	5	2	2	5
15	-53.878902	996	1000	226.9	4	1	0	10	-54.253944	601	1000	252.3	5	2	2	6
16	-58.595339	997	1000	277.3	4	2	0	10	-59.470682	64	1000	232.4	4	0	0	12
17	-63.395255	108	1000	321.1	5	0	3	9	-64.857005	83	1000	253.2	2	6	0	9
18	-69.174605	273	1000	321.0	2	5	0	11	-70.151377	523	1000	281.9	7	0	0	11
19	-75.814195	28	1000	302.7	2	5	0	12	-76.859376	611	1000	298.9	7	0	0	12
20	-80.662264	135	1000	293.9	4	0	4	12	-81.867655	685	1000	327.1	7	2	0	11
21	-85.610194	677	1000	298.1	3	2	2	14	-86.839591	15	1000	326.2	7	4	0	10
22	-91.431774	177	1000	305.1	3	2	2	15	-92.809846	692	1000	367.2	9	0	2	11
23	-98.240730	516	1000	328.0	3	2	2	16	-99.737798	410	1000	361.3	9	2	0	12
24	-103.189478	683	1000	387.0	4	0	4	16	-104.746825	81	1000	376.7	9	0	3	12
25	-109.146936	735	1000	338.7	4	0	4	17	-110.733850	252	1000	410.4	10	2	0	13
26	-116.107925	1000	1000	351.4	4	0	4	18	-117.802258	671	1000	425.3	7	6	1	12
27	-120.925098	314	1000	419.2	5	0	4	18	-122.817316	100	1000	444.2	9	4	1	13
28	-126.863835	1000	1000	485.3	5	0	5	18	-128.776803	78	1000	474.8	7	7	1	13
29	-133.793912	1000	1000	463.3	5	0	6	18	-135.798297	263	1000	470.9	7	8	2	12
30	-138.716374	928	1000	412.7	5	2	2	21	-140.841900	173	1000	502.7	7	7	3	13
31	-144.568775	368	1000	385.0	6	1	0	24	-146.812565	28	1000	529.5	7	9	1	14
32	-151.480019	1000	1000	445.6	6	1	0	25	-153.814189	12	1000	502.3	7	10	2	13
33	-157.272375	960	1000	427.3	7	0	0	26	-160.033096	253	1000	543.8	7	9	3	14
34	-164.222021	997	1000	477.3	7	0	0	27	-167.246186	469	1000	521.3	7	10	3	14
35	-169.166124	231	1000	448.1	7	0	3	25	-172.327478	207	1000	590.6	7	10	3	15
36	-174.906348	978	1000	443.2	8	0	2	26	-178.304300	218	1000	625.5	7	10	3	16
37	-181.754627	989	1000	482.0	8	0	2	27	-185.308869	76	1000	617.7	8	8	5	16
38	-187.367687	844	1000	462.9	9	0	0	29	-191.534314	42	1000	630.0	12	1	8	17
39	-194.229977	974	1000	508.1	9	0	0	30	-198.672258	509	1000	633.9	9	6	6	18
40	-199.703534	337	1000	545.5	10	0	0	30	-205.423603	14	1000	697.4	13	0	10	17
41	-206.479560	261	1000	538.2	10	0	0	31	-212.614534	126	1000	651.8	13	0	10	18
42	-212.864370	683	1000	630.1	13	0	0	29	-219.757516	152	1000	677.7	13	0	11	18
43	-219.440909	558	1000	611.0	13	0	0	30	-226.908091	101	1000	699.3	13	0	11	19
44	-226.066862	563	1000	588.2	13	0	0	31	-234.120506	50	1000	766.3	13	0	12	19
45	-232.763363	411	1000	649.0	13	0	0	32	-241.418555	202	1000	792.1	13	0	10	22
46	-237.126607	181	1000	681.5	13	0	0	33	-246.331165	48	1000	792.1	13	2	6	25
47	-242.723641	335	1000	729.2	14	0	0	33	-252.336165	237	1000	836.0	13	1	8	25
48	-249.375588	272	1000	759.3	14	0	0	34	-259.353775	254	1000	824.4	13	1	8	26
49	-254.328385	258	1000	807.1	15	0	0	34	-265.183204	673	1000	842.6	14	1	6	28
50	-260.903328	75	1000	812.8	15	0	0	35	-272.279534	843	1000	901.4	15	0	8	27

Table S2 (continued)

	S_D = 1.45								S_D = 1.6							
N	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C	N_D	E_N/ε	N_{hit}	N_{ini}	N_{ls}	N_A	N_B	N_C	N_D
5	-9.176377	999	1000	31.0	3	0	0	2	-9.201428	1000	1000	31.0	3	0	0	2
6	-12.873253	1000	1000	51.5	2	0	0	4	-13.138655	1000	1000	51.7	2	0	0	4
7	-16.602938	261	1000	93.9	3	0	1	3	-16.634759	245	1000	70.2	3	0	0	4
8	-20.589075	493	1000	90.5	2	0	0	6	-20.902561	960	1000	95.9	2	0	0	6
9	-25.812862	834	1000	107.1	1	0	0	8	-26.148194	411	1000	93.2	3	0	0	6
10	-30.786233	1000	1000	105.9	2	0	0	8	-31.451692	995	1000	113.4	4	0	0	6
11	-35.418435	927	1000	131.6	3	0	0	8	-35.739540	550	1000	150.0	2	2	2	5
12	-39.851273	439	1000	145.0	5	0	0	7	-40.313289	236	1000	175.3	4	0	1	7
13	-45.637971	62	1000	189.7	7	0	5	1	-45.639330	151	1000	179.0	1	6	0	6
14	-50.007538	214	1000	205.0	4	0	0	10	-51.095901	21	1000	199.7	6	0	0	8
15	-54.966921	71	1000	215.2	5	0	0	10	-56.181783	248	1000	209.7	4	0	0	11
16	-60.661713	149	1000	250.1	4	2	0	10	-61.799365	144	1000	241.2	5	0	0	11
17	-66.003247	155	1000	259.2	3	0	1	13	-67.602491	175	1000	264.6	3	3	0	11
18	-71.378149	616	1000	289.6	3	1	0	14	-73.165711	96	1000	288.0	6	0	0	12
19	-77.602571	82	1000	284.6	7	0	0	12	-79.045725	37	1000	283.1	5	0	0	14
20	-82.984456	72	1000	287.7	7	0	0	13	-84.872674	283	1000	307.0	3	4	0	13
21	-88.668709	270	1000	314.4	4	1	0	16	-90.636387	60	1000	308.5	7	2	0	12
22	-94.367275	62	1000	341.4	4	1	0	17	-96.860677	32	1000	319.8	6	4	0	12
23	-101.304781	72	1000	359.8	11	0	0	12	-103.276147	28	1000	337.2	11	0	0	12
24	-106.544565	37	1000	390.0	11	0	0	13	-109.119972	104	1000	365.4	8	3	0	13
25	-112.329084	116	1000	407.2	9	3	0	13	-115.179710	48	1000	401.2	10	2	0	13
26	-119.675798	57	1000	422.2	13	1	0	12	-122.006208	117	1000	425.1	14	0	0	12
27	-124.999460	48	1000	458.3	13	1	0	13	-127.430425	14	1000	435.1	14	0	0	13
28	-130.661554	66	1000	465.9	14	1	0	13	-133.265243	41	1000	449.0	13	2	0	13
29	-137.744649	55	1000	479.1	13	4	0	12	-140.051257	36	1000	465.9	14	3	0	12
30	-143.100786	43	1000	505.4	12	4	1	13	-145.639380	20	1000	484.7	14	3	0	13
31	-149.249774	14	1000	525.6	13	4	0	14	-152.530780	5	5000	509.0	13	0	0	18
32	-155.819429	19	1000	542.0	13	5	2	12	-158.700621	10	5000	546.1	13	0	0	19
33	-161.991640	30	1000	567.4	12	7	1	13	-165.783355	19	15000	553.6	13	0	0	20
34	-169.304194	50	1000	587.5	12	8	2	12	-172.003855	16	1000	584.7	17	5	0	12
35	-174.946800	6	5000	606.2	12	1	0	22	-178.296544	37	1000	598.2	12	3	1	19
36	-181.768430	25	5000	632.9	13	0	0	23	-184.964394	24	1000	624.0	12	3	1	20
37	-188.421639	21	5000	659.8	12	1	0	24	-191.050865	5	5000	663.1	14	2	2	19
38	-195.299487	36	5000	686.9	13	0	0	25	-198.192375	38	5000	682.1	17	3	3	15
39	-201.946746	34	5000	695.1	12	1	0	26	-204.935543	21	1000	712.5	16	4	2	17
40	-208.875202	45	5000	737.5	13	0	0	27	-211.877989	18	5000	746.9	13	14	0	13
41	-214.728766	30	1000	743.1	13	10	6	12	-218.070870	22	5000	759.8	15	10	2	14
42	-221.696645	27	5000	762.3	15	9	2	16	-224.605848	10	5000	776.0	17	6	2	17
43	-228.827386	7	5000	800.9	13	14	3	13	-231.453073	8	5000	796.6	20	4	3	16
44	-236.199979	37	1000	824.3	13	13	5	13	-238.718490	5	15000	828.1	13	20	0	11
45	-243.606804	117	1000	841.2	13	12	8	12	-246.845169	39	5000	853.9	13	20	0	12
46	-248.738035	107	1000	879.3	13	12	8	13	-252.002059	17	5000	876.4	14	19	0	13
47	-254.779313	46	1000	898.7	13	12	8	14	-258.844169	8	15000	909.1	20	6	0	21
48	-261.813840	9	5000	928.5	13	10	10	15	-265.388314	16	15000	932.4	20	6	0	22
49	-267.948832	15	1000	924.8	13	10	11	15	-271.973689	2	15000	964.1	24	0	0	25
50	-274.978552	29	1000	966.0	13	10	11	16	-278.643848	13	5000	987.4	20	3	0	27

Table S3. The global-minimum geometries of the ternary Lennard-Jones (TLJ_N) clusters.

TLJ (S_C = 1.1)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124079	0.000000	0.000000
3A	0.562040	-0.973481	0.000000
4C	0.562040	-0.324494	0.980584
5C	0.562040	-0.324494	-0.980584

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.571934	0.000000	0.000000
3C	0.785967	-0.870196	0.000000
4C	0.785967	0.000000	-0.870196
5C	0.785967	0.000000	0.870196
6C	0.785967	0.870196	0.000000

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.123670	0.000000	0.000000
3C	0.561835	-1.035488	0.000000
4C	0.561835	0.820404	0.631801
5C	0.561835	-0.310775	-0.987671
6C	0.561835	0.848848	-0.592902
7A	0.561835	-0.312955	0.919295

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.198906	0.000000	0.000000
3C	0.599453	-0.991395	0.000000
4C	0.599452	0.496506	0.858106
5C	1.207441	-0.578185	1.002536
6C	-0.008538	-0.578185	1.002536
7C	0.599453	-0.175085	-0.972933
8C	0.599453	0.929811	-0.335715

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.123768	0.000000	0.000000
3A	0.567954	-0.969682	0.000000
4C	0.568280	-0.325733	0.978932
5A	0.569637	-0.326512	-0.911461
6C	-0.419567	-0.886677	-0.634781
7C	0.553050	0.810165	-0.634782
8C	-0.444213	-0.902568	0.595324
9C	0.554306	0.839463	0.595323

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.176058	0.000000	0.000000
3C	0.535118	-1.047264	0.000000
4C	0.535118	-0.327500	0.994739
5C	0.530081	0.842284	0.618855
6C	-0.508849	-0.855280	0.618855
7C	0.530082	-0.324418	-0.993568
8C	-0.517148	-0.843201	-0.610823
9C	-0.517148	0.316500	0.991928
10C	0.515551	0.844178	-0.610823

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.169122	0.000000	0.000000
3C	0.525570	-1.044329	0.000000
4C	0.519424	-0.320087	0.995927
5C	0.519424	-0.320087	-0.995927
6C	0.520225	0.847599	-0.612808
7C	0.520225	0.847599	0.612808
8C	-0.523261	-0.845728	0.612808
9C	-0.523261	-0.845728	-0.612808
10C	-0.536036	0.330323	-0.969831
11C	-0.536036	0.330323	0.969831

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.169433	0.000000	0.000000
3C	0.524602	-1.045105	0.000000
4C	0.524602	-0.322955	0.993954
5C	0.524601	0.845507	0.614298
6C	0.524602	-0.322955	-0.993954
7C	0.524602	0.845508	-0.614296
8C	-0.523592	-0.842627	-0.612204
9C	-0.523593	0.321854	0.990567
10C	-0.523593	0.321855	-0.990567
11C	-0.523593	1.041544	0.000001
12C	-0.523592	-0.842627	0.612204

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.167838	0.000000	0.000000
3C	0.522274	-1.044546	0.000000
4C	-0.522272	-0.845056	-0.613969
5C	0.522272	0.845055	-0.613968
6C	-0.522273	0.322781	-0.993422
7C	-1.167838	-0.000002	0.000000
8C	0.522272	0.845055	0.613968
9C	0.522273	-0.322782	0.993422
10C	0.522273	-0.322782	-0.993422
11C	-0.522274	1.044545	0.000000
12C	-0.522272	-0.845056	0.613969
13C	-0.522273	0.322781	0.993422

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.166805	0.000000	0.000000
3B	0.510686	-1.009512	0.000000
4B	0.510686	-0.314351	0.959322
5C	-0.502074	-0.854510	0.619211
6C	0.525212	-0.326903	-0.988682
7C	0.525212	0.837734	0.618514
8C	-0.513853	0.311257	1.000489
9C	-0.513853	-0.853825	-0.607323
10C	0.518779	0.844028	-0.611615
11C	-1.163694	-0.013887	0.010063
12C	-0.524989	1.037533	0.008241
13C	-0.524989	0.315245	-0.988516
14C	1.482384	-0.958755	0.694751

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2B	1.130610	0.000000	0.000000
3A	0.500525	-0.974559	0.000000
4C	0.530674	-0.326478	-0.984422
5B	0.523346	-0.321067	0.950908
6C	-0.487915	-0.863318	0.617146
7C	-0.499129	-0.860980	-0.606655
8C	0.531991	0.831794	0.618393
9C	0.524689	0.839657	-0.609315
10C	-0.505539	0.301871	1.002617
11C	-0.521524	0.310831	-0.987619
12C	-1.158476	-0.024242	0.011689
13C	-0.522492	1.033060	0.011202
14C	1.483363	-0.955315	0.630077
15C	1.500898	-0.966432	-0.602220

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094550	0.000000	0.000000
3A	0.516010	-0.967498	0.000000
4A	0.516010	-0.312676	-0.915580
5C	0.537117	-0.320853	0.981716
6C	0.537117	0.825341	-0.620907
7C	0.531093	0.839563	0.600454
8C	-0.469209	-0.868537	-0.621177
9C	-0.489911	-0.862524	0.603468
10C	-0.489912	0.292333	-1.011268
11C	-0.519760	0.312623	0.982012
12C	-0.519760	1.030348	-0.021521
13C	-1.152979	-0.030914	-0.022109
14C	1.484023	-0.902456	-0.645436
15C	1.530470	0.255907	-1.049866
16C	1.530469	-0.910824	0.581471

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094689	0.000000	0.000000
3A	0.516326	-0.965272	0.000000
4A	0.516325	-0.309368	-0.914353
5C	0.537203	-0.321875	0.981536
6C	0.537202	0.826598	-0.619477
7C	-0.475499	-0.863571	-0.619475
8C	0.531452	0.838597	0.601560
9C	-0.488790	0.292867	-1.011372
10C	-0.488788	-0.864157	0.601563
11C	-0.519073	0.311016	0.982726
12C	-0.519074	1.030565	-0.020353
13C	-1.153559	-0.028372	-0.020351
14C	1.493091	-0.894617	-0.641747
15C	1.527516	0.257272	-1.053259
16C	1.527517	-0.915243	0.581269
17C	0.493615	-1.468278	-1.053258

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.081957	0.000000	0.000000
3C	0.535443	-1.038187	0.000000
4C	0.535444	0.839911	0.610231
5C	0.535443	-0.320817	-0.987375
6C	0.535444	-0.320817	0.987375
7C	0.535444	0.839911	-0.610231
8C	-0.507777	0.323159	0.994581
9C	-0.507777	1.045765	0.000000
10C	-0.507777	-0.846041	0.614685
11C	-0.507778	0.323159	-0.994581
12C	-0.507778	-0.846041	-0.614685
13C	-1.158636	0.000000	0.000000
14C	1.580340	-0.846706	0.615168
15C	1.580340	0.323413	0.995362
16C	1.580340	-0.846706	-0.615168
17C	1.580341	1.046585	-0.000001
18C	1.580340	0.323412	-0.995363

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.077440	0.000000	0.000000
3C	0.538720	-1.037909	0.000000
4C	0.538720	0.839686	-0.610068
5C	0.538720	-0.320731	0.987110
6C	0.538720	-0.320731	-0.987110
7C	0.538720	0.839686	0.610068
8C	-0.504837	0.323225	0.994783
9C	1.582277	0.323225	-0.994783
10C	-0.504837	1.045976	0.000000
11C	1.582277	-0.846212	-0.614809
12C	-0.504837	-0.846212	0.614810
13C	1.582277	1.045976	0.000000
14C	1.582277	-0.846212	0.614809
15C	-0.504837	0.323225	-0.994783
16C	-0.504837	-0.846212	-0.614810
17C	1.582277	0.323225	0.994783
18C	-1.157027	0.000000	0.000000
19C	2.234467	0.000000	0.000000

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.072616	0.000000	0.000000
3A	0.536307	-0.962486	0.000000
4A	0.536308	-0.291391	-0.917317
5C	0.536308	0.839604	-0.609011
6C	0.536308	-0.326243	0.984579
7C	0.536308	0.835351	0.611131
8C	-0.449759	-0.862227	-0.630793
9C	1.522374	-0.862228	-0.630793
10C	-0.478957	0.298627	-1.010948
11C	1.551573	0.298626	-1.010948
12C	-0.478958	-0.873096	0.590674
13C	1.551573	-0.873097	0.590674
14C	-0.516760	0.301502	0.983758
15C	-0.516759	1.028870	-0.010478
16C	1.589375	0.301501	0.983758
17C	1.589375	1.028870	-0.010477

18C	-1.147868	-0.036891	-0.026990
19C	2.220484	-0.036892	-0.026989
20C	0.536307	-1.447967	-1.059310

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.072658	0.000000	0.000000
3A	0.536329	-0.953967	0.000000
4B	0.536329	-0.301247	0.952802
5B	0.536329	-0.301246	-0.952802
6C	0.536330	0.839091	0.609460
7C	0.536330	0.839091	-0.609459
8C	1.528536	-0.874032	0.612425
9C	1.528536	-0.874032	-0.612426
10C	-0.455879	-0.874032	0.612425
11C	-0.455878	-0.874031	-0.612426
12C	-0.499856	0.296529	0.996581
13C	1.572515	0.296528	0.996581
14C	-0.499856	0.296530	-0.996581
15C	1.572515	0.296530	-0.996581
16C	-0.519903	1.025076	0.000000
17C	1.592562	1.025075	0.000000
18C	2.218546	-0.048355	-0.000001
19C	-1.145888	-0.048354	-0.000001
20C	0.536328	-1.489947	-1.021526
21C	0.536328	-1.489948	1.021526

N = 22

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.074801	0.000000	0.000000
3A	0.540639	-0.941670	0.000000
4B	0.535615	-0.308378	-0.953463
5B	0.535614	-0.308377	0.953463
6C	0.538483	0.834993	-0.610319
7C	0.538482	0.834995	0.610316
8C	-0.457990	-0.874116	-0.611142
9C	-0.457991	-0.874115	0.611142
10C	1.526339	-0.881090	0.612485
11C	1.526339	-0.881091	-0.612484
12C	-0.498601	0.294463	-0.996786
13C	-0.498602	0.294465	0.996784
14C	1.573173	0.289751	-0.997164
15C	1.573171	0.289753	0.997164
16C	-0.517880	1.024285	-0.000002
17C	1.596278	1.021216	-0.000001
18C	-1.145607	-0.049329	-0.000001
19C	2.218838	-0.056378	0.000001
20C	0.527336	-1.505726	0.999333
21C	0.527337	-1.505728	-0.999332
22C	-0.110710	-1.885830	0.000001

N = 23

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.076807	0.000000	0.000000
3A	0.538403	-0.932542	0.000000
4B	0.538403	-0.310847	-0.953715
5B	0.538403	-0.310847	0.953715
6C	-0.452022	-0.882669	-0.610607
7C	0.538403	0.832796	-0.610608
8C	1.528827	-0.882669	-0.610608
9C	-0.452022	-0.882668	0.610608
10C	0.538403	0.832796	0.610608
11C	1.528827	-0.882669	0.610607
12C	-0.498069	0.287560	-0.996896
13C	1.574874	0.287560	-0.996896
14C	0.538402	-1.507662	-0.996896
15C	-0.498068	0.287560	0.996896
16C	0.538402	-1.507662	0.996896
17C	1.574875	0.287560	0.996895
18C	-0.520465	1.020031	0.000000
19C	-1.143605	-0.059279	0.000000
20C	-0.084738	-1.893292	0.000000
21C	1.597271	1.020030	0.000000
22C	2.220411	-0.059280	-0.000001
23C	1.161542	-1.893293	0.000000

N = 24

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.075469	0.000000	0.000000
3A	0.537734	-0.933008	0.000000
4A	0.537734	-0.316357	0.910114
5C	0.537735	-0.310418	-0.989031
6B	0.537734	0.801110	0.587720
7C	-0.446545	-0.873478	0.625765
8C	1.522013	-0.873478	0.625766
9C	0.537734	0.840266	-0.603478
10C	-0.461644	-0.883177	-0.595795
11C	1.537113	-0.883177	-0.595794
12C	1.531932	0.288257	1.019885
13C	-0.456465	0.288257	1.019884
14C	0.537734	-1.484164	1.015459
15C	-0.519668	0.302213	-0.975248
16C	1.595137	0.302214	-0.975247
17C	-0.507006	1.025894	0.030926
18C	1.582474	1.025895	0.030927
19C	0.537734	-1.528509	-0.978799
20C	-1.140465	-0.047522	0.035078
21C	2.215933	-0.047522	0.035079
22C	-0.086704	-1.890465	0.025100
23C	1.162173	-1.890465	0.025101
24C	0.537733	0.488822	1.734575

N = 25

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.078987	0.000000	0.000000
3A	0.537445	-0.935610	0.000000
4A	0.544588	-0.315214	-0.892537
5C	0.541560	-0.313461	0.987281
6C	0.536841	0.828332	-0.616258
7C	-0.450861	-0.878098	-0.616258
8C	1.520418	-0.880036	-0.630946
9C	-0.458415	-0.886402	0.600043
10C	0.540279	0.839018	0.600043
11C	1.537852	-0.890127	0.589875
12C	-0.462510	0.267706	-1.027440
13C	1.537340	0.276645	-1.029871
14C	0.525867	-1.470854	-1.029870
15C	-0.516624	0.299029	0.976668
16C	0.540782	-1.535231	0.973733
17C	1.600593	0.295780	0.973732
18C	-0.520694	1.017542	-0.032041
19C	-1.141688	-0.055334	-0.032040
20C	1.598131	1.018134	-0.032200
21C	-0.086812	-1.892903	-0.032198
22C	2.218633	-0.058739	-0.040520
23C	1.156038	-1.894560	-0.040520
24C	0.528104	0.416262	-1.767632
25C	-0.097900	-0.665269	-1.767632

N = 26

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.081094	0.000000	0.000000
3A	0.540548	-0.936255	0.000000
4A	0.540548	-0.312085	-0.882710
5C	1.525887	-0.880970	-0.622940
6C	0.540547	-0.312085	0.986112
7C	0.540547	0.825686	-0.622941
8C	-0.444791	-0.880971	-0.622941
9C	1.538669	-0.888350	0.594286
10C	-0.457574	0.264180	-1.035641
11C	0.540547	0.840447	0.594285
12C	0.540549	-1.464617	-1.035640
13C	-0.457574	-0.888351	0.594285
14C	1.538669	0.264181	-1.035640
15C	-0.519367	1.016105	-0.041203
16C	0.540548	-1.535967	0.971728
17C	1.600460	1.016106	-0.041202
18C	-0.519367	0.299856	0.971727
19C	1.600460	0.299857	0.971727
20C	-1.139656	-0.058269	-0.041203
21C	1.160839	-0.670210	-1.772033
22C	1.160839	-1.894092	-0.041201
23C	-0.079741	-0.670211	-1.772034
24C	-0.079741	-1.894092	-0.041202
25C	0.540548	0.404164	-1.772034
26C	2.220751	-0.058267	-0.041202

N = 27

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.078454	0.000000	0.000000
3A	0.539227	-0.937885	0.000000
4A	0.539227	-0.315427	-0.879938
5A	0.539227	-0.320996	0.904928
6C	0.539227	0.825084	-0.625350
7C	-0.449095	-0.883450	-0.610283
8C	1.527549	-0.883450	-0.610283
9C	0.539227	0.840177	0.584176
10C	-0.447400	-0.879493	0.610481
11C	1.525854	-0.879493	0.610481
12C	0.539227	-1.471165	-1.023517
13C	-0.462563	0.260627	-1.027347
14C	1.541017	0.260626	-1.027348
15C	-0.466366	0.287779	1.002662
16C	1.544820	0.287779	1.002662
17C	0.539227	-1.499780	0.995261
18C	-0.519861	1.012945	-0.024194
19C	1.598315	1.012945	-0.024194
20C	-1.135306	-0.056129	-0.009946
21C	2.213760	-0.056130	-0.009947
22C	-0.083126	-0.678790	-1.762249
23C	1.161579	-0.678790	-1.762249
24C	-0.080386	-1.892415	-0.016327
25C	1.158839	-1.892415	-0.016327
26C	0.539227	0.395699	-1.770179
27C	0.539228	0.468271	1.736526

N = 28

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.082388	0.000000	0.000000
3A	0.538249	-0.939069	0.000000
4A	0.542191	-0.314170	-0.877734
5A	0.547533	-0.317264	0.887748
6C	0.542366	0.827104	-0.614664
7C	-0.447880	-0.881852	-0.614665
8C	1.529019	-0.885982	-0.604779
9C	0.538089	0.831926	0.600452
10C	-0.454191	-0.880539	0.600452
11C	1.524462	-0.883341	0.615727
12C	-0.458458	0.265652	-1.025082
13C	1.545897	0.262139	-1.021090
14C	0.541313	-1.471560	-1.021090
15C	-0.467115	0.270669	1.009819
16C	0.523752	-1.479731	1.012099
17C	1.544253	0.281436	1.012099
18C	-0.517469	1.012019	-0.010982
19C	-1.135344	-0.054303	-0.010982
20C	1.599295	1.012171	-0.010030
21C	-0.082855	-1.890864	-0.010030
22C	2.215829	-0.058828	-0.001205
23C	1.152924	-1.893178	-0.001205
24C	1.167160	-0.676305	-1.757541
25C	0.546152	0.401576	-1.763058
26C	-0.076813	-0.673529	-1.763058
27C	-0.104604	-0.665161	1.752337
28C	0.525072	0.421526	1.752336

N = 29

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.085580	0.000000	0.000000
3A	0.542790	-0.940140	0.000000
4A	0.542790	-0.313380	0.875974
5A	0.542790	-0.313380	-0.875974
6C	0.542790	0.828334	0.608356
7C	-0.445964	-0.884237	0.608355
8C	1.531544	-0.884237	0.608355
9C	0.542790	0.828334	-0.608356
10C	-0.445964	-0.884237	-0.608355
11C	1.531544	-0.884237	-0.608355
12C	-0.460280	0.265742	1.019671
13C	0.542790	-1.471626	1.019671
14C	1.545860	0.265742	1.019671
15C	0.542790	-1.471626	-1.019671
16C	-0.460280	0.265742	-1.019671
17C	1.545860	0.265742	-1.019671
18C	-1.133208	-0.058298	0.000000
19C	-0.516117	1.010535	0.000000
20C	-0.074302	-1.892378	0.000000
21C	1.601696	1.010536	0.000000
22C	1.159881	-1.892378	0.000000
23C	2.218788	-0.058298	0.000000
24C	0.542790	0.404898	1.758386
25C	-0.079257	-0.672520	1.758386
26C	1.164837	-0.672520	1.758386
27C	0.542790	0.404898	-1.758386
28C	-0.079257	-0.672520	-1.758386
29C	1.164837	-0.672520	-1.758386

N = 30

atom	*X*/σ	*Y*/σ	*Z*/σ

1A	0.000000	0.000000	0.000000
2A	1.083430	0.000000	0.000000
3A	0.541714	-0.938365	0.000000
4A	0.541714	-0.313758	0.876029
5A	0.541714	-0.313758	-0.876029
6B	0.541714	0.783630	0.600712
7B	0.541714	0.783630	-0.600712
8C	-0.450270	-0.875612	-0.608568
9C	-0.450270	-0.875612	0.608568
10C	1.533699	-0.875612	-0.608569
11C	1.533699	-0.875612	0.608569
12C	-0.456049	0.279710	-1.015342
13C	-0.456049	0.279710	1.015342
14C	1.539477	0.279711	-1.015343
15C	1.539477	0.279711	1.015343
16C	0.541714	-1.465841	1.021192
17C	0.541714	-1.465841	-1.021192
18C	-0.465430	1.035542	0.000000
19C	1.548857	1.035543	0.000000
20C	0.541713	0.421153	-1.745431
21C	0.541713	0.421153	1.745431
22C	-1.128508	-0.027240	0.000000
23C	2.211937	-0.027239	0.000000
24C	-0.077279	-1.886322	0.000000
25C	1.160707	-1.886322	0.000000
26C	-0.081325	-0.659680	-1.759281
27C	-0.081325	-0.659680	1.759281
28C	1.164752	-0.659680	-1.759281
29C	1.164752	-0.659680	1.759281
30C	0.541712	1.795539	0.000000

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.088932	0.000000	0.000000
3A	0.545551	-0.933501	0.000000
4A	0.541034	-0.309990	-0.876608
5A	0.544900	-0.299949	0.873629
6A	0.552229	0.736936	-0.575798
7B	0.540035	0.802691	0.579768
8C	-0.448442	-0.874561	-0.608979
9C	1.536027	-0.866286	-0.616456
10C	-0.446678	-0.868920	0.611138
11C	1.540367	-0.865188	0.607503
12C	-0.458692	0.279609	-1.009459
13C	1.533073	0.293156	-1.018081
14C	-0.453928	0.296043	1.006064
15C	1.540417	0.299500	1.005469
16C	-0.460938	1.036405	-0.033967
17C	0.548741	-1.451601	1.024652
18C	0.544617	-1.455946	-1.027153
19C	1.540689	1.044128	-0.022411
20C	0.522469	0.472640	-1.710657
21C	-1.128537	-0.023857	-0.000957
22C	0.543585	0.446750	1.731051
23C	2.215545	-0.014653	-0.008470
24C	-0.070475	-1.881261	0.002546
25C	1.168000	-1.876813	-0.001991
26C	-0.083081	-0.635089	-1.762954
27C	1.170339	-0.635671	1.757100
28C	-0.076629	-0.637978	1.759002
29C	1.157528	-0.626593	-1.769030
30C	0.524156	1.778104	-0.117118
31C	-0.111517	1.444016	-1.161887

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.093141	0.000000	0.000000
3A	0.546570	-0.933145	0.000000
4A	0.546570	-0.315323	-0.878255
5A	0.546571	-0.297877	0.873395
6A	0.546571	0.721362	-0.575487
7C	0.546571	0.837839	0.589391
8C	1.538586	-0.872805	-0.613989
9C	-0.445446	-0.872804	-0.613988
10C	1.541240	-0.867700	0.606878
11C	-0.448099	-0.867699	0.606879
12C	1.541240	0.277972	-1.021732
13C	-0.448100	0.277973	-1.021731
14C	-0.456744	0.294785	1.005106
15C	-0.456745	1.045594	-0.062195
16C	1.549887	0.294784	1.005105
17C	1.549887	1.045593	-0.062196
18C	0.546570	-1.451910	1.022517
19C	0.546570	0.471747	-1.712028
20C	0.546569	-1.459733	-1.026872
21C	-1.125990	-0.016637	-0.011703
22C	2.219131	-0.016639	-0.011705
23C	-0.072314	-1.879787	0.000025
24C	-0.072315	-0.635184	-1.769220
25C	1.165454	-1.879787	0.000024
26C	1.165453	-0.635184	-1.769220
27C	0.546572	0.433847	1.744272
28C	0.546572	1.788272	-0.181088
29C	1.171254	-0.643183	1.755090
30C	-0.078112	-0.643182	1.755091
31C	1.171254	1.434509	-1.198419
32C	-0.078113	1.434510	-1.198418

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.101159	0.000000	0.000000
3A	0.551030	-0.924042	0.000000
4A	0.551030	-0.293045	-0.876343
5A	0.546792	0.737487	-0.547819
6A	0.546792	-0.285658	0.873151
7A	0.561531	0.761669	0.548427
8C	-0.441613	-0.858999	-0.618508
9C	-0.446472	0.308649	-1.006648
10C	-0.446472	-0.856802	0.611960
11C	1.546811	-0.854920	-0.615571
12C	1.544161	-0.852955	0.618502
13C	1.544161	0.316074	-1.005074
14C	-0.451976	0.318513	0.992704
15C	-0.451976	1.042472	-0.012748
16C	1.541095	0.320225	1.003662
17C	1.541095	1.053408	-0.014600
18C	0.548341	-1.430300	1.033498
19C	0.548341	0.526552	-1.684226
20C	0.554382	-1.435290	-1.033456
21C	0.528339	1.764000	-0.042010
22C	0.528339	0.519583	1.686266
23C	-1.127051	-0.010908	-0.007854
24C	2.225554	-0.001320	-0.000950
25C	-0.067087	-0.592482	-1.770315
26C	-0.067087	-1.866829	-0.000471
27C	1.173317	-0.588741	-1.768401
28C	1.173317	-1.863828	0.002470
29C	-0.080618	-0.590543	1.760806
30C	-0.080618	1.482633	-1.118471
31C	1.162331	-0.588017	1.767963
32C	1.162331	1.490222	-1.118345
33C	-0.100033	1.500961	1.080742

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.106895	0.000000	0.000000
3A	0.553448	-0.920301	0.000000
4A	0.553448	-0.284388	0.875258
5A	0.553448	-0.284388	-0.875258
6A	0.553448	0.744539	0.540939
7A	0.553448	0.744539	-0.540939
8C	-0.442295	-0.850999	0.618287
9C	-0.442295	0.325053	1.000410
10C	1.549191	1.051893	0.000000
11C	1.549191	0.325053	-1.000410
12C	-0.442295	-0.850999	-0.618287
13C	-0.442295	1.051893	0.000000
14C	-0.442295	0.325053	-1.000410
15C	1.549191	0.325053	1.000410
16C	1.549191	-0.850999	-0.618287
17C	1.549191	-0.850999	0.618287
18C	0.553448	-1.425738	1.035860
19C	0.553448	-1.425738	-1.035860
20C	0.553448	0.544584	1.676056
21C	0.553448	1.762310	0.000000
22C	0.553448	0.544584	-1.676056
23C	-1.124487	0.000000	0.000000
24C	2.231382	0.000000	0.000000
25C	-0.067312	1.504777	1.093284
26C	-0.067312	-0.574773	-1.768971
27C	-0.067312	1.504777	-1.093284
28C	-0.067312	-0.574773	1.768971
29C	-0.067312	-1.860006	0.000000
30C	1.174208	-0.574773	1.768971
31C	1.174208	-1.860006	0.000000
32C	1.174208	1.504777	1.093284
33C	1.174208	-0.574773	-1.768971
34C	1.174208	1.504777	-1.093284

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.088848	0.000000	0.000000
3A	0.555048	-0.936755	0.000000
4A	0.555048	-0.316288	-0.881744
5A	0.536169	0.716558	-0.581626
6A	-0.343152	-0.826546	-0.581626
7A	0.536168	-0.305530	0.870859
8C	-0.449277	0.256016	-1.026552
9C	0.527907	0.835019	0.587588
10C	-0.449278	-0.879825	0.587587
11C	1.538543	-0.876721	-0.616933
12C	1.535217	-0.874827	0.606694
13C	0.545410	-1.461310	-1.028297
14C	1.535218	0.275687	-1.028297
15C	-0.484097	1.022241	-0.073618
16C	-1.126224	-0.104617	-0.073618
17C	-0.484097	0.275858	0.987065
18C	-0.120802	-0.688798	-1.721081
19C	0.531006	0.455049	-1.721081
20C	1.532225	0.290657	1.009435
21C	1.532226	1.048293	-0.067239
22C	0.531005	-1.466366	1.009435
23C	-0.120803	-1.852577	-0.067240
24C	1.139115	-0.649112	-1.781134
25C	2.211581	-0.013652	-0.009606
26C	1.139114	-1.895704	-0.009606
27C	-1.268721	-0.635321	-1.208466
28C	-0.100162	-0.659612	1.740274
29C	0.516419	1.780700	-0.189984
30C	-0.100161	1.415364	-1.208466
31C	0.516418	0.422413	1.740274
32C	-1.268722	-1.352008	-0.189984
33C	1.150639	1.429222	-1.209258
34C	-0.643040	-1.718471	-1.209258
35C	1.150637	-0.655678	1.753587

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.104006	0.000000	0.000000
3A	0.555851	-0.920939	0.000000
4A	0.555851	-0.280165	-0.877289
5A	0.547936	-0.288517	0.874334
6A	0.547936	0.745121	-0.540828
7A	0.544873	0.741777	0.541796
8A	-0.348816	-0.818498	-0.597833
9C	-0.443378	-0.851868	0.608841
10C	-0.443378	0.320831	-0.996711
11C	-0.458806	0.314057	0.991155
12C	-0.458805	1.039718	-0.002354
13C	1.541422	-0.854738	-0.624302
14C	1.540206	0.321268	1.002515
15C	1.540206	1.052733	0.001061
16C	1.542685	-0.858777	0.614480
17C	1.542686	0.324101	-1.005007
18C	0.539547	-1.423434	-1.039679
19C	-1.121190	-0.062641	-0.045753
20C	0.540190	-1.434103	1.026878
21C	0.540192	0.541928	-1.678524
22C	0.536956	0.537037	1.674557
23C	0.536957	1.758563	0.002157
24C	-0.120364	-1.827627	-0.043495
25C	-0.120364	-0.597429	-1.727771
26C	2.225820	-0.002108	-0.001539
27C	-0.079159	-0.583697	1.761836
28C	-0.079158	1.500760	-1.092010
29C	-0.084747	1.494941	1.091910
30C	1.143201	-1.873658	-0.010048
31C	1.143201	-0.579570	-1.781794
32C	1.160141	1.501825	1.096938
33C	1.164211	-0.584988	1.766740
34C	1.164213	1.505039	-1.094731
35C	-1.281104	-0.546673	-1.184046
36C	-1.281104	-1.294233	-0.160555

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.101571	0.000000	0.000000
3A	0.559630	-0.924554	0.000000
4A	0.559630	-0.285487	0.879373
5A	0.542929	-0.291199	-0.872736
6A	0.542929	0.740170	0.546455
7A	0.537518	0.741437	-0.538824

8A	-0.338493	-0.808040	0.587226
9C	-0.444539	-0.865675	-0.596721
10C	-0.444539	0.300253	1.007630
11C	1.546348	-0.854364	0.620892
12C	-0.470077	0.304380	-0.983603
13C	-0.470077	1.029524	0.014216
14C	1.541737	0.322775	1.005617
15C	1.541737	-0.856807	-0.617520
16C	1.530841	0.325077	-1.004109
17C	1.530841	1.055418	0.000861
18C	0.551284	-1.428814	1.038361
19C	-1.123756	-0.087169	0.063348
20C	-0.117902	-0.639913	1.720165
21C	-0.117902	-1.833699	0.077481
22C	0.521886	1.754440	0.006723
23C	0.521886	0.535349	-1.670780
24C	0.539439	0.529556	1.684446
25C	0.539438	-1.438612	-1.023807
26C	2.222895	0.003959	-0.002877
27C	1.145921	-0.589453	1.781882
28C	1.145922	-1.876820	0.010432
29C	-0.089267	1.484941	1.105041
30C	-0.089267	-0.592514	-1.753594
31C	-1.262791	-0.595879	1.205170
32C	-1.262791	-1.330274	0.194622
33C	-0.103041	1.488879	-1.082012
34C	1.155421	-0.584001	-1.767943
35C	1.155421	1.501218	1.101374
36C	1.144191	1.505914	-1.094392
37C	-0.639988	-1.686657	1.225743

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.073812	0.000000	0.000000
3A	0.539208	-0.940466	0.000000
4A	0.539207	-0.340174	0.876788
5A	0.512656	0.704427	0.599340
6A	0.512657	-0.303962	-0.873517
7A	-0.388385	0.199454	0.954437
8A	-0.388384	-0.817669	-0.531178
9A	-0.394054	-0.846626	0.579641
10C	0.505687	0.843872	-0.577755
11C	-1.125241	-0.077907	0.053339
12C	-0.514681	1.001289	0.087008
13C	-0.514680	0.281058	-0.964965
14C	1.517222	-0.891423	0.610312
15C	1.500920	-0.878851	-0.624532
16C	1.500920	0.264359	1.045245
17C	0.468830	-1.462401	-1.011284
18C	0.468829	0.413849	1.729174
19C	0.491858	-1.478623	1.012337
20C	-0.164482	-0.655973	1.713175
21C	-0.164481	-1.834449	-0.008112
22C	-0.224224	1.304300	1.241013
23C	-0.224223	-0.685209	-1.664873
24C	1.495274	0.286572	-1.023394
25C	1.495273	1.057758	0.103003
26C	-1.286405	-0.456200	1.207585
27C	-1.286404	-1.290833	-0.011483
28C	1.101827	-0.678260	1.782619
29C	1.101827	-1.907251	-0.012452
30C	0.445425	0.408740	-1.740959
31C	0.445423	1.770926	0.248656
32C	-1.357465	0.773439	0.953679
33C	-1.357463	-0.609347	-1.066025
34C	2.188778	-0.012499	0.008559
35C	1.065396	1.411397	1.271607
36C	1.065398	-0.674993	-1.775783
37C	-0.752773	0.414925	1.993328
38C	-0.752771	-1.708280	-1.107835

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092746	0.000000	0.000000
3A	0.575129	-0.929151	0.000000
4A	0.536509	-0.298882	0.877157
5A	0.536509	-0.298882	-0.877157
6A	0.523476	0.734932	-0.546422
7A	0.523476	0.734932	0.546422
8A	-0.349392	-0.831912	0.546422
9A	-0.349392	-0.831912	-0.546422
10C	-0.483787	0.269511	0.988123
11C	-0.483787	0.269511	-0.988123
12C	-0.494407	1.012562	0.000000
13C	-1.121185	-0.112537	0.000000
14C	1.536897	-0.856185	0.627636
15C	1.536897	-0.856185	-0.627636
16C	1.513069	0.318563	1.014020
17C	1.513069	0.318563	-1.014020
18C	0.525480	-1.454211	-1.014020
19C	0.525480	-1.454211	1.014020
20C	1.509002	1.056986	0.000000
21C	-0.104534	-1.839396	0.000000
22C	0.490838	1.745042	0.000000
23C	-1.225456	-1.335796	0.000000
24C	-0.176224	-0.690743	-1.679442
25C	-0.176224	-0.690743	1.679442
26C	0.494582	0.513390	1.679442
27C	0.494582	0.513390	-1.679442
28C	1.156383	-1.883710	0.000000
29C	2.210320	0.008164	0.000000
30C	-0.131411	1.462173	-1.097312
31C	-0.131411	1.462173	1.097312
32C	-1.312434	-0.657826	1.097312
33C	-1.312434	-0.657826	-1.097312
34C	1.100382	-0.613008	-1.784883
35C	1.100382	-0.613008	1.784883
36C	1.120312	1.499937	-1.105426
37C	1.120312	1.499937	1.105426
38C	-0.685744	-1.742029	1.105426
39C	-0.685744	-1.742029	-1.105426

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.087364	0.000000	0.000000
3A	0.543870	-0.926190	0.000000
4A	0.543870	-0.303259	0.875136
5A	0.526133	-0.282530	-0.878632
6A	0.526133	0.737691	0.554643
7A	0.522329	0.748543	-0.532822
8A	-0.376283	0.260998	0.937486
9A	-0.376283	-0.800352	-0.553569
10B	-0.419173	-0.839577	0.597620
11C	-0.487041	1.020615	0.024654
12C	-0.487041	0.310881	-0.972428
13C	-1.125268	-0.051197	0.036442
14C	1.511952	0.318272	1.016376
15C	1.511952	-0.856139	-0.633516
16C	1.525644	-0.865334	0.615954
17C	1.507048	1.060662	0.018581
18C	1.507047	0.329732	-1.008280
19C	0.491619	0.505863	1.687522
20C	0.491620	-1.428868	-1.030517
21C	-0.155641	-0.559999	1.731612
22C	-0.155640	-1.819518	-0.037845
23C	0.508559	-1.441472	1.026056
24C	-0.194703	1.385317	1.153307
25C	-0.194703	-0.636145	-1.686577
26C	0.488637	1.754038	0.031772
27C	0.488637	0.544297	-1.667753
28C	-1.290442	-1.277799	-0.079436
29C	-1.290442	-0.343328	1.233371
30C	2.203679	0.002704	-0.001925
31C	-0.127304	1.495722	-1.064672
32C	-1.330840	-0.567306	-1.105436
33C	-1.330841	0.858750	0.897981
34C	1.114452	-0.603531	1.785005
35C	1.114452	-1.884222	-0.014194
36C	1.084803	1.500610	1.141910
37C	1.084803	-0.587625	-1.791784
38C	1.123398	1.517862	-1.080431
39C	-0.726328	0.546133	1.962483
40C	-0.726326	-1.675488	-1.158597

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.081811	0.000000	0.000000
3A	0.551098	-0.930917	0.000000
4A	0.551098	-0.314180	-0.876297
5A	-0.366234	-0.810130	-0.570168
6A	0.510562	-0.291070	0.877572
7A	0.510562	0.727848	-0.570168
8A	-0.384483	-0.818435	0.526289
9A	-0.384483	0.219192	-0.948035
10A	0.508413	0.747783	0.526289
11C	-1.123952	-0.071405	-0.050255
12C	-0.511121	0.291388	0.961634
13C	-0.511121	1.003554	-0.050255
14C	1.527689	-0.870931	-0.612960
15C	1.503797	-0.857310	0.640267
16C	0.496414	-1.453678	-1.023096
17C	1.503797	0.313362	-1.023096
18C	-0.157657	-1.821563	-0.029190
19C	-0.157657	-0.642247	-1.704834
20C	0.472349	-1.448601	1.011058
21C	0.472350	0.462840	-1.704835
22C	1.487170	1.063611	-0.029191
23C	1.487170	0.331485	1.011058
24C	-1.266422	-1.285373	-0.050371
25C	-1.266422	-0.481224	-1.192956
26C	-0.231043	-0.672433	1.659217
27C	0.460940	0.541369	1.659216
28C	0.460941	1.744575	-0.050372
29C	-0.231044	1.334922	-1.192957
30C	1.111979	-1.893557	0.005451
31C	1.111979	-0.633936	-1.784296
32C	2.195904	0.007744	0.005450
33C	-1.358707	0.774593	-0.932602
34C	-1.358707	-0.616461	1.043895
35C	-0.161681	1.483228	1.043894
36C	-0.741415	-1.664730	-1.171633
37C	1.054833	-0.601357	1.794281
38C	1.054834	1.486050	-1.171635
39C	-0.752883	-1.719825	1.072580
40C	-0.752883	0.429214	-1.980910
41C	1.096403	1.523986	1.072580

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.078445	0.000000	0.000000
3A	0.540868	-0.925787	0.000000
4A	0.518505	-0.292592	-0.881895
5A	0.518505	-0.292593	0.881895
6A	0.516792	0.741421	-0.549175
7A	0.516792	0.741421	0.549176
8A	-0.387310	-0.800918	-0.548621
9A	-0.387311	-0.800919	0.548620
10C	-0.482663	0.294945	0.982584
11C	-0.482663	0.294946	-0.982584
12A	-0.401155	0.958658	0.000001
13C	-1.129698	-0.014942	0.000000
14C	1.502857	-0.862904	-0.629433
15C	1.502857	-0.862905	0.629432
16C	1.489481	1.065582	0.000001
17C	-0.178118	-1.808456	-0.000002
18C	0.470530	-1.444880	-1.015059
19C	0.470530	-1.444882	1.015057
20C	1.496218	0.324665	-1.015044
21C	1.496219	0.324663	1.015044
22C	0.460187	1.752385	0.000001
23C	-1.286257	-1.247012	-0.000001
24C	-0.206946	1.484742	-1.014810
25C	-0.206947	1.484741	1.014811
26C	-0.211716	-0.663572	-1.680851
27C	-0.211717	-0.663575	1.680850
28C	0.477810	0.534216	-1.678658
29C	0.477810	0.534213	1.678659
30C	-1.344301	1.062950	-0.619216
31C	-1.344301	1.062949	0.619217
32C	-1.350087	-0.568647	-1.083227
33C	-1.350087	-0.568649	1.083226
34C	2.192372	0.002033	0.000000
35C	1.095401	-1.891640	-0.000002
36C	1.073349	1.526830	-1.105917
37C	1.073349	1.526828	1.105919
38C	1.071447	-0.608658	-1.792066
39C	1.071447	-0.608662	1.792064
40C	-0.762868	-1.689602	1.108652
41C	-0.762867	-1.689600	-1.108657
42C	-0.765902	2.015897	0.000001

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069887	0.000000	0.000000
3A	0.523848	-0.932867	0.000000
4A	0.519653	-0.304170	0.875778
5A	0.519653	-0.304170	-0.875778
6A	0.493618	0.742776	0.550661
7A	0.493618	0.742776	-0.550661
8A	-0.405959	-0.794085	0.550662
9A	-0.405959	-0.794085	-0.550662
10A	-0.416772	0.243951	-0.921010

11A	-0.416772	0.243951	0.921010
12C	-0.517746	1.003789	0.000000
13C	-1.128737	-0.040045	0.000000
14C	1.490585	-0.872489	-0.626708
15C	1.490585	-0.872489	0.626708
16C	1.472917	0.326112	-1.021660
17C	1.472917	0.326112	1.021660
18C	0.436836	-1.443955	-1.021660
19C	0.436836	-1.443955	1.021660
20C	0.426825	0.491256	1.685484
21C	0.426825	0.491256	-1.685484
22C	-0.219355	-0.612694	1.685484
23C	-0.219355	-0.612694	-1.685484
24C	1.466442	1.068215	0.000000
25C	-0.213396	-1.801664	0.000000
26C	-0.261159	1.362943	-1.141013
27C	-0.261159	1.362943	1.141013
28C	-1.316263	-0.439623	-1.141013
29C	-1.316263	-0.439623	1.141013
30C	0.438839	1.748316	0.000000
31C	-1.309542	-1.238663	0.000000
32C	-1.385623	0.811053	-0.854514
33C	-1.385623	0.811053	0.854514
34C	2.180619	0.003750	0.000000
35C	1.064426	-1.903184	0.000000
36C	1.057076	-0.618741	-1.795322
37C	1.057076	-0.618741	1.795322
38C	-0.812393	0.475522	-1.935713
39C	-0.812393	0.475522	1.935713
40C	1.030688	1.511354	-1.141311
41C	1.030688	1.511354	1.141311
42C	-0.813142	-1.638690	-1.141312
43C	-0.813142	-1.638690	1.141312

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.057998	0.000000	0.000000
3A	0.489738	-0.929096	0.000000
4A	0.489737	-0.287106	-0.883623
5A	0.489737	-0.287106	0.883623
6A	0.489736	0.751655	-0.546109
7A	0.489736	0.751655	0.546109
8A	-0.445190	-0.761417	-0.553202
9A	-0.445190	-0.761417	0.553202
10A	-0.445192	0.941162	0.000000
11A	-0.445191	0.290834	-0.895099
12A	-0.445191	0.290834	0.895099
13B	-1.103127	-0.000002	0.000000
14C	1.449225	-0.874438	-0.635317
15C	1.449225	-0.874438	0.635317
16C	1.449223	1.080866	0.000000
17C	1.449224	0.334007	-1.027964
18C	1.449224	0.334007	1.027964
19C	0.375257	1.755756	0.000000
20C	0.375261	-1.420436	-1.032008
21C	0.375261	-1.420436	1.032008
22C	0.375258	0.542559	-1.669823
23C	0.375258	0.542559	1.669823
24C	-0.283347	1.430149	-1.039064
25C	-0.283347	1.430149	1.039064
26C	-0.283343	-1.767763	0.000000
27C	-0.283344	-0.546269	-1.681242
28C	-0.283344	-0.546269	1.681242
29C	-1.366307	-0.357818	-1.101245
30C	-1.366307	-0.357818	1.101245
31C	-1.366309	0.936773	-0.680606
32C	-1.366309	0.936773	0.680606
33C	-1.366306	-1.157920	0.000000
34C	2.164752	0.000001	0.000000
35C	1.002859	-1.909550	0.000000
36C	1.002859	-0.590082	-1.816090
37C	1.002859	-0.590082	1.816090
38C	1.002856	1.544859	-1.122406
39C	1.002856	1.544859	1.122406
40C	-0.890897	0.603628	-1.857773
41C	-0.890893	-1.580318	-1.148168
42C	-0.890897	0.603628	1.857773
43C	-0.890893	-1.580318	1.148168
44C	-0.890899	1.953377	0.000000

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.045028	0.000000	0.000000
3A	0.467351	-0.934701	0.000000
4A	0.467351	-0.288839	-0.888954
5A	0.467351	-0.288838	0.888954
6A	0.467351	0.756189	-0.549404
7A	0.467351	0.756189	0.549404
8A	-0.467350	-0.756189	0.549404
9A	-0.467350	0.288838	-0.888954
10A	-0.467350	-0.756189	-0.549404
11A	-0.467350	0.288838	0.888954
12A	-0.467350	0.934701	0.000000
13A	-1.045027	0.000000	0.000000
14C	1.422157	0.335726	-1.033257
15C	1.422157	-0.878940	0.638588
16C	1.422157	-0.878941	-0.638588
17C	-0.335725	1.422156	1.033257
18C	0.335726	0.543215	1.671845
19C	1.422157	1.086431	0.000000
20C	1.422157	0.335726	1.033257
21C	0.335726	1.757882	0.000000
22C	0.335727	-1.422156	1.033257
23C	0.335726	0.543215	-1.671845
24C	0.335727	-1.422156	-1.033257
25C	-0.335724	-1.757882	0.000000
26C	-0.335725	-0.543216	-1.671845
27C	-0.335725	-0.543216	1.671845
28C	-0.335725	1.422156	-1.033258
29C	-1.422155	-1.086432	0.000000
30C	-1.422156	-0.335726	-1.033257
31C	-1.422156	-0.335726	1.033257
32C	-1.422156	0.878941	-0.638588
33C	-1.422156	0.878941	0.638588
34C	2.149706	0.000001	0.000000
35C	0.961381	-1.922754	0.000000
36C	0.961380	-0.594163	-1.828649
37C	0.961380	-0.594163	1.828649
38C	0.961379	1.555541	-1.130167
39C	0.961379	1.555542	1.130167
40C	-0.961375	-1.555543	-1.130168
41C	-0.961376	-1.555543	1.130168
42C	-0.961377	0.594163	-1.828650
43C	-0.961377	0.594163	1.828649
44C	-0.961377	1.922756	0.000000
45C	-2.149706	-0.000001	-0.000001

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.051958	0.000000	0.000000
3A	0.463256	-0.950893	0.000000
4A	0.503328	-0.338894	-0.880499
5A	-0.426243	-0.803589	-0.570577
6A	-0.425996	0.204132	-0.951597
7A	-0.478738	-0.777916	0.520121
8A	-1.043798	-0.051896	-0.081789
9A	0.477901	0.714489	-0.599751
10A	0.439587	-0.304889	0.888402
11A	-0.496789	0.904129	-0.122201
12C	0.476915	0.844835	0.581730
13C	-0.558393	0.327178	0.930130
14A	1.317987	-0.850382	0.605160
15C	1.450815	-0.917293	-0.590228
16C	0.338385	-1.455026	1.012575
17C	-0.244117	-0.657421	-1.697721
18C	0.406102	-1.485520	-1.005923
19C	0.399720	0.427700	-1.724203
20C	-1.357509	-0.451003	-1.131097
21C	-0.298091	-1.801267	-0.008712
22C	-0.318688	1.310593	-1.200026
23C	-1.411769	0.760996	-0.829106
24C	-1.391084	-1.165198	-0.087007
25C	1.440230	0.241261	1.047627
26C	1.456861	0.263498	-1.048616
27C	1.055008	-1.892342	0.083629
28C	0.265530	1.762058	-0.204099
29C	-1.521702	0.865500	0.399429
30C	1.039371	-0.723351	1.739685
31C	-0.344398	-0.646165	1.648450
32C	-1.503957	-0.432668	0.898699
33C	2.154670	-0.186105	0.119046
34C	1.452308	1.066151	-0.105990
35C	-0.511150	1.552620	0.796140
36C	0.385170	0.409867	1.744492
37C	1.519406	-1.763247	1.237945
38C	2.211937	-1.434342	0.239960
39C	1.035382	-0.694032	-1.787525
40C	-0.871803	0.424272	-1.944118
41C	-0.859125	-1.641546	-1.155085
42C	2.212759	-0.706651	1.271815
43C	-1.040411	1.856031	-0.316672
44C	-0.958800	-1.619487	1.057458
45C	-2.144713	-0.111020	-0.193442
46C	0.974936	1.458147	-1.253917

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.083004	0.000000	0.000000
3A	0.506007	-0.919762	0.000000
4A	0.506007	-0.224320	-0.891988
5A	0.551924	0.726990	0.566801
6A	0.526462	-0.313516	0.877539
7A	0.526463	0.774576	-0.518071
8A	-0.394893	-0.761566	-0.593758
9A	1.366789	-0.805698	-0.628166
10A	-0.377927	0.291439	0.925453
11A	-0.377926	0.968587	0.056929
12C	-0.483883	0.363568	-0.966493
13C	-0.483884	-0.848637	0.588305
14A	0.462427	-1.282583	-0.999971
15C	-1.129087	-0.004610	-0.003596
16C	1.499639	-0.906832	0.569398
17C	1.499640	0.331037	-1.018319
18C	-0.164180	1.422977	1.109429
19C	-0.166834	-0.573186	-1.724363
20C	-0.166834	-1.812086	-0.135325
21C	0.488391	0.509246	1.685978
22C	0.488393	1.759266	0.082677
23C	1.523462	0.272509	1.011360
24C	1.523464	1.047281	0.017622
25C	1.092800	-0.612521	-1.761766
26C	1.092800	-1.857953	-0.164350
27C	-1.276125	0.976772	0.761542
28C	-0.202618	-0.516911	1.729759
29C	-0.202615	1.551458	-0.923172
30C	1.482380	-1.701458	-1.326549
31C	2.192770	-0.152003	-0.118509
32C	0.484962	0.609456	-1.662287
33C	0.484960	-1.463452	0.996466
34C	-0.600353	-1.642022	-1.280210
35C	-1.341433	-0.217733	1.201673
36C	-1.341431	1.112286	-0.504235
37C	-1.313143	-1.272198	-0.202510
38C	-1.313142	-0.506668	-1.184392
39C	1.122261	1.479408	1.153427
40C	2.248023	-0.639432	-1.297840
41C	2.248023	-1.414600	-0.303593
42C	0.423142	-1.624611	-2.065096
43C	0.423142	-2.398961	-1.071899
44C	1.093933	-0.640486	1.773029
45C	1.093936	1.563280	-1.053568
46C	-0.747514	2.014735	0.161687
47C	-0.747518	0.648177	1.914460

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1B	0.000000	0.000000	0.000000
2C	1.131944	0.000000	0.000000
3C	-1.129206	-0.064253	0.000000
4A	-0.437086	-0.936137	-0.526669
5A	-0.437084	-0.936153	0.526642
6A	0.493748	-1.053630	-0.000017
7A	0.479597	-0.525440	0.911154
8A	0.479593	-0.525412	-0.911171
9A	-0.460627	-0.017703	-1.046951
10A	-0.460622	-0.017735	1.046953
11A	0.454510	0.530138	0.905054
12A	0.454505	0.530166	-0.905039
13A	-0.493407	0.911183	-0.532827
14A	-0.493404	0.911167	0.532858
15A	0.447538	1.076545	0.000016
16C	-0.302282	-0.982705	-1.672268
17C	-0.302274	-0.982756	1.672240
18C	0.377056	-1.676539	0.966729
19C	0.377051	-1.676509	-0.966782
20C	-0.276566	-1.953443	-0.000029
21C	0.332230	0.002991	1.927626
22C	0.332221	0.003050	-1.927627
23C	1.447181	-1.060370	0.624544
24C	1.447178	-1.060350	-0.624582
25C	-1.380648	-1.302833	-0.000017
26C	1.420432	0.013110	1.249416
27C	1.420426	0.013149	-1.249420
28C	-1.393967	-0.682059	-1.085783

29C	-1.393962	-0.682091	1.085768
30C	-0.343777	0.963888	1.663093
31C	-0.343785	0.963939	-1.663061
32C	1.415826	1.067882	0.618688
33C	1.415823	1.067901	-0.618660
34C	0.332262	1.683442	0.950400
35C	0.332257	1.683471	-0.950350
36C	-1.440639	0.550086	-1.079262
37C	-1.440633	0.550053	1.079286
38C	-1.480013	1.140210	0.000021
39C	-0.415142	1.918759	0.000031
40C	0.983013	-1.022917	1.797040
41C	0.983004	-1.022861	-1.797075
42C	1.013823	-2.060830	-0.000034
43C	-0.904141	-1.834391	1.037508
44C	-0.904146	-1.834360	-1.037560
45C	-0.943897	-0.027353	-2.071666
46C	-0.943887	-0.027416	2.071670
47C	0.950132	1.042487	1.788170
48C	0.950124	1.042542	-1.788142

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1B	0.000000	0.000000	0.000000
2C	1.131332	0.000000	0.000000
3C	-1.130482	-0.043861	0.000000
4A	-0.448972	-0.761342	-0.744073
5A	0.478135	-0.742410	0.745024
6A	-0.444105	-1.035095	0.273132
7A	0.483910	-1.017447	-0.271830
8A	0.469463	-0.271535	-1.015910
9A	-0.458607	-0.288232	1.016258
10A	-0.467878	0.260400	-1.010636
11A	0.457406	0.279637	1.010281
12A	0.452952	0.746807	-0.735569
13A	-0.481584	0.729625	0.734614
14A	-0.491431	1.028642	-0.281161
15A	0.451173	1.047281	0.279823
16C	-0.320843	-0.511341	-1.863847
17C	0.340383	-0.496132	1.864480
18C	0.357030	-1.368302	-1.365626
19C	-0.303745	-1.379367	1.367373
20C	-0.294533	-1.881592	-0.499046
21C	0.367250	-1.868118	0.501434
22C	0.322278	0.501354	-1.860091
23C	-0.341520	0.490861	1.859446
24C	-1.394063	-1.242177	-0.323250
25C	1.441168	-1.186779	0.324791
26C	1.434666	-0.867054	-0.881573
27C	-1.399993	-0.920894	0.882701
28C	1.413620	0.330087	-1.206700
29C	-1.425385	0.276574	1.206297
30C	-1.407459	-0.364493	-1.209396
31C	1.420504	-0.308103	1.209810
32C	-0.343792	1.367480	-1.357806
33C	0.290481	1.381517	1.356037
34C	0.340108	1.874936	-0.486959
35C	-0.412558	1.860961	0.484558
36C	1.418644	1.186807	-0.324048
37C	-1.463600	1.131325	0.322551
38C	-1.447011	0.821707	-0.878454
39C	1.414045	0.878311	0.877349
40C	-0.926986	-1.493532	-1.465686
41C	0.984160	-1.454592	1.467560
42C	0.966232	-0.526966	-2.002283
43C	-0.945125	-0.561470	2.002967
44C	0.997741	-1.992270	-0.535060
45C	-0.919762	-2.028769	0.537621
46C	-0.960600	0.518801	-1.996003
47C	0.939718	0.558207	1.995301
48C	0.950918	1.464265	-1.461223
49C	-1.007012	1.428163	1.459362

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1B	0.000000	0.000000	0.000000
2C	1.131403	0.000000	0.000000
3C	-1.130730	-0.025212	0.000000
4A	0.473972	-0.913285	0.526205
5A	0.473965	-0.912710	-0.527204
6A	-0.453057	-1.063597	-0.000575
7A	-0.457875	-0.535775	0.911344
8A	-0.457887	-0.534780	-0.911918
9A	0.464958	-0.000258	1.052664
10A	0.464944	0.000891	-1.052666
11A	-0.468342	0.520504	0.902955
12A	-0.468355	0.521489	-0.902376
13A	0.458785	0.913502	0.526507
14A	0.458778	0.914077	-0.525512
15A	-0.479801	1.079715	0.000595
16C	0.341515	-0.967860	1.672945
17C	0.341492	-0.966033	-1.674001
18C	-0.330592	-0.006314	1.928320
19C	-0.330618	-0.004209	-1.928317
20C	-0.313550	-1.682222	0.965128
21C	-0.313563	-1.681167	-0.966956
22C	0.351355	-1.934614	-0.001056
23C	0.322654	0.965311	1.670973
24C	0.322631	0.967135	-1.669919
25C	0.359619	1.933003	0.001054
26C	1.420393	1.236877	0.000668
27C	1.418027	0.621788	1.076409
28C	1.418013	0.622962	-1.075741
29C	1.432027	-1.237556	-0.000682
30C	1.425424	-0.617377	1.078506
31C	1.425410	-0.616197	-1.079191
32C	-1.407086	-1.098928	0.622934
33C	-1.407095	-1.098247	-0.624108
34C	-1.414703	-0.023495	1.250414
35C	-1.414720	-0.022130	-1.250412
36C	-0.336706	1.677478	0.960732
37C	-0.336720	1.678525	-0.958892
38C	-1.440822	1.037405	0.622588
39C	-1.440831	1.038083	-0.621429
40C	-0.946232	-1.051954	1.794389
41C	-0.946258	-1.049995	-1.795519
42C	0.978471	-1.790661	1.035079
43C	0.978458	-1.789530	-1.037042
44C	0.961399	0.004577	2.070532
45C	0.961373	0.006838	-2.070533
46C	-0.939727	-2.086185	-0.001131
47C	-0.964400	1.025320	1.786767
48C	-0.964427	1.027269	-1.785628
49C	0.968945	1.786044	1.043489
50C	0.968932	1.787181	-1.041548

TLJ (S_C = 1.2)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124063	0.000000	0.000000
3A	0.562032	-0.973467	0.000000
4C	0.562031	-0.324489	-1.046803
5C	0.562031	-0.324489	1.046803

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.551283	0.000000	0.000000
3C	0.775641	-0.951047	0.000000
4C	0.775641	0.951047	0.000000
5C	0.775641	0.000000	-0.951047
6C	0.775641	0.000000	0.951047

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.125583	0.000000	0.000000
3C	0.562791	-1.097305	0.000000
4C	0.562791	0.897954	0.630679
5A	0.562791	-0.292130	-0.924705
6A	0.562791	0.770535	-0.588809
7A	0.562791	-0.292268	0.924640

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.144795	0.000000	0.000000
3C	0.572398	-1.076215	0.000000
4C	0.572398	0.586914	0.902092
5C	1.237488	-0.577416	1.064545
6C	-0.092690	-0.577416	1.064545
7C	0.572397	-0.207617	-1.054207
8C	0.572397	0.996869	-0.400885

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.230986	0.000000	0.000000
3C	0.493668	-1.127661	0.000000
4C	0.504962	-0.330168	-1.075736
5A	0.520857	-0.340561	0.938786
6C	0.479364	0.862050	0.716879
7C	-0.597450	-0.784840	0.716879
8C	0.485044	0.930139	-0.625023
9C	-0.657546	-0.817349	-0.625023

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.232727	0.000000	0.000000
3C	0.499510	-1.120289	0.000000
4C	0.487652	-0.306984	1.075520
5C	-0.651700	-0.846878	0.618459
6B	0.517486	0.882640	0.584586
7A	0.519297	-0.329033	-0.939137
8C	0.468587	0.872357	-0.698436
9C	-0.597974	-0.776122	-0.716771
10C	-0.630702	0.448300	0.939097

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.204476	0.000000	0.000000
3C	0.440391	-1.121079	0.000000
4C	0.419487	-0.285906	1.081576
5C	0.485115	0.967556	0.572506
6C	-0.723191	-0.805292	0.572507
7C	-0.648731	-0.684681	-0.750662
8C	0.400080	0.854152	-0.750662
9C	-0.706553	0.481560	0.869934
10A	0.502008	-0.342150	-0.944219
11C	-0.905548	0.617188	-0.458682

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.223488	0.000000	0.000000
3C	0.502983	-1.128948	0.000000
4C	0.502983	0.895222	-0.687824
5C	0.497291	-0.341533	1.073696
6C	0.497291	0.924986	0.643326
7B	0.502264	-0.342187	-1.007010
8C	-0.660918	1.029039	-0.035507
9C	-0.660919	-0.837630	0.598797
10A	-0.505629	0.256206	-0.965205
11A	-0.505629	-0.791225	-0.609283
12A	-0.523830	0.320532	0.943282

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.241126	0.000000	0.000000
3C	0.530038	-1.122253	0.000000
4C	-0.620525	-0.879254	-0.618267
5C	0.530040	0.936589	-0.618267
6C	-0.620523	0.393180	-1.000377
7B	-0.528192	-0.832059	0.655910
8B	0.526796	-0.333791	1.006278
9B	0.526797	0.832943	0.655910
10B	-1.180208	0.026729	0.089002
11B	-0.528189	1.055757	0.089002
12A	-0.461305	0.292295	0.973346
13C	0.507455	-0.321536	-1.070722

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.115288	0.000000	0.000000
3A	0.552549	-0.963798	0.000000
4A	0.542142	-0.310542	-0.914165
5C	0.608620	0.879879	-0.662933
6C	-0.466730	-0.947052	-0.667900
7B	0.583125	-0.327514	0.978318
8C	-0.482886	-0.941328	0.655506
9C	-0.508544	0.308494	-1.085380
10B	0.558402	0.835366	0.608087
11C	-0.519558	0.322843	1.068545
12C	-0.535344	1.103614	-0.011682
13C	-1.220683	-0.049084	-0.012341
14C	1.573554	-0.913863	-0.668651

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.112662	0.000000	0.000000
3A	0.558713	-0.962214	0.000000

4A	0.541890	-0.311967	-0.913238
5A	0.541890	-0.311967	0.913238
6C	-0.459745	-0.957381	0.662436
7C	-0.459745	-0.957381	-0.662436
8C	0.597072	0.878321	-0.662436
9C	0.597072	0.878321	0.662436
10C	-0.518030	0.298230	-1.078598
11C	-0.518030	0.298230	1.078598
12C	-1.218249	-0.073064	0.000000
13C	-0.548550	1.090212	0.000000
14C	1.577602	-0.908230	0.673232
15C	1.577602	-0.908230	-0.673232

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.113036	0.000000	0.000000
3A	0.554540	-0.958562	0.000000
4A	0.554540	-0.299399	0.910605
5A	0.538335	-0.303585	-0.912893
6A	0.538335	0.772399	0.573530
7C	0.615476	0.886268	-0.641546
8C	-0.456543	-0.934944	0.676782
9C	-0.474235	0.326830	1.093049
10C	-0.474235	-0.936280	-0.651883
11C	-0.513768	0.325588	-1.062551
12C	-0.513767	1.111087	0.022580
13C	-1.211506	-0.037205	0.026932
14C	1.574597	-0.922276	0.667611
15C	1.574018	-0.902371	-0.675249
16C	1.574018	0.359619	1.068134

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.053332	0.000000	0.000000
3C	0.523601	-1.094374	0.000000
4C	0.514181	0.537912	0.951151
5C	0.543604	0.546428	-0.944647
6C	-0.141812	-0.617158	1.049506
7C	1.213023	-0.610148	-1.038931
8C	-0.120567	1.217176	-0.003757
9C	1.203865	1.204985	0.017754
10B	-0.056798	-0.578129	-1.012106
11A	1.068586	-0.554886	0.955257
12C	1.892500	-0.842609	0.092816
13C	1.886521	0.342415	0.782194
14C	-0.869115	-0.813874	-0.052785
15C	-0.856536	0.380183	-0.737046
16C	-0.929289	0.377319	0.641232
17C	2.027672	0.347029	-0.588488

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.112954	0.000000	0.000000
3A	0.548877	-0.955981	0.000000
4A	0.548877	-0.295414	0.909192
5A	0.548877	0.773404	0.561911
6A	0.548877	-0.295414	-0.909192
7A	0.548877	0.773404	-0.561911
8C	-0.473511	0.350005	-1.077204
9C	-0.473512	-0.916324	-0.665748
10C	-0.473512	-0.916324	0.665748
11C	-0.473511	0.350005	1.077204
12C	-0.473511	1.132639	0.000000
13C	-1.205103	0.000000	0.000000
14C	1.570092	-0.918856	-0.667588
15C	1.570093	0.350971	-1.080179
16C	1.570093	0.350971	1.080179
17C	1.570092	-0.918856	0.667588
18C	1.570092	1.135768	0.000000

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.103101	0.000000	0.000000
3A	0.551550	-0.956917	0.000000
4A	0.551550	-0.295704	-0.910082
5A	0.551550	-0.295704	0.910082
6A	0.551550	0.774162	-0.562462
7A	0.551550	0.774162	0.562462
8C	-0.470793	1.132668	0.000000
9C	1.573893	1.132668	0.000000
10C	-0.470793	0.350013	1.077232
11C	-0.470793	0.350013	-1.077232
12C	1.573893	0.350013	1.077232
13C	1.573893	0.350013	-1.077232
14C	1.573892	-0.916349	0.665766
15C	1.573892	-0.916349	-0.665766
16C	-0.470792	-0.916349	0.665766
17C	-0.470792	-0.916349	-0.665766
18C	-1.203884	-0.000001	0.000000
19C	2.306984	-0.000001	0.000000

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.100188	0.000000	0.000000
3A	0.550603	-0.958619	0.000000
4A	0.550602	-0.311742	-0.906514
5A	0.546105	-0.292748	0.909881
6A	0.546105	0.765223	-0.572728
7A	0.543406	0.778280	0.555371
8C	1.596029	-0.909655	-0.649119
9B	-0.455300	-0.861829	-0.614990
10C	-0.470702	0.323652	-1.085028
11C	-0.470701	-0.920801	0.658911
12C	1.569420	-0.909646	0.674346
13C	1.569420	0.341877	-1.079499
14C	1.562929	1.136097	-0.008922
15C	1.562928	0.361020	1.077247
16C	-0.478725	0.349946	1.069591
17C	-0.478725	1.125255	-0.016904
18C	-1.206115	-0.008948	-0.006384
19C	2.305466	0.014394	0.010272
20C	0.511976	-1.525552	-1.088614

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.097423	0.000000	0.000000
3A	0.548711	-0.958365	0.000000
4A	0.552614	-0.311604	-0.906703
5A	0.544808	-0.311604	0.906703
6A	0.545986	0.768450	0.566077
7A	0.551437	0.768450	-0.566077
8C	1.593670	-0.914856	-0.640824
9C	-0.496248	-0.914855	0.640824
10B	-0.455947	-0.853761	-0.624731
11B	1.553369	-0.853762	0.624731
12C	1.559569	0.335759	1.085495
13C	-0.462146	0.335760	-1.085495
14C	1.573971	0.340268	-1.072073
15C	-0.476548	0.340268	1.072073
16C	-0.469831	1.129170	-0.007332
17C	1.567254	1.129170	0.007332
18C	-1.207527	0.006581	-0.016903
19C	2.304949	0.006580	0.016903
20C	0.587390	-1.531560	1.078263
21C	0.510032	-1.531560	-1.078263

N = 22

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.096153	0.000000	0.000000
3A	0.551617	-0.958782	0.000000
4A	0.542023	-0.315089	-0.905683
5A	0.542022	-0.315089	0.905683
6B	0.520902	0.826170	-0.611712
7B	0.520902	0.826170	0.611713
8A	-0.398341	-0.848473	-0.564597
9A	-0.398341	-0.848473	0.564597
10C	1.574040	-0.932570	0.658701
11C	1.574040	-0.932570	-0.658700
12C	-0.519116	0.253649	-1.077841
13C	-0.519117	0.253649	1.077841
14C	1.580984	0.318205	1.080955
15C	1.580985	0.318205	-1.080953
16C	-1.211767	-0.132340	0.000000
17C	1.604700	1.111027	0.000001
18C	-0.583332	1.058335	0.000000
19C	2.308518	-0.026690	0.000002
20C	0.467129	-1.519691	-1.089047
21C	0.467128	-1.519691	1.089047
22C	-0.203020	-1.914463	0.000000

N = 23

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.098435	0.000000	0.000000
3A	0.549218	-0.951272	0.000000
4A	0.549218	-0.317091	0.907038
5A	0.549218	-0.317091	-0.907038
6B	0.549217	0.824379	-0.611083
7B	0.549217	0.824379	0.611083
8B	1.537760	-0.887825	0.611083
9B	-0.439324	-0.887826	0.611083
10B	1.537760	-0.887825	-0.611083
11B	-0.439324	-0.887826	-0.611083
12C	0.549218	-1.529425	-1.080281
13C	1.599130	0.289077	1.080281
14C	0.549218	-1.529425	1.080281
15C	-0.500695	0.289076	1.080282
16C	-0.500695	0.289076	-1.080282
17C	1.599130	0.289077	-1.080282
18C	-0.543341	1.087520	0.000000
19C	1.219368	-1.965580	0.000000
20C	-0.120931	-1.965580	0.000000
21C	1.641776	1.087521	0.000000
22C	-1.213491	-0.073214	0.000000
23C	2.311926	-0.073212	0.000000

N = 24

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099134	0.000000	0.000000
3A	0.549567	-0.951665	0.000000
4A	0.549567	-0.318399	0.902345
5A	0.549567	-0.317579	-0.906545
6B	0.549568	0.820481	0.616272
7B	-0.439446	-0.887122	0.611047
8B	1.538580	-0.887122	0.611047
9B	0.549568	0.824791	-0.607700
10B	1.537270	-0.888532	-0.611407
11B	-0.438137	-0.888532	-0.611407
12C	-0.513603	0.287056	1.071580
13C	1.612738	0.287055	1.071579
14C	0.549567	-1.523962	1.084964
15C	-0.498162	0.289885	-1.081105
16C	1.597297	0.289884	-1.081106
17C	0.549567	-1.531609	-1.078469
18C	-0.541514	1.087885	0.001267
19C	1.640650	1.087884	0.001267
20C	-1.214833	-0.074607	-0.007283
21C	2.313967	-0.074608	-0.007283
22C	-0.120162	-1.965215	0.004001
23C	1.219295	-1.965216	0.004001
24C	0.549568	0.441130	1.849990

N = 25

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099039	0.000000	0.000000
3A	0.549916	-0.951567	0.000000
4A	0.550146	-0.317474	0.901677
5A	0.549977	-0.317377	-0.906442
6B	0.548565	0.821379	0.612736
7B	-0.436684	-0.885943	0.612736
8B	1.538079	-0.887583	0.610709
9B	0.550291	0.823968	-0.609920
10B	-0.438061	-0.888732	-0.609920
11B	1.537548	-0.887277	-0.612122
12C	-0.517253	0.298492	1.063503
13C	1.608939	0.285381	1.073751
14C	0.557962	-1.535841	1.073751
15C	-0.498045	0.287408	-1.082591
16C	0.548624	-1.529670	-1.080430
17C	1.598924	0.290378	-1.080430
18C	-0.541693	1.089601	-0.006849
19C	-1.214437	-0.076187	-0.006849
20C	-0.120600	-1.964590	0.002694
21C	1.640632	1.087421	0.002693
22C	1.222055	-1.965811	-0.004711
23C	2.313501	-0.074462	-0.004712
24C	0.545434	0.458330	1.844294
25C	-0.123918	-0.701577	1.844294

N = 26

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099114	0.000000	0.000000
3A	0.549557	-0.951860	0.000000
4A	0.549556	-0.317287	0.899258
5B	1.535496	-0.886520	0.612284
6B	0.549557	0.821178	0.612284
7B	-0.436384	-0.886520	0.612281
8A	0.549558	-0.317286	-0.906171

9C	1.612958	0.296668	1.065731
10C	0.549555	-1.545198	1.065729
11C	-0.513846	0.296669	1.065729
12B	-0.438315	-0.887635	-0.610566
13B	0.549558	0.823411	-0.610564
14B	1.537431	-0.887635	-0.610564
15C	-0.499346	0.288300	-1.081566
16C	0.549558	-1.528457	-1.081565
17C	1.598463	0.288299	-1.081564
18C	-0.541252	1.089288	-0.004391
19C	-0.123167	-1.965243	-0.004392
20C	1.222281	-1.965243	-0.004390
21C	1.640367	1.089287	-0.004389
22C	-1.213977	-0.075904	-0.004393
23C	2.313091	-0.075905	-0.004388
24C	-0.121699	-0.704836	1.842834
25C	1.220808	-0.704836	1.842835
26C	0.549555	0.457809	1.842835

N = 27

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099967	0.000000	0.000000
3A	0.549984	-0.952109	0.000000
4A	0.549983	-0.317355	0.898809
5A	0.549983	-0.318316	-0.901678
6B	0.549983	0.821124	0.610009
7B	1.535207	-0.887297	0.612254
8B	-0.435239	-0.887297	0.612254
9B	0.549983	0.819534	-0.615430
10B	1.538222	-0.887006	-0.610716
11B	-0.438254	-0.887006	-0.610716
12C	1.612366	0.297106	1.066034
13C	-0.512400	0.297105	1.066034
14C	0.549984	-1.546466	1.064584
15C	1.612632	0.286409	-1.072419
16C	-0.512666	0.286409	-1.072419
17C	0.549984	-1.523063	-1.086128
18C	-0.539167	1.089614	-0.005207
19C	1.639132	1.089615	-0.005207
20C	-1.215730	-0.077982	0.002387
21C	2.315696	-0.077981	0.002388
22C	1.222039	-1.964856	-0.007966
23C	-0.122071	-1.964856	-0.007966
24C	1.220883	-0.705329	1.842305
25C	-0.120917	-0.705330	1.842305
26C	0.549983	0.458074	1.842265
27C	0.549983	0.441086	-1.849857

N = 28

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099745	0.000000	0.000000
3A	0.550467	-0.952063	0.000000
4A	0.550132	-0.317389	-0.898968
5A	0.550409	-0.317550	0.901160
6B	0.550635	0.820576	-0.611552
7B	-0.434768	-0.887422	-0.611553
8B	1.535616	-0.885949	-0.612772
9B	0.548994	0.820362	0.612195
10B	-0.435404	-0.885896	0.612194
11B	1.537848	-0.887237	0.610503
12C	-0.512294	0.295560	-1.067057
13C	0.549808	-1.545512	-1.065757
14C	1.613172	0.297617	-1.065755
15C	-0.516537	0.298007	1.064127
16C	1.608769	0.284808	1.074648
17C	0.558692	-1.535291	1.074647
18C	-0.539189	1.091925	-0.002280
19C	-1.215180	-0.079769	-0.002280
20C	-0.122420	-1.964208	0.006622
21C	1.639164	1.089147	0.006624
22C	1.225808	-1.965422	-0.000140
23C	2.315058	-0.077424	-0.000139
24C	1.221510	-0.704729	-1.842620
25C	0.550465	0.457700	-1.842895
26C	-0.120705	-0.705639	-1.842896
27C	-0.123607	-0.701703	1.844235
28C	0.545603	0.458238	1.844235

N = 29

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099744	0.000000	0.000000
3A	0.549871	-0.952407	0.000000
4A	0.549872	-0.317469	-0.898836
5A	0.549872	-0.317469	0.898836
6B	1.535061	-0.886270	-0.611889
7B	1.535061	-0.886270	0.611889
8B	-0.435319	-0.886269	-0.611888
9B	0.549872	0.820131	-0.611889
10B	-0.435319	-0.886269	0.611888
11B	0.549872	0.820131	0.611889
12C	0.549871	-1.544933	1.066402
13C	1.612886	0.296262	1.066402
14C	0.549871	-1.544933	-1.066402
15C	-0.513143	0.296263	1.066402
16C	1.612886	0.296262	-1.066402
17C	-0.513143	0.296263	-1.066402
18C	-1.214724	-0.079116	0.000000
19C	-0.538846	1.091539	0.000000
20C	1.638589	1.091539	0.000000
21C	1.225749	-1.964831	0.000000
22C	2.314467	-0.079117	0.000000
23C	-0.126008	-1.964830	0.000000
24C	0.549871	0.457608	1.842815
25C	-0.121366	-0.705008	1.842815
26C	1.221108	-0.705009	-1.842815
27C	0.549871	0.457608	-1.842815
28C	1.221108	-0.705009	1.842815
29C	-0.121366	-0.705008	-1.842815

N = 30

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094922	0.000000	0.000000
3A	0.547461	-0.949261	0.000000
4A	0.547461	-0.317983	-0.893014
5A	0.547461	-0.304359	0.895107
6B	0.547461	0.831740	0.588096
7A	0.547461	0.747937	-0.589813
8B	-0.437619	-0.878218	-0.618991
9B	1.532541	-0.878218	-0.618991
10B	-0.443389	-0.873789	0.607467
11B	1.538311	-0.873789	0.607467
12C	1.613742	0.320717	1.044220
13C	-0.518821	0.320716	1.044220
14B	1.541574	0.277879	-1.025537
15B	-0.446653	0.277879	-1.025537
16C	0.547461	-1.527603	1.067220
17C	0.547461	-1.529324	-1.080032
18C	-0.518720	1.092037	-0.054674
19C	1.613641	1.092037	-0.054674
20C	0.547460	0.511246	-1.785530
21C	-1.208307	-0.057902	-0.035568
22C	2.303229	-0.057900	-0.035568
23C	1.222236	-1.954526	-0.004494
24C	-0.127313	-1.954527	-0.004494
25C	0.547460	0.487750	1.820501
26C	-0.125116	-0.655311	-1.840489
27C	1.220038	-0.655310	-1.840489
28C	-0.125875	-0.675280	1.835452
29C	1.220797	-0.675279	1.835453
30C	0.547460	1.880192	-0.150742

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.097749	0.000000	0.000000
3A	0.545232	-0.949004	0.000000
4A	0.548361	-0.317506	-0.895741
5A	0.543421	-0.307005	0.896148
6A	0.551259	0.744565	-0.588160
7B	0.542713	0.827595	0.592371
8B	-0.440200	-0.877317	-0.615230
9B	1.531389	-0.880635	-0.617975
10B	-0.447154	-0.873992	0.607063
11B	1.531455	-0.878340	0.611840
12B	-0.448935	0.277842	-1.021041
13C	1.594409	0.309182	-1.067363
14C	-0.523931	0.316340	1.046421
15C	1.605152	0.313641	1.056902
16C	0.540498	-1.533275	-1.074798
17C	0.540244	-1.531030	1.067434
18C	-0.522638	1.089216	-0.043208
19C	1.613867	1.098592	-0.022857
20C	0.526364	0.492056	-1.804860
21C	-1.210809	-0.056530	-0.035709
22C	2.307540	-0.066602	-0.007368
23C	1.217347	-1.956744	-0.002646
24C	-0.133282	-1.955242	-0.002272
25C	-0.142885	-0.664299	-1.833598
26C	0.537750	0.481987	1.825914
27C	1.200058	-0.680625	-1.851811
28C	-0.134045	-0.680722	1.835583
29C	1.210554	-0.683180	1.840827
30C	0.544257	1.876180	-0.144824
31C	-0.131471	1.502917	-1.245647

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.095982	0.000000	0.000000
3A	0.547990	-0.948454	0.000000
4A	0.547990	-0.318179	0.893492
5A	0.547991	-0.303599	-0.894750
6A	0.547991	0.741051	0.586168
7B	0.547992	0.831934	-0.586852
8B	1.533245	-0.877061	0.618685
9B	-0.437266	-0.877059	0.618684
10B	1.539553	-0.872850	-0.607215
11B	1.539553	0.279212	1.025972
12B	-0.443572	-0.872848	-0.607216
13B	-0.443573	0.279213	1.025970
14C	-0.518417	0.320529	-1.044516
15C	-0.518417	1.091515	0.048450
16C	1.614401	0.320527	-1.044515
17C	1.614401	1.091513	0.048452
18C	0.547989	-1.529425	1.078868
19C	0.547989	0.493088	1.795919
20C	0.547990	-1.526431	-1.066992
21C	-1.207214	-0.054589	0.038507
22C	2.303196	-0.054592	0.038510
23C	-0.127067	-0.659207	1.838991
24C	-0.127067	-1.953568	0.004079
25C	1.223045	-1.953569	0.004079
26C	1.223045	-0.659208	1.838992
27C	0.547992	1.878079	0.149700
28C	0.547992	0.489015	-1.819465
29C	1.221128	-0.674565	-1.835388
30C	1.221127	1.502731	1.251194
31C	-0.125146	-0.674564	-1.835388
32C	-0.125147	1.502732	1.251192

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.100406	0.000000	0.000000
3A	0.537367	-0.942996	0.000000
4A	0.537368	-0.294045	0.895979
5A	0.534546	0.759567	0.557182
6A	0.534544	-0.292554	-0.895436
7A	0.540972	0.766456	-0.555139
8C	1.580380	-0.904678	0.655250
9C	1.578105	-0.902222	-0.658793
10C	1.578108	0.344614	1.062662
11B	-0.466805	-0.845214	0.612183
12B	-0.469195	0.315843	0.991899
13B	-0.469198	-0.843957	-0.609388
14B	-0.470547	1.039411	0.001968
15B	-0.470549	0.322240	-0.988199
16C	1.572717	0.350990	-1.066530
17C	1.572719	1.122798	-0.000928
18C	0.497608	-1.504412	1.089634
19C	0.493897	-1.503691	-1.089232
20C	0.493901	0.566044	1.768362
21C	0.486166	0.562151	-1.771034
22C	0.486169	1.858022	0.018120
23C	-1.212921	-0.003073	0.002228
24C	2.310473	0.003543	-0.002569
25C	-0.179562	-1.923789	0.000715
26C	-0.179560	-0.600553	1.827649
27C	-0.187538	-0.600949	-1.823875
28C	-0.187533	1.545552	1.139707
29C	1.150720	-1.982171	-0.001760
30C	1.150722	-0.616409	1.883890
31C	1.144173	-0.618155	-1.885210
32C	1.144178	1.598462	1.175179
33C	-0.159092	1.557565	-1.128132

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.101884	0.000000	0.000000
3A	0.537285	-0.941797	0.000000
4A	0.537285	-0.291032	0.895701
5A	0.537284	-0.291032	-0.895702
6A	0.537284	0.761929	0.553574

7A	0.537284	0.761929	-0.553574
8C	1.579039	0.345469	-1.063244
9C	1.579039	1.117961	0.000000
10C	1.579040	-0.904449	-0.657121
11C	1.579040	0.345469	1.063244
12C	1.579041	-0.904449	0.657120
13B	-0.468168	-0.842120	0.611835
14B	-0.468169	-0.842120	-0.611834
15B	-0.468169	0.321659	0.989970
16B	-0.468171	0.321659	-0.989969
17B	-0.468171	1.040914	0.000000
18C	0.494813	-1.501205	1.090689
19C	0.494811	-1.501206	-1.090689
20C	0.494811	0.573408	1.764772
21C	0.494809	0.573408	-1.764772
22C	0.494809	1.855590	0.000000
23C	-1.212082	-0.000002	0.000001
24C	2.312869	0.000001	-0.000001
25C	-0.181065	-1.920919	0.000001
26C	-0.181064	-0.593598	1.826902
27C	-0.181067	-0.593598	-1.826901
28C	-0.181067	1.554054	1.129088
29C	-0.181068	1.554054	-1.129087
30C	1.148391	-1.981990	0.000000
31C	1.148391	-0.612469	1.884984
32C	1.148389	-0.612469	-1.884984
33C	1.148388	1.603463	1.164984
34C	1.148388	1.603463	-1.164985

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094222	0.000000	0.000000
3A	0.550820	-0.945473	0.000000
4A	0.550819	-0.316580	0.890897
5A	0.540827	-0.310834	-0.891525
6A	0.540826	0.735983	0.591409
7A	-0.363689	-0.837793	0.591405
8B	-0.446711	-0.882238	-0.585977
9B	0.537439	0.830097	-0.585972
10B	-0.446713	0.256742	1.027519
11B	1.530632	-0.879719	0.621003
12B	1.535306	0.272802	1.033402
13B	1.535307	-0.882404	-0.603077
14B	0.537136	-1.463925	1.033399
15C	-0.532529	0.306070	-1.035042
16C	-0.532531	1.077778	0.058170
17C	-1.199335	-0.082402	0.058167
18C	0.535761	-1.543062	-1.045758
19C	-0.135307	-0.698879	1.804148
20C	-0.135305	-1.934016	0.054436
21C	1.602996	1.090474	0.054444
22C	0.535758	0.468715	1.804151
23C	1.602997	0.313834	-1.045755
24C	2.297388	-0.054571	0.038524
25C	1.203632	-1.957610	0.038520
26C	1.203629	-0.691780	1.831711
27C	0.530058	0.472664	-1.817373
28C	-1.349601	-1.399705	0.163141
29C	-0.141584	1.479443	1.264285
30C	0.530056	1.870732	0.163150
31C	-1.349603	-0.622402	1.264279
32C	-0.141580	-0.695928	-1.817376
33C	1.205178	-0.692662	-1.827971
34C	1.205175	1.490522	1.264756
35C	-0.681233	-1.791659	1.264747

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099379	0.000000	0.000000
3A	0.538505	-0.941115	0.000000
4A	0.538504	-0.291483	0.894838
5A	0.531602	-0.293498	-0.894461
6A	0.531602	0.759576	0.556099
7A	0.530270	0.760745	-0.552283
8A	-0.394526	-0.812886	0.590136
9B	-0.469359	-0.843384	-0.597879
10B	-0.469359	0.307266	0.987088
11C	1.574643	-0.907663	0.658943
12C	1.573332	0.343165	1.066842
13C	1.573332	-0.908096	-0.656714
14B	-0.478750	0.316015	-0.984456
15B	-0.478750	1.033924	0.004431
16C	1.571191	1.117807	0.002525
17C	1.571191	0.343808	-1.063623
18C	0.481565	-1.498387	1.087794
19C	-1.206363	-0.018895	0.013717
20C	0.483144	0.561787	1.768058
21C	0.483145	-1.507121	-1.081767
22C	0.482750	1.851416	0.005147
23C	0.482750	0.568529	-1.761971
24C	-0.196711	-0.613823	1.802315
25C	-0.196710	-1.903805	0.025424
26C	2.307077	-0.000886	0.000644
27C	-0.194171	1.541107	1.134906
28C	-0.194170	-0.601786	-1.816832
29C	-0.192859	1.548903	-1.124468
30C	1.135947	-0.619245	1.886975
31C	1.135948	-1.985981	0.004359
32C	1.136272	1.598712	1.171461
33C	1.136272	-0.618702	-1.882926
34C	1.137282	1.602141	-1.163117
35C	-1.394114	-1.332360	0.137318
36C	-1.394114	-0.543225	1.224314

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.098561	0.000000	0.000000
3A	0.539001	-0.941990	0.000000
4A	0.539001	-0.295098	0.894574
5A	0.529622	-0.293739	-0.894051
6A	0.529623	0.757028	0.559034
7A	0.527860	0.761240	-0.550474
8A	-0.392996	-0.809814	0.585600
9B	-0.470110	-0.845572	-0.595215
10B	-0.470110	0.300361	0.989473
11C	1.581359	-0.905642	0.654895
12C	1.571911	-0.907027	-0.659125
13C	1.571912	0.341801	1.067856
14B	-0.481504	0.315010	-0.982398
15B	-0.481503	1.031631	0.008604
16C	1.567665	0.345870	-1.063946
17C	1.567665	1.118741	0.004844
18C	0.501188	-1.499737	1.084503
19C	-1.207126	-0.020567	0.014873
20C	0.479703	0.552243	1.770937
21C	0.479702	-1.508792	-1.079228
22C	-0.199808	-0.632825	1.794538
23C	-0.199808	-1.902453	0.038796
24C	0.478294	1.850130	0.010657
25C	0.478293	0.569473	-1.760339
26C	2.306488	0.003318	-0.002400
27C	-0.197818	1.534278	1.140901
28C	-0.197819	-0.602826	-1.814460
29C	-0.197523	1.548638	-1.119864
30C	1.135687	-1.986710	0.001020
31C	1.135687	-0.623348	1.886387
32C	-1.398708	-0.542743	1.221679
33C	-1.398708	-1.330210	0.132708
34C	1.132045	1.594848	1.177020
35C	1.132045	-0.618152	-1.883296
36C	1.132428	1.604269	-1.160091
37C	-0.787202	-1.734691	1.254407

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.088825	0.000000	0.000000
3A	0.537122	-0.943279	0.000000
4A	0.521749	-0.299795	0.894143
5A	0.517646	-0.296948	-0.893152
6A	0.513334	0.756133	0.558938
7A	0.511201	0.758903	-0.554071
8A	-0.403662	-0.812015	0.562930
9A	-0.409231	-0.823090	-0.560156
10B	-0.492535	0.294318	0.977744
11B	-0.500731	0.296342	-0.970667
12B	-0.507837	1.017865	0.005135
13C	1.564449	-0.910231	0.657882
14C	1.559549	-0.908919	-0.663227
15C	1.551169	0.338569	1.071064
16C	1.547324	0.343189	-1.070471
17C	1.548082	1.119064	0.001853
18C	0.470732	-1.509532	1.073144
19B	-1.134080	-0.050973	0.004641
20C	0.458102	-1.506697	-1.075981
21C	-0.215771	-1.891252	0.004340
22C	0.450878	0.543850	1.768073
23C	-0.244663	-0.647458	1.771446
24C	0.444938	0.553412	-1.761672
25C	0.451096	1.843324	0.005309
26C	-0.246225	-0.629974	-1.774354
27C	-1.386656	-1.287413	0.023011
28C	2.290492	0.003338	-0.002528
29C	-0.222045	1.527939	1.135538
30C	-0.227153	1.532095	-1.123667
31C	-1.433609	-0.541818	1.144609
32C	1.122151	-1.991388	-0.003326
33C	1.098892	-0.634988	1.886939
34C	1.095239	-0.626458	-1.888299
35C	1.108952	1.593066	1.176753
36C	1.104748	1.599112	-1.169050
37C	-0.837983	-1.736861	1.189177
38C	-1.433707	-0.567389	-1.127492

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.087407	0.000000	0.000000
3A	0.538806	-0.944533	0.000000
4A	0.518082	-0.300911	-0.893626
5A	0.518081	-0.300911	0.893626
6A	-0.404590	-0.816857	-0.557458
7A	-0.404591	-0.816857	0.557458
8A	0.509057	0.756181	-0.557458
9A	0.509057	0.756181	0.557458
10B	-0.499402	0.290061	-0.974449
11B	-0.499402	0.290061	0.974448
12B	-1.134690	-0.057072	0.000000
13B	-0.512661	1.013882	0.000000
14C	1.563391	-0.908045	0.660682
15C	1.563391	-0.908045	-0.660682
16C	1.545401	0.340961	1.072019
17C	1.545401	0.340961	-1.072019
18C	0.469578	-1.511296	-1.072018
19C	0.469578	-1.511296	1.072019
20C	1.543205	1.119910	0.000000
21C	-0.208113	-1.895355	0.000000
22C	-0.252655	-0.653113	-1.765887
23C	-0.252656	-0.653113	1.765887
24C	0.442110	0.543074	1.765887
25C	0.442111	0.543074	-1.765887
26C	-1.378962	-1.298322	0.000000
27C	0.444465	1.841093	0.000000
28C	1.127822	-1.991494	0.000000
29C	2.288663	0.007141	0.000000
30C	-1.439130	-0.555493	1.130323
31C	-1.439129	-0.555493	-1.130324
32C	-0.230576	1.525287	1.130324
33C	-0.230576	1.525287	-1.130324
34C	1.091822	-0.634150	1.888015
35C	1.091823	-0.634150	-1.888015
36C	-0.840099	-1.746321	1.174530
37C	-0.840098	-1.746321	-1.174530
38C	1.100606	1.595013	1.174530
39C	1.100607	1.595013	-1.174530

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.070518	0.000000	0.000000
3A	0.497133	-0.942919	0.000000
4A	0.497133	-0.295394	-0.895455
5A	0.491041	-0.292244	0.894197
6A	0.491041	0.757632	-0.557663
7A	0.488121	0.761625	0.550749
8A	-0.443491	-0.775849	-0.561036
9A	-0.456159	-0.787379	0.561316
10A	-0.456159	0.286393	-0.923590
11A	-0.464876	0.292058	0.912669
12A	-0.464876	0.958222	-0.008561
13A	-1.061338	-0.013484	-0.009750
14C	1.519459	-0.916190	-0.662520
15C	1.516387	0.347198	-1.076290
16C	1.516387	-0.913344	0.666896
17C	1.510274	0.352635	1.075892
18C	1.510274	1.132206	-0.002167
19C	0.396839	-1.493882	-1.080263
20C	0.392434	0.556685	-1.753542
21C	0.392434	-1.490877	1.078006
22C	-0.304629	-1.852504	-0.009202
23C	-0.304629	-0.589084	-1.756370
24C	0.382730	0.567572	1.745235
25C	0.382730	1.835190	-0.007739
26C	-0.315760	1.482394	-1.095162
27C	-0.315760	-0.575636	1.750861

28C	-0.323039	1.488855	1.076628
29C	-1.453510	-1.166536	-0.018096
30C	-1.453510	-0.382633	-1.102146
31C	-1.468304	-0.371402	1.075795
32C	-1.468304	0.905291	-0.689727
33C	-1.473378	0.913122	0.660301
34C	2.258815	0.003408	0.002464
35C	1.045645	-1.996095	-0.000103
36C	1.045645	-0.625426	-1.895584
37C	1.036651	-0.615572	1.897166
38C	1.036651	1.608823	-1.178922
39C	1.030252	1.616542	1.168962
40C	-0.946113	-1.645877	-1.190174

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.068606	0.000000	0.000000
3A	0.499165	-0.944856	0.000000
4A	0.492661	-0.296914	0.894822
5A	0.492661	-0.296914	-0.894822
6A	0.483948	0.758055	0.555507
7A	0.483948	0.758055	-0.555507
8A	-0.444208	-0.782006	0.555507
9A	-0.444208	-0.782006	-0.555507
10A	-0.465455	0.280518	0.918580
11A	-0.465455	0.280518	-0.918580
12A	-0.473878	0.951920	0.000000
13A	-1.063040	-0.025659	0.000000
14C	1.517750	-0.914710	-0.664940
15C	1.517750	-0.914710	0.664940
16C	0.394837	-1.497237	-1.077106
17C	0.394837	-1.497237	1.077106
18C	1.508285	0.350273	1.077106
19C	1.508285	0.350273	-1.077106
20C	-0.300545	-1.857980	0.000000
21C	1.502427	1.133636	0.000000
22C	-0.313629	-0.595429	1.750139
23C	-0.313629	-0.595429	-1.750139
24C	0.379974	0.555445	1.750139
25C	0.379974	0.555445	-1.750139
26C	0.371158	1.831576	0.000000
27C	-1.446096	-1.183739	0.000000
28C	-1.460681	-0.397980	-1.086486
29C	-1.460681	-0.397980	1.086486
30C	-0.330418	1.477430	-1.086486
31C	-0.330418	1.477430	1.086486
32C	-1.479566	0.891697	-0.675734
33C	-1.479566	0.891697	0.675734
34C	2.255862	0.006860	0.000000
35C	1.047688	-1.997826	0.000000
36C	1.037286	-0.625146	-1.896253
37C	1.037286	-0.625146	1.896253
38C	1.022832	1.611734	-1.176074
39C	1.022832	1.611734	1.176074
40C	-0.947303	-1.657253	-1.176074
41C	-0.947303	-1.657253	1.176074

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.066317	0.000000	0.000000
3A	0.494253	-0.944853	0.000000
4A	0.494253	-0.299247	0.896212
5A	0.484673	-0.293448	-0.895058
6A	0.484674	0.756043	0.561817
7A	-0.445269	-0.779901	0.561818
8A	-0.453604	-0.777898	-0.549282
9A	0.479036	0.762499	-0.549283
10A	-0.453603	0.274636	0.911817
11A	-0.475356	0.287805	-0.909134
12A	-0.475356	0.953484	0.014943
13A	-1.065207	-0.020745	0.014944
14C	1.515675	-0.917671	0.661063
15C	1.508766	0.346191	1.078658
16C	0.392577	-1.497366	1.078658
17C	1.508765	-0.913488	-0.669995
18C	-0.309973	-1.854334	0.004825
19C	0.380771	-1.493006	-1.077315
20C	1.499429	0.354630	-1.077316
21C	-0.309972	-0.591868	1.757347
22C	1.499430	1.134172	0.004824
23C	0.380772	0.549002	1.757347
24C	0.367051	0.564273	-1.743226
25C	-1.453360	-0.387983	1.108684
26C	-0.329865	-0.586790	-1.743226
27C	-1.453361	-1.174490	0.016876
28C	0.367052	1.832200	0.016875
29C	-0.329864	1.467643	1.108683
30C	-0.338992	1.484757	-1.069577
31C	-1.472756	0.891686	0.706611
32C	-1.472757	-0.387828	-1.069576
33C	-1.486796	0.900186	-0.648468
34C	2.252355	0.005783	-0.004167
35C	1.038872	-1.998469	-0.004166
36C	1.038873	-0.628990	1.896910
37C	1.021969	-0.618757	-1.899302
38C	-0.948973	-1.649757	1.188437
39C	1.021971	1.605560	1.188436
40C	1.014223	1.619172	-1.166406
41C	-0.964627	-1.649202	-1.166404
42C	-0.964626	0.584037	1.933718

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.063682	0.000000	0.000000
3A	0.488544	-0.944851	0.000000
4A	0.485396	-0.295463	-0.896594
5A	0.485396	-0.295463	0.896594
6A	0.479271	0.760698	-0.555624
7A	0.479271	0.760698	0.555624
8A	-0.455589	-0.775111	-0.555624
9A	-0.455589	-0.775111	0.555624
10A	-0.463592	0.282194	-0.901929
11A	-0.463592	0.282194	0.901929
12A	-0.477253	0.955447	0.000000
13A	-1.067908	-0.014892	0.000000
14C	1.505681	-0.916519	0.666300
15C	1.505681	-0.916519	-0.666300
16C	0.377127	-1.492574	1.079149
17C	0.377127	-1.492574	-1.079149
18C	1.499043	0.350536	1.079149
19C	1.499043	0.350536	-1.079149
20C	1.496086	1.134608	0.000000
21C	-0.320710	-1.850067	0.000000
22C	0.366285	0.558414	1.750594
23C	0.366285	0.558414	-1.750594
24C	-0.327796	-0.581839	1.750595
25C	-0.327796	-0.581839	-1.750595
26C	0.362788	1.833131	0.000000
27C	-1.461714	-1.164203	0.000000
28C	-0.338857	1.475624	1.091757
29C	-0.338857	1.475624	-1.091757
30C	-1.466408	-0.376742	1.091758
31C	-1.466408	-0.376742	-1.091758
32C	-1.480055	0.900923	0.680443
33C	-1.480055	0.900923	-0.680443
34C	2.248342	0.004398	0.000000
35C	1.028745	-1.999185	0.000000
36C	1.022075	-0.622144	1.900342
37C	1.022075	-0.622144	-1.900342
38C	1.012926	1.613087	1.178930
39C	1.012926	1.613087	-1.178930
40C	-0.967649	-1.640645	1.178931
41C	-0.967649	-1.640645	-1.178931
42C	-0.982364	0.597975	1.916537
43C	-0.982364	0.597975	-1.916537

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.061268	0.000000	0.000000
3A	0.480028	-0.944073	0.000000
4A	0.480028	-0.291735	0.897867
5A	0.480028	-0.291735	-0.897867
6A	0.480026	0.763772	-0.554913
7A	0.480027	0.763772	0.554913
8A	-0.465361	-0.765788	0.556377
9A	-0.465362	-0.765788	-0.556376
10A	-0.465363	0.292503	0.900236
11A	-0.465363	0.292503	-0.900236
12A	-0.465364	0.946563	0.000000
13A	-1.070526	-0.000002	0.000000
14C	1.496079	1.135043	0.000000
15C	1.496081	0.350748	1.079489
16C	1.496082	-0.918267	-0.667161
17C	1.496082	-0.918268	0.667161
18C	1.496080	0.350748	-1.079490
19C	0.362517	-1.487130	-1.080463
20C	0.362517	-1.487130	1.080463
21C	0.362513	1.838193	0.000000
22C	0.362515	0.568033	1.748226
23C	0.362514	0.568033	-1.748226
24C	-0.337799	1.489170	-1.081946
25C	-0.337796	-0.568814	-1.750625
26C	-0.337795	-0.568814	1.750625
27C	-0.337794	-1.840717	0.000000
28C	-0.337798	1.489170	1.081946
29C	-1.474181	-0.354020	1.089556
30C	-1.474182	-0.354021	-1.089554
31C	-1.474183	0.926829	-0.673382
32C	-1.474180	-1.145628	0.000001
33C	-1.474182	0.926829	0.673383
34C	2.244608	0.000002	0.000000
35C	1.012471	-2.000234	0.000000
36C	1.012468	-0.618106	1.902337
37C	1.012468	-0.618106	-1.902337
38C	1.012466	1.618225	1.175709
39C	1.012465	1.618225	-1.175709
40C	-0.985138	-1.624534	-1.180291
41C	-0.985137	-1.624534	1.180292
42C	-0.985140	0.620514	1.909752
43C	-0.985141	0.620513	-1.909752
44C	-0.985141	2.008031	0.000000

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.056965	0.000000	0.000000
3A	0.472689	-0.945378	0.000000
4A	0.472690	-0.292138	-0.899108
5A	0.472690	0.764827	-0.555679
6A	0.472689	-0.292138	0.899108
7A	0.472689	0.764827	0.555679
8A	-0.472689	-0.764827	-0.555679
9A	-0.472688	0.292138	-0.899108
10A	-0.472689	-0.764827	0.555680
11A	-0.472689	0.945378	0.000000
12A	-0.472689	0.292138	0.899108
13A	-1.056965	0.000000	0.000000
14C	0.351124	0.568131	1.748527
15C	1.487386	0.351124	1.080649
16C	1.487386	-0.919255	0.667878
17C	1.487387	-0.919255	-0.667877
18C	1.487387	0.351124	-1.080649
19C	0.351125	-1.487386	1.080649
20C	-1.487385	-0.351124	-1.080649
21C	0.351125	-1.487386	-1.080649
22C	-1.487385	0.919255	-0.667879
23C	-0.351124	-0.568131	1.748527
24C	-0.351124	1.487386	1.080649
25C	-0.351123	-0.568132	-1.748527
26C	1.487387	1.136261	0.000000
27C	-1.487386	0.919255	0.667877
28C	-0.351124	-1.838510	0.000001
29C	-1.487386	-0.351124	1.080649
30C	0.351125	1.838510	0.000000
31C	0.351125	0.568130	-1.748527
32C	-1.487386	-1.136262	0.000000
33C	-0.351123	1.487386	-1.080649
34C	2.238454	0.000000	0.000000
35C	1.001067	-2.002134	0.000001
36C	1.001068	-0.618694	-1.904142
37C	1.001067	-0.618693	1.904143
38C	1.001068	1.619760	-1.176825
39C	1.001067	1.619760	1.176825
40C	-1.001067	-1.619761	-1.176824
41C	-1.001067	-1.619760	1.176826
42C	-1.001065	0.618693	-1.904143
43C	-1.001066	2.002134	0.000000
44C	-1.001067	0.618694	1.904143
45C	-2.238454	0.000000	-0.000001

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.057244	0.000000	0.000000
3A	0.475427	-0.944317	0.000000
4A	0.467917	-0.288295	0.902194
5A	0.467917	-0.288295	-0.902194
6A	0.472587	0.765238	0.555458
7A	0.472587	0.765238	-0.555458
8A	-0.470986	-0.766224	0.555458
9A	-0.470986	-0.766224	-0.555458
10A	-0.474657	0.292449	0.898655
11A	-0.474657	0.292449	-0.898655
12A	-0.473409	0.944971	0.000000

13A	-1.056921	-0.002095	0.000000
14C	1.472624	-0.907321	-0.687180
15C	1.472624	-0.907321	0.687180
16C	1.487474	0.353902	1.081831
17C	0.352793	-1.487738	1.081831
18C	1.487474	0.353902	-1.081831
19C	0.352793	-1.487738	-1.081831
20C	0.348079	0.571872	1.749009
21C	0.348079	0.571872	-1.749009
22C	-0.354263	-0.568061	1.749009
23C	-0.354263	-0.568061	-1.749009
24C	0.353167	1.837326	0.000000
25C	-1.482263	-1.141661	0.000000
26C	-0.352539	1.487919	1.079517
27C	-1.487522	-0.354210	1.079517
28C	-0.352539	1.487919	-1.079517
29C	-1.487522	-0.354210	-1.079517
30C	-1.489140	0.917498	-0.667111
31C	-1.489140	0.917498	0.667111
32C	1.493205	1.128567	0.000000
33C	-0.336552	-1.841211	0.000000
34C	2.240022	-0.050676	0.000000
35C	1.052567	-1.977971	0.000000
36C	0.992502	-0.611506	1.912829
37C	0.992502	-0.611506	-1.912829
38C	-1.004036	0.618613	1.903133
39C	-1.004036	0.618613	-1.903133
40C	1.001461	1.620739	1.175093
41C	1.001461	1.620739	-1.175093
42C	-0.997283	-1.623313	1.175093
43C	-0.997283	-1.623313	-1.175093
44C	-1.001641	2.001584	0.000000
45C	-2.238213	-0.005426	0.000000
46C	2.416143	-1.488643	0.000000

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.055220	0.000000	0.000000
3A	0.468966	-0.943893	0.000000
4A	0.468967	-0.282811	0.900529
5A	0.474821	0.766871	0.552686
6A	0.474820	-0.297523	-0.897236
7A	-0.465796	-0.765843	0.562209
8A	0.477663	0.759966	-0.557894
9A	-0.469114	0.293895	0.901310
10A	-0.469115	-0.771844	-0.550444
11A	-0.470069	0.943832	-0.002185
12A	-0.470070	0.284879	-0.899814
13A	-1.054245	-0.005121	0.003761
14A	1.352989	-0.848213	0.622677
15C	1.484222	0.349248	1.073895
16C	1.484221	-0.919916	-0.654966
17C	0.378030	-1.475477	1.083155
18C	0.363026	0.568291	1.750410
19C	0.363024	-1.499720	-1.066643
20C	0.359719	1.834295	-0.006568
21C	0.359717	0.555862	-1.748055
22C	-0.344670	1.488026	1.078441
23C	-0.344673	-0.583049	-1.742786
24C	-1.476343	-0.354811	1.089969
25C	-1.476344	-1.146201	0.011934
26C	-0.345758	1.478714	-1.085529
27C	1.500717	1.122724	-0.001091
28C	1.500716	0.337433	-1.070817
29C	-1.484257	0.910682	-0.668533
30C	-1.482969	0.916631	0.669000
31C	-1.482971	-0.363619	-1.074963
32C	-0.330695	-0.567002	1.756268
33C	-0.330697	-1.845467	0.014737
34C	2.228428	-0.093995	0.069001
35C	1.064864	-0.636052	1.855101
36C	1.064863	-1.960450	0.051002
37C	1.009774	1.618920	1.171034
38C	1.009771	-0.632170	-1.895411
39C	-0.977529	-1.622625	1.191177
40C	-0.990152	0.619578	1.908426
41C	-0.990155	-1.635108	-1.162918
42C	1.012535	1.607638	-1.180174
43C	-0.995995	1.999491	-0.005202
44C	-0.995997	0.604056	-1.906069
45C	-2.233646	-0.010304	0.007567
46C	2.315213	-1.446944	0.227469
47C	2.315214	-0.650554	1.312313

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.054337	0.000000	0.000000
3A	0.465578	-0.945973	0.000000
4A	0.465577	-0.289769	-0.900499
5A	0.476596	-0.296627	0.896529
6A	0.476596	0.762570	-0.556990
7A	-0.473737	-0.764349	-0.556989
8A	0.481683	0.760913	0.554487
9A	-0.470004	-0.768182	0.554487
10A	-0.470005	0.292524	-0.901103
11A	-0.465807	0.289912	0.900454
12A	-0.465808	0.945973	0.000152
13A	-1.054439	0.000207	0.000153
14A	1.353610	-0.842468	-0.613916
15C	1.482774	-0.922857	0.651541
16C	1.482773	0.337534	-1.078073
17C	0.351925	-1.479424	-1.078073
18C	1.505232	0.336123	1.066814
19C	0.363106	0.556376	-1.753678
20C	0.363108	-1.498951	1.066814
21C	-0.338851	-0.571473	-1.753678
22C	-0.338849	-1.844431	-0.006818
23C	1.505231	1.118492	-0.006818
24C	0.367417	0.559968	1.745334
25C	-0.340170	-0.576927	1.745334
26C	0.367416	1.832962	-0.001574
27C	-1.482327	-1.139057	-0.001574
28C	-1.482328	-0.350414	-1.083818
29C	-0.340172	1.484711	-1.083818
30C	-0.336531	1.484299	1.081629
31C	-1.480350	-0.353498	1.081629
32C	-1.480351	0.921350	-0.667825
33C	-1.477939	0.919848	0.670307
34C	2.228223	-0.095311	-0.069455
35C	1.069460	-1.957119	-0.069455
36C	1.069460	-0.665616	-1.841763
37C	1.014067	-0.631141	1.893176
38C	1.014065	1.608841	-1.180713
39C	-0.995692	-1.620276	-1.180713
40C	1.022126	1.608365	1.172037
41C	-0.991705	-1.627299	1.172036
42C	-0.991707	0.617224	-1.908087
43C	-0.986830	0.614189	1.907528
44C	-0.986832	2.003967	0.000358
45C	-2.233769	0.000489	0.000359
46C	2.321260	-1.444719	-0.222427
47C	1.612059	-1.793764	-1.307137
48C	2.321259	-0.654277	-1.307137

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.049397	0.000000	0.000000
3A	0.473362	-0.946433	0.000000
4A	0.482161	0.750806	0.568618
5A	0.446831	-0.304173	0.898499
6A	0.486622	-0.288952	-0.894553
7A	0.490912	0.767222	-0.541530
8A	-0.475499	-0.770343	0.550739
9A	-0.469686	0.287461	0.905119
10A	-0.461595	-0.763785	-0.560282
11A	-0.454001	0.950757	0.013490
12A	-0.455355	0.302543	-0.897504
13A	-1.050831	0.005015	-0.000993
14A	1.354482	-0.817642	0.626232
15A	1.358176	0.259883	1.011630
16C	1.504791	-0.907863	-0.637320
17C	0.363881	-1.482399	1.084082
18C	1.517497	1.099149	0.036378
19C	0.379321	0.530219	1.756471
20C	1.517067	0.348165	-1.055647
21C	-0.347989	-0.584501	1.753959
22C	0.383835	0.579086	-1.733623
23C	-1.483016	-0.353842	1.078080
24C	-0.324140	-0.559832	-1.747594
25C	-0.315896	1.501930	-1.058255
26C	-1.477698	-1.136291	-0.012164
27C	-1.468559	0.926101	0.678050
28C	-1.467973	-0.338369	-1.087390
29C	-1.462612	0.936046	-0.660933
30C	0.397282	1.828718	0.040729
31C	0.383551	-1.488353	-1.068194
32C	-0.325740	-1.843367	-0.000116
33C	-0.312029	1.474707	1.108950
34C	2.215140	-0.039477	0.094367
35C	1.060271	-0.623833	1.846161
36C	1.118514	-1.933466	0.098465
37C	2.275631	-0.485709	1.330599
38C	1.118350	1.496768	1.225448
39C	1.034623	-0.614841	-1.886342
40C	1.044783	1.619810	-1.138152
41C	-0.993465	-1.629696	1.168636
42C	-0.981880	0.607012	1.916849
43C	-0.968954	0.640365	-1.901443
44C	-2.227907	0.011448	-0.005525
45C	-0.960272	2.013340	0.029458
46C	-0.975365	-1.618505	-1.185291
47C	2.359955	-1.362032	0.275762
48C	1.651030	-1.720654	1.349127
49C	2.360656	0.886924	1.060613

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.059098	0.000000	0.000000
3A	-0.455449	-0.956166	0.000000
4A	0.471625	-0.747043	-0.563947
5A	0.471624	-0.747042	0.563948
6A	0.476324	0.290058	-0.900993
7A	0.476324	0.290060	0.900993
8A	-0.466704	-0.305295	-0.900993
9A	-0.466704	-0.305294	0.900993
10A	0.476084	0.939960	-0.000001
11A	-1.053340	-0.025597	-0.000001
12A	-0.475239	0.752770	-0.558248
13A	-0.475239	0.752771	0.558246
14A	1.335261	-1.054714	0.000000
15A	0.378001	-1.659054	0.000000
16C	1.488666	-0.374278	-1.072046
17C	1.488666	-0.374278	1.072046
18C	-0.302276	-1.504937	1.072046
19C	-0.302275	-1.504938	-1.072046
20C	0.368453	-0.583620	-1.750770
21C	0.368452	-0.583618	1.750770
22C	-0.347075	0.549760	-1.750747
23C	-0.347075	0.549763	1.750745
24C	0.354115	1.476725	-1.080848
25C	0.354115	1.476727	1.080845
26C	-1.485487	0.315346	-1.080848
27C	-1.485487	0.315348	1.080846
28C	-0.355986	1.823187	-0.000002
29C	-1.492906	1.105426	-0.000002
30C	1.502581	0.896688	-0.665009
31C	1.502581	0.896689	0.665008
32C	-1.455703	-0.970939	-0.665009
33C	-1.455703	-0.970938	0.665009
34C	1.029660	-1.630957	-1.092052
35C	1.029659	-1.630957	1.092053
36C	1.428150	-2.262157	0.000001
37C	2.230294	-0.174697	0.000000
38C	-0.801384	-2.088662	0.000000
39C	1.013168	0.603746	-1.902213
40C	1.013168	0.603748	1.902212
41C	-0.980766	-0.655068	-1.902213
42C	-0.980767	-0.655065	1.902213
43C	-1.008657	1.597694	-1.180345
44C	-1.008657	1.597696	1.180341
45C	1.009734	1.988868	-0.000002
46C	-2.229795	-0.056314	-0.000001
47C	2.270308	-1.381014	0.666508
48C	2.270309	-1.381013	-0.666507
49C	0.270486	-2.643546	-0.666507
50C	0.270484	-2.643545	0.666508

TLJ (S_C = 1.3)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124044	0.000000	0.000000
3A	0.562022	-0.973450	0.000000
4C	0.562022	-0.324483	-1.111850
5C	0.562022	-0.324483	1.111850

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.512770	0.000000	0.000000
3C	0.756385	-1.033689	0.000000
4C	0.756385	0.000000	-1.033689
5C	0.756385	0.000000	1.033689

6C	0.756385	1.033689	0.000000

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2B	1.206218	0.000000	0.000000
3C	0.509459	-1.186589	0.000000
4C	0.509881	0.940273	0.723193
5C	0.509881	0.940273	-0.723193
6A	0.522159	-0.319983	0.940716
7A	0.522159	-0.319983	-0.940716

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.122610	0.000000	0.000000
3C	0.561305	-1.153397	0.000000
4C	0.561305	0.663861	-0.943193
5C	1.285717	-0.582634	-1.122567
6C	-0.163110	-0.582634	-1.122566
7C	0.561305	1.058833	0.457163
8C	0.561305	-0.235587	1.128993

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.279801	0.000000	0.000000
3C	0.434894	-1.203644	0.000000
4B	0.479150	-0.336343	-1.054882
5A	0.499135	-0.350371	0.950562
6C	0.424621	0.912132	0.772162
7C	-0.713560	-0.709309	0.772162
8C	0.435230	0.977760	-0.684958
9C	-0.771678	-0.741587	-0.684958

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.255488	0.000000	0.000000
3C	0.387708	-1.194124	0.000000
4C	0.387707	-0.281749	-1.160410
5C	-0.098448	0.983916	0.773607
6C	-0.966228	0.702165	-0.386804
7C	-0.966227	-0.210210	0.773606
8C	0.432408	-0.314234	1.156443
9C	-0.864814	-0.735416	-0.578222
10C	0.432407	1.049650	-0.578221

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.254360	0.000000	0.000000
3C	0.278272	-1.223104	0.000000
4C	-0.968470	-0.642795	-0.471487
5C	0.411930	-0.328737	-1.138273
6C	-0.697818	-0.444143	0.942977
7C	0.278271	0.778961	0.942976
8C	0.411929	1.086937	-0.471488
9C	-0.968470	0.772880	0.195297
10A	-0.562818	0.449152	-0.953612
11A	0.562819	-0.449153	0.953613

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.237327	0.000000	0.000000
3C	0.333635	-1.206011	0.000000
4C	-0.803366	0.585732	-0.780174
5A	-0.229070	-0.552421	-0.944349
6A	0.445643	0.326372	-0.968718
7C	0.321118	1.229349	-0.093570
8C	-0.810866	0.677824	0.673451
9C	-1.086119	-0.627953	-0.000276
10C	-0.222716	-0.563935	1.151607
11A	0.456784	0.470001	0.907573
12C	1.007325	-0.788197	-1.199759

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.130336	0.000000	0.000000
3A	0.590718	-0.963697	0.000000
4C	-0.527980	0.295640	1.159077
5C	-0.527980	0.295640	-1.159077
6C	-1.283988	-0.112099	0.000000
7C	-0.575444	1.153280	0.000000
8B	-0.414899	-0.947613	0.637426
9B	0.591084	0.848959	-0.637426
10B	0.591084	0.848959	0.637426
11B	-0.414899	-0.947613	-0.637426
12A	0.567748	-0.317908	-0.907333
13A	0.567748	-0.317908	0.907333

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.119572	0.000000	0.000000
3A	0.562984	-0.967724	0.000000
4A	0.562984	-0.323801	0.911945
5B	-0.421283	-0.939110	0.663106
6B	0.599893	0.836382	0.663105
7B	0.599892	-0.345029	-1.010048
8B	-0.462033	0.265739	1.083234
9B	-0.462034	-0.931880	-0.612872
10B	0.573152	0.867970	-0.612872
11C	-1.291952	-0.088922	0.062788
12C	-0.572806	1.161437	0.062788
13C	-0.572807	0.329450	-1.115501
14C	1.648201	-0.947966	0.669358

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.123139	0.000000	0.000000
3A	0.583544	-0.959644	0.000000
4A	0.563906	-0.317077	-0.912565
5A	0.538850	-0.302987	0.911874
6C	-0.471053	-1.040837	0.687346
7C	0.644581	0.943267	0.687344
8B	0.595361	0.838024	-0.661553
9B	-0.406705	-0.944104	-0.661552
10C	-0.565276	0.317848	1.126366
11B	-0.467078	0.262630	-1.079175
12C	-1.285606	-0.104873	-0.052960
13C	-0.578350	1.152949	-0.052962
14C	1.630086	-0.916576	0.740793
15C	1.652953	-0.929432	-0.707395

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.054978	0.000000	0.000000
3C	0.527489	-1.203548	0.000000
4C	0.527488	1.156827	0.000000
5A	0.527489	-0.370190	-0.921289
6A	0.527489	-0.370190	0.921289
7C	1.279155	0.618543	-1.093748
8C	-0.224176	0.618543	1.093749
9C	-0.224176	0.618543	-1.093749
10C	1.279154	0.618543	1.093748
11C	1.735769	-0.748604	0.732949
12C	1.735770	-0.748604	-0.732948
13C	-0.680793	-0.748603	0.732949
14C	-0.680792	-0.748603	-0.732949
15C	-1.168097	0.439406	-0.000001
16C	2.223076	0.439403	0.000001

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.062083	0.000000	0.000000
3C	0.536276	-1.170526	0.000000
4C	0.536276	0.575328	1.019376
5C	0.507120	0.587011	-1.005356
6B	1.162618	-0.610084	1.044872
7B	1.151783	1.206970	0.002947
8B	1.151783	-0.595808	-1.049666
9B	-0.125767	1.197734	0.021912
10B	-0.125767	-0.607784	-1.032301
11A	-0.036266	-0.558370	0.956303
12C	-0.902665	-0.876313	0.056251
13C	-0.902665	0.381731	0.790803
14C	1.992236	0.424424	0.732838
15C	1.992236	-0.846817	-0.009419
16C	1.980422	0.434003	-0.743303
17C	-0.966519	0.402503	-0.689355

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.150346	0.000000	0.000000
3A	0.570382	-0.948112	0.000000
4A	0.570382	0.767039	0.557286
5A	0.570382	-0.292983	-0.901708
6A	0.570382	0.767039	-0.557286
7A	0.570382	-0.292983	0.901708
8C	-0.475032	0.376909	-1.160005
9C	-0.475032	0.376909	1.160005
10C	-0.475032	-0.986759	0.716922
11C	-0.475032	1.219701	0.000000
12C	-0.475032	-0.986759	-0.716922
13C	-1.266964	0.000000	0.000000
14C	1.617651	1.218319	0.000000
15C	1.617651	-0.985640	-0.716110
16C	1.617651	-0.985640	0.716110
17C	1.617651	0.376481	1.158689
18C	1.617651	0.376481	-1.158689

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.141477	0.000000	0.000000
3A	0.570738	-0.948804	0.000000
4A	0.570738	-0.293196	-0.902366
5A	0.570739	0.767599	-0.557693
6A	0.570738	-0.293196	0.902366
7A	0.570739	0.767599	0.557693
8C	1.615692	0.376906	1.159996
9C	1.615692	-0.986752	0.716917
10C	1.615692	-0.986752	-0.716917
11C	1.615692	1.219693	0.000000
12C	-0.474215	0.376907	1.159997
13C	-0.474216	-0.986751	0.716917
14C	1.615692	0.376906	-1.159996
15C	-0.474216	-0.986751	-0.716917
16C	-0.474214	1.219694	0.000000
17C	-0.474215	0.376907	-1.159997
18C	-1.266465	0.000003	0.000000
19C	2.407942	0.000000	0.000000

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.126475	0.000000	0.000000
3A	0.565160	-0.955971	0.000000
4A	0.565159	-0.328720	0.897677
5A	0.557091	-0.293650	-0.901823
6A	0.557090	0.745857	0.585842
7A	0.552691	0.776315	-0.542451
8B	1.578960	-0.909905	0.635796
9A	-0.392576	-0.835265	0.583640
10C	-0.478236	0.297882	1.182284
11C	-0.478234	-1.007762	-0.686258
12C	1.603867	0.331811	1.172607
13C	1.603868	-0.987007	-0.714789
14C	-0.500328	0.364873	-1.132051
15C	-0.500329	1.188484	0.046639
16C	1.599522	0.385431	-1.146166
17C	1.599522	1.208808	0.032190
18C	-1.269146	-0.049510	0.034593
19C	2.395113	-0.008070	0.005639
20C	0.493620	-1.582728	1.105929

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.132759	0.000000	0.000000
3A	0.565026	-0.943255	0.000000
4A	0.562516	-0.335758	-0.900043
5A	0.576106	-0.284662	0.902895
6A	0.577663	0.740390	-0.589718
7A	0.586090	0.779510	0.536594
8C	-0.514685	-1.002255	-0.665504
9C	-0.471514	-0.962750	0.754115
10A	1.531660	-0.837008	-0.568446
11C	1.592386	-1.022069	0.695646
12C	1.614167	0.283496	-1.179509
13C	-0.478977	0.335797	-1.163083
14C	1.635000	0.361423	1.132777
15C	-0.453081	0.412218	1.156790
16C	1.640544	1.181729	-0.051769
17C	-0.456525	1.220214	-0.032382
18C	2.402124	-0.062306	-0.021984
19C	-1.267362	0.016808	0.023765
20C	0.700180	-1.588819	-1.125047
21C	0.121876	-2.107693	0.098880

N = 22

atom	X/σ	Y/σ	Z/σ
1A	0.000000	0.000000	0.000000
2A	1.112774	0.000000	0.000000
3A	0.554815	-0.970876	0.000000
4A	0.553931	-0.322103	0.892958
5A	0.553931	-0.322103	-0.892958
6A	0.540069	0.758918	0.569683
7A	0.540069	0.758918	-0.569684
8A	-0.390856	-0.844452	0.570136
9A	-0.390857	-0.844452	-0.570135
10B	1.565450	-0.909459	-0.633682
11B	1.565450	-0.909459	0.633682
12C	-0.502928	0.293155	1.155011
13C	-0.502929	0.293154	-1.155011
14C	1.589676	0.342788	-1.158699
15C	1.589676	0.342788	1.158699
16C	-0.530197	1.157917	0.000000
17C	1.586401	1.199897	0.000000
18C	-1.267965	-0.112231	0.000001
19C	2.383335	-0.017159	0.000000
20C	0.495828	-1.555959	-1.150821
21C	0.495829	-1.555959	1.150822
22C	-0.258538	-1.972692	0.000001

N = 23

atom	X/σ	Y/σ	Z/σ
1A	0.000000	0.000000	0.000000
2A	1.113583	0.000000	0.000000
3A	0.554440	-0.965746	0.000000
4A	0.554868	-0.321256	-0.892879
5A	0.554868	-0.321256	0.892879
6B	1.565518	-0.906397	-0.635914
7B	1.565518	-0.906397	0.635914
8A	-0.389062	-0.846402	-0.569471
9A	-0.389062	-0.846402	0.569471
10A	0.540324	0.758824	0.569471
11A	0.540324	0.758824	-0.569471
12C	-0.502783	0.291099	-1.154777
13C	-0.502783	0.291099	1.154777
14C	0.493802	-1.550294	1.158926
15C	1.590336	0.343627	1.158926
16C	0.493802	-1.550294	-1.158926
17C	1.590336	0.343627	-1.158926
18C	-1.267283	-0.115326	0.000000
19C	-0.530951	1.156459	0.000000
20C	1.587754	1.198645	0.000000
21C	-0.248990	-1.973758	0.000000
22C	1.204678	-2.056739	0.000000
23C	2.383483	-0.020719	0.000000

N = 24

atom	X/σ	Y/σ	Z/σ
1A	0.000000	0.000000	0.000000
2A	1.112625	0.000000	0.000000
3A	0.552087	-0.963275	0.000000
4A	0.556750	-0.324359	0.889990
5A	0.548446	-0.319277	-0.893494
6B	0.555338	0.834463	0.658646
7B	0.550344	0.851348	-0.620168
8A	-0.369361	-0.870632	0.580860
9A	1.483804	-0.878690	0.562246
10A	1.474708	-0.875461	-0.576734
11A	-0.379900	-0.872847	-0.561699
12C	1.671262	0.227770	1.148147
13B	-0.499603	0.213840	1.056294
14C	0.561669	-1.537688	1.163117
15C	0.540849	-1.543748	-1.151943
16C	-0.547519	0.251261	-1.142517
17C	1.638128	0.249426	-1.159756
18C	-1.277946	-0.186429	0.019319
19C	2.388374	-0.194533	-0.017681
20C	-0.184806	-1.997744	0.012772
21C	1.283177	-2.002807	-0.002022
22C	-0.618567	1.108571	0.031157
23C	1.727346	1.109325	0.008553
24C	0.494099	0.349730	1.957311

N = 25

atom	X/σ	Y/σ	Z/σ
1A	0.000000	0.000000	0.000000
2A	1.100881	0.000000	0.000000
3A	0.539267	-0.959755	0.000000
4A	0.540615	-0.316347	0.912272
5A	0.527980	-0.308956	-0.897649
6A	-0.386650	-0.833908	0.589017
7A	0.537607	0.745575	0.589016
8B	1.556813	-0.910991	0.614080
9B	1.535978	-0.898800	-0.658931
10A	0.522238	0.773607	-0.552652
11A	-0.418618	-0.834242	-0.552651
12A	-0.425048	0.248724	0.959851
13C	1.618092	0.319398	1.141972
14C	0.514170	-1.567119	1.141973
15C	-0.533996	1.156406	0.066018
16C	-1.269740	-0.100923	0.066020
17C	-0.539327	0.315594	-1.114282
18C	0.448638	-1.535948	-1.163232
19C	1.558815	0.361257	-1.163234
20C	1.576219	1.197092	0.011674
21C	-0.271522	-1.960553	0.011677
22C	1.186631	-2.055538	-0.034246
23C	2.373304	-0.027608	-0.034248
24C	-0.315928	-0.647525	1.842502
25C	0.409761	0.592621	1.842501

N = 26

atom	X/σ	Y/σ	Z/σ
1A	0.000000	0.000000	0.000000
2A	1.100032	0.000000	0.000000
3A	0.543723	-0.956261	0.000000
4A	0.543724	-0.316314	0.902431
5B	1.549060	-0.901172	0.639054
6A	0.535919	0.744104	0.591188
7A	0.535918	-0.311772	-0.897771
8A	-0.381958	-0.833671	0.591189
9B	0.503353	-1.496273	1.061063
10B	1.549510	-0.901434	-0.635991
11B	1.549512	0.302010	1.061063
12A	0.526653	0.774637	-0.549323
13A	-0.413079	0.240310	0.975089
14A	-0.413080	-0.840707	-0.549324
15C	-0.535248	1.151099	0.073519
16C	-0.535249	0.311384	-1.110618
17C	-1.265216	-0.103671	0.073519
18C	-0.259244	-0.684730	1.838485
19C	1.576987	0.359340	-1.140209
20C	0.467100	0.563810	1.838485
21C	0.467096	-1.548493	-1.140210
22C	-0.259247	-1.961487	0.038048
23C	1.576987	1.194886	0.038049
24C	1.190396	-0.692518	1.928049
25C	2.369230	-0.022239	0.015769
26C	1.190393	-2.048587	0.015769

N = 27

atom	X/σ	Y/σ	Z/σ
1A	0.000000	0.000000	0.000000
2A	1.104438	0.000000	0.000000
3A	0.544501	-0.960886	0.000000
4A	0.540573	-0.315008	0.902031
5A	0.539698	-0.314498	-0.887469
6B	1.547149	-0.901570	0.639977
7C	1.626791	-0.947980	-0.707263
8A	-0.386035	-0.826388	0.592932
9A	0.528656	0.743278	0.592932
10B	0.494165	-1.490296	1.068316
11B	1.540220	0.304799	1.068316
12A	-0.416996	-0.838928	-0.544512
13A	0.524302	0.776397	-0.544513
14A	-0.418802	0.244048	0.972152
15C	0.422841	-1.574271	-1.128221
16C	1.578116	0.408252	-1.128222
17C	-0.520860	0.303520	-1.123388
18C	-1.266707	-0.098723	0.063899
19C	-0.538610	1.150735	0.063898
20C	-0.286269	-1.957501	0.059093
21C	1.561936	1.214131	0.059092
22C	-0.268019	-0.677694	1.840063
23C	0.457472	0.567293	1.840063
24C	1.157299	-2.073361	0.039013
25C	2.374433	0.015315	0.039013
26C	1.183150	-0.689457	1.930803
27C	1.029251	-0.599777	-2.006928

N = 28

atom	X/σ	Y/σ	Z/σ
1A	0.000000	0.000000	0.000000
2A	1.099335	0.000000	0.000000
3A	0.549351	-0.949692	0.000000
4A	0.538491	-0.317518	0.903356
5A	0.542210	-0.337515	-0.906719
6B	0.542816	0.845175	0.635762
7B	0.550530	0.836502	-0.638999
8A	-0.371641	-0.858843	0.579393
9A	1.453892	-0.854102	0.604426
10A	-0.374561	-0.876853	-0.568268
11B	-0.505207	0.240554	1.047406
12B	1.575687	0.244113	1.068312
13A	1.492321	-0.886034	-0.531817
14B	-0.511356	0.243737	-1.027763
15A	0.533389	-1.422312	0.978312
16C	0.599583	-1.595212	-1.087593
17C	1.663335	0.218300	-1.128460
18C	-0.177813	-1.986195	0.061040
19C	-1.272705	-0.185759	0.006743
20C	1.281711	-1.992171	0.110127
21C	2.374729	-0.184569	0.059571
22C	1.248527	-0.822333	1.848036
23C	-0.196960	-0.822713	1.830831
24C	-0.620933	1.114329	0.005640
25C	1.716521	1.108500	0.014926
26C	0.525578	0.434373	1.925293
27C	0.490409	0.426148	-1.931328
28C	-0.279250	-0.788155	-1.840802

N = 29

atom	X/σ	Y/σ	Z/σ
1A	0.000000	0.000000	0.000000
2A	1.092536	0.000000	0.000000
3A	0.542329	-0.948428	0.000000
4A	0.537447	-0.311787	0.901416
5A	0.528356	-0.306511	-0.902857
6B	1.545647	-0.896670	0.639497
7B	1.544667	-0.896100	-0.632273
8A	-0.401253	-0.830457	-0.573942
9A	0.521739	0.760562	-0.573940
10A	0.532533	0.750356	0.580259
11A	-0.387036	-0.834763	0.580258
12B	1.544451	0.311479	1.051727
13B	0.496262	-1.495351	1.051726
14B	0.495639	-1.495100	-1.043516
15B	1.543927	0.311899	-1.043514
16B	-0.518465	0.300777	-0.999124
17A	-0.421781	0.244686	0.965863
18C	-0.533627	1.151927	0.054963
19C	-1.264873	-0.108569	0.054962
20C	1.566764	1.189072	0.001873
21C	-0.254496	-1.950351	0.001869
22C	0.458501	0.570675	1.828578
23C	-0.267805	-0.681304	1.828577
24C	2.362186	-0.019171	0.003753
25C	1.189219	-2.041090	0.003751
26C	-0.248343	-0.704675	-1.842564
27C	0.488452	0.565388	-1.842562
28C	1.182068	-0.685749	1.923993
29C	1.196779	-0.694279	-1.914362

N = 30

atom	X/σ	Y/σ	Z/σ
1A	0.000000	0.000000	0.000000
2A	1.097331	0.000000	0.000000
3A	0.538502	-0.947321	0.000000
4A	0.538607	-0.311740	-0.905839
5A	0.520936	-0.308750	0.903728
6A	0.535503	0.740022	-0.578072
7B	1.543319	-0.898606	-0.639174
8B	1.533600	-0.903349	0.638131
9A	0.518333	0.756632	0.578109
10C	1.622939	0.362452	-1.116535
11A	-0.409603	-0.827251	0.571202
12A	-0.391271	-0.832306	-0.575872
13B	1.533332	0.300581	1.059597
14B	0.486991	-1.498146	-1.046633
15B	0.481003	-1.496897	1.043308
16B	-0.523986	0.307004	0.994195
17A	-0.424778	0.243361	-0.962924
18C	1.566723	1.194681	0.042618
19C	0.418418	0.557479	-1.846144
20C	-0.520256	1.161278	-0.064439
21C	-1.267815	-0.097505	-0.057741
22C	-0.265206	-1.949363	-0.000927
23C	-0.291738	-0.693579	-1.820382
24C	2.368927	-0.030294	0.037589
25C	1.179425	-2.043460	-0.002042
26C	0.475740	0.561336	1.847665
27C	-0.265863	-0.703005	1.838009
28C	1.151207	-0.712753	-1.939174
29C	1.178001	-0.704299	1.920892

30C	1.033563	1.703718	-1.205392

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.086705	0.000000	0.000000
3A	0.516295	-0.951460	0.000000
4A	0.534083	-0.287151	-0.902791
5A	0.513859	-0.297773	0.909239
6A	0.532338	0.779477	-0.562432
7A	0.527689	0.768392	0.556735
8B	1.528093	-0.890012	-0.643736
9B	1.521819	-0.900621	0.632551
10B	-0.525343	-0.845140	0.603069
11A	-0.411469	-0.799184	-0.602151
12A	-0.395478	0.303338	-0.964295
13B	-0.514989	0.370561	0.984981
14B	1.549177	0.320189	-1.041430
15B	1.546419	0.314464	1.032233
16C	0.466828	-1.579918	1.115911
17B	0.477124	-1.458192	-1.080883
18A	-0.435658	0.982395	-0.034082
19C	1.605087	1.176204	-0.002948
20C	0.498936	0.604025	-1.827759
21C	-1.272146	0.018847	-0.107866
22C	-0.271247	-0.612533	-1.842492
23C	0.508596	0.635160	1.817363
24C	-0.270636	-1.964503	-0.082519
25C	2.363467	-0.046521	-0.001180
26C	1.175286	-2.040838	-0.049562
27C	1.184284	-0.660031	-1.930075
28C	-0.242786	-0.596519	1.900556
29C	1.203444	-0.640100	1.928289
30C	0.395535	1.923717	0.055941
31C	-0.313339	1.561154	-1.149010

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.088431	0.000000	0.000000
3A	0.538870	-0.951159	0.000000
4A	0.525758	-0.293552	-0.907365
5A	0.543256	-0.292026	0.903638
6A	0.527174	0.780799	-0.548595
7A	0.539116	0.764231	0.567760
8B	1.547984	-0.881264	-0.630159
9B	1.552409	-0.871797	0.647347
10B	1.543846	0.339304	-1.024330
11B	-0.495764	-0.869763	-0.603688
12B	-0.514018	0.339491	-0.987757
13A	-0.387444	-0.819575	0.600647
14B	-0.493830	1.063803	0.066864
15B	1.550098	0.337016	1.044649
16B	1.556651	1.080037	0.017311
17C	0.501569	0.614202	-1.825465
18C	0.510481	-1.582415	-1.114854
19B	0.513869	-1.462019	1.081966
20A	-0.402253	0.276048	0.969913
21C	-1.274201	-0.040709	0.102291
22C	2.367043	-0.005094	0.002399
23C	0.475763	0.617561	1.818427
24C	-0.252967	-0.636375	1.844880
25C	-0.222988	-1.983202	0.082860
26C	0.527948	1.933688	0.078829
27C	1.223632	-2.027481	0.051222
28C	1.230121	-0.627013	-1.922237
29C	-0.221240	-0.622590	-1.901529
30C	1.197068	-0.638684	1.933760
31C	-0.215881	1.651456	-1.126391
32C	1.233308	1.657746	-1.160145

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.089899	0.000000	0.000000
3A	0.551353	-0.946940	0.000000
4A	0.534598	-0.298918	0.901752
5A	0.540742	-0.304215	-0.899435
6A	0.522897	0.772263	0.562371
7A	0.528763	0.765994	-0.562377
8B	1.554369	-0.886966	-0.641116
9B	1.555087	-0.888658	0.629261
10B	1.546281	0.316144	1.035338
11B	-0.510880	0.301322	0.997030
12B	1.540922	0.321151	-1.043033
13B	1.550357	1.074191	-0.000591
14A	-0.386790	-0.835329	0.577910
15A	-0.375031	-0.842850	-0.581184
16C	-0.596403	1.109914	-0.087077
17C	0.498690	0.554818	1.847039
18B	0.511705	-1.490995	1.044553
19B	0.513257	-1.491099	-1.053212
20A	-0.428607	0.223567	-0.968121
21C	0.444907	0.578004	-1.815142
22C	0.533145	1.942612	-0.000481
23C	-1.268201	-0.151929	-0.042892
24C	2.365144	-0.004858	-0.006178
25C	-0.236173	-1.954234	-0.000560
26C	-0.236948	-0.702358	1.842813
27C	-0.256383	-0.689793	-1.832293
28C	1.206853	-2.034615	-0.004820
29C	1.211698	-0.689670	1.910469
30C	1.190029	-0.664953	-1.923306
31C	1.240910	1.617626	1.208287
32C	-0.209711	1.615115	1.196222
33C	1.229491	1.623001	-1.208533

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.087894	0.000000	0.000000
3A	0.545530	-0.944694	0.000000
4A	0.537367	-0.300362	0.904879
5A	0.537367	-0.300361	-0.904880
6A	0.526574	0.766973	0.566823
7A	0.526574	0.766973	-0.566822
8B	1.552563	-0.889296	0.631528
9B	1.552563	-0.889295	-0.631529
10B	1.548064	0.317156	1.036210
11B	1.548064	0.317157	-1.036210
12B	1.544829	1.075632	0.000001
13B	-0.497599	0.296058	1.015528
14B	-0.497599	0.296059	-1.015527
15B	-0.512663	1.048990	0.000001
16A	-0.387451	-0.831650	0.584168
17A	-0.387450	-0.831649	-0.584168
18C	0.507367	1.925826	0.000001
19C	0.509362	0.555330	1.855130
20C	0.509362	0.555333	-1.855129
21B	0.509744	-1.491285	-1.045465
22B	0.509744	-1.491286	1.045463
23C	-1.269925	-0.120598	0.000000
24C	2.365156	-0.004229	0.000000
25C	-0.246196	-1.946036	-0.000001
26C	-0.227943	-0.707468	1.853654
27C	-0.227943	-0.707466	-1.853655
28C	1.199212	-2.036581	-0.000001
29C	1.217799	-0.691667	1.912284
30C	1.217799	-0.691664	-1.912285
31C	1.234890	1.621412	-1.204682
32C	1.234891	1.621410	1.204684
33C	-0.216840	1.607056	-1.198307
34C	-0.216840	1.607054	1.198309

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.084512	0.000000	0.000000
3A	0.528109	-0.949341	0.000000
4A	0.536999	-0.288681	-0.905316
5A	0.535962	0.761757	-0.566743
6A	0.526656	0.769435	0.554596
7A	0.515674	-0.294673	0.908347
8B	-0.521596	-0.859266	0.590896
9A	-0.398552	-0.801630	-0.599163
10B	-0.517576	0.342740	0.985766
11B	1.542940	-0.871410	-0.645553
12B	1.541218	1.085206	-0.013539
13B	1.537669	-0.878550	0.633860
14B	1.543401	0.336876	-1.045839
15B	1.535818	0.344155	1.028614
16A	-0.392382	0.308172	-0.964620
17A	-0.401575	1.004228	-0.016831
18C	0.489463	-1.574084	1.112779
19C	0.481903	0.589766	-1.841014
20B	0.495479	-1.457506	-1.078745
21C	0.487287	0.624527	1.824351
22B	0.494832	1.812921	-0.026024
23C	-1.260478	0.056957	-0.103026
24C	-0.222805	-1.983953	-0.078824
25C	-0.277847	-0.627254	-1.833295
26C	2.356336	0.002132	-0.002230
27C	-0.272742	1.575467	-1.128895
28C	-0.245731	1.647468	1.085070
29C	-0.240882	-0.617107	1.894903
30C	1.216300	-2.023892	-0.047699
31C	1.187977	-0.654246	-1.931332
32C	1.202268	1.672368	1.144814
33C	1.189268	1.655353	-1.187727
34C	1.211678	-0.621636	1.925136
35C	-1.490748	-1.345669	-0.262290

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.085006	0.000000	0.000000
3A	0.525762	-0.948718	0.000000
4A	0.532579	-0.285841	0.903958
5A	0.538939	0.765226	0.563093
6A	0.529956	0.769428	-0.556570
7A	0.520547	-0.292864	-0.909649
8A	-0.410357	-0.806430	0.599631
9B	-0.511014	-0.854177	-0.600794
10B	1.538484	-0.871158	0.648018
11B	-0.512937	0.345284	-0.989293
12B	1.539695	-0.878707	-0.631112
13B	1.545626	1.084258	0.010620
14B	1.543953	0.337945	1.044012
15B	1.540986	0.343706	-1.027605
16B	0.486032	-1.452994	1.076776
17A	-0.391200	0.318978	0.960916
18A	-0.398370	1.006506	0.012651
19C	0.499517	-1.571283	-1.120487
20C	0.490893	0.606994	1.836317
21C	0.494538	0.625950	-1.826345
22C	-0.218960	-1.984729	0.052668
23B	0.500231	1.814879	0.019402
24C	-1.257207	0.056808	0.100577
25C	-0.270718	-0.590199	1.841764
26C	2.357979	-0.001023	0.005317
27C	-0.267202	1.585655	1.121167
28C	1.213947	-2.022961	0.051090
29C	1.182333	-0.650219	1.930637
30C	-0.239925	1.649036	-1.090300
31C	-0.231655	-0.613450	-1.901825
32C	1.208930	1.671874	-1.147640
33C	1.197466	1.663099	1.178071
34C	1.221561	-0.618286	-1.925779
35C	-1.503148	-1.346030	0.177595
36C	-0.802098	-1.806087	1.342885

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.084366	0.000000	0.000000
3A	0.534171	-0.939931	0.000000
4A	0.517838	-0.290688	-0.905290
5A	0.522339	-0.299453	0.903940
6A	0.522117	0.764196	-0.562053
7A	0.531330	0.761294	0.559853
8A	-0.418551	-0.815004	-0.570137
9B	-0.518322	0.316489	-0.985134
10A	-0.415084	-0.819032	0.562335
11B	1.535649	-0.878269	-0.639219
12B	1.532221	-0.888896	0.641757
13B	1.532148	0.335601	-1.038278
14B	1.536938	1.083110	0.002140
15B	1.532698	0.330486	1.041729
16B	0.481197	-1.466087	-1.056124
17A	-0.411395	0.997590	0.006184
18A	-0.402052	0.318642	0.950882
19C	-1.255355	0.027316	0.090587
20C	0.456119	-1.569631	1.109288
21C	0.474120	0.595006	-1.834260
22C	-0.248791	-0.664614	-1.853995
23C	0.468443	0.596437	1.830519
24B	-0.177514	-1.866775	-0.034775
25B	0.486787	1.807974	0.007765
26C	-0.319847	-0.603376	1.813393
27C	2.350429	-0.003917	0.003560
28C	-0.278084	1.583762	1.111637
29C	-0.259127	1.623121	-1.102297
30C	1.183218	-2.032485	-0.037651
31C	1.189659	-0.659300	-1.918294
32C	-1.422055	-1.382874	0.016521
33C	1.189443	1.657343	-1.165639
34C	1.184254	1.655626	1.173492
35C	1.170688	-0.643966	1.934807

36C	-1.518929	-0.574743	-1.184676
37C	-0.814753	-1.836590	-1.227897

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.067347	0.000000	0.000000
3A	0.500787	-0.955636	0.000000
4A	0.504954	-0.300819	-0.899520
5A	0.503157	-0.299092	0.899065
6A	0.495618	0.771312	-0.557081
7A	0.495251	0.773159	0.554353
8A	-0.445684	-0.789336	-0.573034
9A	-0.450999	-0.792599	0.575249
10A	-0.440387	0.288837	-0.937010
11A	-0.441302	0.293216	0.933428
12B	-0.560561	1.020419	-0.002920
13C	0.441089	-1.546836	-1.135911
14B	1.511657	-0.883716	-0.641703
15B	1.508433	0.336956	-1.033620
16B	1.509418	-0.883256	0.644324
17B	1.506344	0.338855	1.033923
18B	1.502999	1.097115	-0.000883
19A	-1.064409	-0.037530	-0.004166
20C	0.433933	-1.545786	1.136353
21C	-0.305812	-1.938097	-0.000769
22C	-0.296802	-0.569583	-1.852360
23C	0.429551	1.922772	-0.003041
24B	0.453542	0.547184	-1.721972
25B	0.449733	0.550537	1.719760
26C	-0.304223	-0.567640	1.848200
27C	-1.521970	-1.214511	0.003897
28C	2.327305	0.003036	0.001555
29C	-1.518000	-0.339593	-1.141031
30C	-0.301708	1.533819	-1.209120
31C	-0.303009	1.538027	1.202577
32C	1.160309	-0.601460	-1.941101
33C	1.164049	-2.035832	0.001257
34C	1.155631	-0.598349	1.942030
35C	1.150200	1.623965	-1.220809
36C	1.148553	1.626651	1.217370
37C	-0.993499	-1.695965	-1.259920
38C	-1.522561	-0.326099	1.134835

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.083806	0.000000	0.000000
3A	0.541585	-0.938788	0.000000
4A	0.526935	-0.304345	0.904279
5A	0.526935	-0.304345	-0.904279
6A	0.520288	0.765094	0.567659
7A	-0.402729	-0.832992	0.567659
8A	-0.402729	-0.832992	-0.567659
9A	0.520288	0.765094	-0.567658
10B	-0.502964	0.290500	1.011210
11B	-0.502965	0.290501	-1.011209
12B	-0.519764	1.045582	0.000001
13B	-1.165407	-0.072267	0.000000
14B	1.545134	-0.892433	-0.630873
15B	1.545134	-0.892433	0.630872
16B	1.539232	0.313538	1.037091
17B	0.497578	-1.489951	-1.037091
18B	0.497578	-1.489951	1.037091
19B	1.539231	0.313539	-1.037091
20B	-0.162604	-1.869454	0.000000
21B	1.538058	1.075025	0.000000
22C	0.499868	0.550322	-1.854711
23C	-0.226898	-0.707982	-1.854712
24C	-0.226898	-0.707983	1.854712
25C	0.499870	0.550321	1.854712
26C	-1.416479	-1.392157	0.000000
27C	0.498057	1.922617	0.000001
28C	1.183532	-2.039439	0.000000
29C	2.357971	-0.006050	0.000000
30C	1.209696	-0.698692	1.909638
31C	1.209696	-0.698691	-1.909638
32C	-0.227718	1.600403	-1.198745
33C	-0.227716	1.600402	1.198747
34C	-1.500052	-0.602483	1.198746
35C	-1.500052	-0.602483	-1.198746
36C	-0.789608	-1.869806	1.205958
37C	1.225044	1.618309	-1.205957
38C	1.225046	1.618308	1.205958
39C	-0.789608	-1.869806	-1.205958

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.076472	0.000000	0.000000
3A	0.485037	-0.952897	0.000000
4A	0.485037	-0.292299	-0.906958
5A	0.479659	-0.301305	0.907851
6A	0.479659	0.771661	-0.565258
7A	0.478634	0.771474	0.561918
8A	-0.472982	-0.771027	-0.561590
9A	-0.479364	-0.782095	0.553461
10A	-0.479364	0.286875	-0.914162
11A	-0.483170	0.287936	0.907331
12A	-0.483171	0.951913	-0.004264
13A	-1.081030	-0.007225	-0.005262
14C	1.550811	-0.972042	-0.708003
15C	1.540979	1.202029	-0.002577
16C	1.540979	0.366263	1.144872
17C	1.544328	0.368384	-1.150508
18C	1.544328	-0.982044	0.703539
19B	0.350954	-1.464748	-1.066874
20C	0.318489	0.575440	-1.841520
21C	0.318489	-1.576230	1.112580
22C	0.315942	1.925294	-0.004890
23C	0.315943	0.585919	1.833980
24B	-0.329813	-0.598420	-1.720999
25B	-0.329813	-1.821596	-0.041659
26C	-1.532855	-0.379903	-1.156648
27C	-1.532855	-1.217422	-0.006790
28B	-0.342627	1.463263	-1.079674
29B	-0.342627	-0.578776	1.723908
30B	-0.345981	1.466813	1.068381
31C	-1.537801	0.969386	-0.716121
32C	-1.537801	-0.384244	1.142322
33C	-1.540323	0.968381	0.705340
34C	0.996781	-2.112726	-0.044264
35C	0.996781	-0.690202	-1.997296
36C	2.344748	0.001248	0.000910
37C	-0.967272	-1.713667	-1.248178
38C	0.999878	-0.669586	2.004947
39C	0.999878	1.702898	-1.252313
40C	0.999648	1.706487	1.242952

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.067035	0.000000	0.000000
3A	0.494607	-0.957819	0.000000
4A	0.487631	-0.293185	0.904928
5A	0.487630	-0.293186	-0.904928
6A	0.475343	0.777118	0.553081
7A	0.475342	0.777117	-0.553082
8A	-0.463478	-0.776852	0.564790
9A	-0.463479	-0.776853	-0.564789
10A	-0.468632	0.301260	0.912232
11A	-0.468634	0.301258	-0.912231
12A	-0.483527	0.967699	0.000000
13A	-1.064991	-0.001559	0.000001
14C	1.582937	-0.929235	-0.703670
15C	1.582937	-0.929234	0.703670
16C	-0.360708	-1.917137	0.000002
17C	0.385190	-1.536076	-1.149731
18C	0.385191	-1.536074	1.149733
19B	1.475246	0.365984	-1.047993
20B	1.475247	0.365986	1.047991
21B	1.465522	1.122890	-0.000002
22C	-0.357136	-0.537403	-1.839676
23C	-0.357134	-0.537400	1.839678
24C	-1.562861	-1.156897	0.000002
25C	0.376799	1.923909	-0.000002
26B	0.396755	0.576223	1.712281
27B	0.396753	0.576220	-1.712282
28C	-0.353816	1.541539	-1.153399
29C	-0.353814	1.541541	1.153397
30B	-1.452097	-0.358615	1.076942
31B	-1.452098	-0.358616	-1.076940
32C	-1.558205	0.930943	-0.711404
33C	-1.558204	0.930944	0.711407
34C	2.327154	0.088735	-0.000001
35C	1.098448	1.650321	-1.218806
36C	1.098450	1.650324	1.218801
37C	1.082078	-0.559935	1.990555
38C	1.082076	-0.559939	-1.990555
39C	1.073873	-2.085195	0.000001
40C	-1.051876	-1.661788	1.251723
41C	-1.051878	-1.661789	-1.251720

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.074904	0.000000	0.000000
3A	0.485785	-0.956039	0.000000
4A	0.490066	-0.300931	0.895045
5A	0.495027	0.757627	0.573799
6A	-0.461458	-0.778410	0.577300
7A	-0.450900	0.279111	0.930125
8A	0.484920	-0.294032	-0.906002
9A	0.485941	0.785268	-0.542393
10A	-0.479751	-0.783930	-0.544268
11A	-0.470447	0.961157	0.040163
12A	-1.073099	-0.002368	0.042625
13A	-0.489701	0.305005	-0.894942
14C	1.574054	-0.962870	-0.670176
15C	1.569484	1.182830	0.054239
16C	-0.339644	-1.931002	0.047955
17B	1.473588	-0.903268	0.676040
18C	1.573476	0.378514	-1.104674
19B	0.384285	-1.454682	1.085085
20C	0.379844	-1.567023	-1.108450
21B	1.476613	0.316033	1.085868
22B	0.396897	0.512277	1.740116
23B	-0.281160	-0.572493	1.745035
24C	0.358603	1.922062	0.082916
25C	-1.506363	-0.369140	1.203319
26C	-0.376829	-0.590608	-1.807424
27C	0.362273	0.613569	-1.804962
28C	-1.546858	-1.197736	0.064648
29B	-0.285942	1.428031	1.154576
30C	-1.499406	0.983877	0.785445
31C	-1.568654	-0.367466	-1.081480
32C	-0.377417	1.573321	-1.077865
33C	-1.566730	0.966824	-0.626836
34C	1.067179	-0.655783	1.955500
35C	2.340110	-0.023798	0.088047
36C	1.082920	-2.071703	0.087438
37C	1.059504	1.609270	1.323529
38C	-0.943339	-1.684634	1.321084
39C	-0.906351	0.612770	2.064668
40C	1.059645	-0.643331	-1.984298
41C	1.055423	1.725226	-1.178144
42C	-1.051733	-1.716319	-1.192046

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.074199	0.000000	0.000000
3A	0.484525	-0.955906	0.000000
4A	0.488186	-0.300110	0.895185
5A	0.493871	0.758457	0.572504
6A	-0.463532	-0.777273	0.575973
7A	0.484429	-0.294071	-0.906524
8A	-0.452977	0.280717	0.927817
9A	0.485559	0.784819	-0.544002
10A	-0.480328	-0.782902	-0.545842
11A	-0.486735	0.303435	-0.893310
12A	-0.470769	0.961491	0.036448
13A	-1.073527	-0.001149	0.038832
14C	1.573246	-0.963454	-0.669025
15C	1.568924	1.182546	0.053713
16C	-0.374327	-0.593821	-1.807724
17C	-0.341504	-1.930073	0.047467
18C	0.366877	0.612423	-1.805265
19C	1.574626	0.377262	-1.103982
20C	0.379889	-1.567859	-1.107759
21B	1.471440	-0.902960	0.677279
22B	0.381242	-1.453517	1.085410
23B	1.474517	0.316729	1.086202
24B	0.393776	0.514115	1.738868
25B	-0.284846	-0.570250	1.743739
26C	0.359175	1.922531	0.081229
27C	-1.509061	-0.366514	1.199535
28C	-1.569463	-0.369542	-1.081759
29C	-0.374402	1.575329	-1.078170
30C	-1.548171	-1.197145	0.062980
31B	-0.287793	1.429594	1.151186
32C	-1.500625	0.985862	0.780238
33C	-1.565926	0.967387	-0.630746
34C	1.063419	-0.654230	1.956331
35C	2.339153	-0.024452	0.089809
36C	1.081035	-2.071636	0.089198
37C	1.057821	1.610171	1.322476
38C	-0.946709	-1.682478	1.320010
39C	-0.910069	0.615739	2.061101

40C	1.059748	-0.644124	-1.984027
41C	1.056117	1.723898	-1.179961
42C	-1.051990	-1.715265	-1.193811
43C	-1.069378	0.664420	-1.961871

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.071236	0.000000	0.000000
3A	0.484217	-0.957984	0.000000
4A	0.484217	0.765273	-0.576273
5A	0.487502	-0.299390	-0.895283
6A	-0.455012	-0.781420	-0.572459
7A	-0.455012	0.279865	-0.927363
8A	0.480411	-0.298219	0.906613
9A	0.480410	0.783599	0.544844
10A	-0.481801	-0.786640	0.544219
11A	-0.481801	0.955771	-0.038459
12A	-0.491577	0.298517	0.892671
13A	-1.070869	-0.011991	-0.035857
14C	0.359463	0.604158	1.806647
15C	1.569027	1.175752	-0.047509
16C	1.569028	-0.967813	0.669318
17C	-0.348112	1.511239	-1.205634
18C	-0.348111	-1.932480	-0.054023
19C	-0.380834	1.567382	1.079860
20C	-0.380833	-0.602498	1.805487
21C	1.569143	0.370452	1.107782
22C	0.373693	1.921704	-0.065047
23C	0.373693	-1.574258	1.104034
24B	1.468973	0.315692	-1.085360
25B	1.468973	-0.905081	-0.677123
26B	0.381260	-1.457700	-1.086276
27B	0.381260	0.511019	-1.744633
28B	-0.282664	-0.581346	-1.738429
29C	-1.554208	0.899161	-0.778338
30C	-1.554207	-1.186491	-0.080877
31C	-1.574751	-0.379763	1.080363
32C	-1.574751	0.953258	0.634589
33B	-1.406825	-0.384341	-1.149313
34C	1.062826	-0.654189	-1.956256
35C	1.076644	-2.075508	-0.089797
36C	1.076643	1.603976	-1.320249
37C	2.336264	-0.029754	-0.088976
38C	-0.961752	-1.667806	-1.322381
39C	-0.961752	0.536830	-2.059632
40C	1.052491	-0.652926	1.984183
41C	1.052491	1.715161	1.192274
42C	-1.076127	0.655891	1.961347
43C	-1.060928	-1.721160	1.180137
44C	-1.060928	2.084834	-0.092621

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.073474	0.000000	0.000000
3A	0.487003	-0.956647	0.000000
4A	0.487004	0.766257	-0.572733
5A	-0.461926	0.283184	-0.926702
6A	-0.461926	-0.781630	-0.572733
7A	0.485144	-0.297416	-0.894691
8A	0.486223	0.781439	0.547601
9A	0.486223	-0.298078	0.906456
10A	-0.475810	0.958874	-0.033041
11A	-0.475810	-0.787822	0.547601
12A	-1.070379	-0.010984	-0.033041
13A	-0.485700	0.297758	0.895722
14C	-1.562942	0.958160	0.643561
15C	-1.562943	-0.382178	1.089119
16C	0.369749	0.601701	1.810049
17C	-0.368474	-0.602482	1.810049
18C	-0.368473	1.566231	1.089120
19C	-1.508722	-0.397489	-1.195734
20C	-0.330231	-1.937256	-0.044849
21C	-0.330231	1.524858	-1.195733
22C	1.576608	-0.966537	0.666438
23C	1.576609	1.173167	-0.044848
24C	-1.537782	-1.217632	-0.054396
25C	-1.537782	0.942736	-0.772551
26C	0.387472	-1.572719	1.107604
27C	0.387472	1.922829	-0.054395
28C	1.577344	0.368192	1.107604
29B	0.386061	0.515647	-1.738682
30B	-0.284384	-0.577977	-1.738682
31B	1.470862	-0.901709	-0.679291
32B	1.470862	0.315570	-1.083942
33B	0.386060	-1.453951	-1.083943
34C	1.061181	-0.650554	-1.957008
35C	2.341500	-0.030623	-0.092119
36C	-0.936126	-1.699171	-1.314734
37C	1.089558	-2.072781	-0.092119
38C	1.089558	1.605111	-1.314733
39C	-0.936126	0.573892	-2.070351
40C	-1.066552	0.653849	1.966920
41C	1.064908	-0.652840	1.984280
42C	1.064908	1.710877	1.198528
43C	-1.041565	-1.725186	1.198527
44C	-1.041565	2.099388	-0.072848
45C	-2.343437	-0.024216	-0.072848

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.073312	0.000000	0.000000
3A	0.484394	-0.942798	0.000000
4A	0.485085	-0.300786	0.908792
5A	0.485086	-0.300782	-0.908792
6A	-0.461608	-0.790564	0.561062
7A	-0.461607	-0.790562	-0.561064
8A	0.487083	0.765764	0.568839
9A	0.487083	0.765767	-0.568834
10A	-0.475966	0.271239	0.920289
11A	-0.475965	0.271244	-0.920287
12A	-1.070100	-0.035078	0.000000
13A	-0.485014	0.943971	0.000003
14B	1.462427	-0.923690	-0.646327
15B	1.462426	-0.923692	0.646326
16C	1.578200	0.326753	1.127554
17C	1.578201	0.326759	-1.127550
18B	0.386630	-1.488121	-1.037904
19B	0.386629	-1.488126	1.037900
20C	0.371780	1.906557	0.000006
21C	-0.367309	1.527420	-1.142602
22C	-0.367309	1.527414	1.142612
23C	-1.562393	0.913054	-0.706173
24C	-1.562393	0.913051	0.706179
25C	-0.330215	-0.654079	-1.824393
26C	-0.330216	-0.654088	1.824392
27C	-1.507406	-1.260933	-0.000003
28C	1.579682	1.164723	0.000005
29B	-0.281514	-1.833484	-0.000003
30C	0.388277	0.554850	-1.842016
31C	0.388276	0.554841	1.842022
32C	-1.537380	-0.436046	-1.138169
33C	-1.537381	-0.436052	1.138167
34C	1.069051	-2.057404	-0.000003
35C	2.340446	-0.106920	0.000002
36C	1.089102	-0.741089	1.939652
37C	1.089103	-0.741080	-1.939653
38C	-0.935041	-1.784420	-1.197361
39C	-0.935042	-1.784425	1.197353
40C	1.066667	1.676022	1.245107
41C	1.066668	1.676028	-1.245095
42C	-1.064996	2.072843	0.000006
43C	-1.040950	0.593051	2.015127
44C	-1.040948	0.593062	-2.015123
45C	-2.342805	-0.077246	0.000000
46C	2.452039	-1.568639	-0.000001

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.060587	0.000000	0.000000
3A	0.491867	-0.947458	0.000000
4A	0.491867	-0.291050	0.901647
5A	0.495066	0.768280	0.563908
6A	0.495066	-0.300633	-0.904360
7A	0.492926	0.768454	-0.559442
8A	-0.453245	-0.784145	0.570865
9A	-0.452986	0.291124	0.926650
10A	-0.452986	-0.792414	-0.561707
11A	-0.458371	0.962176	0.006491
12A	-0.458371	0.289395	-0.917647
13A	-1.059520	-0.011400	0.008299
14A	1.410017	-0.838069	0.610123
15B	1.500282	0.316306	1.034843
16B	1.500282	-0.887640	-0.618906
17C	0.450164	-1.567321	-1.106095
18C	0.450164	0.571146	1.831321
19C	-1.521929	-0.391629	-1.130984
20C	-1.521929	0.955993	0.720121
21C	-1.527624	0.955977	-0.695960
22B	1.503769	1.085643	0.002989
23B	1.503770	0.330656	-1.034067
24C	-0.291301	-0.618722	1.840374
25C	-0.291300	-1.941454	0.023459
26C	0.431308	0.580939	-1.820721
27C	0.431308	1.911145	0.006461
28C	-1.513379	-1.221360	0.016286
29C	-1.513380	-0.390690	1.157301
30B	0.415701	-1.456988	1.060702
31C	-0.307446	-0.618292	-1.830689
32C	-0.307446	1.552237	1.150769
33C	-0.319153	1.556181	-1.132914
34C	2.311547	-0.012812	0.009327
35C	1.157379	-2.006574	0.083190
36C	1.157379	-0.695568	1.883997
37C	1.168271	-0.643283	-1.922767
38C	1.168270	1.632186	1.202837
39C	1.156475	1.641649	-1.195136
40C	-0.985042	0.632860	2.027732
41C	-0.985041	-1.735278	-1.225162
42C	-1.004603	0.635029	-2.008232
43C	-1.004603	2.106205	0.012588
44C	-2.324685	-0.021750	0.015833
45C	-0.950551	-1.730408	1.259754
46C	2.461812	-0.591642	1.317714
47C	2.461811	-1.435746	0.158247

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.067903	0.000000	0.000000
3A	0.483110	-0.952377	0.000000
4A	0.489361	-0.300485	-0.891125
5A	0.494864	0.761827	-0.572819
6A	-0.455540	-0.785973	-0.572819
7A	-0.454026	0.278788	-0.928812
8A	0.488326	-0.299850	0.904078
9A	0.494095	0.776663	0.548635
10A	-0.469120	-0.791999	0.548635
11A	-0.467927	0.957423	-0.032891
12A	-1.065535	-0.015822	-0.032891
13A	-0.477776	0.293371	0.899056
14A	1.392797	-0.855227	-0.621234
15B	0.407957	-1.452283	-1.069408
16B	1.479732	0.293176	-1.069408
17B	1.487496	-0.913376	0.613597
18C	1.587934	0.343138	1.099693
19C	0.412349	-1.571385	1.099692
20C	-0.312214	-1.944468	-0.044509
21C	1.592872	1.158098	-0.044507
22B	-0.268593	-0.587002	-1.738411
23B	0.401992	0.505092	-1.738410
24C	-0.353732	1.559408	1.092412
25C	-1.550736	-0.389997	1.092412
26C	-1.552026	0.953000	0.646162
27C	-0.315773	1.518953	-1.196969
28C	-1.497485	-0.405547	-1.196969
29C	-0.350154	-0.612158	1.811778
30C	0.387527	0.589207	1.811779
31C	-1.525016	-1.226667	-0.053421
32C	0.404063	1.914972	-0.053420
33C	-1.527191	0.937750	-0.772780
34C	1.082277	-0.664556	-1.929223
35C	2.316240	-0.079045	-0.067490
36C	1.118340	-2.029909	-0.067491
37C	1.109255	1.586960	-1.314731
38C	-0.913466	-1.707181	-1.314732
39C	-0.921250	0.565681	-2.071760
40C	1.101528	-0.676379	1.951226
41C	1.084591	1.694020	1.198953
42C	-1.020103	-1.733620	1.198951
43C	-1.051004	0.645353	1.970924
44C	-1.027126	2.095240	-0.071599
45C	-2.333239	-0.031856	-0.071599
46C	1.658368	-1.862263	-1.380354
47C	2.411035	-0.636494	-1.380354
48C	2.427229	-1.490406	-0.203283

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.055611	0.000000	0.000000
3A	0.496439	-0.949061	0.000000
4A	0.487232	-0.302224	0.890567
5A	0.497224	0.751868	0.578573
6A	-0.443860	-0.789871	0.572188

7A	-0.446578	0.277751	0.933259
8A	0.502479	-0.289553	-0.902987
9A	0.504165	0.780172	-0.538398
10A	-0.452583	-0.789068	-0.554062
11A	-0.451973	0.963633	0.041365
12A	-1.057525	-0.011935	0.033320
13A	-0.460257	0.306244	-0.899499
14A	1.402920	-0.822699	0.624063
15A	1.404949	0.263877	1.002254
16B	0.439412	-1.450109	1.075286
17B	1.509346	-0.887808	-0.608080
18B	1.515520	1.070332	0.063758
19C	1.621358	0.361036	-1.062535
20C	0.444277	-1.558736	-1.101272
21C	-0.279575	-1.942796	0.040908
22C	0.450628	1.905593	0.081232
23B	0.422647	0.503259	1.735273
24C	-1.527922	-0.376814	-1.098567
25C	-1.527344	0.968433	-0.641994
26C	-1.484682	-0.407852	1.194812
27C	0.424710	0.611687	-1.796917
28C	-0.318343	1.578190	-1.075231
29C	-0.321215	-0.593712	-1.815132
30C	-0.283484	1.519172	1.213044
31B	-0.254062	-0.591154	1.742320
32C	-1.507178	0.944811	0.779397
33C	-1.504843	-1.226215	0.043932
34B	2.197088	-0.041069	0.103850
35C	1.110957	-0.622999	1.914267
36C	1.174071	-1.998641	0.076907
37C	1.183612	1.518789	1.292666
38C	2.400565	-0.481519	1.351716
39C	-0.891324	-1.711349	1.308629
40C	-0.903306	0.561615	2.076192
41C	1.137302	-0.647991	-1.938989
42C	1.140393	1.695290	-1.139553
43C	2.474051	-1.367170	0.205411
44C	-0.989741	-1.724920	-1.209028
45C	-0.988192	2.105409	0.090312
46C	-1.016971	0.670393	-1.967898
47C	-2.316753	-0.024137	0.067289
48C	1.734907	-1.788746	1.379931
49C	2.478141	0.929643	1.012319

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.055694	0.000000	0.000000
3A	0.479554	-0.940487	0.000000
4A	0.497798	-0.304949	-0.898553
5A	0.497798	-0.304950	0.898553
6A	0.509108	0.760981	-0.564867
7A	0.509107	0.760981	0.564867
8A	-0.446672	-0.799229	-0.564868
9A	-0.446672	-0.799230	0.564867
10A	-0.447778	0.274307	-0.925700
11A	-0.447778	0.274307	0.925700
12A	-0.452276	0.954246	0.000000
13A	-1.055560	-0.030552	0.000000
14A	1.399192	-0.857140	-0.572630
15A	1.399192	-0.857140	0.572630
16B	0.439111	-1.480494	-1.034205
17B	0.439111	-1.480494	1.034205
18B	1.518399	0.281331	-1.034205
19B	1.518398	0.281330	1.034206
20C	1.631694	1.115271	0.000001
21C	-0.252358	-1.960247	0.000000
22C	-0.275593	-0.652876	1.829842
23C	0.456440	0.542089	-1.829842
24C	-0.275592	-0.652876	-1.829843
25C	0.456439	0.542089	1.829842
26C	-1.518823	0.930425	0.709943
27C	-1.518823	0.930425	-0.709944
28C	-1.491843	-1.252880	-0.000001
29C	0.438477	1.898168	0.000000
30C	-0.308113	1.531270	1.146852
31C	-1.504127	-0.421099	1.146852
32C	-0.308112	1.531270	-1.146853
33C	-1.504127	-0.421099	-1.146853
34B	2.197574	-0.125565	0.000000
35B	1.110121	-1.900718	0.000000
36C	1.182589	-0.724450	-1.862874
37C	1.182588	-0.724450	1.862875
38C	2.377481	-1.456437	0.000000
39C	2.475466	-0.663360	-1.213469
40C	2.475466	-0.663361	1.213470
41C	1.715461	-1.903988	1.213470
42C	1.715462	-1.903988	-1.213470
43C	-0.923071	-1.763705	-1.235962
44C	-0.923071	-1.763705	1.235961
45C	1.151925	1.623510	-1.235961
46C	1.151923	1.623510	1.235961
47C	-0.980387	0.600582	-2.022947
48C	-0.980389	0.600582	2.022946
49C	-1.001828	2.087191	-0.000001
50C	-2.314505	-0.055619	-0.000001

TLJ (S_C = 1.4)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124022	0.000000	0.000000
3A	0.562011	-0.973432	0.000000
4C	0.562011	-0.324478	-1.175919
5C	0.562011	-0.324478	1.175919

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.428479	0.000000	0.000000
3C	0.714240	-1.123439	0.000000
4C	0.714240	0.000000	1.123439
5C	0.714240	0.000000	-1.123439
6C	0.714240	1.123439	0.000000

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2B	1.229611	0.000000	0.000000
3C	0.485463	-1.261053	0.000000
4C	0.486497	0.992239	-0.776620
5C	0.486497	0.992239	0.776620
6A	0.507959	-0.327212	-0.948016
7A	0.507959	-0.327212	0.948016

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.129529	0.000000	0.000000
3C	0.564765	-1.207598	0.000000
4A	0.564764	0.485415	0.828600
5C	1.343740	-0.545946	1.190464
6C	-0.214210	-0.545947	1.190464
7C	0.564764	1.157968	-0.339096
8C	0.564764	-0.174674	-1.194419

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.307282	0.000000	0.000000
3C	0.341600	-1.261862	0.000000
4C	0.341241	-0.261145	1.234644
5C	0.341600	0.739021	-1.022812
6C	-0.624083	-0.522841	-1.022812
7C	0.341240	1.153692	0.511407
8C	-1.024440	-0.630849	0.511407
9C	-1.024440	0.783988	-0.211830

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.309426	0.000000	0.000000
3C	0.245227	-1.286259	0.000000
4C	0.245228	0.880477	0.937668
5C	-0.818973	-0.405782	0.937669
6C	-1.022483	-0.587102	-0.609167
7C	0.385226	1.114344	-0.609168
8C	0.385226	-0.318721	-1.229335
9C	-1.022483	0.845963	0.011001
10A	0.500591	-0.414169	0.957050

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.323266	0.000000	0.000000
3C	0.344389	-1.277665	0.000000
4C	0.344390	0.749961	1.034401
5C	-0.634488	-0.527703	1.034402
6C	0.400682	-0.306981	-1.218638
7C	-1.022315	-0.690543	-0.466781
8C	0.400683	1.166804	-0.466782
9C	-1.022314	0.783242	0.285076
10A	-0.614657	0.470916	-0.923086
11A	0.684511	-0.524435	1.027994

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.311589	0.000000	0.000000
3C	0.364074	-1.260046	0.000000
4C	-0.857165	0.644561	-0.772968
5A	-0.226991	-0.525013	-0.954438
6A	0.441372	0.363806	-0.954437
7C	-1.127451	-0.699252	0.008299
8C	0.358811	1.277244	0.008301
9C	-0.845321	0.635653	0.793882
10A	-0.205900	-0.536058	0.959505
11A	0.457837	0.346608	0.959506
12C	1.027666	-0.772772	-1.322644

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.147826	0.000000	0.000000
3C	-0.512039	-1.273281	0.000000
4C	-0.512039	-0.340396	1.226936
5C	-1.340523	0.043387	-0.032990
6A	0.591456	0.956089	-0.026898
7A	0.591456	0.281517	-0.914099
8B	-0.423389	0.927733	-0.705389
9B	-0.435926	-0.348356	-1.098668
10B	-0.435926	0.965550	0.629392
11A	0.582960	0.325963	0.893465
12A	0.582960	-0.773803	-0.552956
13A	0.577398	-0.754269	0.573498

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.144604	0.000000	0.000000
3A	0.575959	-0.950705	0.000000
4A	0.569805	-0.269466	-0.907975
5C	-0.504088	-1.035061	-0.749942
6A	0.592059	-0.308011	0.905860
7A	0.583919	0.787386	-0.534134
8C	-0.513604	0.443701	-1.195377
9A	0.591282	0.758748	0.581440
10B	-0.437998	-0.926541	0.686080
11C	-1.339070	0.011969	0.048016
12B	-0.423879	0.337603	1.113619
13B	-0.435899	1.150043	0.054163
14C	1.676730	-0.978692	-0.738713

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.079526	0.000000	0.000000
3C	0.556965	-1.240618	0.000000
4A	0.558971	-0.302088	-0.927172
5A	0.558971	-0.302088	0.927172
6A	0.523314	0.964169	0.000000
7C	-0.213255	0.746780	-1.084870
8C	-0.213255	0.746780	1.084870
9C	-0.692886	-0.762094	-0.807401
10C	-0.692886	-0.762094	0.807401
11C	1.359862	0.766281	1.018760
12C	1.359862	0.766281	-1.018760
13C	-1.266296	0.443605	0.000000
14C	1.817040	-0.738622	0.793369
15C	1.817040	-0.738622	-0.793369

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.078297	0.000000	0.000000
3C	0.539146	-1.288154	0.000000
4C	0.539149	1.212605	0.000001
5A	0.539148	-0.361462	0.908853
6A	0.539148	-0.361462	-0.908854
7C	1.326482	0.646524	-1.187848
8C	1.326482	0.646523	1.187849
9C	-0.248182	0.646526	-1.187850
10C	-0.248182	0.646525	1.187851
11C	1.800064	-0.787222	-0.781958
12C	1.800064	-0.787223	0.781957
13C	-0.721770	-0.787218	0.781957
14C	-0.721770	-0.787218	-0.781958

15C	-1.222175	0.491477	0.000000
16C	2.300476	0.491469	0.000000

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.077076	0.000000	0.000000
3C	0.538536	-1.224158	0.000000
4C	0.538538	0.712228	-0.995637
5A	0.538538	0.440928	0.857548
6C	1.313673	-0.608287	-1.183038
7C	-0.236600	-0.608286	-1.183039
8A	1.085593	-0.530407	0.981631
9A	-0.008518	1.106981	0.139731
10A	1.085595	1.106981	0.139731
11A	-0.008519	-0.530406	0.981632
12C	-0.822488	0.495210	0.963118
13C	1.899563	0.495208	0.963118
14C	2.084741	-0.829217	0.144188
15C	-1.007666	0.599719	-0.590531
16C	-1.007668	-0.829214	0.144188
17C	2.084743	0.599716	-0.590531

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.068583	0.000000	0.000000
3C	0.472375	-1.290041	0.000000
4A	0.539432	-0.354732	-0.886332
5C	-0.716191	-0.673693	-0.892452
6C	0.509703	1.215967	-0.025335
7C	1.274939	0.641772	-1.219720
8C	1.755297	-0.813445	-0.806258
9A	0.501198	-0.371929	0.911803
10A	-0.085764	0.535832	-0.977634
11C	1.307560	0.637843	1.157044
12C	-0.272188	0.653715	1.168567
13C	1.762088	-0.811401	0.759516
14C	-0.818083	-0.727973	0.687868
15C	-1.109768	0.658640	-0.137896
16C	2.284610	0.467287	-0.044597
17C	0.170159	-0.088562	-2.114292
18C	0.507956	-1.495442	-1.532933

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.173890	0.000000	0.000000
3A	0.586944	-0.941322	0.000000
4A	0.586944	-0.290885	0.895251
5A	0.586944	-0.290885	-0.895251
6A	0.586944	0.761546	0.553295
7A	0.586944	0.761546	-0.553295
8C	1.647866	0.404931	1.246252
9C	1.647867	1.310386	0.000000
10C	1.647866	-1.060126	0.770226
11C	1.647866	-1.060126	-0.770226
12C	-0.473978	1.310386	0.000000
13C	1.647866	0.404931	-1.246252
14C	-0.473978	0.404931	1.246252
15C	-0.473978	0.404931	-1.246252
16C	-0.473977	-1.060126	-0.770226
17C	-0.473977	-1.060126	0.770226
18C	-1.324398	-0.000001	0.000000
19C	2.498287	-0.000001	0.000000

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.149505	0.000000	0.000000
3A	0.574752	-0.952629	0.000000
4A	0.574752	-0.340219	0.889804
5A	0.574753	0.728611	0.597329
6A	0.574752	-0.297721	-0.893889
7A	0.574753	0.772526	-0.531691
8A	-0.373469	-0.851865	0.586298
9A	1.522973	-0.851866	0.586298
10C	1.632356	0.296433	1.276762
11C	-0.482851	0.296433	1.276762
12C	1.632355	-1.086694	-0.732864
13C	-0.482851	-1.086692	-0.732864
14C	-0.500644	0.390722	-1.205834
15C	-0.500643	1.265853	0.065697
16C	1.650149	0.390721	-1.205834
17C	1.650149	1.265853	0.065696
18C	-1.329482	-0.061374	0.042242
19C	2.478987	-0.061375	0.042242
20C	0.574752	-1.634602	1.125019

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.142004	0.000000	0.000000
3A	0.626161	-0.955038	0.000000
4A	0.573880	-0.309969	-0.861479
5C	0.737094	0.973946	-0.820734
6C	-0.410345	-1.150433	-0.820734
7A	0.551295	-0.297770	0.891759
8C	0.723417	1.000749	0.723904
9C	-0.440258	-1.153692	0.723904
10C	1.939621	-1.047646	-0.029679
11C	1.800165	-0.080639	-1.221677
12C	1.054467	-1.461230	-1.221678
13B	-0.459338	0.248101	-1.139778
14C	1.807154	-0.069681	1.160029
15C	1.049135	-1.473084	1.160030
16C	-0.575870	0.311044	1.198559
17C	-0.593513	1.203910	-0.070239
18C	-1.332231	-0.163761	-0.070239
19C	0.418177	-2.243301	-0.038472
20C	2.105317	0.880289	-0.038472
21C	0.487275	-0.263188	-2.134844

N = 22

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.134715	0.000000	0.000000
3A	0.562775	-0.985446	0.000000
4A	0.573035	-0.334334	0.878979
5A	0.562357	-0.329495	-0.878467
6A	0.560134	0.749246	0.568915
7A	0.554512	0.747961	-0.572964
8A	-0.370764	-0.856671	-0.580566
9A	-0.380045	-0.853028	0.562789
10B	1.597220	-0.970130	0.614924
11A	1.509106	-0.843653	-0.595060
12C	-0.504974	0.291845	1.236297
13C	-0.508998	0.300277	-1.242327
14C	1.609135	0.323272	-1.263087
15C	1.642362	0.334621	1.220095
16C	-0.539078	1.226211	0.000884
17C	-1.331775	-0.136108	-0.007671
18C	1.633012	1.259233	-0.020352
19C	2.469843	-0.060118	-0.048430
20C	0.585312	-1.591858	-1.194763
21C	0.479184	-1.586692	1.248270
22C	-0.290798	-2.042927	-0.007021

N = 23

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.132338	0.000000	0.000000
3A	0.566169	-0.980633	0.000000
4A	0.566169	-0.326878	0.876160
5A	0.566169	-0.326878	-0.876160
6A	-0.366534	-0.865374	0.572054
7A	-0.366534	-0.865374	-0.572054
8A	1.498873	-0.865374	-0.572054
9A	1.498873	-0.865374	0.572054
10A	0.566169	0.750115	-0.572054
11A	0.566169	0.750115	0.572054
12C	-0.507801	0.293180	-1.236889
13C	-0.507801	0.293180	1.236889
14C	0.566170	-1.566992	1.236889
15C	0.566170	-1.566992	-1.236889
16C	1.640140	0.293180	1.236889
17C	1.640140	0.293180	-1.236889
18C	-0.534702	1.223018	0.000000
19C	-1.326514	-0.148441	0.000000
20C	2.458853	-0.148441	0.000000
21C	-0.225643	-2.055208	0.000000
22C	1.667041	1.223017	0.000000
23C	1.357982	-2.055207	0.000000

N = 24

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.135260	0.000000	0.000000
3A	0.567630	-0.983165	0.000000
4A	0.567630	-0.327721	0.866997
5A	0.567630	-0.327722	-0.874624
6A	-0.362664	-0.864827	0.578367
7A	1.497924	-0.864827	0.578366
8A	0.567630	0.746490	0.578366
9A	-0.365454	-0.866438	-0.569122
10A	1.500714	-0.866438	-0.569122
11A	0.567630	0.749711	-0.569123
12C	1.643979	0.293709	1.236023
13C	-0.508718	0.293709	1.236024
14C	0.567630	-1.570581	1.236025
15C	0.567630	-1.568646	-1.233754
16C	-0.507041	0.292740	-1.233755
17C	1.642300	0.292739	-1.233756
18C	1.666830	1.223130	0.003321
19C	1.361107	-2.055083	0.003323
20C	-0.531570	1.223130	0.003322
21C	-0.225847	-2.055083	0.003324
22C	-1.325047	-0.151212	0.003323
23C	2.460307	-0.151212	0.003322
24C	0.567630	-0.327721	2.174919

N = 25

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.109977	0.000000	0.000000
3A	0.550810	-0.963669	0.000000
4A	0.549428	-0.318805	0.909393
5A	0.541399	-0.314146	-0.886207
6A	-0.361719	-0.849553	0.592364
7A	0.558074	0.735618	0.592364
8A	1.476268	-0.856602	0.579748
9A	-0.396616	-0.856142	-0.551508
10A	0.546478	0.769185	-0.551508
11A	1.477067	-0.857066	-0.578269
12A	-0.405137	0.235080	0.977319
13B	1.593553	0.247121	1.095733
14B	0.576230	-1.506134	1.095733
15C	-0.543601	1.219586	0.086551
16C	-1.328584	-0.133254	0.086551
17C	-0.552387	0.320522	-1.181440
18C	0.527822	-1.563990	-1.219216
19C	1.619762	0.317858	-1.219216
20C	1.651636	1.220495	0.040519
21C	-0.240020	-2.039584	0.040519
22C	1.341642	-2.042761	0.005478
23C	2.439271	-0.151109	0.005478
24C	-0.305303	-0.715113	1.895444
25C	0.469351	0.619923	1.895444

N = 26

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.106665	0.000000	0.000000
3A	0.553332	-0.958401	0.000000
4A	0.553332	-0.319466	0.903589
5A	0.553332	0.730748	0.597204
6A	1.462844	-0.844574	0.597205
7A	-0.356180	-0.844573	0.597204
8A	0.553332	-0.319467	-0.888023
9A	-0.391933	0.226283	0.997703
10A	0.553332	-1.410965	0.997704
11A	1.498597	0.226283	0.997703
12A	0.553333	0.772031	-0.545909
13A	-0.391933	-0.865216	-0.545908
14A	1.498597	-0.865216	-0.545908
15C	-1.323784	-0.134588	0.095168
16C	1.331781	-0.768904	1.889286
17C	-0.545335	1.213725	0.095168
18C	-0.225117	-0.768904	1.889286
19C	0.553332	0.579409	1.889285
20C	1.652000	1.213724	0.095168
21C	1.652000	0.314848	-1.176033
22C	-0.545335	0.314849	-1.176034
23C	2.430449	-0.134589	0.095169
24C	0.553332	-1.588099	-1.176033
25C	1.331781	-2.037537	0.095170
26C	-0.225117	-2.037536	0.095169

N = 27

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.118600	0.000000	0.000000
3A	0.551269	-0.973329	0.000000
4A	0.550811	-0.321055	0.912021
5A	0.545533	-0.317980	-0.871801
6B	1.584260	-0.923429	0.646019
7A	0.542733	0.734854	0.586919
8A	-0.371950	-0.834399	0.586920

9B	1.575823	-0.918513	-0.680051
10A	0.529169	0.765179	-0.555028
11A	-0.405021	-0.837543	-0.555027
12B	1.581262	0.325253	1.082928
13B	0.496264	-1.536196	1.082929
14A	-0.411920	0.240100	0.969013
15C	-0.543528	0.316809	-1.199560
16C	0.438572	-1.574247	-1.241547
17C	1.585938	0.394203	-1.241549
18C	-1.335403	-0.121491	0.072300
19C	-0.552400	1.221849	0.072299
20C	1.587862	1.291063	0.024434
21C	-0.340865	-2.017910	0.024437
22C	-0.339586	-0.699803	1.890096
23C	0.441567	0.640362	1.890095
24C	1.209530	-2.139771	-0.014067
25C	2.457962	0.002071	-0.014069
26C	1.211973	-0.706432	2.014294
27C	0.535577	-0.312179	-2.166765

N = 28

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.095550	0.000000	0.000000
3A	0.544576	-0.950614	0.000000
4A	0.519439	-0.301066	0.910088
5A	0.546520	-0.316762	-0.912096
6A	-0.389978	-0.832851	0.580298
7A	0.528819	0.752379	0.580298
8A	1.435837	-0.832209	0.616430
9A	-0.367767	-0.858912	-0.579589
10A	0.562473	0.746061	-0.579589
11B	-0.534760	0.309947	1.033890
12A	1.506610	-0.873228	-0.513140
13A	1.470544	0.239623	0.997536
14A	0.523055	-1.395110	0.997536
15A	-0.416978	0.241680	-0.958184
16C	0.613547	-1.607726	-1.156109
17C	1.700013	0.266790	-1.156110
18C	-1.330412	-0.139018	-0.068337
19C	-0.540693	1.223509	-0.068338
20C	-0.235019	-2.023264	0.074968
21C	1.638773	1.209650	0.074968
22C	1.326044	-2.036962	0.144171
23C	2.426631	-0.138083	0.144170
24C	1.310357	-0.759481	1.898777
25C	-0.237643	-0.784698	1.897403
26C	0.562760	0.596261	1.897403
27C	0.413477	0.653577	-1.886312
28C	-0.361579	-0.683656	-1.886313

N = 29

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094580	0.000000	0.000000
3A	0.531207	-0.957039	0.000000
4A	0.517716	-0.304760	0.916065
5A	0.517716	-0.304760	-0.916065
6B	1.552559	-0.913932	-0.662765
7B	1.552559	-0.913932	0.662765
8A	0.518999	0.753102	0.572869
9A	0.518999	0.753102	-0.572869
10A	-0.406596	-0.819269	-0.572869
11A	-0.406596	-0.819269	0.572869
12B	0.453084	-1.518846	-1.081789
13B	0.453084	-1.518846	1.081789
14B	1.547878	0.340955	1.081789
15B	1.547878	0.340955	-1.081789
16A	-0.449273	0.264470	0.940964
17A	-0.449273	0.264470	-0.940964
18C	-1.341011	-0.102630	0.000000
19C	-0.561067	1.222312	0.000000
20C	1.569935	1.288383	0.000000
21C	-0.364590	-1.997924	0.000000
22C	0.397361	0.665003	1.873890
23C	-0.388600	-0.670162	1.873890
24C	-0.388600	-0.670162	-1.873890
25C	0.397361	0.665003	-1.873890
26C	1.183509	-2.130693	0.000000
27C	2.437324	-0.000754	0.000000
28C	1.162289	-0.684196	2.022228
29C	1.162289	-0.684196	-2.022228

N = 30

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.098813	0.000000	0.000000
3A	0.532469	-0.953753	0.000000
4A	0.520137	-0.306505	-0.918329
5A	0.519296	-0.296107	0.914701
6A	0.525569	0.733114	-0.570542
7B	1.555621	-0.908144	-0.664783
8B	1.556089	-0.906810	0.663156
9A	0.521907	0.759943	0.563771
10A	-0.406427	-0.815691	-0.575106
11A	-0.407776	-0.813419	0.573970
12B	1.548612	0.351361	-1.085013
13B	1.550243	0.352417	1.075688
14B	0.455543	-1.515553	-1.083654
15B	0.455084	-1.508879	1.084262
16A	-0.441598	0.273229	-0.943309
17C	-0.546258	1.236790	-0.016278
18A	-0.446579	0.279328	0.935911
19C	1.566521	1.299723	-0.009083
20C	0.400822	0.679166	-1.872719
21C	-1.335357	-0.086893	-0.004778
22C	-0.360832	-1.992497	0.001628
23C	-0.383723	-0.659609	-1.875837
24C	0.401530	0.682207	1.865431
25C	-0.385463	-0.652637	1.872899
26C	2.437912	0.010411	-0.004865
27C	1.186566	-2.123653	0.001750
28C	1.164852	-0.673700	-2.023991
29C	1.164987	-0.668437	2.020986
30C	0.499458	1.962906	-0.960737

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.105066	0.000000	0.000000
3A	0.534281	-0.949080	0.000000
4A	0.522849	-0.290739	-0.916173
5A	0.522850	-0.290735	0.916173
6A	0.529580	0.747801	-0.553102
7A	0.529581	0.747804	0.553097
8B	1.557107	-0.902385	-0.667526
9B	1.557107	-0.902382	0.667528
10A	-0.403870	-0.809347	-0.580313
11A	-0.403869	-0.809345	0.580316
12C	-0.565062	1.226662	-0.000004
13C	1.595761	1.292682	-0.000004
14B	1.553777	0.361691	-1.076357
15B	1.553777	0.361696	1.076353
16B	0.457777	-1.500334	1.090973
17B	0.457776	-1.500339	-1.090968
18A	-0.441388	0.286642	-0.936034
19A	-0.441387	0.286647	0.936032
20C	0.404901	0.729987	-1.844512
21C	0.404903	0.729997	1.844507
22C	-1.336682	-0.096793	0.000001
23C	-0.356408	-1.983551	0.000004
24C	-0.375290	-0.626269	1.879815
25C	-0.375292	-0.626278	-1.879813
26C	2.446405	0.001257	-0.000001
27C	1.186648	-2.115563	0.000004
28C	1.164822	-0.640695	-2.025640
29C	1.164824	-0.640685	2.025641
30C	0.492890	2.010009	-0.822629
31C	0.492890	2.010016	0.822613

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.089963	0.000000	0.000000
3A	0.565029	-0.951600	0.000000
4A	0.524934	-0.299383	-0.903279
5A	0.564128	-0.293523	0.915903
6A	0.525836	0.777049	-0.566770
7A	0.544982	0.763841	0.551535
8B	1.620460	-0.861920	0.630167
9B	-0.530497	0.327000	-1.016409
10A	1.466683	-0.823205	-0.611979
11A	-0.376721	-0.839891	-0.588869
12A	1.436527	0.286815	-0.991753
13A	-0.346564	-0.851158	0.584267
14C	1.707877	0.484670	1.087322
15C	-0.617913	1.184592	0.117977
16B	0.531087	0.537323	-1.777858
17B	0.558876	-1.518533	1.069370
18B	0.544981	-1.499702	-1.082869
19A	-0.425414	0.207608	0.967005
20A	1.515379	0.983216	-0.107164
21C	-1.333762	-0.186458	0.058743
22C	2.423725	-0.002903	-0.195472
23C	1.341059	-0.644020	-1.914957
24C	-0.251097	-2.020331	-0.008853
25C	0.687147	1.979025	0.053147
26C	0.402818	0.673070	1.861812
27C	-0.305929	-0.718749	1.890019
28C	1.395893	1.567919	-1.276871
29C	1.322733	-2.058024	-0.046958
30C	-0.232771	-0.692046	-1.938747
31C	-0.146727	1.698049	-1.255369
32C	1.236691	-0.657400	2.006775

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.075218	0.000000	0.000000
3A	0.502095	-0.956471	0.000000
4A	0.502095	-0.297496	-0.909029
5A	0.501332	-0.291852	0.916727
6A	0.501331	0.780480	-0.562510
7A	0.492884	0.779153	0.564825
8B	1.525270	-0.917059	-0.664797
9B	1.525856	0.342483	-1.074312
10B	1.525857	-0.914500	0.659643
11A	-0.442204	-0.792356	-0.574396
12A	-0.441416	-0.794017	0.571287
13A	-0.441417	0.295983	-0.932322
14A	-0.447312	0.289576	0.930152
15A	-0.447313	0.974083	-0.014097
16B	1.530253	1.125009	-0.000085
17B	1.530254	0.349838	1.069232
18B	0.412411	-1.500978	-1.088092
19B	0.414521	0.560922	-1.765280
20B	0.414524	-1.503253	1.082164
21C	-1.336533	-0.002563	-0.001857
22C	0.410152	0.673527	1.876506
23C	0.410150	1.992919	0.056459
24C	-0.407164	-0.616521	-1.874897
25C	-0.407163	-1.973659	-0.002780
26C	-0.409858	1.581981	-1.183744
27C	-0.409855	-0.632977	1.871699
28C	2.418577	-0.007854	-0.005695
29C	1.138243	-2.128912	-0.002975
30C	1.138242	-0.664993	-2.022390
31C	1.146459	1.705195	-1.274998
32C	1.146462	-0.681380	2.017183
33C	-0.591722	1.571996	1.139576

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.078146	0.000000	0.000000
3A	0.503049	-0.956039	0.000000
4A	0.503050	-0.295432	0.909248
5A	0.503050	0.773452	0.561946
6A	0.503050	-0.295432	-0.909248
7A	0.503050	0.773452	-0.561946
8B	1.527663	0.348841	-1.073620
9B	1.527662	-0.913275	-0.663534
10B	1.527663	0.348841	1.073620
11B	1.527662	-0.913275	0.663534
12B	1.527663	1.128871	0.000000
13A	-0.441650	-0.790852	-0.574588
14A	-0.441650	-0.790852	0.574588
15A	-0.441650	0.302079	0.929702
16A	-0.441650	0.302079	-0.929702
17A	-0.441650	0.977547	0.000000
18B	0.414530	0.572249	-1.761197
19B	0.414530	0.572249	1.761197
20B	0.414529	-1.498163	1.088480
21B	0.414529	-1.498163	-1.088480
22B	0.414530	1.851833	0.000000
23C	-1.334089	0.000000	0.000000
24C	-0.404673	-0.608892	1.873981
25C	-0.404673	1.594104	1.158184
26C	-0.404673	1.594104	-1.158184
27C	-0.404673	-0.608892	-1.873981
28C	-0.404674	-1.970419	0.000000
29C	2.417248	0.000000	0.000000
30C	1.139383	-0.656812	2.021462
31C	1.139383	1.719559	1.249332
32C	1.139382	-2.125490	0.000000
33C	1.139383	1.719559	-1.249332
34C	1.139383	-0.656812	-2.021462

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.075416	0.000000	0.000000
3A	0.506905	-0.958202	0.000000
4A	0.506905	-0.296011	0.911334
5A	0.495316	0.771228	0.565231
6A	0.495316	-0.299334	-0.908118
7A	0.492157	0.772598	-0.561384
8A	-0.413724	-0.788235	0.572746
9B	1.526993	-0.914708	0.664644
10B	1.523692	-0.915045	-0.664858
11B	1.523691	0.349660	1.075677
12B	1.516107	0.349053	-1.075450
13B	1.516106	1.130677	0.000252
14A	-0.445723	-0.797337	-0.564564
15A	-0.445724	0.290634	0.932744
16A	-0.456373	0.968122	0.005382
17A	-0.456373	0.293956	-0.922432
18C	-1.339559	-0.026168	0.019013
19B	0.411881	-1.503224	1.092270
20B	0.405351	-1.504328	-1.081653
21B	0.405350	0.564026	1.764894
22B	0.397397	0.566959	-1.758238
23B	0.397397	1.847384	0.003933
24C	-0.418641	-1.970836	0.015058
25C	-0.418642	-0.623157	1.869785
26C	-0.418669	-0.618257	-1.864460
27C	-0.418670	1.582271	1.163990
28C	-0.422835	1.586178	-1.152546
29C	2.410375	0.003860	-0.002804
30C	1.131119	-0.660804	2.023499
31C	1.131120	-2.128661	0.003378
32C	1.125294	-0.661164	-2.020230
33C	1.125293	1.717166	1.252919
34C	1.120898	1.719043	-1.249087
35C	-1.526569	-1.305952	0.948929

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.126202	0.000000	0.000000
3A	-1.125875	-0.027118	0.000000
4A	-0.523393	-0.948771	0.000051
5A	0.546086	-0.935893	0.000051
6A	-0.532400	-0.300821	-0.890286
7A	0.539490	-0.287914	-0.890286
8A	-0.532402	-0.300724	0.890318
9A	0.539488	-0.287817	0.890318
10C	0.017877	-1.484612	-1.076261
11C	0.017875	-1.484494	1.076423
12A	-0.555100	0.748760	-0.551903
13A	0.536910	0.761909	-0.551903
14A	-0.555101	0.748820	0.551819
15A	0.536909	0.761969	0.551819
16C	1.572696	-1.077456	-0.783421
17C	-1.546295	-1.115013	-0.783423
18C	1.572695	-1.077370	0.783542
19C	-1.546297	-1.114927	0.783540
20C	-0.007109	0.590481	-1.726484
21C	-0.007113	0.590670	1.726418
22C	1.578462	0.401286	-1.257390
23C	-1.587667	0.363161	-1.257390
24C	1.578460	0.401423	1.257348
25C	-1.587669	0.363299	1.257347
26C	-1.616068	1.270583	-0.000072
27C	1.585005	1.309128	-0.000071
28C	-0.021883	1.817376	-0.000100
29C	-0.773492	-2.241727	0.000121
30C	0.827246	-2.222452	0.000122
31C	-0.790034	-0.689909	-2.114317
32C	0.806419	-0.670685	-2.114316
33C	-0.790039	-0.689678	2.114390
34C	0.806414	-0.670454	2.114390
35C	-2.426352	-0.079800	0.000002
36C	2.427570	-0.021352	0.000003

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.137670	0.000000	0.000000
3B	-1.273927	-0.013462	0.000000
4A	0.552465	-0.753886	0.549491
5A	0.552464	-0.753806	-0.549600
6A	0.548394	0.292564	0.887768
7A	0.548393	0.292693	-0.887725
8C	0.037480	-1.831458	-0.000132
9A	-0.521206	-0.768585	0.556569
10A	-0.521207	-0.768505	-0.556679
11C	0.032955	-0.562641	-1.742331
12C	0.032955	-0.562893	1.742250
13A	-0.525709	0.290731	0.898634
14A	-0.525710	0.290861	-0.898591
15A	0.552644	0.935516	0.000068
16A	-0.537112	0.942371	0.000069
17C	1.589346	-1.320668	-0.000096
18C	1.586512	-0.405049	-1.260264
19C	1.586513	-0.405232	1.260206
20C	0.021258	1.501822	1.044505
21C	0.021257	1.501973	-1.044287
22C	1.592853	1.066797	-0.775377
23C	1.592853	1.066685	0.775531
24C	-1.516034	-1.419039	-0.000102
25C	-1.519397	-0.441953	1.342247
26C	-1.519398	-0.441758	-1.342309
27C	-1.541907	1.117927	0.827174
28C	-1.541908	1.118047	-0.827010
29C	0.847049	-1.791673	-1.305463
30C	0.847049	-1.791862	1.305204
31C	-0.748549	-1.816764	-1.319879
32C	-0.748548	-1.816955	1.319617
33C	0.832490	0.703378	2.100342
34C	0.832489	0.703682	-2.100240
35C	2.439305	-0.006571	0.000000
36C	-0.752718	0.703199	2.123713
37C	-0.752718	0.703506	-2.123611

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124935	0.000000	0.000000
3A	-1.124843	-0.014460	0.000000
4A	-0.531146	-0.763081	-0.550348
5A	-0.531146	-0.763093	0.550332
6A	0.540910	-0.756191	-0.550348
7A	0.540910	-0.756203	0.550332
8A	-0.538764	0.285181	0.889364
9A	-0.538764	0.285201	-0.889357
10A	0.535053	0.292082	0.889364
11A	0.535053	0.292102	-0.889357
12C	0.011763	-1.830324	-0.000019
13C	0.003624	-0.563967	-1.738729
14C	0.003624	-0.564006	1.738717
15A	-0.551529	0.932054	0.000011
16A	0.539503	0.939067	0.000011
17C	-1.555807	-1.346107	-0.000014
18C	1.572980	-1.325998	-0.000014
19C	-1.563703	-0.428363	1.264773
20C	-1.563703	-0.428335	-1.264782
21C	1.569079	-0.408229	1.264774
22C	1.569079	-0.408201	-1.264782
23C	-0.009623	1.497183	1.042958
24C	-0.009623	1.497206	-1.042924
25C	1.577881	1.064123	0.778356
26C	1.577881	1.064140	-0.778332
27C	-1.591429	1.043754	0.778356
28C	-1.591429	1.043771	-0.778332
29C	0.816290	-1.794420	1.306744
30C	0.816290	-1.794392	-1.306782
31C	-0.793160	-1.804764	1.306744
32C	-0.793159	-1.804735	-1.306782
33C	-0.805358	0.692647	2.102470
34C	-0.805358	0.692693	-2.102454
35C	0.796388	0.702941	2.102470
36C	0.796387	0.702987	-2.102454
37C	-2.423376	-0.042343	0.000000
38C	2.423719	-0.011191	0.000000

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.136194	0.000000	0.000000
3B	-1.272885	-0.000001	0.000000
4A	0.549937	0.288375	0.888273
5A	0.549937	0.288813	-0.888131
6A	0.549938	-0.755685	0.548753
7A	0.549938	-0.755414	-0.549125
8A	0.549937	0.933911	0.000230
9A	-0.525073	-0.765109	0.555595
10A	-0.525073	-0.764835	-0.555973
11A	-0.525074	0.291971	0.899350
12A	-0.525074	0.292414	-0.899206
13A	-0.525074	0.945556	0.000233
14C	0.029658	-1.830251	-0.000451
15C	0.029656	1.480969	-1.075429
16C	0.029656	1.480438	1.076159
17C	0.029657	-0.565149	-1.740811
18C	0.029657	-0.566008	1.740532
19C	1.587717	-0.408063	-1.256944
20C	1.587717	-0.408682	1.256743
21C	1.587718	-1.321523	-0.000326
22C	1.587716	1.069327	-0.776508
23C	1.587716	1.068944	0.777036
24C	-1.525053	-1.406220	-0.000347
25C	-1.525054	1.137450	0.826835
26C	-1.525054	1.137858	-0.826274
27C	-1.525054	-0.434876	1.337286
28C	-1.525053	-0.434217	-1.337500
29C	0.841967	2.217698	0.000547
30C	0.841969	-1.793834	-1.303973
31C	0.841969	-1.794476	1.303088
32C	0.841968	0.685827	-2.108987
33C	0.841967	0.684786	2.109325
34C	2.436544	0.000001	0.000000
35C	-0.758102	-1.813077	-1.317961
36C	-0.758102	-1.813727	1.317066
37C	-0.758104	2.241487	0.000553
38C	-0.758103	0.693183	-2.131611
39C	-0.758104	0.692132	2.131952

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.123359	0.000000	0.000000
3A	-1.123359	0.000000	0.000000
4A	0.537062	-0.756985	-0.550232
5A	0.537062	-0.757223	0.549904
6A	0.537061	0.289380	-0.889966
7A	0.537062	0.288995	0.890091
8A	0.537061	0.935831	0.000202
9A	-0.537061	-0.756985	-0.550232
10A	-0.537061	-0.757223	0.549904
11A	-0.537061	0.289380	-0.889966
12A	-0.537062	0.288995	0.890091
13A	-0.537062	0.935831	0.000202
14C	0.000000	-1.826900	-0.000396
15C	0.000000	1.478224	-1.073505
16C	0.000000	1.477760	1.074144
17C	0.000000	-0.564168	-1.737607
18C	0.000000	-0.564920	1.737362
19C	1.570538	-1.325050	-0.000287
20C	1.570538	-0.409736	1.260109
21C	1.570538	-0.409191	-1.260286
22C	1.570537	1.071820	0.779077
23C	1.570538	1.072156	-0.778613
24C	-1.570538	-1.325051	-0.000287
25C	-1.570538	-0.409736	1.260109
26C	-1.570537	1.071819	0.779077
27C	-1.570538	-0.409191	-1.260286
28C	-1.570538	1.072156	-0.778613
29C	0.808693	-1.795938	1.304230
30C	0.808694	-1.795372	-1.305009
31C	-0.808693	-1.795938	1.304230
32C	-0.808693	-1.795373	-1.305009
33C	0.808693	0.685421	2.111067
34C	0.808693	0.686335	-2.110771
35C	-0.808693	0.685421	2.111067
36C	-0.808693	0.686335	-2.110771
37C	0.808693	2.219551	0.000480
38C	-0.808693	2.219551	0.000480
39C	2.420332	0.000000	0.000000
40C	-2.420332	0.000000	0.000000

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.065436	0.000000	0.000000
3A	0.478081	-0.952152	0.000000
4A	0.478081	-0.294914	0.905328
5A	0.479564	0.767992	0.561306
6A	0.479564	-0.295829	-0.904081
7A	-0.471145	-0.773185	0.561307
8A	0.473345	0.775288	-0.562833
9A	-0.480456	-0.770901	-0.562833
10A	-0.480456	0.296380	0.907319
11A	-0.474112	0.292467	-0.909575
12A	-0.474112	0.955432	0.003643
13A	-1.066586	-0.005018	0.003643

14B	1.493272	-0.921158	0.668730
15B	0.359988	-1.491548	1.082814
16B	1.494490	-0.921909	-0.665865
17B	1.494490	0.347572	1.082814
18B	-0.344598	-0.572823	1.752331
19B	-0.344597	-1.843579	0.001898
20B	0.357291	-1.491158	-1.079967
21B	1.492931	1.135205	0.001898
22B	0.357291	0.564994	1.752330
23B	1.492931	0.349808	-1.079967
24B	-0.342640	1.491730	1.089165
25B	0.358829	0.563577	-1.755723
26B	-0.342640	-0.573563	-1.755723
27B	-1.486868	-0.363157	1.089165
28B	-1.486868	-1.148086	0.007947
29B	0.358830	1.843941	0.007947
30C	-1.619767	0.999189	0.627007
31C	-0.470610	1.576186	-1.144257
32C	-1.619767	-0.286691	-1.144258
33C	2.384861	-0.001160	0.000842
34C	1.071166	-0.660772	2.025722
35C	1.071166	-2.130767	0.000842
36C	1.077530	-0.664698	-2.021492
37C	1.077531	1.716201	1.258136
38C	-1.050216	-1.733050	1.258137
39C	1.079703	1.721026	-1.249406
40C	-1.053554	0.649908	2.038712
41C	-1.053553	-1.737157	-1.249407

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.071101	0.000000	0.000000
3A	0.488520	-0.949289	0.000000
4A	0.483022	-0.294649	0.903185
5A	0.490021	-0.295027	-0.902577
6A	0.488284	0.765761	0.558520
7A	-0.471192	-0.777121	0.562578
8A	0.482469	0.773204	-0.563941
9A	-0.467336	-0.775191	-0.566166
10A	-0.482493	0.297880	0.909716
11A	-0.466846	0.290374	-0.915134
12A	-0.464559	0.959269	0.000544
13A	-1.069505	-0.008056	0.004675
14B	1.505301	-0.917554	0.668718
15B	1.509249	-0.918667	-0.663677
16B	0.378581	-1.489031	1.079767
17B	1.505492	0.345149	1.080670
18B	1.505139	1.131168	0.001914
19B	-0.314714	-1.849978	-0.005235
20B	1.505796	0.347294	-1.077941
21B	0.383223	-1.490028	-1.081035
22B	0.375864	0.563180	1.747716
23B	-0.334631	-0.574699	1.752579
24C	-1.619147	-0.386002	1.146599
25B	0.377816	1.843173	0.005363
26B	-0.321837	-0.578387	-1.758946
27B	0.374846	0.560567	-1.756771
28B	-0.313290	1.498180	1.088553
29B	-1.461953	-1.186342	-0.012166
30C	-1.602590	-0.335992	-1.157210
31C	-0.426648	1.588074	-1.156324
32C	-1.592816	1.049363	0.655797
33C	1.096387	-2.127528	0.001692
34C	1.082218	-0.661100	2.024965
35C	2.396975	-0.000448	0.002007
36C	1.100349	1.713702	1.255364
37C	1.097551	-0.663374	-2.020946
38C	-1.005888	-1.782682	1.249388
39C	-1.010192	-1.763823	-1.264154
40C	1.110673	1.715600	-1.249548
41C	-1.006781	0.685717	2.066567
42A	-1.379597	0.849857	-0.626358

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.072243	0.000000	0.000000
3A	0.490828	-0.953306	0.000000
4A	0.493535	-0.301002	0.898845
5A	0.493532	-0.301002	-0.898846
6A	0.484085	0.772253	0.560224
7A	0.484083	0.772253	-0.560223
8A	-0.464998	-0.783891	0.560226
9A	-0.465000	-0.783891	-0.560222
10A	-0.464472	0.283281	0.917837
11A	-0.464476	0.283281	-0.917834
12A	-0.485178	0.956460	0.000002
13A	-1.072460	-0.006464	0.000003
14B	1.513849	-0.923287	-0.661172
15B	1.513851	-0.923287	0.661168
16B	1.510797	0.340341	-1.074514
17B	0.388993	-1.499009	1.074512
18B	0.388989	-1.499009	-1.074512
19B	1.510801	0.340340	1.074511
20B	1.499870	1.137720	-0.000001
21B	-0.324944	-1.854298	0.000001
22B	-0.301169	-0.596012	-1.757692
23B	0.392039	0.540591	-1.757693
24B	-0.301162	-0.596013	1.757695
25B	0.392045	0.540590	1.757694
26C	-1.612796	-1.208249	0.000004
27C	0.335959	1.986986	0.000001
28B	-1.451720	-0.381906	1.138372
29B	-0.324993	1.465515	-1.138365
30B	-1.451724	-0.381905	-1.138364
31B	-0.324989	1.465515	1.138370
32C	-1.598170	0.974715	-0.750177
33C	-1.598167	0.974715	0.750186
34C	1.111040	-0.677614	2.016482
35C	1.111033	-0.677613	-2.016484
36C	2.400296	0.003750	-0.000003
37C	1.095420	-2.135764	-0.000001
38C	1.108918	1.692969	1.292496
39C	1.108914	1.692970	-1.292496
40C	-0.997563	-1.760880	1.292499
41C	-0.997569	-1.760879	-1.292494
42C	-0.990630	0.604183	2.109224
43C	-0.990638	0.604184	-2.109217

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.071527	0.000000	0.000000
3A	0.489535	-0.949457	0.000000
4A	0.489534	-0.293361	0.903000
5A	0.486486	0.766582	-0.556981
6A	0.483522	-0.295388	-0.902829
7A	0.483521	0.767385	0.559886
8A	-0.473602	0.293401	-0.910105
9A	-0.473603	0.956226	0.002153
10A	-0.457086	-0.776582	0.564245
11A	-0.474259	-0.775193	-0.559819
12A	-0.474261	0.292911	0.910232
13A	-1.070742	-0.002767	0.002009
14B	1.508419	-0.916504	0.665910
15B	1.503964	1.133839	0.002521
16B	1.503965	0.347931	-1.079139
17B	1.504698	0.352392	1.079420
18B	1.504700	-0.917723	-0.668663
19B	0.372288	0.565439	1.749288
20B	0.372291	-1.488990	-1.078260
21B	0.384484	-1.490805	1.083183
22B	0.376244	1.836583	0.003261
23B	0.376246	0.564356	-1.747728
24B	-0.320131	-0.579661	1.755149
25B	-0.320129	-1.848372	0.008999
26B	-0.315402	1.494923	-1.086177
27B	-0.339647	-0.574026	-1.751108
28B	-0.339650	1.488066	1.086986
29C	-1.624023	0.964760	0.702859
30C	-1.624021	-0.370384	-1.134724
31B	-1.466013	-0.386622	1.104316
32B	-1.466012	-1.169740	0.026495
33B	-1.461313	0.965546	-0.701545
34C	1.093389	-2.126856	-0.001422
35C	1.093387	-0.655794	2.023229
36C	1.093887	1.718265	-1.248451
37C	1.078964	-0.661531	-2.023682
38C	1.078961	1.720267	1.254430
39C	2.395663	0.001226	-0.000889
40C	-1.016271	-1.748999	1.270779
41C	-1.009008	0.691242	-2.059425
42C	-1.009011	2.172232	-0.021112
43C	-1.019372	-1.772959	-1.240048
44C	-1.019375	0.631571	2.069350

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.064413	0.000000	0.000000
3A	0.476020	-0.952040	0.000000
4A	0.476020	-0.294196	0.905444
5A	0.476020	-0.294197	-0.905444
6A	0.476020	0.770217	0.559595
7A	-0.476020	-0.770217	0.559595
8A	-0.476020	-0.770217	-0.559595
9A	0.476020	0.770216	-0.559595
10A	-0.476020	0.294196	-0.905444
11A	-0.476020	0.294197	0.905444
12A	-1.064413	0.000000	0.000000
13A	-0.476020	0.952040	0.000000
14B	-1.489767	0.920727	0.668947
15B	-1.489767	-0.351687	-1.082379
16B	-0.351686	1.489767	-1.082379
17B	0.351687	-1.489767	1.082379
18B	-0.351686	-0.569041	-1.751326
19B	-1.489767	0.920727	-0.668947
20B	1.489767	-0.920727	-0.668947
21B	1.489767	0.351687	1.082379
22B	0.351686	1.841453	0.000000
23B	-1.489767	-0.351686	1.082379
24B	1.489767	-0.920726	0.668947
25B	-0.351686	-0.569040	1.751326
26B	0.351687	-1.489767	-1.082379
27B	1.489767	1.138081	0.000000
28B	-0.351686	-1.841453	0.000000
29B	1.489767	0.351686	-1.082379
30B	0.351686	0.569040	-1.751326
31B	0.351686	0.569041	1.751326
32B	-0.351686	1.489767	1.082379
33B	-1.489767	-1.138081	0.000000
34C	2.380993	0.000000	0.000000
35C	1.064813	-2.129624	0.000000
36C	1.064813	-0.658090	2.025394
37C	1.064812	-0.658090	-2.025394
38C	-1.064812	-1.722903	-1.251761
39C	1.064812	1.722902	-1.251762
40C	1.064812	1.722903	1.251762
41C	-1.064812	-1.722903	1.251762
42C	-1.064812	0.658091	2.025393
43C	-1.064812	0.658090	-2.025393
44C	-2.380993	0.000000	0.000000
45C	-1.064812	2.129625	0.000000

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.064219	0.000000	0.000000
3A	0.476056	-0.951806	0.000000
4A	0.474147	-0.292997	0.906454
5A	0.474147	-0.292996	-0.906455
6A	0.476637	0.770006	0.559587
7A	0.476637	0.770007	-0.559587
8A	-0.475457	-0.770736	0.559587
9A	-0.475457	-0.770736	-0.559587
10A	-0.476194	0.294262	0.905471
11A	-0.476194	0.294262	-0.905470
12A	-0.475604	0.951971	0.000000
13A	-1.064165	-0.000478	0.000000
14B	1.482088	-0.915849	0.673982
15B	1.482089	-0.915849	-0.673982
16B	1.490623	0.351407	1.082501
17B	0.352510	-1.490362	-1.082501
18B	0.352510	-1.490363	1.082500
19B	1.490623	0.351408	-1.082500
20B	1.491982	1.135685	0.000001
21B	-0.348315	-1.842408	0.000000
22B	-0.351882	-0.569438	-1.751615
23B	-0.351883	-0.569439	1.751614
24B	0.351882	0.569440	-1.751614
25B	0.351882	0.569439	1.751615
26B	0.353093	1.840803	0.000001
27B	-1.488409	-1.139239	0.000000
28B	-0.351023	1.489676	-1.082282
29B	-1.489344	-0.352429	-1.082283
30B	-1.489344	-0.352430	1.082283
31B	-0.351023	1.489676	1.082283
32B	-1.489572	0.920475	-0.668805
33B	-1.489572	0.920474	0.668805
34C	2.380379	-0.008932	0.000000
35C	1.072802	-2.124942	-0.000001
36C	1.064133	-0.657576	2.027063
37C	1.064133	-0.657575	-2.027064
38C	1.066124	1.722319	-1.251251
39C	-1.063481	-1.723951	1.251252
40C	1.066124	1.722318	1.251253
41C	-1.063481	-1.723951	-1.251252

42C	-1.064740	0.657951	2.025260
43C	-1.064740	0.657952	-2.025259
44C	-1.063848	2.129507	0.000001
45C	-2.380456	-0.001114	0.000000
46C	2.553999	-1.578230	0.000000

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.063609	0.000000	0.000000
3A	0.469178	-0.954048	0.000000
4A	0.469178	-0.289286	-0.909132
5A	0.478223	-0.298488	0.903616
6A	0.478222	0.770568	-0.558429
7A	-0.477824	-0.768438	-0.561885
8A	0.479396	0.767400	0.561127
9A	-0.475906	-0.772189	0.558298
10A	-0.475907	0.297871	-0.905121
11A	-0.472904	0.291506	0.907045
12A	-0.472904	0.952733	0.002749
13A	-1.063544	0.001177	0.000861
14B	1.454588	-0.915601	-0.669492
15B	1.491320	0.351099	-1.080986
16B	1.491321	-0.923634	0.662346
17B	0.345041	-1.489369	-1.089034
18B	1.493992	0.345055	1.081067
19B	1.493991	1.134799	0.001009
20B	0.355384	-1.496057	1.076231
21B	0.355383	0.571929	-1.751957
22B	-0.350825	-0.564452	-1.755351
23B	-0.350824	-1.843863	-0.005621
24B	0.357469	1.840059	0.003944
25B	0.357470	0.561700	1.752235
26B	-0.347059	-0.575567	1.749644
27B	-0.347060	1.492749	-1.078996
28B	-1.489597	-0.346327	-1.083023
29B	-1.489596	-1.137049	-0.001628
30B	-0.345774	1.486397	1.086861
31B	-1.485555	0.920573	0.673128
32B	-1.487241	0.925062	-0.665464
33B	-1.487241	-0.353638	1.083293
34C	2.379465	-0.002725	-0.001993
35C	1.076069	-0.655003	-2.023358
36C	1.076069	-2.126710	-0.010644
37C	1.071253	-0.668328	2.019159
38C	1.071252	1.721449	-1.249112
39C	1.071646	1.716186	1.254884
40C	-1.069466	-1.717720	-1.256005
41C	-1.062208	-1.726789	1.247462
42C	-1.062209	0.665136	-2.023747
43C	-1.058569	0.652341	2.028607
44C	-1.058570	2.130904	0.006517
45C	-2.379048	0.002925	0.002140
46C	2.567867	-0.564721	-1.445406
47C	2.567867	-1.548592	-0.099860

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.063199	0.000000	0.000000
3A	0.479891	-0.948735	0.000000
4A	0.479891	-0.295051	0.901689
5A	-0.471282	-0.772286	0.559872
6A	0.476420	0.769125	0.559874
7A	0.476421	-0.292916	-0.905103
8A	-0.472886	0.290742	0.907712
9A	0.475693	0.770555	-0.558617
10A	-0.472886	-0.772281	-0.558618
11A	-1.063186	-0.003928	0.002848
12A	-0.476380	0.950495	0.002848
13A	-0.476380	0.292892	-0.904247
14A	1.395759	-0.858152	0.622122
15B	1.486994	0.338422	1.072686
16B	0.369189	-1.479657	1.072684
17B	1.486994	-0.914245	-0.655240
18B	-0.342610	-1.843054	0.000525
19B	1.489987	1.137614	0.000528
20B	0.357273	-1.489037	-1.081367
21B	-0.342611	-0.573680	1.751497
22B	0.357272	0.564661	1.751498
23B	1.489987	0.353291	-1.081366
24B	-1.483669	-1.144577	0.003789
25B	0.351675	0.568801	-1.750466
26B	-0.348830	1.486226	1.086642
27B	0.351674	1.840558	0.003791
28B	-0.348829	-0.570549	-1.750467
29B	-1.483669	-0.359559	1.086641
30B	-1.487917	-0.356470	-1.079187
31B	-1.487917	0.914811	0.674414
32B	-0.353501	1.488625	-1.079186
33B	-1.490750	0.916555	-0.664461
34C	1.071519	-0.658802	2.008188
35C	2.369595	-0.002204	0.001599
36C	1.071520	-2.113489	0.001596
37C	1.072390	-0.659334	-2.018525
38C	1.072389	1.713381	1.254390
39C	-1.044878	-1.730298	1.254387
40C	-1.058518	0.650803	2.029592
41C	-1.058517	-1.726552	-1.249724
42C	1.062894	1.723862	-1.249721
43C	-1.066181	2.125835	0.005897
44C	-2.378204	-0.008133	0.005896
45C	-1.066181	0.655518	-2.022253
46C	2.487909	-0.621236	1.406166
47C	1.677307	-1.939658	1.406164
48C	2.487910	-1.529636	0.153120

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.062285	0.000000	0.000000
3A	0.481797	-0.948399	0.000000
4A	0.470453	-0.301610	-0.903012
5A	0.473804	0.767468	-0.563466
6A	0.478874	0.772930	0.553881
7A	0.480088	-0.290037	0.904570
8A	-0.472903	-0.775048	-0.556457
9A	-0.476033	0.288478	-0.907477
10A	-0.469428	-0.771099	0.561856
11A	-0.474402	0.951659	-0.005208
12A	-0.472134	0.296522	0.904464
13A	-1.062382	-0.003509	0.000217
14A	1.396384	-0.853874	-0.624645
15B	1.463438	0.321471	-1.075374
16B	1.491297	-0.911551	0.653755
17B	0.370119	-1.483261	-1.073424
18B	1.492641	1.135099	-0.010171
19B	0.349255	0.560001	-1.755908
20B	1.493284	0.358280	1.077784
21B	-0.349446	-0.579201	-1.750645
22B	0.364218	-1.486437	1.082289
23B	-0.337666	-1.843635	0.004163
24B	0.357860	1.840725	-0.014728
25B	-0.346613	1.484427	-1.092077
26C	2.368768	0.002628	0.001922
27B	0.358457	0.575695	1.746934
28B	-1.486678	-0.362732	-1.080826
29B	-0.341704	-0.565137	1.752503
30B	-0.346628	1.493638	1.073705
31B	-1.481982	-1.145134	0.004267
32B	-1.487839	0.914621	-0.672806
33B	-1.482576	-0.352874	1.084556
34B	-1.486261	0.920281	0.665539
35C	1.065463	-0.659887	-2.015353
36C	1.081878	-2.108071	-0.006445
37C	1.086228	1.698734	-1.264526
38C	2.492872	-0.576520	-1.409883
39C	1.079475	-0.652947	2.017038
40C	1.071110	1.728927	1.236801
41C	-1.046674	-1.734839	-1.246183
42C	-1.065834	0.646058	-2.027941
43C	-1.051177	-1.723546	1.256887
44C	-1.060844	2.127591	-0.011219
45C	-1.057839	0.663223	2.022471
46C	-2.376531	-0.007025	0.001746
47C	2.497138	-1.513048	-0.164490
48C	1.691953	-1.918742	-1.411882
49C	2.572440	1.172978	-0.997320

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.055046	0.000000	0.000000
3A	0.474834	-0.944109	0.000000
4A	0.484328	-0.310854	0.897861
5A	0.484328	-0.310853	-0.897861
6A	-0.461239	-0.792802	0.556522
7A	-0.461238	-0.792802	-0.556523
8A	0.488230	0.770703	0.562417
9A	0.488230	0.770704	-0.562416
10A	-0.469333	0.266970	0.909781
11A	-0.469333	0.266971	-0.909780
12A	-1.058749	-0.032927	0.000000
13A	-0.477672	0.944475	0.000001
14A	1.392038	-0.873240	-0.586971
15A	1.392038	-0.873241	0.586971
16B	0.387848	-1.504822	-1.054803
17B	0.387847	-1.504822	1.054803
18B	1.499596	0.299914	1.073599
19B	1.499596	0.299916	-1.073599
20C	1.657282	1.189449	0.000001
21B	-0.304201	-1.871528	0.000000
22C	0.370561	1.980331	0.000001
23B	-0.325362	-0.613292	1.748106
24B	-0.325361	-0.613291	-1.748106
25B	0.360302	0.518305	-1.758208
26B	0.360301	0.518303	1.758209
27B	-1.462563	-1.184772	0.000000
28B	-1.473828	-0.401003	-1.084780
29B	-1.473828	-0.401003	1.084780
30B	-1.493252	0.869463	-0.675550
31B	-1.493252	0.869463	0.675551
32B	-0.364599	1.454948	1.101370
33B	-0.364599	1.454949	-1.101369
34B	1.063514	-1.957868	0.000000
35B	2.220262	-0.128274	0.000000
36C	1.111964	-0.714550	1.976340
37C	1.111965	-0.714549	-1.976339
38C	2.417593	-1.527135	0.000000
39C	-1.021317	-1.767768	-1.245705
40C	-1.021318	-1.767768	1.245705
41C	-1.058594	0.601908	2.035413
42C	-1.058593	0.601909	-2.035413
43C	-2.371543	-0.060598	0.000000
44C	1.067819	1.671554	1.344866
45C	1.067819	1.671556	-1.344864
46C	-1.147436	2.081599	0.000000
47C	2.516321	-0.670093	-1.294523
48C	2.516321	-0.670094	1.294523
49C	1.701120	-1.984753	1.290505
50C	1.701121	-1.984752	-1.290505

TLJ (S_C = 1.5)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.123998	0.000000	0.000000
3A	0.562000	-0.973411	0.000000
4C	0.562000	-0.324470	-1.239161
5C	0.562000	-0.324470	1.239161

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.184180	0.000000	0.000000
3C	0.592090	-1.242964	0.000000
4C	0.592090	0.000000	-1.242964
5C	0.592090	0.000000	1.242964
6C	0.592090	1.242964	0.000000

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.409860	0.000000	0.000000
3C	0.394643	-1.341452	0.000000
4C	0.396357	1.048084	0.837272
5C	0.396357	1.048084	-0.837272
6A	0.454748	-0.338539	0.966493
7A	0.454748	-0.338539	-0.966493

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.372615	0.000000	0.000000
3C	0.234630	-1.361777	0.000000
4C	0.234630	0.916203	-1.007477
5A	0.494380	-0.428603	-0.969103
6C	0.359385	1.191352	0.630439
7C	0.359384	-0.335126	1.305551
8C	-0.886537	-0.420728	-0.951296

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.381971	0.000000	0.000000
3C	0.352502	-1.336259	0.000000
4C	0.352502	-0.285471	1.305409

5C	-0.650090	0.949986	-0.764691
6C	-1.084382	-0.664517	-0.540720
7C	0.365940	-0.268028	-1.305410
8C	-1.084383	0.386271	0.764691
9C	0.365940	1.218012	0.540721

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.364329	0.000000	0.000000
3C	0.232880	-1.344307	0.000000
4C	0.284442	1.012551	-0.860671
5C	0.284442	1.012551	0.860671
6C	-0.949138	-0.453101	-0.860672
7C	-0.949138	-0.453101	0.860672
8B	-0.964833	0.812061	0.000000
9A	0.433717	-0.365042	0.967822
10A	0.433717	-0.365042	-0.967822

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.391721	0.000000	0.000000
3C	0.392031	-1.335365	0.000000
4B	-0.448612	-0.545383	1.021855
5B	0.396929	0.584074	1.021855
6C	-1.030587	0.771524	0.504433
7C	0.382137	1.269399	-0.361285
8C	-1.110351	-0.724238	-0.361286
9C	0.354045	-0.265047	-1.291725
10A	-0.669973	0.501559	-0.794461
11C	1.005157	-0.752488	1.435705

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.353576	0.000000	0.000000
3C	-1.011156	-0.943525	0.000000
4C	-1.011156	0.599714	0.728412
5A	0.398240	0.409974	0.949630
6A	0.398240	-0.993708	0.287090
7A	-0.233240	-0.485510	1.028619
8C	0.249760	1.383609	-0.007340
9C	0.249759	-0.873768	-1.072826
10C	-0.887620	0.443738	-0.940117
11A	0.490165	0.457249	-0.968746
12C	1.054579	-0.698142	1.479108

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.413487	0.000000	0.000000
3A	-1.149552	0.000000	0.000000
4B	0.450784	1.162837	-0.218219
5B	0.450784	0.566875	1.038490
6B	0.450784	0.151798	-1.173357
7B	0.450784	-0.812488	0.860041
8B	0.450784	-1.069020	-0.506955
9A	-0.587073	0.653909	-0.692180
10A	-0.587073	0.860372	0.408009
11A	-0.587073	-0.122170	0.944344
12A	-0.587073	-0.935877	0.175628
13A	-0.587073	-0.456234	-0.835800

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094025	0.000000	0.000000
3C	0.547012	-1.254802	0.000000
4C	0.547012	0.004238	1.254794
5A	0.547012	0.942228	0.183854
6A	0.547012	-0.187034	-0.941602
7C	-0.283449	0.941507	-0.944692
8C	1.377475	0.941506	-0.944691
9C	-0.755146	-0.676769	-0.915917
10C	-0.755146	0.918197	0.673672
11C	1.849170	-0.676771	-0.915916
12C	1.849170	0.918196	0.673674
13C	-0.862167	-0.757488	0.760050
14C	1.956190	-0.757488	0.760051

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.122549	0.000000	0.000000
3C	0.598790	-1.252248	0.000000
4C	0.598789	-0.069270	-1.250331
5C	-0.257106	0.966307	0.914257
6A	0.579436	-0.148326	0.935716
7A	0.579435	0.926079	-0.199857
8C	1.412326	0.970902	0.918602
9C	-0.632828	-0.774613	0.990755
10C	-0.632828	0.946391	-0.828230
11C	-0.830795	-0.784894	-0.742614
12C	1.868912	0.909467	-0.704019
13C	1.868914	-0.652633	0.947016
14C	2.028665	-0.758144	-0.717306
15A	-1.133718	0.194063	0.183610

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.067367	0.000000	0.000000
3C	0.534505	-1.284850	0.000000
4C	0.563525	1.355588	0.033886
5A	0.523979	0.343103	0.919357
6A	0.557427	0.389994	-0.905499
7C	1.861652	0.671898	0.898128
8B	-0.149632	-0.585694	-1.139991
9B	1.255391	-0.596927	-1.125775
10C	-0.776180	0.773456	-0.830734
11C	-0.801036	0.752285	0.830447
12C	1.913979	0.735353	-0.774206
13C	-0.201279	-0.718602	1.335049
14A	1.162096	-0.545656	0.977156
15C	2.192137	-0.760863	0.063936
16C	-1.168010	-0.689796	-0.015468

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.371942	0.000000	0.000000
3C	-0.837031	-1.125136	0.000000
4A	0.423916	-0.832273	0.539254
5A	0.423916	-0.832273	-0.539254
6B	-0.494558	-0.213870	1.137205
7B	0.399418	-1.969009	0.000000
8B	-0.494558	-0.213870	-1.137205
9C	1.581350	-1.497257	-0.828552
10C	0.282682	1.052410	-0.823451
11C	0.282682	1.052411	0.823450
12C	0.934021	-0.226360	1.652003
13C	0.934021	-0.226360	-1.652003
14C	1.581349	-1.497257	0.828552
15C	-0.043329	-1.670737	1.466011
16C	-1.195785	0.591876	0.000000
17C	-0.043329	-1.670737	-1.466011

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.073870	0.000000	0.000000
3C	0.515392	-1.346854	0.000000
4A	0.553802	-0.342107	0.908386
5C	0.540260	1.278442	0.011077
6C	-0.757510	-0.710789	0.918388
7C	1.859751	-0.772655	0.837372
8C	1.286409	0.706095	1.337872
9A	0.511261	-0.356794	-0.913105
10A	-0.086085	0.539856	0.975613
11C	1.847463	-0.771983	-0.832097
12C	-0.849679	-0.756164	-0.750681
13C	-0.270660	0.697247	-1.283182
14B	1.255132	0.600572	-1.126895
15C	-1.149805	0.719154	0.118646
16C	2.261757	0.661939	0.005374
17C	0.088509	-0.047018	2.204809
18C	0.574318	-1.517763	1.635768

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.106133	0.000000	0.000000
3A	0.553067	-0.922179	0.000000
4C	0.553067	0.562672	1.157945
5C	0.553066	0.562673	-1.157945
6C	1.887729	-1.271141	-0.000001
7C	-0.781595	-1.271141	0.000001
8A	0.006883	-0.666108	-0.923839
9A	1.099250	-0.666108	-0.923840
10A	1.099251	-0.666108	0.923839
11A	0.006884	-0.666108	0.923840
12C	1.392642	1.374025	0.000000
13C	-0.286508	1.374024	0.000001
14C	0.553067	-1.957967	-0.854951
15C	0.553067	-1.957968	0.854950
16C	-1.079203	0.169300	0.840166
17C	2.185337	0.169300	0.840165
18C	-1.079204	0.169300	-0.840164
19C	2.185337	0.169301	-0.840166

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.197703	0.000000	0.000000
3A	0.598851	-0.912246	0.000000
4A	0.598851	-0.295459	-0.892984
5A	0.598852	-0.295459	0.892984
6A	0.598851	0.751775	-0.554424
7A	0.598852	0.751774	0.554425
8C	-0.433865	-1.188889	-0.829698
9C	-0.433863	-1.188890	0.829699
10C	1.631567	-1.188890	0.829698
11C	1.631566	-1.188889	-0.829699
12C	-0.482039	0.394640	-1.330825
13C	1.679741	0.394638	1.330828
14C	1.679741	0.394640	-1.330826
15C	-0.482037	0.394638	1.330828
16C	1.692956	1.362047	0.000001
17C	-0.495252	1.362047	0.000002
18C	2.568256	-0.077969	0.000000
19C	-1.370553	-0.077969	0.000002
20C	0.598852	-2.261996	0.000000

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.198969	0.000000	0.000000
3A	0.599484	-0.917150	0.000000
4A	0.599484	-0.289503	0.870259
5C	1.604290	-1.202290	0.867113
6C	-0.405322	-1.202290	0.867113
7A	0.599484	0.752681	0.563269
8A	0.599485	-0.296883	-0.891998
9A	0.599484	0.756326	-0.545475
10C	1.646633	0.383238	1.380256
11C	-0.447665	0.383237	1.380255
12C	1.646634	-1.188717	-0.799329
13C	-0.447664	-1.188718	-0.799329
14C	1.701885	1.350821	0.037987
15C	-0.502917	1.350821	0.037987
16C	-0.502917	0.390349	-1.293750
17C	1.701885	0.390350	-1.293749
18C	-1.364218	-0.091214	0.065785
19C	2.563187	-0.091213	0.065786
20C	0.599485	-2.266918	0.014296
21C	0.599484	-0.729130	2.146507

N = 22

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.078302	0.000000	0.000000
3A	0.513392	-0.948242	0.000000
4C	1.290066	-0.768552	-1.161495
5A	0.518345	0.321203	-0.905029
6A	-0.035673	-0.608755	-0.905028
7C	0.377393	1.323254	0.001139
8C	-0.983970	-0.961888	0.001142
9C	-0.851960	0.507551	-0.919352
10C	1.274691	-0.759390	1.155039
11C	1.763209	0.844947	-0.862659
12C	0.096445	-1.952830	-0.862656
13A	0.496499	0.339245	0.923410
14A	-0.061938	-0.598130	0.923410
15C	0.158465	-0.094407	-2.168585
16C	-0.902936	0.537921	0.821506
17C	2.402193	-0.448337	-0.003976
18C	1.537969	-1.898997	-0.003975
19C	0.093059	-1.961575	0.824231
20C	1.769289	0.852092	0.824229
21C	0.374213	1.464750	-1.644586
22C	-1.109917	-1.026461	-1.644582

N = 23

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.161112	0.000000	0.000000
3A	0.580555	-1.005553	0.000000

4A	0.580556	-0.335184	0.857080
5A	0.580556	-0.335185	-0.857080
6A	1.512318	-0.873138	0.571010
7A	1.512318	-0.873139	-0.571009
8A	-0.351208	-0.873137	-0.571010
9A	-0.351208	-0.873137	0.571010
10A	0.580556	0.740722	-0.571010
11A	0.580556	0.740723	0.571010
12C	-0.504937	0.291526	1.324519
13C	0.580554	-1.588604	-1.324519
14C	1.666048	0.291524	-1.324519
15C	1.666048	0.291525	1.324519
16C	0.580554	-1.588603	1.324519
17C	-0.504936	0.291525	-1.324520
18C	-0.545327	1.288795	-0.000001
19C	-1.388792	-0.172128	0.000000
20C	1.706439	1.288794	0.000000
21C	-0.262912	-2.122217	0.000000
22C	2.549904	-0.172131	0.000000
23C	1.424018	-2.122218	0.000001

N = 24

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.064716	0.000000	0.000000
3A	0.445813	-0.966887	0.000000
4A	-0.026788	-0.625174	-0.916753
5A	0.556516	0.286097	-0.916753
6C	0.391846	1.299667	0.015123
7C	-1.016179	-0.900032	0.015122
8A	1.057531	-0.676924	-0.848531
9C	-0.827466	0.529661	-0.907052
10C	1.347272	-0.862387	1.009390
11C	1.380448	-1.894418	-0.346333
12C	2.298369	-0.460389	-0.346333
13C	0.634758	-1.405960	-1.902777
14C	1.542560	0.012262	-1.902777
15B	0.035130	-0.022486	-2.009978
16B	1.637712	0.873227	-0.693417
17B	-0.107258	-1.852868	-0.693417
18A	0.548266	0.294108	0.933239
19A	-0.037518	-0.621037	0.933239
20C	-0.847777	0.542661	0.879191
21C	1.850157	0.750222	0.808787
22C	0.093397	-1.994289	0.808787
23C	0.519742	1.396811	-1.664632
24C	-1.050844	-1.056853	-1.664633

N = 25

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.111543	0.000000	0.000000
3A	0.515864	-0.940312	0.000000
4A	0.595680	0.326584	0.881777
5A	1.097602	-0.662253	0.844222
6A	0.013942	-0.561658	0.914238
7C	1.937705	0.343967	1.193988
8C	-0.826161	-1.239125	0.092134
9C	0.409840	-1.827282	1.109252
10C	0.701703	-0.405559	2.098790
11C	1.454047	-0.844554	-1.009690
12C	-0.342503	1.240162	0.441299
13C	0.555773	0.705559	-1.013715
14B	1.148955	1.246511	0.281785
15B	-0.037411	-0.697175	-1.071047
16A	2.016983	-0.621752	0.232067
17A	-0.905439	-0.001677	0.663647
18A	1.415052	-1.537374	0.211529
19A	-0.303508	0.335592	1.515138
20C	-1.133374	0.277023	-0.684711
21C	2.244918	0.545872	-0.497587
22C	0.428059	-2.139081	-0.591233
23C	0.683486	1.297361	1.800577
24C	2.045417	-1.354509	1.463240
25C	-0.933873	-0.901711	1.778392

N = 26

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.118543	0.000000	0.000000
3A	0.559270	-0.968688	0.000000
4A	0.559271	-0.322896	-0.913287
5A	-0.344399	-0.844630	-0.597243
6A	0.559272	0.720572	-0.597244
7A	0.559271	-0.322896	0.878443
8A	1.462940	-0.844631	-0.597243
9A	-0.386586	0.223194	-1.000610
10A	-0.386586	-0.868986	0.543967
11A	0.559270	-1.415078	-1.000610
12A	0.559272	0.769286	0.543966
13A	1.505128	0.223193	-1.000611
14A	1.505127	-0.868987	0.543967
15C	1.390850	-2.097898	-0.110000
16C	0.559270	0.637329	-1.941250
17C	1.390850	-0.803011	-1.941250
18C	-1.393716	-0.155564	-0.110000
19C	-0.272311	-0.803010	-1.941249
20C	1.680678	0.324548	1.247964
21C	1.680679	1.284773	-0.110003
22C	-0.562134	0.324550	1.247964
23C	-0.272311	-2.097897	-0.110000
24C	-0.562134	1.284775	-0.110002
25C	2.512258	-0.155568	-0.110002
26C	0.559270	-1.617784	1.247965

N = 27

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.119144	0.000000	0.000000
3A	0.559572	-0.969208	0.000000
4A	0.559572	-0.323069	-0.913182
5A	0.559572	-0.323070	0.876086
6A	0.559572	0.719562	-0.596549
7A	-0.343372	-0.844384	-0.596551
8A	1.462516	-0.844385	-0.596550
9A	1.502963	-0.867737	0.548725
10A	0.559572	0.766266	0.548725
11A	-0.383821	-0.867737	0.548724
12A	-0.385934	0.222820	-1.001119
13A	1.505079	0.222820	-1.001118
14A	0.559572	-1.414846	-1.001119
15C	-0.573609	0.331172	1.235276
16C	1.692752	0.331172	1.235277
17C	0.559571	-1.631553	1.235276
18C	-1.394363	-0.158031	-0.114973
19C	2.513507	-0.158032	-0.114971
20C	-0.560322	1.286570	-0.114972
21C	1.679467	1.286570	-0.114971
22C	1.393612	-2.097746	-0.114972
23C	-0.274470	-2.097745	-0.114973
24C	1.391379	-0.803311	-1.940815
25C	-0.272232	-0.803311	-1.940816
26C	0.559573	0.637418	-1.940815
27C	0.559570	-0.323070	2.250493

N = 28

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124603	0.000000	0.000000
3A	0.562302	-0.963801	0.000000
4A	0.562302	-0.313790	-0.912747
5A	0.562302	-0.313844	0.878177
6A	0.562302	0.751681	0.548015
7A	0.562302	0.726461	-0.588572
8A	-0.339604	-0.840672	-0.600696
9A	1.464208	-0.840672	-0.600696
10C	1.721040	0.306148	1.231921
11C	-0.596438	0.306147	1.231920
12A	-0.383954	-0.869556	0.541977
13A	1.508558	-0.869556	0.541977
14A	0.562302	-1.406078	-1.004399
15A	1.505478	0.239229	-0.996615
16A	-0.380874	0.239228	-0.996615
17C	0.562302	-1.612533	1.245337
18C	-0.546030	1.294628	-0.080451
19C	1.670633	1.294629	-0.080451
20C	2.518565	-0.151916	-0.130909
21C	-1.393962	-0.151918	-0.130910
22C	-0.267917	-2.093931	-0.113360
23C	1.392520	-2.093931	-0.113359
24C	1.393616	-0.783259	-1.942985
25C	-0.269011	-0.783260	-1.942985
26C	0.562302	0.657394	-1.934244
27C	0.562301	-0.270899	2.249663
28C	0.562300	1.368918	1.752056

N = 29

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092690	0.000000	0.000000
3A	0.539597	-0.950161	0.000000
4A	0.528558	-0.321516	0.916470
5A	0.540593	-0.300843	-0.916470
6A	0.548735	0.752517	-0.575986
7A	-0.383382	-0.848770	0.575985
8A	-0.377208	-0.826064	-0.575301
9A	0.532039	0.735936	0.575300
10A	1.457873	-0.829539	-0.592909
11A	1.441268	-0.858065	0.592909
12B	0.522661	-1.573799	1.064335
13B	1.626618	0.322693	-1.064336
14A	0.517981	-1.400437	-0.985919
15A	1.473557	0.241153	0.985919
16A	-0.428402	0.241395	-0.961632
17A	-0.421464	0.253315	0.961631
18C	-0.568384	1.277356	-0.007746
19C	-1.391422	-0.136545	0.007744
20C	2.476673	-0.159386	0.090697
21C	1.361637	-2.074912	-0.090698
22C	-0.310469	-2.076025	-0.087223
23C	1.651915	1.295163	0.087222
24C	0.521251	0.696603	1.911710
25C	-0.348334	-0.797260	-1.911710
26C	1.372311	-0.721331	1.962104
27C	1.304922	-0.837100	-1.962104
28C	0.451321	0.647256	-1.943189
29C	-0.339957	-0.712083	1.943188

N = 30

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.095712	0.000000	0.000000
3A	0.554182	-0.952540	0.000000
4A	0.542616	-0.321789	0.923302
5A	0.556293	-0.313831	-0.917062
6A	-0.356203	-0.844717	0.577412
7A	-0.352809	-0.842741	-0.577166
8A	0.558385	0.740376	-0.587315
9A	1.473784	-0.833029	-0.587316
10A	0.525748	0.739857	0.579336
11A	1.457204	-0.861146	0.579335
12B	-0.554932	0.302887	1.053471
13B	0.543232	-1.584656	1.053470
14B	1.637634	0.315287	-1.066563
15C	-1.407938	-0.192103	-0.075062
16C	-0.308662	-2.081563	-0.075062
17A	-0.412615	0.210927	-0.980663
18A	0.533621	-1.415484	-0.980664
19A	1.494119	0.231791	0.975881
20C	-0.244912	-0.779971	2.009883
21C	-0.578833	1.272184	-0.096863
22C	1.374058	-2.084486	-0.096867
23C	1.649901	1.291250	0.084672
24C	2.492134	-0.156394	0.084672
25C	-0.329940	-0.829435	-1.914475
26C	1.440010	-0.754271	1.937525
27C	0.610161	0.672088	1.937526
28C	1.324772	-0.855877	-1.955277
29C	0.464877	0.622128	-1.955277
30C	-1.439558	-1.475003	1.042362

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.116943	0.000000	0.000000
3A	0.552121	-0.946031	0.000000
4A	0.518484	-0.292016	0.920043
5A	0.559413	-0.311384	-0.924635
6A	0.527469	0.741324	0.563009
7A	0.566175	0.727503	-0.559691
8B	1.629453	-0.909613	-0.643139
9C	1.778258	0.506191	-1.135987
10A	-0.363638	-0.847561	-0.571361
11A	1.443085	-0.833619	0.612700
12A	-0.392488	-0.809733	0.589193
13C	-0.558335	1.315460	-0.129419
14B	-0.560189	0.365487	1.035271
15B	1.596617	1.160198	0.182309
16B	0.513381	-1.577889	-1.065378
17A	1.455606	0.249591	1.010696
18A	-0.410934	0.231879	-0.958913
19A	0.509571	-1.380574	1.003183
20C	0.575477	0.707110	1.938403
21C	0.374108	0.757993	-1.918174
22C	-1.410227	-0.145765	-0.090772
23C	-0.337715	-2.056085	0.098059
24C	2.521048	-0.069282	0.233703
25C	1.360551	-0.768672	1.949972

26C	1.307114	-2.124832	0.163848
27C	-0.285992	-0.781533	1.959168
28C	-0.421449	-0.726290	-1.922358
29C	1.215195	-0.698441	-2.093768
30C	0.839319	2.007244	-0.829150
31C	0.559379	2.049793	0.867057

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.095935	0.000000	0.000000
3A	0.574917	-0.953470	0.000000
4A	0.521018	-0.294565	-0.906827
5A	0.530395	0.781801	-0.576378
6A	0.565539	-0.306653	0.921623
7A	0.547967	0.754530	0.548245
8B	1.657822	-0.880992	0.634105
9B	-0.561888	0.330911	-1.033796
10A	-0.336554	-0.877390	0.568882
11A	1.432489	0.269992	-1.010220
12A	1.462637	-0.812979	-0.615895
13A	-0.366702	-0.836928	-0.582935
14C	-0.667717	1.230504	0.167905
15C	1.763651	0.539843	1.118438
16B	0.564639	-1.583615	1.060354
17B	0.531296	0.519241	-1.833733
18A	0.547967	-1.382851	-1.004785
19A	-0.437973	0.164427	0.965353
20A	1.533906	0.968929	-0.141852
21C	-1.418668	-0.244774	0.072882
22C	2.514602	-0.006302	-0.255316
23C	1.377093	-0.739342	-1.951755
24C	-0.281159	-2.084690	-0.100199
25C	0.752341	2.036010	0.108339
26C	0.343591	0.732043	1.902941
27C	1.366020	-2.107946	-0.169071
28C	-0.270085	-0.812030	-1.952596
29C	-0.393140	-0.787103	1.928763
30C	1.489072	1.591245	-1.344470
31C	1.243681	-0.682584	2.083814
32C	-0.147748	1.770998	-1.292967

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.074970	0.000000	0.000000
3A	0.514009	-0.955118	0.000000
4A	0.490354	-0.300529	-0.905823
5A	0.508818	0.769446	-0.579552
6A	0.526719	-0.308212	0.916245
7A	0.510054	0.762637	0.564922
8B	1.596730	-0.908431	0.631330
9A	-0.422110	-0.817758	0.560802
10A	-0.435149	0.293983	-0.948909
11A	1.395147	0.277730	-1.022559
12A	-0.432582	-0.793720	-0.572330
13A	1.407937	-0.831710	-0.619803
14C	1.725676	0.518699	1.120752
15A	-0.428629	0.271849	0.935709
16A	-0.414243	0.991514	-0.013223
17B	0.446308	0.521035	-1.817343
18B	0.459926	-1.563968	1.063689
19C	-1.388027	0.008840	0.002818
20A	0.447216	-1.380151	-1.009987
21A	1.486304	0.990221	-0.134088
22C	0.591221	2.014135	0.073887
23B	0.399660	0.570081	1.806411
24C	2.460638	-0.020242	-0.253206
25C	1.273692	-0.747722	-1.959224
26C	-0.396570	-0.723935	-1.913330
27C	-0.393827	-2.044574	-0.091869
28C	-0.455860	-0.682875	1.910420
29C	-0.366620	1.643167	-1.219858
30C	1.252230	-2.124507	-0.170922
31C	1.341141	1.620174	-1.342159
32C	1.192511	-0.710418	2.082031
33C	-0.526711	1.598492	1.202658

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.059177	0.000000	0.000000
3A	0.529589	-0.955780	0.000000
4A	0.529589	-0.295352	0.909001
5A	0.529589	-0.295352	-0.909001
6A	0.529589	0.773242	0.561794
7A	0.529588	0.773243	-0.561793
8A	-0.400602	-0.808734	0.587580
9A	-0.400603	-0.808734	-0.587580
10A	-0.400603	0.308909	0.950724
11A	1.459780	0.308910	-0.950723
12A	1.459781	0.999650	0.000000
13A	1.459781	-0.808733	-0.587580
14A	1.459781	-0.808733	0.587579
15A	1.459781	0.308909	0.950723
16A	-0.400603	0.308909	-0.950723
17A	-0.400603	0.999650	0.000001
18B	0.529589	1.874192	0.000001
19B	0.529588	0.579158	-1.782461
20B	0.529589	-1.516252	1.101622
21B	0.529590	0.579158	1.782462
22B	0.529590	-1.516252	-1.101622
23C	-1.360216	0.000000	0.000001
24C	2.419394	0.000000	0.000000
25C	-0.340034	1.660020	-1.206073
26C	1.399209	1.660021	-1.206074
27C	1.399211	1.660020	1.206074
28C	1.399211	-0.634069	-1.951470
29C	-0.340032	-0.634070	1.951470
30C	-0.340032	-2.051896	0.000000
31C	-0.340032	1.660020	1.206075
32C	-0.340032	-0.634070	-1.951470
33C	1.399212	-0.634070	1.951469
34C	1.399211	-2.051896	0.000000

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.158024	0.000000	0.000000
3B	-1.305150	-0.004204	0.000000
4A	0.555857	0.758157	-0.560113
5A	0.555858	0.757927	0.560422
6C	0.024805	1.894497	0.000388
7A	0.555003	-0.957351	-0.000197
8A	-0.530653	0.769173	-0.571502
9A	-0.530652	0.768939	0.571817
10A	-0.526472	-0.971373	-0.000199
11A	0.565237	-0.296148	-0.875160
12A	0.565238	-0.296507	0.875038
13A	-0.533363	-0.302337	-0.893527
14A	-0.533362	-0.302704	0.893404
15C	1.636952	1.378612	0.000281
16C	0.030316	0.493154	-1.833180
17C	0.030318	0.492403	1.833381
18C	0.028930	-1.502955	-1.176894
19C	0.028932	-1.503438	1.176276
20C	1.640895	0.406156	1.331522
21C	1.640893	0.406702	-1.331359
22C	1.638282	-1.138951	0.824013
23C	1.638281	-1.138614	-0.824484
24C	-1.594060	1.452763	0.000298
25C	-1.595944	0.417802	-1.401062
26C	-1.595942	0.417228	1.401234
27C	-1.594352	-1.185993	-0.867770
28C	-1.594350	-1.186349	0.867285
29C	0.864083	1.851739	1.399011
30C	0.864081	1.852312	-1.398254
31C	2.542089	-0.013058	-0.000006
32C	-0.800777	1.860044	1.411532
33C	-0.800778	1.860622	-1.410770
34C	0.851859	-2.330300	-0.000480
35C	-0.791747	-2.341000	-0.000481

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.142878	0.000000	0.000000
3A	-1.142879	-0.000416	0.000000
4A	-0.542777	0.613973	0.717920
5A	0.542553	0.614171	0.717920
6A	-0.542830	0.866214	-0.376761
7A	0.542514	0.866412	-0.376761
8C	-0.000336	1.843356	0.424773
9A	-0.540254	-0.933496	-0.215052
10A	0.540593	-0.933300	-0.215052
11A	-0.550593	-0.486530	0.789490
12A	0.550769	-0.486329	0.789490
13A	-0.550682	-0.092003	-0.922707
14A	0.550714	-0.091803	-0.922707
15C	-1.619132	1.347057	0.310489
16C	1.618641	1.347646	0.310489
17C	-0.000162	0.888069	-1.672383
18C	-0.000013	0.066659	1.892429
19C	0.000217	-1.194789	-1.482057
20C	0.000313	-1.722890	0.809809
21C	1.623124	0.098618	1.391161
22C	-1.623161	0.098027	1.391161
23C	1.623029	0.697478	-1.207798
24C	-1.623284	0.696887	-1.207798
25C	-1.619847	-1.296815	0.548082
26C	1.620317	-1.296225	0.548082
27C	1.620260	-0.925659	-1.060127
28C	-1.619924	-0.926249	-1.060127
29C	0.834789	1.488678	1.780144
30C	-0.835333	1.488374	1.780144
31C	-0.835450	2.117275	-0.949204
32C	0.834678	2.117579	-0.949203
33C	2.523363	-0.011322	-0.002680
34C	-2.523360	-0.012241	-0.002680
35C	0.823273	-2.268109	-0.522633
36C	-0.822450	-2.268408	-0.522633

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.157069	0.000000	0.000000
3B	-1.299118	-0.001400	0.000000
4A	0.554898	-0.752970	0.547523
5A	0.554898	-0.753007	-0.547472
6A	0.561498	0.294416	-0.901453
7A	0.561498	0.294476	0.901434
8C	0.050077	-0.617241	1.802589
9C	0.050077	-0.617362	-1.802547
10A	-0.529738	-0.769860	0.563625
11A	-0.529738	-0.769898	-0.563573
12A	-0.522123	0.297512	0.918097
13A	-0.522123	0.297450	-0.918116
14B	0.006875	-1.721037	0.000058
15A	0.569585	0.923129	-0.000031
16A	-0.529358	0.942792	-0.000031
17C	1.643562	-0.442994	-1.310397
18C	1.643562	-0.442906	1.310427
19C	0.037779	1.581478	-1.053731
20C	0.037780	1.581548	1.053626
21B	1.553469	-1.213365	0.000041
22C	1.651490	1.125551	-0.810038
23C	1.651490	1.125605	0.809963
24C	-1.577947	-0.469187	-1.395636
25C	-1.577947	-0.469093	1.395668
26C	-1.597020	-1.454158	0.000049
27C	-1.588632	1.189313	0.849507
28C	-1.588632	1.189257	-0.849586
29C	0.910721	-1.920766	-1.188122
30C	0.910721	-1.920686	1.188252
31C	-0.747796	-1.943768	-1.301420
32C	-0.747797	-1.943680	1.301552
33C	2.542369	-0.030678	0.000001
34C	-0.782227	0.736756	2.218504
35C	-0.782227	0.736608	-2.218552
36C	0.876858	0.735268	2.203195
37C	0.876858	0.735120	-2.203244

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.138584	0.000000	0.000000
3A	-1.138580	-0.003195	0.000000
4C	-0.002639	1.880904	0.007979
5A	-0.546031	0.749710	0.564389
6A	0.543924	0.751240	0.564389
7A	-0.546039	0.754470	-0.557997
8A	0.543919	0.755999	-0.557998
9C	-0.000776	0.553138	1.812893
10C	-0.000799	0.568492	-1.808129
11A	0.542404	-0.314652	0.899427
12A	-0.541520	-0.316172	0.899427
13A	0.542394	-0.307013	-0.902063
14A	-0.541532	-0.308534	-0.902063
15A	-0.548807	-0.932745	-0.003949
16A	0.551421	-0.931202	-0.003949
17C	-1.626339	1.371883	0.005831
18C	1.622483	1.376441	0.005831
19C	-1.621390	0.394358	1.330894
20C	1.620277	0.398906	1.330893
21C	-1.621408	0.405630	-1.327474
22C	1.620262	0.410178	-1.327474
23C	0.002243	-1.599518	-1.040850
24C	0.002255	-1.608288	1.027254

25C	1.621649	-1.161922	0.806644
26C	-1.618384	-1.166466	0.806645
27C	1.621639	-1.155039	-0.816482
28C	-1.618394	-1.159584	-0.816481
29C	-2.520567	-0.026366	-0.000093
30C	2.520630	-0.019294	-0.000093
31C	-0.856291	1.868176	1.390472
32C	0.851045	1.870572	1.390471
33C	-0.856308	1.879901	-1.374561
34C	0.851028	1.882296	-1.374562
35C	0.834533	-0.791311	2.197859
36C	-0.832310	-0.793648	2.197859
37C	0.834506	-0.772643	-2.204494
38C	-0.832337	-0.774981	-2.204494

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.059480	0.000000	0.000000
3A	0.444908	-0.966399	0.000000
4A	0.444907	-0.298536	0.919132
5A	0.461750	-0.299976	-0.925838
6A	0.461747	0.787887	0.571311
7A	0.463866	0.786903	-0.571782
8A	-0.548778	-0.752301	0.546638
9A	-0.494801	-0.756340	-0.570033
10A	-0.494803	0.308505	0.895438
11A	-0.467537	0.296106	-0.910232
12A	-0.467539	0.957183	-0.000439
13A	-1.073386	0.041476	-0.030140
14B	1.477334	-0.953420	0.692779
15B	1.490839	0.355514	1.116182
16B	1.490842	-0.951763	-0.682931
17B	1.497447	1.172271	-0.001740
18B	1.497449	0.363791	-1.114394
19B	0.272082	-1.516401	1.101853
20C	-0.642526	1.604182	-1.165637
21B	-0.437041	-1.864096	-0.024177
22B	-0.437044	-0.552857	1.780389
23B	0.315973	0.587466	1.797423
24B	0.315978	-1.528032	-1.113986
25B	0.315366	0.589297	-1.804191
26B	0.315363	1.897990	-0.003129
27C	-0.579141	-0.626380	-1.915715
28C	-0.579147	1.628515	1.187538
29C	-1.746773	-1.121368	-0.217171
30C	-1.746776	-0.139863	1.133604
31C	-1.780714	0.246787	-1.193473
32C	-1.780716	1.211333	0.133963
33C	2.455240	-0.008283	0.006022
34C	1.044026	-0.700296	2.119691
35C	1.044029	-2.232347	0.011239
36C	1.045301	1.809039	-1.314488
37C	1.075987	1.804815	1.308058
38C	1.075993	-0.686541	-2.120619
39C	-1.236631	-1.726332	1.254391

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.059162	0.000000	0.000000
3A	0.432616	-0.966782	0.000000
4A	0.453496	-0.293899	-0.920962
5A	0.453497	-0.293898	0.920962
6A	0.465330	0.790024	-0.569148
7A	0.465330	0.790025	0.569148
8A	-0.531055	-0.747430	-0.569148
9A	-0.531055	-0.747430	0.569149
10A	-0.478541	0.310130	-0.903023
11A	-0.478541	0.310131	0.903022
12A	-0.466098	0.958016	0.000000
13A	-1.064836	0.034143	0.000000
14B	1.475048	-0.955940	0.687202
15B	1.475048	-0.955940	-0.687202
16B	0.281353	-1.512968	1.113757
17B	0.281353	-1.512969	-1.113756
18B	1.495927	0.361161	1.113756
19B	1.495927	0.361159	-1.113756
20B	-0.457172	-1.849414	0.000001
21B	1.501378	1.172692	-0.000001
22B	-0.419904	-0.539376	-1.797685
23B	0.320821	0.603588	-1.797685
24B	0.320821	0.603590	1.797684
25B	-0.419903	-0.539374	1.797685
26B	-1.605489	-1.064680	0.000000
27B	0.316057	1.900329	-0.000001
28C	-1.733436	-0.096711	-1.168203
29C	-1.733436	-0.096710	1.168203
30C	-0.619747	1.621749	1.168202
31C	-0.619747	1.621748	-1.168203
32C	-1.796188	1.164062	0.000000
33C	1.017124	-2.232264	0.000001
34C	2.453012	-0.016641	0.000000
35C	1.059276	-0.686487	2.120092
36C	1.059276	-0.686490	-2.120092
37C	-1.222507	-1.710842	-1.305748
38C	1.062289	1.814675	-1.305750
39C	-1.222507	-1.710840	1.305750
40C	1.062289	1.814676	1.305747

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.063889	0.000000	0.000000
3A	0.450359	-0.963865	0.000000
4A	0.450358	-0.286667	0.920249
5A	0.469923	-0.299120	-0.918359
6A	-0.514845	-0.759245	0.558717
7A	0.469922	0.787840	0.558717
8A	0.473643	0.783173	-0.576327
9A	-0.509042	-0.760641	-0.576327
10A	-0.509043	0.324022	0.897627
11A	-0.465776	0.959123	-0.011757
12A	-0.465775	0.296480	-0.912225
13A	-1.066118	0.015975	-0.011757
14B	1.485305	-0.945442	0.695738
15B	1.498154	0.365327	1.112622
16B	0.303209	-1.511950	1.112622
17B	1.498155	-0.953622	-0.679704
18B	0.317794	0.610850	1.782423
19B	-0.418893	-0.546497	1.782423
20B	1.511704	1.168694	-0.008351
21B	-0.418892	-1.864303	-0.008351
22B	0.317796	-1.520092	-1.113325
23B	1.511705	0.355559	-1.113325
24B	0.339086	1.898139	-0.026540
25B	-1.576142	-1.110714	-0.026540
26B	-0.390874	1.557071	1.068344
27B	-1.576143	-0.305004	1.068344
28B	-0.390872	-0.556907	-1.804353
29B	0.339087	0.589870	-1.804353
30C	-0.605027	1.608855	-1.183935
31C	-1.713711	-0.132907	-1.183936
32C	-1.713712	1.090831	0.479009
33C	1.054091	-0.670962	2.125476
34C	1.054092	-2.228849	0.008454
35C	2.465511	-0.011487	0.008454
36C	-1.183378	-1.756270	1.292413
37C	1.090212	1.815573	1.292413
38C	1.090213	-0.693954	-2.117798
39C	-1.173945	0.747252	2.059401
40C	1.083060	1.801819	-1.325934
41C	-1.173942	-1.743969	-1.325934

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.061191	0.000000	0.000000
3A	0.473338	-0.949777	0.000000
4A	0.487209	-0.301552	0.902997
5A	-0.458048	0.959355	-0.016320
6A	-1.062943	-0.017955	-0.016319
7A	0.475593	-0.294362	-0.917128
8A	-0.445266	0.275592	-0.934877
9A	0.486410	0.796339	0.548238
10A	-0.495772	-0.790544	0.548238
11A	-0.472057	-0.773260	-0.573772
12A	0.481519	0.767403	-0.573772
13A	-0.483048	0.298977	0.897487
14B	1.535383	-0.950307	0.640913
15B	1.555261	0.349959	1.061788
16B	0.380496	-1.548073	1.061788
17C	0.451392	0.698544	-1.914382
18C	-0.423864	-0.715580	-1.914382
19A	-1.333299	0.825231	-0.653930
20C	-1.682303	-0.280792	1.182963
21C	-0.499067	1.630927	1.182963
22A	1.373740	-0.850260	-0.609473
23C	0.372819	2.058136	-0.158157
24C	-1.675762	-1.251693	-0.158157
25B	1.546694	1.130752	-0.081148
26B	-0.322144	-1.888672	-0.081147
27B	0.380570	0.572834	1.771041
28B	-0.342942	-0.596123	1.771041
29A	1.404339	0.265178	-1.003366
30A	0.389059	-1.375180	-1.003366
31A	-1.395651	-0.241718	-1.037707
32A	-0.406179	1.356940	-1.037707
33A	-1.422009	0.880137	0.485403
34C	-1.211791	0.750025	-1.998508
35C	1.161585	-2.147737	-0.167567
36C	2.440366	-0.081648	-0.167567
37C	1.242688	-0.769147	-1.950877
38C	-1.278588	2.088191	-0.208802
39C	-2.439260	0.212929	-0.208802
40C	1.139623	-0.705356	2.077008
41C	-1.080224	-1.833569	1.261989
42C	1.159240	1.784664	1.261989

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.072293	0.000000	0.000000
3A	0.489920	-0.946968	0.000000
4A	0.489922	-0.276082	-0.905829
5A	0.487303	0.763476	0.565456
6A	-0.460054	-0.780053	-0.577734
7A	-0.480802	0.274268	0.909142
8A	-0.480801	0.949608	-0.002699
9A	0.483055	-0.324174	0.911039
10A	0.483056	0.776952	-0.575697
11A	-1.077635	-0.036540	-0.027064
12A	-0.467033	-0.798739	0.540509
13A	-0.467032	0.284164	-0.921622
14B	1.539583	0.323980	1.093655
15B	1.539584	1.140597	-0.008937
16B	-0.357089	1.500066	1.110998
17B	0.366372	1.870644	0.005643
18B	0.366370	0.550767	1.787736
19B	-1.523892	0.907855	0.672386
20B	1.517350	0.332563	-1.130690
21B	1.517349	-0.984616	0.647760
22A	1.390635	-0.843641	-0.624827
23C	0.304546	0.549628	-2.011012
24C	0.304543	-1.763412	1.112044
25C	-1.545401	-1.410860	-0.013663
26C	-1.545399	-0.424391	-1.345589
27A	0.382498	-1.349858	-0.999749
28B	-1.516466	0.925955	-0.700809
29B	-1.516468	-0.400409	1.090043
30B	-0.363184	1.524449	-1.106281
31B	-0.363187	-0.613782	1.780750
32A	-0.220004	-1.757807	-0.144201
33A	-0.220002	-0.650409	-1.639404
34C	1.146686	-0.866959	-1.990766
35C	1.146684	-2.157039	-0.248905
36C	-0.783968	-1.895181	-1.403636
37C	2.462079	-0.086043	-0.063724
38C	1.126354	1.768171	1.309568
39C	-1.115596	2.208902	0.013939
40C	-1.115598	0.657320	2.108879
41C	1.123809	1.794256	-1.302977
42C	1.123806	-0.723276	2.096183
43C	-2.477694	-0.037531	-0.027799

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.066188	0.000000	0.000000
3A	0.485747	-0.955985	0.000000
4A	0.479149	-0.303370	-0.903067
5A	0.501667	-0.287564	0.906874
6A	0.495917	0.787164	0.538424
7A	0.480367	0.766382	-0.578838
8A	-0.459803	-0.780902	0.566828
9A	-0.461634	0.307717	0.907524
10A	-1.066557	-0.009349	-0.000682
11A	-0.468698	-0.785076	-0.575671
12A	-0.473422	0.964255	-0.034319
13A	-0.469809	0.278269	-0.920571
14B	0.399690	0.606339	1.764542
15B	-0.320590	-0.569650	1.790000
16B	-0.332146	1.541296	1.062387
17B	-1.495453	-0.360525	1.116962
18B	-0.317069	-1.890706	-0.007380
19B	0.403936	-1.521838	1.098055
20B	-1.497722	-1.180980	0.008426
21B	-1.506721	0.943039	0.672849

22B	1.545009	1.139673	-0.048500
23B	1.552085	-0.925059	0.649258
24B	0.399399	-1.496760	-1.130742
25B	1.566507	0.370513	1.067530
26B	0.384913	1.880035	-0.086527
27C	-0.344971	-0.520960	-2.010087
28C	-0.369152	1.547615	-1.366724
29A	1.386803	-0.855178	-0.616821
30A	1.390274	0.308130	-0.988666
31B	-1.523675	-0.379471	-1.105670
32B	-1.534115	0.915284	-0.697014
33A	0.480105	0.495242	-1.638110
34C	1.306701	-0.606713	-1.976012
35C	2.439443	-0.060910	-0.189562
36C	1.185319	-2.166740	-0.066022
37C	-1.070716	0.712819	2.103273
38C	-1.065547	-1.803167	1.315508
39C	1.252774	1.615093	-1.415450
40C	1.140792	1.820605	1.236489
41C	1.159436	-0.665479	2.092436
42C	-2.478538	-0.025642	0.021864
43C	-1.100249	2.218579	-0.043798
44C	-1.080077	-1.820138	-1.303435

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.073894	0.000000	0.000000
3A	0.480261	-0.960519	0.000000
4A	0.480261	-0.296817	-0.913508
5A	0.480261	-0.296817	0.913508
6A	0.480260	0.777076	-0.564579
7A	0.480261	0.777076	0.564579
8A	-0.480258	-0.777077	-0.564579
9A	-0.480258	-0.777077	0.564579
10A	-0.480259	0.296816	-0.913508
11A	-0.480259	0.296816	0.913508
12A	-0.480259	0.960519	0.000000
13A	-1.073893	-0.000001	0.000000
14B	-1.525059	0.942538	-0.684794
15B	-1.525058	0.942538	0.684794
16B	-1.525058	-0.360019	1.108021
17B	-1.525058	-0.360019	-1.108020
18B	-0.360017	1.525059	-1.108021
19B	-0.360017	1.525059	1.108020
20B	-1.525058	-1.165043	0.000000
21B	0.360019	0.582521	1.792815
22B	-0.360016	-0.582521	1.792815
23B	0.360019	1.885077	0.000000
24B	0.360018	0.582520	-1.792815
25B	-0.360016	-0.582522	-1.792815
26B	1.525060	0.360018	-1.108021
27B	-0.360016	-1.885078	0.000000
28B	1.525060	1.165042	-0.000001
29B	0.360020	-1.525060	1.108020
30B	1.525061	0.360018	1.108020
31B	0.360020	-1.525060	-1.108020
32B	1.525061	-0.942538	-0.684794
33B	1.525061	-0.942538	0.684794
34C	-2.490763	-0.000001	0.000000
35C	-1.113903	2.227807	0.000000
36C	-1.113902	0.688430	2.118771
37C	-1.113903	0.688429	-2.118771
38C	-1.113902	-1.802335	1.309472
39C	1.113904	1.802334	-1.309473
40C	-1.113902	-1.802335	-1.309472
41C	1.113905	1.802334	1.309472
42C	1.113905	-0.688430	2.118771
43C	1.113905	-0.688431	-2.118771
44C	1.113906	-2.227807	0.000000
45C	2.490766	0.000000	-0.000001

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.064960	0.000000	0.000000
3A	0.477240	-0.952041	0.000000
4A	0.473467	-0.292283	-0.915740
5A	0.485926	-0.299975	0.909188
6A	0.496775	0.769101	-0.566536
7A	-0.464933	-0.788757	-0.566536
8A	0.499908	0.767920	0.565108
9A	-0.462473	-0.791028	0.565109
10A	-0.470883	0.290689	-0.917361
11A	-0.463029	0.285842	0.921039
12A	-0.465198	0.957696	0.002777
13A	-1.064619	-0.013297	0.002777
14B	0.410790	-1.524419	-1.093582
15B	1.546871	0.315903	-1.093582
16A	1.357501	-0.838021	-0.622234
17B	-0.331863	-0.599417	-1.797771
18B	0.387143	0.565292	-1.797771
19B	-1.494018	-1.190532	0.000632
20B	0.394787	1.869118	0.000632
21B	-0.336264	1.514822	-1.109184
22B	-1.504893	-0.378224	-1.109184
23B	-1.503978	0.928448	0.693879
24B	-1.509344	0.931760	-0.681141
25B	-1.497751	-0.382799	1.115829
26B	-0.328973	1.510488	1.115828
27B	-0.318872	-0.607817	1.794655
28B	0.400475	0.557444	1.794655
29B	0.411623	-1.533895	1.081463
30B	1.555716	0.319406	1.081463
31B	-0.305929	-1.907170	-0.006031
32B	1.567857	1.128150	-0.006031
33A	1.383381	-0.853998	0.619864
34C	1.296920	-2.069206	-0.015666
35C	2.430993	-0.232135	-0.015666
36C	1.171621	-0.723273	-2.068935
37C	1.189476	-0.734294	2.049060
38C	-1.067372	-1.820675	-1.308845
39C	1.149307	1.770094	-1.308846
40C	-1.091451	0.673783	-2.117087
41C	-2.465927	-0.023628	0.007328
42C	-1.083928	2.215053	0.007327
43C	-1.075936	0.664207	2.125719
44C	-1.062913	-1.826633	1.303698
45C	1.156633	1.768780	1.303697
46C	2.388831	-1.474691	-1.185100

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.063320	0.000000	0.000000
3A	0.461815	-0.957797	0.000000
4A	0.479384	-0.301056	-0.911010
5A	0.479383	-0.301056	0.911010
6A	0.505467	0.764890	-0.566870
7A	0.505466	0.764890	0.566870
8A	-0.469452	-0.787506	-0.566870
9A	-0.469453	-0.787507	0.566869
10A	-0.461776	0.290001	-0.920677
11A	-0.461777	0.290000	0.920676
12A	-0.456004	0.960863	0.000000
13A	-1.063557	-0.006565	-0.000001
14A	1.357221	-0.852346	-0.599827
15A	1.357220	-0.852345	0.599827
16B	0.404225	-1.535544	-1.084176
17B	1.558720	0.302799	1.084176
18B	0.404224	-1.535544	1.084176
19B	1.558721	0.302799	-1.084176
20B	-0.321107	-0.605662	-1.797024
21B	-0.321108	-0.605663	1.797023
22B	0.406097	0.552290	1.797023
23B	0.406098	0.552290	-1.797023
24B	-1.501712	-1.180605	-0.000001
25B	0.411230	1.865438	0.000000
26B	-1.500679	-0.370932	-1.114430
27B	-0.317644	1.512857	1.114429
28B	-1.500680	-0.370933	1.114428
29B	-0.317643	1.512857	-1.114429
30B	-1.496332	0.939710	0.688636
31B	-1.496331	0.939710	-0.688638
32B	-0.321871	-1.908418	0.000000
33B	1.579238	1.118782	0.000000
34C	1.273747	-2.088892	0.000000
35C	2.434800	-0.240105	0.000000
36C	1.197121	-0.751801	-2.041933
37C	1.197120	-0.751802	2.041933
38C	-1.075078	-1.816953	1.307448
39C	1.169722	1.757517	-1.307448
40C	-1.075077	-1.816953	-1.307449
41C	1.169721	1.757517	1.307448
42C	-2.462802	-0.006047	-0.000001
43C	-1.064181	2.221024	0.000000
44C	-1.071266	0.672765	2.123244
45C	-1.071264	0.672766	-2.123245
46C	2.404528	-1.510061	1.106142
47C	2.404528	-1.510061	-1.106141

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.072294	0.000000	0.000000
3A	0.468318	-0.964621	0.000000
4A	0.468317	-0.293227	0.918973
5A	0.485082	0.774704	0.566004
6A	0.485083	-0.303723	-0.910098
7A	-0.485057	-0.774720	0.566003
8A	0.488400	0.772939	-0.564702
9A	-0.482020	0.301806	0.911826
10A	-0.482019	-0.776933	-0.564703
11A	-0.472856	0.962966	-0.003512
12A	-0.472856	0.296069	-0.916329
13A	-1.072787	0.004806	-0.003512
14B	1.481668	-0.927714	0.677781
15B	1.528508	0.351447	1.116721
16B	1.528509	-0.957042	-0.674278
17B	0.351410	-1.528516	1.116721
18B	-0.369074	-1.885190	0.005430
19B	0.358984	-1.531722	-1.102336
20B	-0.369075	-0.578237	1.794327
21B	0.358982	0.584555	1.794327
22B	1.534699	1.155359	0.005431
23B	1.534700	0.346034	-1.102335
24B	-1.529468	-1.158271	-0.001677
25B	-1.529468	-0.350496	1.103967
26B	-0.352682	-0.586949	-1.792198
27B	0.373980	0.573616	-1.792197
28B	-0.352684	1.528965	1.103968
29B	0.373979	1.881756	-0.001676
30B	-1.520639	-0.355787	-1.112936
31B	-1.520640	0.952116	0.677261
32B	-0.344068	1.523335	-1.112935
33B	-1.514436	0.948232	-0.692771
34C	1.097467	-2.236188	0.007762
35C	1.097467	-0.687155	2.128008
36C	2.490956	-0.010624	0.007763
37C	-1.123849	-1.795235	1.311582
38C	1.124136	-0.703852	-2.108808
39C	1.124134	1.795056	1.311584
40C	-1.115555	-1.801133	-1.307886
41C	-1.115558	0.698482	2.113472
42C	1.133063	1.790173	-1.307885
43C	-2.488314	0.012672	-0.009260
44C	-1.098153	0.687586	-2.124438
45C	-1.098155	2.232918	-0.009258
46C	2.658785	-0.650478	1.539878
47C	2.658786	-1.664740	0.151603
48C	1.746370	-2.107713	1.539878

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.071858	0.000000	0.000000
3A	0.461161	-0.966799	0.000000
4A	0.470291	-0.297649	0.917136
5A	0.480627	-0.302158	-0.912099
6A	0.487748	0.772276	0.567373
7A	-0.486104	-0.775575	0.565437
8A	0.491842	0.771535	-0.564945
9A	-0.485426	-0.774629	-0.566140
10A	-0.478957	0.300064	0.913412
11A	-0.472063	0.298985	-0.916186
12A	-0.469161	0.963991	-0.001758
13A	-1.072225	0.007359	-0.002432
14B	1.483697	-0.931941	0.671009
15B	1.501299	-0.957254	-0.669482
16B	1.530014	0.345932	1.118298
17B	0.353532	-1.535145	1.110967
18B	1.540773	0.338694	-1.103101
19B	0.348286	-1.532506	-1.108097
20B	1.535568	1.154112	0.005588
21C	2.488823	0.002032	0.015553
22B	-0.374514	-1.885978	0.001297
23B	-0.364336	-0.583840	1.793199
24B	0.364054	0.577213	1.796117
25B	0.378857	0.572761	-1.792424
26B	-0.355015	-0.583089	-1.794729
27B	0.379177	1.880784	0.000214
28B	-0.346580	1.526486	1.107542
29B	-1.532197	-1.154407	-0.002073
30B	-1.527432	-0.349845	1.105642
31B	-0.337855	1.525036	-1.111260
32B	-1.521976	-0.348967	-1.112744
33B	-1.515902	0.953974	0.680828
34B	-1.510929	0.953632	-0.690150

35C	1.093383	-2.240572	-0.004584
36C	1.106124	-0.701271	2.120460
37C	1.125414	-0.707650	-2.108639
38C	1.129469	1.789653	1.314379
39C	1.141430	1.784249	-1.307902
40C	-1.124091	-1.796189	1.309129
41C	2.655102	-1.637622	0.068238
42C	-1.125263	-1.794978	-1.310861
43C	-1.109251	0.694575	2.116445
44C	-1.094671	0.694466	-2.123056
45C	-2.486875	0.019441	-0.006379
46C	-1.090950	2.234902	-0.004750
47C	2.669908	-0.669128	1.520628
48C	1.768207	-2.117567	1.509001
49C	2.699313	-0.648352	-1.485687

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.060971	0.000000	0.000000
3A	0.490783	-0.940633	0.000000
4A	0.497067	-0.301309	-0.908316
5A	0.497067	-0.301309	0.908316
6A	0.491631	0.770423	-0.565193
7A	0.491631	0.770423	0.565193
8A	-0.455623	-0.792248	-0.565194
9A	-0.455623	-0.792248	0.565194
10A	-0.464811	0.281759	-0.919606
11A	-0.464811	0.281759	0.919606
12A	-0.472612	0.953316	0.000000
13A	-1.063809	-0.021971	0.000000
14A	1.417476	-0.859239	0.598515
15A	1.417476	-0.859239	-0.598515
16B	1.541954	0.330422	1.084702
17B	1.541954	0.330422	-1.084702
18B	0.420328	-1.519908	1.084703
19B	0.420328	-1.519908	-1.084703
20B	-0.296732	-1.904153	0.000000
21B	1.550923	1.143896	0.000000
22B	-0.318794	-0.605564	1.793666
23B	-0.318794	-0.605564	-1.793666
24B	0.389416	0.562759	1.793665
25B	0.389416	0.562759	-1.793665
26B	-1.485223	-1.200952	0.000000
27B	0.377712	1.872303	0.000000
28B	-1.496946	-0.392692	1.112465
29B	-1.496946	-0.392692	-1.112465
30B	-0.344297	1.508815	1.112464
31B	-0.344297	1.508815	-1.112464
32B	-1.511923	0.916495	0.688072
33B	-1.511923	0.916495	-0.688072
34B	2.264946	-0.065363	0.000000
35B	1.105662	-1.977817	0.000000
36C	1.177329	-0.713667	-2.066378
37C	1.177329	-0.713667	2.066378
38B	2.358968	-1.429949	0.000000
39C	-1.049288	-1.831602	1.307502
40C	-1.049288	-1.831602	-1.307502
41C	1.138486	1.777536	1.307502
42C	1.138486	1.777536	-1.307502
43C	-1.087429	0.659176	2.121797
44C	-1.087429	0.659176	-2.121797
45C	-2.465178	-0.042204	0.000000
46C	-1.102913	2.205103	0.000000
47C	2.658113	-0.659080	-1.306140
48C	2.658113	-0.659080	1.306140
49C	1.813910	-2.051749	-1.306141
50C	1.813910	-2.051749	1.306141

TLJ (S_C = 1.6)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.123972	0.000000	0.000000
3A	0.561986	-0.973388	0.000000
4C	0.561986	-0.324463	1.301696
5C	0.561986	-0.324463	-1.301696

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.161602	0.000000	0.000000
3C	0.580800	-1.312441	0.000000
4C	0.580800	0.000000	-1.312441
5C	0.580800	0.000000	1.312441
6C	0.580800	1.312441	0.000000

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.462463	0.000000	0.000000
3C	0.351121	-1.413251	0.000000
4C	0.354328	1.096113	0.891532
5C	0.354329	1.096110	-0.891536
6A	0.435898	-0.346079	0.973719
7A	0.435898	-0.346081	-0.973719

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.422607	0.000000	0.000000
3C	0.210329	-1.439661	0.000000
4C	0.210330	0.964520	1.068797
5A	0.454392	-0.431816	0.971339
6C	-0.989290	-0.415741	0.935180
7C	0.313550	1.261605	-0.664799
8C	0.313550	-0.351684	-1.381999

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.411876	0.000000	0.000000
3C	0.113789	-1.407282	0.000000
4C	0.210698	1.063726	0.906118
5C	0.210698	1.063726	-0.906118
6C	-1.043285	-0.295741	-0.906118
7C	-1.043285	-0.295741	0.906118
8A	0.405251	-0.373806	-0.974335
9A	0.405251	-0.373806	0.974335

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.418215	0.000000	0.000000
3C	0.240118	-1.397740	0.000000
4C	0.240118	-0.202383	-1.383010
5C	0.152582	1.066749	0.922008
6C	-1.025515	-0.330992	0.922006
7C	-1.025516	0.864365	-0.461002
8A	-0.835834	-0.567627	-0.490609
9A	0.417918	-0.352246	0.981216
10A	0.417917	0.919873	-0.490606

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2B	1.274896	0.000000	0.000000
3B	-0.384816	-1.215433	0.000000
4B	0.445040	-0.607717	-1.028582
5B	0.445040	-0.607717	1.028582
6C	-1.084027	-0.090387	-0.927992
7C	-1.084027	-0.090387	0.927992
8C	0.413375	1.006183	-0.927993
9C	0.413375	1.006183	0.927993
10A	-0.674032	0.920413	0.000000
11C	1.176787	-1.606939	0.000000

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2B	1.265253	0.000000	0.000000
3A	0.444412	-0.997835	0.000000
4A	0.444412	-0.346146	-0.935873
5C	-0.968758	-0.989126	0.386459
6C	-0.968758	0.019336	-1.061766
7C	0.391990	-0.384221	1.323143
8C	0.391991	1.107695	-0.819359
9C	-0.969323	0.823759	0.573619
10C	-0.237288	-1.601768	-1.115381
11A	0.479219	0.835944	0.582103
12C	1.519527	-1.306066	-0.909472

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.484860	0.000000	0.000000
3A	-1.162150	0.000001	0.000000
4A	-0.599725	0.739029	0.597171
5A	-0.599725	0.796316	-0.518321
6A	-0.599726	-0.246877	-0.917511
7A	-0.599726	-0.339570	0.887394
8A	-0.599726	-0.948894	-0.048732
9B	0.450107	1.224840	0.062903
10B	0.450106	0.438321	-1.145454
11B	0.450107	0.318672	1.184330
12B	0.450106	-0.953943	-0.770833
13B	0.450106	-1.027890	0.669053

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069407	0.000000	0.000000
3A	0.534704	-0.972693	0.000000
4A	0.534703	0.333352	-0.913788
5A	0.534703	0.972693	0.000001
6A	0.534703	-0.333351	0.913788
7C	1.438224	0.778884	1.113232
8C	-0.368818	-0.778883	-1.113232
9C	-0.368821	0.778883	1.113231
10C	1.438226	-0.778883	-1.113231
11C	-0.754620	0.966557	-0.676262
12C	1.824026	0.966558	-0.676261
13C	-0.754619	-0.966558	0.676261
14C	1.824027	-0.966556	0.676262

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.150794	0.000000	0.000000
3C	0.575397	-1.315325	0.000000
4C	0.575397	-0.042743	1.302121
5A	0.575397	-0.155420	-0.897577
6C	1.451029	0.989924	-1.010309
7C	-0.300233	0.989924	-1.010310
8A	0.575397	0.925001	0.148998
9C	-0.711677	-0.718680	-1.070073
10C	1.862470	-0.718681	-1.070074
11C	-0.750446	0.997973	0.710124
12C	1.901241	0.997973	0.710125
13C	-0.965179	-0.774524	0.710306
14C	2.115974	-0.774524	0.710306
15C	0.575398	-0.000199	-2.278691

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092840	0.000000	0.000000
3A	0.540056	-0.950074	0.000000
4C	0.476564	-0.277281	-1.288451
5C	0.480135	1.303233	-0.183257
6C	-0.895709	-1.061437	-0.183260
7C	1.380717	-0.803348	1.168291
8A	0.538168	0.333021	0.903160
9A	-0.023567	-0.632433	0.903159
10C	1.875397	-1.091167	-0.504612
11C	-0.898209	0.522610	0.937410
12C	1.890490	0.856723	0.820910
13C	0.189430	-2.066892	0.820911
14C	0.410169	-2.017893	-0.948801
15C	1.956972	0.640611	-0.948802
16C	-1.009680	0.587467	-0.845460

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.429316	0.000000	0.000000
3A	0.418747	-1.010788	0.000000
4A	0.418746	-0.418655	0.920011
5C	-0.916937	-0.971997	0.625592
6B	0.384638	-1.702530	1.095774
7B	-0.513303	0.464964	1.095773
8B	-0.513303	-0.804783	-0.877061
9C	1.630284	-0.854969	1.593039
10C	0.966788	0.746611	1.593038
11C	1.630284	-1.804088	0.118371
12C	0.295588	0.479439	-1.339375
13C	0.295587	1.417666	0.118368
14C	0.966788	-1.140735	-1.339374
15C	-0.073981	-2.278825	-0.352759
16C	-1.245106	0.548093	-0.352762
17C	-0.073981	-0.622780	2.220276

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.093196	0.000000	0.000000
3A	0.546599	-0.936196	0.000000

4A	0.546599	0.301579	-0.886291
5C	0.546598	1.301887	0.131556
6C	0.546598	-0.294840	1.274867
7A	1.108508	-0.644819	-0.900541
8A	-0.015309	-0.644820	-0.900541
9C	-0.848073	0.522692	-0.997919
10C	-0.848071	-1.113101	0.173369
11C	1.941270	-1.113099	0.173370
12C	1.941270	0.522696	-0.997916
13C	0.546601	-1.958604	-0.963004
14C	0.546600	-0.280738	-2.164415
15C	-0.972928	0.587369	0.820308
16C	2.066123	0.587370	0.820310
17C	0.546598	1.471551	-1.666401
18C	0.546600	-2.051610	0.856304

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094865	0.000000	0.000000
3A	0.543810	-0.950263	0.000000
4A	0.543810	0.319555	-0.894921
5A	-0.007246	-0.630707	-0.894921
6C	1.401248	-0.812581	-1.152983
7C	0.475302	-0.275627	1.286097
8C	0.475302	1.303884	0.172918
9C	-0.895599	0.519358	-0.940264
10C	-0.895599	-1.060156	0.172917
11C	0.187818	-2.052638	-0.848600
12C	0.187819	-0.108915	-2.218463
13C	1.874829	-1.087210	0.521263
14C	1.874830	0.856513	-0.848599
15C	-1.013065	0.587473	0.833578
16C	-1.149665	-1.122644	-1.592940
17C	0.403350	1.555433	-1.592940
18C	1.956360	0.654843	0.929172
19C	0.403349	-2.023234	0.929171

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.089526	0.000000	0.000000
3A	1.089526	-1.089526	0.000000
4A	0.544763	-0.544763	0.770411
5A	0.544763	-0.544763	-0.770411
6A	0.000000	-1.089526	0.000000
7C	0.544763	0.856273	0.990681
8C	0.544763	0.856273	-0.990681
9C	-0.856273	-0.544763	0.990681
10C	-0.856273	-0.544763	-0.990681
11C	1.945798	-0.544762	0.990682
12C	1.945798	-0.544762	-0.990682
13C	0.544764	-1.945799	-0.990681
14C	0.544764	-1.945799	0.990681
15C	-0.986360	0.986360	0.000000
16C	0.544762	-0.544762	-2.165335
17C	0.544762	-0.544762	2.165335
18C	2.075886	0.986360	0.000000
19C	-0.986360	-2.075886	0.000000
20C	2.075888	-2.075883	0.000000

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.222400	0.000000	0.000000
3A	0.611200	-0.918299	0.000000
4A	0.611200	-0.306202	-0.865744
5B	1.633943	-1.034074	-0.731111
6B	-0.411542	-1.034075	-0.731111
7A	0.611200	-0.294268	0.882829
8A	0.611199	0.734182	-0.571802
9A	0.611199	0.753013	0.532393
10C	1.658648	0.378544	-1.475698
11C	-0.436249	0.378543	-1.475698
12C	1.658652	-1.265016	0.848941
13C	-0.436251	-1.265017	0.848941
14C	-0.481318	0.432739	1.387866
15C	-0.481317	1.452734	-0.054807
16C	1.703717	0.432741	1.387866
17C	1.703714	1.452736	-0.054806
18C	-1.433182	-0.043445	-0.030719
19C	2.655581	-0.043442	-0.030720
20C	0.611200	-1.154481	-1.968579
21C	0.611200	-2.240870	-0.432001

N = 22

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.090316	0.000000	0.000000
3A	0.528192	-0.953836	0.000000
4A	0.528192	0.331277	-0.894460
5A	-0.033932	-0.622559	-0.894460
6A	1.048035	-0.617638	-0.887390
7C	2.019496	-1.190151	-0.093343
8C	2.019497	0.325818	-1.148482
9C	0.693291	-1.924545	-1.148484
10C	0.693292	-0.408576	-2.203622
11C	-1.348638	-0.248380	-0.356859
12C	-0.436046	1.300146	-0.356858
13C	-0.436047	-0.786198	1.095272
14C	0.476547	0.762327	1.095274
15B	1.140931	-0.672386	1.093622
16B	-0.548754	-1.608060	-0.250705
17B	1.140932	1.259071	-0.250703
18B	-0.548753	0.323398	-1.595031
19C	0.685323	1.370926	-1.815569
20C	-0.867320	-1.263667	-1.815572
21C	2.237966	0.455904	0.655021
22C	0.685321	-2.178688	0.655019

N = 23

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.210249	0.000000	0.000000
3A	0.605124	-1.048106	0.000000
4A	0.605124	-0.349369	-0.826000
5A	0.605124	-0.349369	0.826000
6A	1.536853	-0.887303	0.567185
7A	1.536853	-0.887303	-0.567185
8A	-0.326605	-0.887302	0.567185
9A	-0.326605	-0.887302	-0.567185
10A	0.605124	0.726500	0.567185
11A	0.605124	0.726500	-0.567185
12C	1.690884	0.277495	-1.413657
13C	1.690884	0.277495	1.413657
14C	-0.480636	0.277495	-1.413657
15C	0.605123	-1.603096	-1.413657
16C	-0.480636	0.277495	1.413657
17C	0.605123	-1.603096	1.413657
18C	-0.545626	1.349942	0.000000
19C	1.755874	1.349942	0.000000
20C	2.652145	-0.202445	0.000000
21C	-0.291148	-2.195602	0.000000
22C	-1.441897	-0.202445	0.000000
23C	1.501394	-2.195603	0.000000

N = 24

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.217398	0.000000	0.000000
3A	0.608698	-1.044293	0.000000
4A	0.608699	-0.352782	-0.826095
5A	0.608699	-0.344442	0.826467
6A	0.608699	0.703938	-0.555585
7A	0.608699	0.732035	0.561267
8C	-0.447072	0.294688	-1.438839
9C	1.664469	0.294687	-1.438839
10A	1.540276	-0.881023	-0.577263
11A	-0.322879	-0.881022	-0.577263
12A	1.546847	-0.883012	0.560582
13A	-0.329450	-0.883011	0.560582
14C	-0.517358	1.375849	-0.035496
15C	1.734756	1.375848	-0.035496
16C	1.705099	0.297950	1.387466
17C	-0.487700	0.297951	1.387466
18C	0.608698	-1.597189	-1.426568
19C	0.608698	-1.604417	1.400654
20C	-1.431993	-0.174482	-0.033153
21C	2.649391	-0.174483	-0.033153
22C	-0.287948	-2.190092	-0.013678
23C	1.505344	-2.190093	-0.013678
24C	0.608700	1.787590	-1.431848

N = 25

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124432	0.000000	0.000000
3A	0.000257	-1.080104	0.000000
4A	0.604210	-0.538387	-0.778545
5A	1.072890	-1.113757	0.006980
6A	0.569348	-0.505013	0.767181
7C	1.978287	-0.717416	1.001464
8C	0.580669	-1.855477	1.143943
9C	-0.781698	-0.714556	1.167513
10C	2.176698	-0.646888	-0.763177
11C	0.524359	1.329020	0.042998
12C	-0.287942	-1.484608	-1.371696
13C	-0.322839	0.381249	-1.324077
14A	1.134104	0.437829	1.009131
15A	0.482841	-2.030275	-0.272804
16B	-1.115516	-0.615654	-0.366186
17B	1.246432	0.569871	-1.120321
18A	0.039183	0.428402	1.036536
19A	1.094459	-1.517824	-1.023144
20C	1.895031	-2.248491	-0.022569
21C	0.653983	-0.314053	2.153103
22C	2.237679	0.860959	0.168592
23C	-0.895739	-2.167178	0.156376
24C	-1.137799	0.823327	0.291181
25C	1.020299	-0.610557	-2.149276

N = 26

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.129285	0.000000	0.000000
3A	0.564641	-0.977990	0.000000
4A	0.564642	-0.325996	0.922058
5A	-0.333259	-0.844399	0.597081
6A	0.564642	0.710810	0.597081
7A	1.462542	-0.844400	0.597081
8A	0.564642	-0.325997	-0.869185
9A	-0.381527	0.220275	1.003058
10A	0.564641	-1.418538	1.003058
11A	0.564643	0.766546	-0.542029
12A	1.510811	-0.872268	-0.542029
13A	1.510811	0.220274	1.003058
14A	-0.381528	-0.872267	-0.542029
15C	-1.462795	-0.178738	0.126388
16C	0.564642	0.697287	1.990037
17C	1.450830	-0.837639	1.990037
18C	1.705891	1.356186	0.126387
19C	2.592079	-0.178740	0.126388
20C	-0.321550	-2.155437	0.126389
21C	-0.576605	0.332903	-1.320754
22C	1.450830	-2.155438	0.126389
23C	-0.576605	1.356187	0.126387
24C	1.705890	0.332902	-1.320753
25C	-0.321549	-0.837638	1.990037
26C	0.564641	-1.643796	-1.320753

N = 27

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.126458	0.000000	0.000000
3A	0.560490	-0.977118	0.000000
4A	0.570968	-0.330717	0.922478
5A	-0.332678	-0.845785	0.599911
6A	0.568124	0.709410	0.599911
7A	1.462523	-0.847126	0.599264
8A	0.552726	-0.320152	-0.870640
9A	-0.355743	0.206054	0.991281
10A	-0.398351	-0.867712	-0.529367
11A	0.553286	-1.418921	1.008134
12A	1.506105	0.226077	1.008133
13A	0.554468	0.777285	-0.529368
14A	1.503249	-0.870716	-0.545375
15C	-0.588081	1.361622	0.187106
16C	-1.473715	-0.167385	0.187107
17C	-0.358133	-0.813553	1.989484
18C	0.527501	0.715453	1.989483
19C	-0.607711	0.351999	-1.276118
20C	1.419668	-0.822301	1.999392
21C	1.703369	1.362544	0.131404
22C	-0.334362	-2.155504	0.131407
23C	2.585063	-0.173565	0.124137
24C	1.693125	0.343064	-1.316913
25C	0.544861	-1.639358	-1.316912
26C	1.436800	-2.155988	0.124138
27C	-1.328676	0.769598	1.795512

N = 28

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.116599	0.000000	0.000000
3A	0.558366	-0.976233	0.000000
4A	0.537960	-0.323016	0.922791
5A	0.555642	-0.324471	-0.880691
6A	-0.354635	-0.841614	0.582730

7A	-0.359744	-0.858445	-0.550106
8A	1.440916	-0.842137	0.609010
9A	0.545358	0.715763	0.592242
10C	0.571624	-1.663007	-1.310116
11B	-0.513268	0.304687	-1.114177
12A	0.555584	0.757973	-0.562355
13A	1.503032	-0.874750	-0.535609
14A	0.526970	-1.417773	0.999828
15A	1.482115	0.223680	1.010598
16A	-0.419910	0.216071	0.982405
17C	1.725252	0.324492	-1.302669
18C	-1.474616	-0.209303	0.043659
19C	-0.364013	-2.140270	0.090793
20C	-0.598770	1.341320	0.095943
21C	1.422348	-2.157748	0.147739
22C	2.577927	-0.182147	0.155421
23C	1.689197	1.354970	0.126867
24C	1.402491	-0.835933	2.000167
25C	0.514133	0.697721	1.983790
26C	-0.369618	-0.837233	1.975574
27C	0.373822	-0.231246	-2.303443
28C	-1.110380	-1.082315	-1.693959

N = 29

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.098971	0.000000	0.000000
3A	0.541195	-0.946902	0.000000
4A	0.528564	-0.326012	-0.923450
5A	0.540815	-0.319009	0.922406
6A	0.552068	0.738749	0.583078
7A	1.457919	-0.846173	0.583079
8A	-0.374288	-0.842030	-0.574380
9A	-0.374364	-0.842073	0.562386
10A	0.532201	0.720854	-0.590805
11A	1.432416	-0.854210	-0.590805
12B	1.655915	0.318318	1.085036
13A	1.478222	0.216757	-0.999611
14A	-0.426450	0.230377	-0.972220
15A	0.523251	-1.431269	-0.972220
16A	-0.433629	0.219690	0.961067
17A	0.510399	-1.432029	0.961068
18C	-0.584622	1.333303	0.004345
19C	1.393281	-2.127337	0.004346
20C	-1.466839	-0.166632	-0.008171
21C	-0.346866	-2.126195	-0.008170
22C	1.671506	1.355291	-0.113777
23C	2.557311	-0.194560	-0.113775
24C	0.520243	0.690422	-1.982801
25C	1.400125	-0.849067	-1.982801
26C	-0.368523	-0.838734	-1.964879
27C	-0.420883	-0.868659	1.942633
28C	0.425394	0.670789	2.004424
29C	1.335068	-0.920824	2.004425

N = 30

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.084462	0.000000	0.000000
3A	0.508667	-0.950134	0.000000
4A	0.511084	-0.320236	0.915810
5A	0.488190	-0.324972	-0.931579
6A	0.536760	0.741091	0.584325
7C	-0.843851	0.522363	0.951334
8C	-0.872764	0.494148	-0.944726
9B	1.616470	0.338220	1.093766
10A	-0.413223	-0.829229	-0.567233
11A	-0.404949	-0.820611	0.567766
12A	1.425352	-0.848148	0.584613
13A	0.521565	0.717232	-0.599839
14A	1.396632	-0.860825	-0.589708
15C	1.674797	1.339799	-0.153973
16C	-0.403207	-2.109367	0.005889
17A	1.459199	0.189819	-1.005051
18A	0.481243	-1.435287	-0.965678
19A	0.477702	-1.431251	0.961683
20C	1.344818	-2.133679	0.007757
21C	2.528077	-0.213934	-0.094659
22B	0.434728	0.449028	1.896520
23C	0.539398	0.673633	-2.001399
24C	1.375461	-0.885495	-1.978768
25C	-0.437911	-0.899548	1.952188
26C	-0.388510	-0.866842	-1.969590
27C	1.319744	-0.923579	1.997460
28C	-0.120017	1.832490	-0.037761
29C	-1.696906	-0.761060	0.023756
30C	0.974299	1.841776	1.378880

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.111655	0.000000	0.000000
3A	0.549157	-0.966542	0.000000
4A	-0.543361	-0.968463	0.000000
5A	0.573622	0.950853	0.000000
6C	1.345602	0.766207	-1.249307
7C	1.345602	0.766207	1.249307
8C	-0.001460	-1.548456	-1.249306
9C	-0.001460	-1.548456	1.249306
10A	-0.544466	0.967868	0.000000
11A	-1.110490	-0.004732	0.000000
12A	0.537141	-0.312599	-0.883861
13A	0.537141	-0.312599	0.883861
14A	-0.002248	0.627667	0.882948
15A	-0.002248	0.627667	-0.882948
16A	-0.546843	-0.308113	0.882948
17A	-0.546843	-0.308113	-0.882948
18C	1.731068	-1.007427	0.878622
19C	1.731068	-1.007427	-0.878622
20C	-1.384140	0.805528	1.146672
21C	-1.384140	0.805528	-1.146672
22C	-1.731778	-1.013872	-0.877598
23C	0.026027	2.006569	-0.877599
24C	0.026027	2.006569	0.877599
25C	-1.731778	-1.013872	0.877598
26C	-0.034041	0.019811	2.161164
27C	-0.034041	0.019811	-2.161164
28C	2.496928	0.358898	0.000000
29C	0.921437	-2.348278	0.000000
30C	1.593942	1.958899	0.000000
31C	-0.915781	-2.353566	0.000000

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.109418	0.000000	0.000000
3A	-0.546426	-0.969307	0.000000
4A	0.573322	-0.953146	0.000004
5A	-1.111541	-0.033922	-0.000005
6A	0.546825	0.970668	-0.000003
7A	-0.571168	0.951844	-0.000006
8C	1.348079	-0.760769	-1.248365
9C	1.348072	-0.760760	1.248373
10C	-1.328887	-0.801592	1.249080
11C	-1.328877	-0.801602	-1.249087
12A	0.008754	-0.623299	-0.882505
13A	0.008748	-0.623293	0.882508
14A	0.534474	0.326491	0.881746
15A	0.534479	0.326486	-0.881748
16A	-0.549210	0.303552	-0.881237
17A	-0.549216	0.303559	0.881230
18C	-0.042723	1.582390	-1.178329
19C	-0.042729	1.582398	1.178314
20C	0.027592	-2.004223	-0.878577
21C	0.027586	-2.004217	0.878587
22C	1.741790	0.991776	-0.883208
23C	1.741785	0.991782	0.883207
24C	-1.762316	0.959535	-0.876636
25C	-1.762322	0.959542	0.876612
26C	-0.001357	0.028457	-2.160626
27C	-0.001370	0.028472	2.160623
28C	1.591462	-1.959549	0.000009
29C	-1.537651	-2.003468	0.000000
30C	2.500097	-0.368706	0.000006
31C	-2.489406	-0.431079	-0.000009
32C	1.012491	2.343451	-0.000007

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.110416	0.000000	0.000000
3A	0.540982	-0.969723	0.000000
4A	-1.110296	0.016357	0.000000
5A	-0.555209	-0.961649	0.000000
6A	-0.555208	0.961649	0.000000
7A	0.569314	0.953366	0.000000
8C	1.349259	0.765800	-1.245128
9C	-1.337831	0.785593	1.245128
10C	-0.011428	-1.551391	1.245128
11C	-1.337831	0.785593	-1.245128
12C	-0.011428	-1.551391	-1.245128
13C	1.349259	0.765800	1.245128
14A	0.004607	0.625383	0.881185
15A	0.004607	0.625383	-0.881185
16A	0.539294	-0.316681	-0.881185
17A	0.539294	-0.316681	0.881185
18A	-0.543901	-0.308702	-0.881186
19A	-0.543901	-0.308702	0.881186
20C	1.728173	-1.014807	0.877167
21C	1.728173	-1.014807	-0.877167
22C	0.014762	2.004046	0.877167
23C	-1.742935	-0.989239	-0.877167
24C	0.014762	2.004046	-0.877167
25C	-1.742935	-0.989239	0.877167
26C	0.000000	0.000001	-2.163217
27C	0.000000	0.000001	2.163217
28C	2.498055	0.353020	0.000000
29C	1.583853	1.963750	0.000000
30C	-1.554753	1.986869	0.000000
31C	-2.492583	0.389781	0.000000
32C	-0.943301	-2.339890	0.000000
33C	0.908729	-2.353532	0.000000

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.059428	0.000000	0.000000
3A	0.529715	-0.958691	0.000000
4A	0.529715	-0.322072	0.902972
5A	0.529712	0.783986	-0.552730
6A	0.529713	-0.288120	-0.908059
7A	0.529713	0.758489	0.576437
8A	-0.401406	-0.826584	0.582764
9A	1.460836	-0.826583	0.582763
10A	1.457193	1.001559	0.035711
11A	1.457193	0.302839	-0.955345
12A	-0.397769	1.001557	0.035712
13A	-0.397769	0.302837	-0.955343
14A	-0.393487	-0.800458	-0.582964
15A	-0.393487	0.280168	0.949782
16A	1.452915	-0.800456	-0.582966
17A	1.452915	0.280171	0.949781
18C	-1.425426	0.001001	-0.000706
19C	2.484853	0.001006	-0.000709
20B	0.529716	-1.568123	1.105569
21B	0.529711	1.904673	0.065696
22B	0.529711	0.577999	-1.816043
23A	0.529714	-1.374269	-1.006591
24A	0.529713	0.486402	1.632560
25C	-0.359198	1.612329	1.355654
26C	-0.359198	-0.735199	-1.974052
27C	1.418621	1.612332	1.355653
28C	1.418621	-0.735198	-1.974055
29C	-0.358105	-0.609349	2.021058
30C	-0.358104	-2.108304	-0.105040
31C	1.417535	-0.609347	2.021057
32C	1.417536	-2.108303	-0.105042
33C	-0.396844	1.706691	-1.203261
34C	1.456264	1.706693	-1.203262

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.109481	0.000000	0.000000
3A	0.565809	-0.954363	0.000000
4A	-0.554483	-0.960887	-0.013836
5A	-1.109066	-0.012919	-0.027399
6A	0.543770	0.966990	-0.013835
7A	-0.554485	0.960594	-0.027399
8C	-1.379087	-0.790022	1.172589
9C	1.358816	-0.774077	1.206403
10C	-0.023735	1.589166	1.172590
11A	0.529189	0.322333	0.890859
12A	-0.007393	-0.619585	0.890859
13A	-0.554744	0.316021	0.877472
14C	1.357619	-0.773394	-1.249035
15C	-1.317258	-0.788972	-1.282071
16C	0.006893	1.535448	-1.282070
17A	0.014592	-0.628662	-0.884970
18A	-0.529735	0.301774	-0.898283
19A	0.548209	0.308052	-0.884970
20C	1.731990	1.025137	0.830607
21C	0.001464	-2.012634	0.830606
22C	-1.763793	1.004780	0.787433
23C	0.022956	-2.003297	-0.914030
24C	1.734920	1.001889	-0.914028
25C	-1.723365	0.981750	-0.956739
26C	0.026961	-0.015358	-2.175624

27C	-0.911301	0.519140	2.251537
28C	-0.022248	-1.000549	2.273280
29C	0.849313	0.529392	2.273281
30C	-1.554681	-1.997919	-0.058389
31C	-2.502565	-0.377669	-0.081571
32C	0.925736	2.356210	-0.058387
33C	1.578811	-1.979671	-0.019689
34C	-0.951383	2.345279	-0.081570
35C	2.508047	-0.348488	-0.019688

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.061995	0.000000	0.000000
3A	0.468244	-0.965113	0.000000
4A	0.468244	-0.257365	-0.930165
5A	0.457110	0.787632	0.599296
6A	-0.518726	-0.752338	-0.572442
7A	0.466352	-0.297336	0.890964
8A	0.466351	0.779410	-0.524162
9A	-0.491707	-0.756357	0.562860
10A	-0.491708	0.340780	-0.879065
11A	-0.482334	0.306902	0.917278
12A	-0.482335	0.965903	0.051178
13A	-1.053250	0.006990	0.005319
14B	0.326174	-1.504662	-1.144873
15B	1.557125	-0.908093	-0.690954
16B	1.534057	0.483342	-1.085311
17B	1.534057	-0.917117	0.755258
18B	-0.428378	-0.476833	-1.823363
19B	-0.428377	-1.884492	0.026669
20C	0.383575	0.375017	2.080035
21C	0.383574	2.104719	-0.193246
22C	0.243557	0.985311	-1.888145
23C	0.243559	-1.557021	1.453140
24C	-1.824299	-1.131938	0.249387
25C	-1.824300	-0.061498	-1.157451
26A	1.371708	1.049069	0.054369
27A	1.371708	0.332156	0.996582
28C	-0.458688	1.691456	1.287001
29C	-1.860940	0.873268	0.664458
30C	-1.192435	1.583977	-0.959053
31C	-1.192432	-0.501927	1.782370
32C	2.500255	0.170220	0.129517
33C	1.307403	1.718269	1.307402
34C	1.109847	-2.266490	0.034767
35C	1.109846	-0.570894	-2.193688
36C	-1.259484	-1.739791	-1.323779

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.146328	0.000000	0.000000
3A	-1.137932	-0.002539	0.000000
4A	-0.544987	0.759871	-0.545694
5A	-0.544989	0.760560	0.544731
6A	0.541915	0.770442	-0.539651
7A	0.541914	0.771123	0.538676
8A	-0.542416	-0.268021	-0.892017
9A	-0.542419	-0.266893	0.892354
10A	0.546282	-0.276406	-0.885090
11A	0.546280	-0.275287	0.885439
12C	-0.073801	1.969605	-0.001246
13A	0.535506	-0.944412	0.000597
14A	-0.565602	-0.937553	0.000591
15C	1.632382	1.505780	-0.000951
16A	0.016022	0.500580	1.454548
17A	0.016025	0.498741	-1.455181
18C	-0.045750	-1.543973	-1.190202
19C	-0.045753	-1.542468	1.192151
20C	-1.741560	1.321343	-0.000838
21B	1.574399	0.409302	1.153390
22B	1.574402	0.407844	-1.153904
23C	1.650503	-1.156725	-0.876415
24C	1.650501	-1.155616	0.877879
25C	-1.725268	-1.046144	0.867663
26C	-1.725265	-1.047241	-0.866345
27C	-0.973909	1.540331	-1.623657
28C	-0.973911	1.542383	1.621704
29C	-0.958497	-0.196549	-2.235835
30C	-0.958502	-0.193721	2.236078
31A	-1.457082	0.344602	-1.004679
32A	-1.457084	0.345873	1.004239
33C	0.771112	1.709838	-1.572719
34C	0.771110	1.711825	1.570556
35C	0.788746	-0.382629	-2.277282
36C	0.788741	-0.379751	2.277764
37C	2.609303	0.038113	-0.000022

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.053447	0.000000	0.000000
3A	0.523240	-0.972707	0.000000
4A	0.501057	-0.308675	0.903214
5A	0.501058	-0.308675	-0.903214
6A	0.481283	0.791093	-0.565730
7A	0.481282	0.791093	0.565730
8B	-0.662967	1.055168	-0.000001
9A	-0.398654	-0.818488	-0.574692
10A	-0.398655	-0.818488	0.574691
11A	-0.449400	0.251009	0.927992
12A	-0.449398	0.251009	-0.927993
13A	-1.066753	-0.165845	-0.000001
14B	1.589870	1.127617	0.000000
15A	1.415616	0.299654	-0.962048
16A	1.415615	0.299654	0.962048
17A	1.420072	-0.816484	0.628066
18A	1.420072	-0.816484	-0.628065
19C	-0.437440	-2.114924	0.000000
20C	-0.451609	-0.591640	-2.015637
21C	-0.451609	-0.591640	2.015637
22B	0.483069	-1.543700	1.147325
23B	0.483069	-1.543701	-1.147325
24C	0.423308	2.157057	0.000000
25A	0.450019	0.480361	-1.625656
26A	0.450017	0.480361	1.625656
27C	-0.449416	1.565534	-1.470138
28C	-0.449419	1.565533	1.470137
29C	2.486192	-0.146850	0.000000
30C	1.342154	-0.565410	-2.059874
31C	1.342154	-0.565410	2.059874
32C	-1.839305	0.567951	-0.943247
33C	-1.839308	0.567952	0.943241
34C	1.430526	-2.096404	0.000000
35C	-1.705151	-1.174872	0.876946
36C	-1.705151	-1.174873	-0.876946
37C	1.305462	1.613770	1.479189
38C	1.305465	1.613769	-1.479189

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.143547	0.000000	0.000000
3A	-1.138799	-0.001984	0.000000
4A	-0.546473	0.765635	-0.542699
5A	-0.546473	0.765700	0.542607
6A	0.539908	0.776303	-0.537730
7A	0.539908	0.776368	0.537636
8A	0.545633	-0.268195	-0.886545
9A	0.545633	-0.268088	0.886577
10A	-0.546200	-0.260582	-0.887979
11A	-0.546200	-0.260475	0.888010
12A	0.530786	-0.951616	0.000057
13C	-0.049524	-1.503043	1.253849
14C	-0.049523	-1.503193	-1.253669
15A	-0.562587	-0.945828	0.000057
16C	-0.077943	1.976461	-0.000120
17C	1.654763	-1.133086	-0.885024
18C	1.654763	-1.132979	0.885161
19C	1.627067	1.521923	-0.000091
20A	0.010589	0.507205	-1.451164
21A	0.010589	0.507380	1.451103
22C	-1.745239	1.324816	-0.000080
23C	-1.735333	-1.027375	0.870621
24C	-1.735332	-1.027479	-0.870498
25B	1.576650	0.424889	-1.146188
26B	1.576648	0.425027	1.146137
27C	-0.954653	-0.187242	-2.236322
28C	-0.954654	-0.186973	2.236344
29C	-0.975939	1.551209	1.619376
30C	-0.975938	1.551014	-1.619562
31C	0.766973	1.716067	1.573131
32C	0.766975	1.715877	-1.573338
33C	0.801798	-0.334649	2.287794
34C	0.801799	-0.334923	-2.287754
35A	-1.456441	0.355367	-1.005537
36A	-1.456441	0.355488	1.005493
37C	2.612056	0.053104	-0.000002
38C	0.802400	-2.388290	0.000144
39C	-0.956042	-2.345806	0.000140

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.137824	0.000000	0.000000
3A	-1.141298	-0.003734	0.000000
4A	0.538626	-0.764759	0.539614
5A	0.538625	-0.764719	-0.539670
6A	0.555558	0.250802	0.890263
7A	0.555558	0.250868	-0.890244
8A	-0.542527	-0.781397	0.536861
9A	-0.542528	-0.781358	-0.536919
10A	-0.539293	0.259310	0.889133
11A	-0.539293	0.259376	-0.889114
12C	0.070736	-1.982395	-0.000074
13A	0.563096	0.941815	0.000035
14A	-0.531078	0.947370	0.000035
15C	0.049073	1.495253	-1.252951
16C	0.049073	1.495160	1.253062
17C	1.719982	1.040351	0.881021
18C	1.719982	1.040416	-0.880944
19C	-1.651043	1.122531	0.888745
20C	-1.651043	1.122597	-0.888662
21C	-1.628449	-1.526721	-0.000057
22B	1.522290	-1.300849	-0.000048
23A	-0.004138	-0.523622	1.449899
24A	-0.004138	-0.523515	-1.449937
25B	-1.570636	-0.432456	1.153998
26B	-1.570636	-0.432370	-1.154030
27A	1.490396	-0.386071	-0.951945
28A	1.490397	-0.386141	0.951917
29C	1.004834	-1.583168	-1.557861
30C	1.004834	-1.583282	1.557745
31C	0.997901	0.125138	2.216316
32C	0.997901	0.125301	-2.216307
33C	-0.753425	-1.726872	-1.572928
34C	-0.753425	-1.726989	1.572799
35C	-0.771999	0.321797	-2.292724
36C	-0.772000	0.321628	2.292748
37C	2.593023	-0.181718	-0.000007
38C	-2.605268	-0.060804	-0.000002
39C	-0.808680	2.381177	0.000088
40C	0.947010	2.348878	0.000087

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.068521	0.000000	0.000000
3A	0.473271	-0.956419	0.000000
4A	0.473271	-0.239750	-0.925882
5A	0.469423	-0.300699	0.926529
6A	0.469423	0.821570	-0.523353
7A	-0.512337	-0.738961	-0.571985
8A	-0.504593	-0.753775	0.592107
9A	-0.504593	0.384250	-0.878133
10A	0.498041	0.742364	0.574620
11A	-1.060064	0.032015	0.024782
12A	-0.455136	0.308859	0.927578
13A	-0.455136	0.975385	0.066479
14B	0.339914	-1.486706	-1.150770
15C	0.367103	2.100470	0.418567
16C	0.367103	0.931734	1.928483
17B	-0.408068	-0.465631	-1.819037
18B	-0.408068	-1.877680	0.005221
19B	1.556288	-0.933854	0.698661
20B	1.556288	0.442262	-1.079173
21B	0.352147	0.741358	-1.768636
22B	0.352146	-1.526329	1.161038
23B	1.565868	-0.913685	-0.707229
24A	1.378075	1.063006	0.029084
25A	1.378075	0.294622	1.021776
26B	-0.368160	-0.501804	1.867874
27B	-0.368160	1.682447	-0.954008
28C	-1.780104	-0.088979	1.221167
29C	-1.780104	1.159873	-0.392252
30B	-1.602395	-1.111291	0.026697
31B	-1.602395	-0.252727	-1.082501
32C	2.505992	0.204431	0.158239
33C	-1.111398	1.541759	1.193384
34C	1.199119	-0.572186	2.172288
35C	1.199120	1.959499	-1.098451
36C	1.126380	-0.589123	-2.208302
37C	1.126380	-2.285473	-0.016750
38C	-1.207210	-1.772609	-1.372070
39C	-1.198452	0.912776	-2.068347
40C	-1.198452	-1.773501	1.402113
41C	1.866306	1.595951	1.235332

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.057115	0.000000	0.000000
3A	-0.476800	-0.943480	0.000000
4A	0.467765	-0.760495	0.587488
5A	0.467764	-0.760494	-0.587489
6A	-0.504594	-0.243982	0.929680
7A	0.445346	0.340307	0.929680
8A	0.445346	0.340309	-0.929679
9A	-0.504595	-0.243981	-0.929679
10A	-1.047340	0.006851	0.000001
11A	0.466276	0.937845	0.000001
12A	-0.490610	0.797636	0.548571
13A	-0.490610	0.797636	-0.548569
14B	1.529632	-0.306927	-1.128397
15B	-0.415990	-1.503639	-1.128397
16B	1.529633	-0.306928	1.128395
17B	-0.415989	-1.503641	1.128395
18B	1.551752	-1.156311	-0.000002
19B	0.332113	-1.906487	-0.000002
20C	-1.895853	0.558762	-0.918588
21C	0.356406	1.944080	-0.918589
22C	0.356406	1.944079	0.918591
23C	-1.895852	0.558761	0.918591
24B	0.311252	-0.506036	-1.858049
25B	0.311254	-0.506038	1.858048
26A	1.355004	0.863228	-0.612400
27A	-1.381594	-0.819998	-0.612399
28A	1.355004	0.863227	0.612400
29A	-1.381593	-0.819999	0.612400
30C	-0.518254	0.842580	1.947755
31C	-0.518256	0.842583	-1.947753
32C	2.487171	0.250990	-0.000001
33C	-1.345820	-2.106606	-0.000001
34C	-1.170786	1.903470	0.000001
35C	-1.358280	-0.676817	-2.043882
36C	-1.358278	-0.676820	2.043883
37C	1.216701	0.906998	2.043883
38C	1.216698	0.907000	-2.043883
39C	1.116533	-1.815265	-1.390013
40C	1.116534	-1.815267	1.390009
41C	-2.647798	-0.772432	0.000001
42C	1.883659	2.014774	0.000001

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.063942	0.000000	0.000000
3A	-1.063185	-0.040124	0.000000
4A	0.492395	-0.919701	0.287255
5A	-0.457359	-0.937637	-0.287188
6A	0.467475	0.571759	-0.759861
7A	-0.488706	0.553778	0.759819
8A	0.448508	-0.566033	-0.780948
9A	-0.426843	-0.582488	0.780989
10A	-0.511977	0.902833	-0.312480
11A	0.477566	0.921521	0.312412
12A	-0.490023	-0.012219	-0.942498
13A	0.490135	0.006338	0.942498
14C	0.565092	-1.089295	1.772052
15C	-0.523606	-1.109959	-1.771974
16B	1.567846	1.084401	-0.348752
17B	-1.607625	1.024528	0.348673
18B	0.358432	-1.815334	-0.646310
19B	-0.289718	-1.827513	0.646441
20B	0.358564	1.806447	-0.611732
21B	-0.426433	1.791684	0.611600
22C	1.748287	0.596902	1.155520
23C	-1.769551	0.530462	-1.155562
24A	-1.310762	-1.057068	0.383828
25A	1.349695	-1.006913	-0.383754
26A	1.351477	0.000602	-1.046559
27A	-1.350539	-0.050290	1.046559
28B	0.313600	1.061932	1.599502
29B	-0.353421	1.049233	-1.599581
30A	0.379148	0.005177	-1.695956
31A	-0.379074	-0.009002	1.695955
32A	-1.440908	-0.761230	-0.715572
33A	1.468591	-0.706297	0.715624
34C	1.251677	-1.166509	-1.812572
35C	-1.206797	-1.212750	1.812658
36C	2.492758	-0.221769	-0.215046
37C	-2.482621	-0.315603	0.215064
38C	-1.247302	1.110481	1.876698
39C	1.204540	1.156593	-1.876783
40C	-1.244117	-2.152747	-0.551077
41C	1.324417	-2.104258	0.551231
42C	1.109073	2.172147	0.741093
43C	-1.190198	2.128722	-0.741252

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.077972	0.000000	0.000000
3A	-0.458637	-0.975538	0.000000
4A	0.483470	-0.761533	0.590125
5A	0.504938	0.230362	-0.932816
6A	-0.423303	-0.358946	-0.932816
7A	0.496809	-0.782542	-0.497151
8A	0.489486	0.315740	0.898797
9A	-0.493996	-0.308638	0.898796
10A	0.495333	0.955747	-0.076989
11A	-1.075674	-0.041628	-0.076990
12A	-0.498643	0.785432	0.508450
13A	-0.457343	0.720381	-0.631073
14B	-0.387277	0.610015	1.771099
15B	-1.579505	0.336952	1.031144
16B	0.367087	1.572774	1.031146
17B	1.571747	-0.371577	1.104453
18B	-0.332453	-1.580486	1.104453
19B	-1.446593	-1.050501	-0.803456
20B	1.566151	0.862183	-0.803455
21B	1.590068	0.956006	0.618972
22B	-1.541678	-1.032228	0.618971
23B	0.376672	-0.593313	1.825426
24C	-1.505583	0.387622	-1.509042
25C	0.289784	1.527436	-1.509041
26A	1.397069	-0.428550	-0.969125
27A	-0.206573	-1.446645	-0.969125
28A	0.441103	-0.694796	-1.554517
29A	0.368719	-1.711367	0.026482
30A	1.391870	-1.061805	0.026483
31B	-0.373037	1.895224	-0.135007
32B	-1.556418	1.143938	-0.135008
33C	1.172364	-1.846636	-1.149997
34A	-0.136385	0.214828	-1.820474
35C	-0.738732	-1.033462	-2.228619
36C	1.249564	0.228836	-2.228618
37C	-0.895181	-2.367320	-0.134001
38C	2.523235	-0.197090	-0.133999
39C	1.205393	-1.898663	1.166556
40C	1.156398	0.759836	2.144469
41C	-1.179640	-0.723231	2.144467
42C	-1.188595	1.872202	1.237318
43C	1.170558	2.268671	-0.165842
44C	-2.551121	-0.094090	-0.165845

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.081707	0.000000	0.000000
3A	0.500709	-0.958842	0.000000
4A	0.500708	0.757137	-0.588323
5A	-0.439365	-0.794304	-0.588325
6A	-0.439365	0.266229	-0.951928
7A	0.496811	-0.301034	-0.878037
8A	0.496697	-0.300967	0.904439
9A	0.496697	0.792597	0.529512
10A	-0.472657	-0.807165	0.529509
11A	-1.071751	-0.026447	-0.077138
12A	-0.472657	0.962260	-0.077137
13A	-0.498675	0.302164	0.881333
14B	-0.372128	1.571178	1.034034
15B	-1.564974	0.948273	0.572661
16B	-1.564973	-0.397421	1.034031
17B	-0.372127	-0.606201	1.780547
18B	0.365092	0.610460	1.780549
19B	-1.448170	-0.431367	-1.258181
20B	-0.287968	1.483360	-1.258178
21B	1.589279	1.154791	-0.083345
22B	-0.287967	-1.943302	-0.083349
23B	1.589280	-0.963002	0.642739
24B	0.407812	1.917379	-0.115397
25B	-1.510825	-1.249023	-0.115402
26B	-1.510826	0.915465	-0.857495
27B	1.593596	0.372108	1.085338
28B	0.407814	-1.584836	1.085336
29A	0.404038	-1.362159	-1.026562
30A	1.394466	0.272385	-1.026561
31A	1.394466	-0.844957	-0.643481
32A	0.404038	0.445737	-1.646398
33A	-0.208082	-0.564467	-1.646400
34C	1.163203	-0.704823	-2.055782
35C	-0.833343	0.504957	-2.353640
36C	-0.833342	-1.842869	-1.548690
37C	2.534029	-0.084424	-0.246246
38C	1.247806	1.591737	-1.548684
39C	1.247808	-2.207126	-0.246247
40C	-1.192560	0.722612	2.107669
41C	-1.133402	2.292929	-0.165384
42C	-2.557128	-0.056704	-0.165388
43C	-1.133400	-1.912056	1.276293
44C	1.170240	1.889731	1.276298
45C	1.170241	-0.709093	2.167303

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.096126	0.000000	0.000000
3C	0.560784	-2.165422	0.000000
4A	0.551330	-0.861354	0.326656
5A	0.547697	0.940826	-0.318519
6A	-0.556120	-0.950133	0.321745
7A	1.658000	-0.949627	0.319643
8A	0.552701	0.000703	-0.935918
9A	0.544604	0.588134	0.720937
10A	-0.004298	-0.294873	1.041020
11A	1.096970	-0.289888	1.043916
12C	-0.361835	0.829750	1.763353
13A	0.018627	-0.897812	-0.619892
14A	-0.391342	0.980634	0.278728
15A	1.088608	-0.896106	-0.620601
16A	-0.927027	0.073606	0.578413
17C	0.555090	-0.674521	2.285184
18C	-1.114569	-0.794907	1.748633
19A	1.476734	0.979615	0.278167
20C	0.553794	1.984810	0.776075
21A	2.018528	0.067444	0.579879
22A	-0.907085	-0.317926	-0.497088
23A	-0.365687	0.608301	-0.809224
24A	1.473843	0.612709	-0.803247
25A	2.012833	-0.307860	-0.494048
26C	-1.682406	0.851106	-0.389843
27C	1.505206	0.851600	1.725968
28A	0.020102	-1.377978	1.134731
29A	1.092693	-1.371958	1.139749
30C	-0.489243	-0.341193	-1.852336
31C	1.597798	-0.340573	-1.849884
32C	2.231168	-0.764227	1.744100
33C	0.558945	1.074836	-1.835850
34C	-2.005943	-0.819376	0.247789
35C	-0.352104	2.026725	-0.714906
36C	-1.037180	-1.748277	-0.867884
37C	2.148654	-1.743619	-0.862297
38C	0.555468	-1.724991	-1.674744
39C	1.464648	2.031668	-0.697577
40C	2.781055	0.877486	-0.306991
41C	3.114682	-0.805167	0.249987
42C	-1.017637	-2.263238	0.799550
43C	2.135922	-2.250867	0.810432
44C	0.557256	-2.504384	1.779979
45C	-2.062066	0.603268	1.308702
46C	-1.205895	2.054250	0.819533

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.059382	0.000000	0.000000
3A	0.529692	-0.917452	0.000000
4A	0.529692	-0.305817	-0.941540
5A	0.529690	-0.305817	0.941539
6A	-0.394633	-0.839476	-0.604693
7A	0.529690	0.761501	-0.604692
8A	0.529690	0.761501	0.604692
9A	1.454017	-0.839475	-0.604693
10A	1.454016	-0.839475	0.604693
11A	-0.394634	-0.839477	0.604691
12B	0.529693	-1.619905	-1.028327
13B	-0.608343	0.351227	-1.028326
14B	1.667723	0.351228	1.028326
15B	1.667725	0.351229	-1.028326
16B	0.529692	-1.619905	1.028325
17B	-0.608344	0.351226	1.028325
18A	-1.049850	-0.207331	-0.000001
19A	-0.345373	1.012861	-0.000001
20A	1.234171	-1.722982	0.000000
21A	-0.174786	-1.722984	-0.000001

22A	1.404753	1.012862	0.000000
23A	2.109232	-0.207328	0.000000
24C	1.415249	-0.817093	2.041146
25C	0.529688	0.716739	2.041145
26C	-0.355870	-0.817096	2.041144
27C	1.415252	-0.817092	-2.041146
28C	0.529691	0.716740	-2.041145
29C	-0.355866	-0.817095	-2.041146
30A	2.252212	-1.300311	0.000000
31A	-1.192827	-1.300315	-0.000002
32A	0.529690	1.683177	0.000000
33C	1.431867	1.915021	1.067005
34C	-1.844699	-0.634928	-1.067007
35C	2.001907	-2.197541	-1.067006
36C	-0.372488	1.915020	-1.067005
37C	1.431869	1.915021	-1.067004
38C	-0.942519	-2.197546	-1.067007
39C	2.001905	-2.197542	1.067006
40C	2.904081	-0.634923	1.067006
41C	-1.844700	-0.634930	1.067003
42C	-0.372489	1.915020	1.067004
43C	2.904083	-0.634922	-1.067005
44C	-0.942521	-2.197547	1.067003
45C	2.796226	1.002771	0.000001
46C	-1.736846	1.002766	-0.000001
47C	0.529694	-2.922987	-0.000002

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.097566	0.000000	0.000000
3C	0.548781	-2.166060	0.000000
4A	0.548784	0.939781	-0.318826
5A	0.548782	-0.861152	0.326707
6A	-0.559828	-0.948190	0.323346
7A	1.657392	-0.948191	0.323348
8A	0.548784	-0.005239	-0.936912
9A	0.548782	0.588939	0.717850
10A	1.100695	-0.292087	1.040860
11A	-0.003133	-0.292086	1.040859
12C	-0.367091	0.834446	1.756107
13C	1.464651	0.834445	1.756111
14A	-0.391347	0.980746	0.274904
15A	1.488912	0.980745	0.274907
16A	0.013555	-0.900281	-0.618337
17A	1.084011	-0.900282	-0.618336
18A	-0.927957	0.076023	0.577559
19A	2.025520	0.076022	0.577563
20C	0.548782	1.982605	0.765252
21C	0.548779	-0.677535	2.283625
22C	-1.118903	-0.787579	1.747438
23C	2.216463	-0.787581	1.747443
24A	-0.365282	0.605894	-0.810355
25A	1.462850	0.605894	-0.810354
26A	-0.909077	-0.317203	-0.495072
27A	2.006644	-0.317204	-0.495069
28C	2.780491	0.851668	-0.395068
29C	-1.682925	0.851669	-0.395076
30A	1.084370	-1.376462	1.135204
31A	0.013190	-1.376461	1.135203
32C	-0.501054	-0.346523	-1.850326
33C	1.598623	-0.346525	-1.850324
34C	0.548785	1.060264	-1.848362
35C	1.451041	2.022764	-0.725522
36C	-0.353472	2.022764	-0.725526
37C	3.107698	-0.815195	0.247484
38C	-2.010134	-0.815193	0.247478
39C	2.141313	-1.749664	-0.864399
40C	-1.043747	-1.749662	-0.864402
41C	0.548784	-1.725166	-1.674686
42C	2.124807	-2.259719	0.804301
43C	-1.027247	-2.259717	0.804297
44C	0.548779	-2.504171	1.781013
45C	2.305130	2.058350	0.809088
46C	-1.207567	2.058352	0.809081
47C	-2.065943	0.609919	1.303009
48C	3.163504	0.609916	1.303017

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.105833	0.000000	0.000000
3C	0.555387	-2.168164	0.000000
4A	0.551700	0.941726	-0.312341
5A	0.556085	-0.861018	0.320100
6A	-0.551743	-0.946900	0.316264
7A	1.666205	-0.949806	0.313360
8A	0.559260	0.582708	0.721369
9A	0.557641	0.006773	-0.928350
10A	0.008205	-0.297757	1.041360
11A	1.112580	-0.299254	1.037612
12C	-0.344037	0.821828	1.772401
13C	1.481784	0.821162	1.758683
14A	0.019284	-0.894806	-0.625081
15A	1.497178	0.979096	0.279040
16A	1.088214	-0.899190	-0.625132
17A	-0.380200	0.979353	0.292907
18A	-0.918682	0.070584	0.587444
19A	2.036008	0.072463	0.573387
20C	0.564196	1.976742	0.784489
21A	-0.913943	-0.317336	-0.509559
22C	-1.669841	0.871933	-0.347145
23C	0.570893	-0.690919	2.281068
24C	-0.423861	-0.351264	-1.871943
25A	-0.367516	0.605354	-0.810888
26C	2.232220	-0.799395	1.736308
27C	-1.094820	-0.797477	1.766701
28A	1.469811	0.613765	-0.807356
29A	2.010984	-0.313964	-0.504608
30C	-1.993933	-0.825155	0.285663
31C	-1.031756	-1.751340	-0.860098
32C	2.788081	0.854114	-0.394407
33C	1.578737	-0.342829	-1.856726
34A	0.023882	-1.379978	1.127615
35A	1.095642	-1.382585	1.124553
36C	0.556103	1.085030	-1.833568
37C	-0.349878	2.026127	-0.698232
38C	1.458958	2.031693	-0.707058
39C	3.116837	-0.814904	0.233470
40C	2.149832	-1.743540	-0.876377
41C	0.561917	-1.753040	-1.670837
42C	-1.017503	-2.263260	0.807519
43C	2.135903	-2.264962	0.788550
44C	0.560512	-2.505062	1.779172
45C	-2.045128	0.602491	1.338634
46C	-1.186310	2.061219	0.853102
47C	2.320270	2.051582	0.821269
48C	3.179145	0.599701	1.299994
49C	-2.091834	-0.442777	-1.416180

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.105597	0.000000	0.000000
3A	0.565174	-0.947598	0.000000
4A	0.546247	0.994536	0.000856
5A	-0.575824	-0.976992	-0.000038
6A	1.707219	-0.966529	0.003224
7A	0.559433	0.313574	0.867075
8A	0.017871	-0.637446	0.868648
9A	0.555438	0.310117	-0.868838
10A	0.015270	-0.639684	-0.868630
11A	1.107640	-0.633850	-0.871642
12A	1.112393	-0.631203	0.868274
13C	-0.335140	0.186075	1.934601
14C	-1.666683	0.947483	-0.003065
15C	-0.325107	0.182791	-1.940963
16A	-0.371836	0.839232	0.593148
17A	-0.370430	0.839495	-0.595338
18A	-0.912319	-0.110546	0.593054
19A	-0.911058	-0.110463	-0.595994
20C	0.572174	1.613064	1.388468
21A	1.481850	0.851575	0.569337
22C	1.469180	0.192819	1.929553
23A	2.033825	-0.081597	0.577981
24A	1.468310	0.845653	-0.576470
25C	-0.338611	2.144378	-0.001933
26C	0.577211	1.614764	-1.392517
27C	-1.094808	-1.322560	1.386837
28A	0.026593	-1.701271	-0.571485
29A	0.025818	-1.700547	0.570670
30C	-1.093575	-1.324856	-1.390120
31C	-2.017482	-0.804629	-0.002892
32A	1.121146	-1.693809	-0.572044
33A	1.120429	-1.693582	0.574474
34A	2.021313	-0.102624	-0.582028
35C	0.576355	-1.423855	1.896506
36C	1.511413	0.225166	-1.902797
37C	0.577219	-1.420698	-1.900234
38C	2.253528	-1.273466	1.382270
39C	2.250262	-1.283587	-1.383539
40C	1.457472	2.159574	-0.005274
41C	2.787235	0.968747	-0.093902
42C	-1.112013	-2.357634	-0.000750
43C	3.160452	-0.754753	-0.001464
44C	2.270035	-2.328396	0.003110
45C	0.582851	-2.885863	0.001147
46C	-1.166275	1.677132	1.497019
47C	-1.161080	1.674155	-1.503401
48C	-2.033213	0.140333	-1.503883
49C	-2.039899	0.141539	1.496061
50C	2.338083	1.622682	1.452100

Table S4. The global-minimum geometries of the quaternary Lennard-Jones (QLJ_N) clusters.

QLJ (S_D = 1.15)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124071	0.000000	0.000000
3A	0.562035	-0.973474	0.000000
4D	0.562036	-0.324491	1.013854
5D	0.562036	-0.324491	-1.013854

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.563360	0.000000	0.000000
3D	0.781680	-0.910483	0.000000
4D	0.781680	0.910483	0.000000
5D	0.781680	0.000000	0.910483
6D	0.781680	0.000000	-0.910483

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.122338	0.000000	0.000000
3D	0.561169	-1.068500	0.000000
4D	0.561169	0.855515	0.639904
5D	0.561169	0.855515	-0.639904
6A	0.561169	-0.306789	0.922346
7A	0.561169	-0.306789	-0.922346

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.163725	0.000000	0.000000
3D	0.581862	-1.036026	0.000000
4D	0.581862	0.544322	-0.881512
5D	1.218036	-0.576809	-1.034087
6D	-0.054312	-0.576809	-1.034087
7D	0.581862	-0.192305	1.015521
8D	0.581862	0.965102	0.369924

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.123750	0.000000	0.000000
3A	0.567940	-0.969670	0.000000
4A	0.568672	-0.325960	-0.911256
5A	0.568672	-0.325960	0.911256
6D	-0.447742	-0.901541	0.643795
7D	-0.447742	-0.901541	-0.643795
8D	0.551640	0.841988	0.643795
9D	0.551640	0.841988	-0.643795

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.203124	0.000000	0.000000
3D	0.518859	-1.085491	0.000000
4D	0.508459	-0.320518	-1.035473
5D	0.525762	0.894056	-0.616837
6D	-0.579901	-0.859928	-0.616838
7B	0.526185	-0.331693	0.967693
8D	-0.558956	-0.812906	0.664248
9D	0.492370	0.854879	0.664249
10D	-0.586710	0.369847	-0.968917

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.167263	0.000000	0.000000
3D	0.426307	-1.086630	0.000000
4D	0.426309	-0.290692	-1.047025
5D	0.488128	0.914063	-0.599212
6D	-0.672647	-0.788241	-0.599213
7D	0.488126	-0.332846	1.041047
8D	0.389557	0.881549	0.670144
9D	-0.678380	-0.684604	0.670144
10D	-0.678378	0.462576	-0.838929
11D	-0.876772	0.597858	0.454485

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.204621	0.000000	0.000000
3C	0.527312	-1.053872	0.000000
4C	0.527312	-0.342761	0.996575
5D	0.521558	0.862301	0.656197
6D	0.521558	-0.340065	-1.028840
7D	0.519750	0.880611	-0.628364
8D	-0.564504	-0.877165	-0.592401
9D	-0.564505	0.274903	1.022147
10D	-0.572652	1.061745	0.022400
11D	-0.572652	0.324140	-1.011304
12A	-0.457869	-0.831193	0.593101

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.180155	0.000000	0.000000
3D	-0.522823	-1.086960	0.000000
4D	-0.522823	-0.335889	1.033760
5D	-0.522823	-0.335889	-1.033760
6D	-0.522823	0.879369	0.638899
7D	-0.522823	0.879369	-0.638899
8C	0.541413	0.322294	0.991921
9C	0.541413	1.042967	0.000000
10C	0.541413	0.322294	-0.991921
11C	0.541413	-0.843778	0.613041
12C	0.541413	-0.843778	-0.613041
13D	-1.200983	0.000000	0.000000

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.105888	0.000000	0.000000
3A	0.534680	-0.968042	0.000000
4A	0.534680	-0.315496	-0.915187
5D	0.573686	0.847014	-0.650057
6D	-0.464067	-0.911696	-0.650056
7D	0.573687	-0.338512	1.012628
8D	-0.495921	-0.903912	0.621136
9D	0.551473	0.871135	0.621135
10D	-0.495921	0.292625	-1.056995
11D	-1.189910	-0.044852	-0.031980
12D	-0.536040	0.316301	1.015645
13D	-0.536041	1.063277	-0.031981
14D	1.536615	-0.906703	-0.646496

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.105161	0.000000	0.000000
3A	0.538879	-0.964878	0.000000
4B	0.540437	-0.317179	0.948356
5A	0.531607	-0.311998	-0.914582
6D	0.570363	0.849503	-0.642540
7D	-0.463562	-0.912184	-0.642539
8D	-0.476036	-0.909074	0.631159
9D	0.561565	0.858878	0.631158
10D	-0.503259	0.295359	-1.045733
11D	-0.520888	0.305707	1.028784
12D	-0.533736	1.060648	-0.013127
13D	-1.186266	-0.051188	-0.013127
14D	1.534917	-0.900834	-0.659707
15D	1.555906	-0.913153	0.627742

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.103758	0.000000	0.000000
3A	0.536666	-0.962861	0.000000
4A	0.536666	-0.305593	-0.913079
5B	0.538357	-0.313576	0.947859
6B	0.538356	0.799331	-0.598195
7D	0.570737	0.861973	0.620480
8D	-0.461604	-0.902456	-0.649620
9D	-0.482655	-0.900322	0.626312
10D	-0.482656	0.308186	-1.052552
11D	-0.518691	0.317776	1.021612
12D	-0.518691	1.069649	-0.022892
13D	-1.182755	-0.035755	-0.025737
14D	1.530092	-0.913312	-0.657436
15D	1.555889	0.306455	-1.059276
16D	1.555890	-0.907247	0.626804

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.100942	0.000000	0.000000
3A	0.531459	-0.964170	0.000000
4A	0.531459	-0.313904	0.911640
5C	0.552172	0.820690	0.627517
6C	0.552173	-0.326138	-0.980278
7C	-0.452184	-0.879748	0.627518
8D	-0.488902	0.288768	1.058795
9D	-0.488902	-0.907096	-0.617746
10D	0.558398	0.866048	-0.617746
11D	-1.186365	-0.047092	0.033590
12D	-0.531454	0.313901	-1.014806
13D	-0.531454	1.061714	0.033590
14A	1.456179	-0.860086	0.613493
15D	1.573954	-0.929649	-0.576550
16D	0.547446	-1.495469	1.066707
17D	1.573954	0.242474	1.066707

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.096623	0.000000	0.000000
3B	0.542137	-0.997550	0.000000
4B	0.542136	-0.308260	-0.948726
5B	0.542136	-0.308260	0.948726
6B	0.542136	0.807035	-0.586345
7B	0.542136	0.807035	0.586345
8D	-0.493562	1.088984	0.000000
9D	-0.493562	0.336514	1.035685
10D	-0.493562	-0.881007	0.640089
11D	-0.493562	0.336514	-1.035685
12D	-0.493562	-0.881007	-0.640089
13D	-1.183293	0.000000	0.000000
14D	1.578581	1.090373	0.000000
15D	1.578581	0.336944	1.037006
16D	1.578581	0.336944	-1.037006
17D	1.578582	-0.882130	0.640905
18D	1.578582	-0.882130	-0.640905

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.090363	0.000000	0.000000
3B	0.545181	-0.997670	0.000000
4B	0.545181	-0.308297	0.948840
5B	0.545181	-0.308297	-0.948840
6B	0.545181	0.807132	0.586416
7B	0.545181	0.807132	-0.586416
8D	-0.490637	-0.881104	0.640160
9D	-0.490637	0.336552	-1.035800
10D	1.580999	1.089105	0.000000
11D	-0.490637	0.336552	1.035800
12D	-0.490637	1.089105	0.000000
13D	1.580999	0.336552	1.035800
14D	1.580999	-0.881105	-0.640160
15D	1.580999	0.336552	-1.035800
16D	1.580999	-0.881105	0.640160
17D	-0.490637	-0.881104	-0.640160
18D	-1.181820	0.000001	0.000000
19D	2.272182	0.000000	0.000000

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.089964	0.000000	0.000000
3A	0.544982	-0.961900	0.000000
4A	0.544982	-0.308177	-0.911197
5C	0.544982	0.828184	-0.618706
6C	0.544982	-0.320756	0.982752
7D	0.544982	0.869058	0.623491
8C	1.531439	-0.877739	-0.629720
9C	-0.441476	-0.877739	-0.629720
10D	1.572087	0.288035	-1.060512
11D	-0.482122	0.288035	-1.060512
12D	-0.482123	-0.912328	0.612622
13D	1.572086	-0.912328	0.612622
14D	-0.538900	1.058779	-0.032520

15D	-0.538901	0.308409	1.013387
16D	1.628865	1.058779	-0.032520
17D	1.628864	0.308409	1.013387
18D	-1.185042	-0.054173	-0.038866
19D	2.275006	-0.054173	-0.038866
20D	0.544982	-1.494108	-1.071923

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092245	0.000000	0.000000
3A	0.546123	-0.955338	0.000000
4B	0.546123	-0.312095	0.947486
5B	0.546123	-0.312095	-0.947486
6C	0.546122	0.834208	0.609542
7C	0.546122	0.834208	-0.609542
8D	-0.477389	-0.897859	0.632206
9D	1.569635	-0.897858	-0.632206
10D	1.569635	-0.897858	0.632206
11D	-0.477389	-0.897859	-0.632206
12D	-0.503009	0.311894	1.037249
13D	1.595254	0.311895	-1.037249
14D	1.595254	0.311895	1.037249
15D	-0.503009	0.311894	-1.037249
16D	1.613899	1.070314	0.000000
17D	-0.521655	1.070314	0.000000
18D	-1.185421	-0.031300	0.000000
19D	2.277666	-0.031299	0.000000
20D	0.546123	-1.539849	-1.034737
21D	0.546123	-1.539849	1.034737

N = 22

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092322	0.000000	0.000000
3A	0.548737	-0.951883	0.000000
4B	0.543557	-0.315531	-0.947100
5B	0.543557	-0.315530	0.947100
6D	0.539800	0.861925	0.633076
7D	0.539801	0.861924	-0.633076
8C	-0.450256	-0.887400	-0.609366
9C	-0.450257	-0.887400	0.609366
10D	1.560525	-0.912813	0.632302
11D	1.560525	-0.912813	-0.632302
12D	-0.520424	0.282448	-1.037263
13D	-0.520426	0.282448	1.037262
14D	1.604089	0.294239	1.037949
15D	1.604089	0.294239	-1.037949
16D	-1.187296	-0.078309	-0.000001
17D	-0.560290	1.045299	-0.000001
18D	1.636548	1.056032	0.000000
19D	2.278807	-0.057072	0.000000
20D	0.526268	-1.536644	1.038400
21D	0.526269	-1.536646	-1.038398
22D	-0.118691	-1.932656	0.000001

N = 23

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.093701	0.000000	0.000000
3A	0.546850	-0.946526	0.000000
4B	0.546850	-0.313436	-0.947105
5B	0.546850	-0.313436	0.947105
6D	1.569418	-0.897676	0.633081
7D	-0.475717	-0.897676	0.633081
8D	1.569418	-0.897676	-0.633081
9D	-0.475717	-0.897676	-0.633081
10C	0.546850	0.832916	-0.609457
11C	0.546850	0.832916	0.609457
12D	-0.502207	0.310363	1.037353
13D	-0.502207	0.310363	-1.037353
14D	1.595908	0.310363	1.037353
15D	1.595908	0.310363	-1.037353
16D	0.546850	-1.536943	1.038019
17D	0.546850	-1.536943	-1.038019
18D	-0.521998	1.068388	0.000000
19D	1.615699	1.068388	0.000000
20D	1.189686	-1.945080	0.000000
21D	-0.095986	-1.945080	0.000000
22D	-1.184290	-0.035558	0.000000
23D	2.277991	-0.035558	0.000000

N = 24

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092283	0.000000	0.000000
3A	0.546141	-0.946758	0.000000
4A	0.546142	-0.318518	0.904073
5C	0.546141	-0.316655	-0.982862
6C	0.546142	0.822447	0.620538
7C	-0.438850	-0.882804	0.626088
8C	1.531133	-0.882804	0.626087
9D	0.546141	0.870056	-0.619291
10D	-0.481070	-0.909228	-0.616151
11D	1.573352	-0.909229	-0.616152
12D	1.574276	0.278277	1.060469
13D	-0.481993	0.278278	1.060469
14D	0.546142	-1.498374	1.066338
15D	-0.537229	0.309279	-1.011719
16D	1.629512	0.309278	-1.011719
17D	0.546141	-1.568321	-1.009849
18D	1.630826	1.055280	0.039357
19D	-0.538543	1.055280	0.039357
20D	-1.183411	-0.060391	0.038958
21D	2.275694	-0.060392	0.038957
22D	1.190178	-1.940269	0.042924
23D	-0.097895	-1.940268	0.042924
24D	0.546142	0.437249	1.813202

N = 25

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.093247	0.000000	0.000000
3A	0.546019	-0.947127	0.000000
4A	0.548700	-0.317026	-0.897886
5C	0.547350	-0.316244	0.982270
6C	0.545463	0.821275	-0.623192
7C	-0.439078	-0.882742	-0.623191
8C	1.530016	-0.884006	-0.628333
9D	-0.480564	-0.908855	0.617096
10D	0.547367	0.870260	0.617094
11D	1.573968	-0.909400	0.614229
12D	-0.483411	0.279303	-1.058562
13D	1.572092	0.275718	-1.064682
14D	0.546309	-1.499681	-1.064681
15D	-0.536278	0.309850	1.011168
16D	0.546482	-1.568347	1.009171
17D	1.631669	0.309866	1.009170
18D	-0.538119	1.055412	-0.039660
19D	-1.183112	-0.060925	-0.039659
20D	1.631067	1.054384	-0.044151
21D	-0.098829	-1.939674	-0.044149
22D	2.275603	-0.061351	-0.043340
23D	1.189695	-1.940814	-0.043339
24D	-0.102493	-0.685491	-1.814348
25D	0.542681	0.431161	-1.814348

N = 26

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.093963	0.000000	0.000000
3A	0.546981	-0.947401	0.000000
4A	0.546981	-0.315800	-0.893218
5C	0.546981	0.820380	-0.625005
6C	0.546981	-0.315801	0.981797
7C	1.530941	-0.883890	-0.625006
8C	-0.436980	-0.883889	-0.625005
9D	1.574288	0.277316	-1.062098
10D	-0.480326	-0.908916	0.615488
11D	0.546981	-1.502032	-1.062098
12D	1.574288	-0.908917	0.615488
13D	-0.480326	0.277317	-1.062097
14D	0.546981	0.870432	0.615489
15D	1.191579	-1.940259	-0.043707
16D	-0.537542	0.310349	1.008920
17D	0.546981	0.428519	-1.814725
18D	-1.182141	-0.061809	-0.043706
19D	1.631504	1.054668	-0.043706
20D	1.631504	0.310349	1.008919
21D	0.546981	-1.568100	1.008919
22D	-0.097618	-0.687959	-1.814725
23D	-0.097619	-1.940259	-0.043707
24D	-0.537542	1.054668	-0.043705
25D	1.191579	-0.687959	-1.814726
26D	2.276103	-0.061810	-0.043707

N = 27

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.091453	0.000000	0.000000
3A	0.545726	-0.946730	0.000000
4A	0.545726	-0.314634	-0.889746
5A	0.545726	-0.320714	0.903230
6C	0.545726	0.823664	-0.619221
7C	-0.442109	-0.882180	-0.614766
8C	1.533562	-0.882180	-0.614766
9C	0.545727	0.832084	0.595771
10D	1.562742	-0.897082	0.629201
11D	-0.471290	-0.897082	0.629201
12D	-0.484377	0.281929	-1.050136
13D	1.575829	0.281929	-1.050136
14D	0.545726	-1.502630	-1.051259
15D	-0.489346	0.302904	1.033067
16D	1.580799	0.302904	1.033067
17D	0.545727	-1.529467	1.032051
18D	-0.525086	1.057283	-0.016505
19D	1.616540	1.057283	-0.016505
20D	-1.176950	-0.050755	-0.016675
21D	2.268402	-0.050755	-0.016675
22D	0.545726	0.429979	-1.806936
23D	-0.100596	-0.686629	-1.804803
24D	1.192049	-0.686629	-1.804803
25D	-0.097621	-1.934807	-0.021829
26D	1.189074	-1.934806	-0.021830
27D	0.545727	0.459983	1.787658

N = 28

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092182	0.000000	0.000000
3A	0.544831	-0.946584	0.000000
4A	0.544693	-0.314962	0.888014
5A	0.550063	-0.318068	-0.893191
6C	0.543241	0.824523	0.613403
7C	-0.443612	-0.882132	0.613403
8C	1.531959	-0.885837	0.610549
9C	0.541547	0.827696	-0.604580
10C	-0.447208	-0.882247	-0.604580
11D	1.557944	-0.900863	-0.634630
12D	-0.487681	0.281996	1.045114
13D	0.541977	-1.505316	1.046333
14D	1.575006	0.281196	1.046333
15D	-0.490688	0.283735	-1.037000
16D	1.577330	0.298798	-1.039134
17D	0.527880	-1.516111	-1.039134
18D	-0.530696	1.050637	0.005639
19D	-1.175313	-0.064158	0.005640
20D	1.613901	1.055897	0.008884
21D	-0.110047	-1.925483	0.008884
22D	2.266531	-0.054005	0.010650
23D	1.177457	-1.937441	0.010650
24D	0.543979	0.430732	1.802072
25D	-0.101948	-0.686330	1.802073
26D	1.190449	-0.688362	1.800648
27D	-0.109640	-0.685414	-1.795364
28D	0.539348	0.436940	-1.795364

N = 29

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092372	0.000000	0.000000
3A	0.546186	-0.946022	0.000000
4A	0.546186	-0.315341	-0.886767
5A	0.546186	-0.315341	0.886767
6C	1.533860	-0.885574	0.609582
7C	1.533860	-0.885574	-0.609582
8C	-0.441487	-0.885574	0.609582
9C	-0.441487	-0.885574	-0.609582
10C	0.546186	0.825126	-0.609582
11C	0.546186	0.825126	0.609582
12D	-0.486409	0.280828	-1.042149
13D	-0.486409	0.280828	1.042149
14D	1.578781	0.280828	-1.042149
15D	1.578781	0.280828	1.042149
16D	0.546186	-1.507679	1.042149
17D	0.546186	-1.507679	-1.042149
18D	-1.172784	-0.067412	0.000000
19D	1.620384	1.049367	0.000000
20D	1.190959	-1.927976	0.000000
21D	-0.528011	1.049367	0.000000
22D	2.265156	-0.067412	0.000000
23D	-0.098586	-1.927976	0.000000
24D	0.546187	0.430772	1.798554
25D	1.192339	-0.688397	1.798554
26D	0.546187	0.430772	-1.798554
27D	-0.099966	-0.688397	1.798554
28D	1.192339	-0.688397	-1.798554
29D	-0.099966	-0.688397	-1.798554

N = 30

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094056	0.000000	0.000000
3A	0.548611	-0.944022	0.000000
4A	0.545118	-0.311432	-0.887457
5A	0.545119	-0.311433	0.887457
6B	0.540930	0.786678	-0.594898
7B	0.540931	0.786678	0.594898
8D	1.566269	-0.892339	-0.629680
9D	1.566270	-0.892339	0.629679
10C	-0.446719	-0.873711	0.609674
11C	-0.446720	-0.873711	-0.609673
12D	-0.486469	0.298429	1.034054
13D	-0.486470	0.298429	-1.034053
14D	1.566675	0.307215	-1.041344
15D	1.566676	0.307214	1.041344
16D	0.535239	-1.497743	-1.049681
17D	0.535241	-1.497744	1.049681
18D	1.572607	1.074344	0.000000
19D	-0.496132	1.065537	0.000001
20D	-1.172424	-0.044677	0.000001
21D	-0.111489	-1.915896	0.000000
22D	2.266165	-0.015044	-0.000001
23D	0.534646	0.461576	1.780856
24D	0.534644	0.461577	-1.780855
25D	1.171453	-1.938216	-0.000001
26D	-0.111642	-0.664801	-1.798466
27D	-0.111640	-0.664802	1.798467
28D	1.175229	-0.659439	1.817352
29D	1.175227	-0.659438	-1.817352
30D	0.534824	1.843054	0.000000

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.100568	0.000000	0.000000
3A	0.551127	-0.941090	0.000000
4A	0.547700	-0.306797	-0.888471
5A	0.550960	-0.299180	0.886657
6A	0.555144	0.746458	-0.572295
7B	0.548467	0.801664	0.577641
8D	-0.473841	-0.888777	-0.628699
9D	1.573472	-0.880923	-0.634730
10D	-0.472395	-0.882718	0.630891
11D	1.576911	-0.880485	0.627557
12D	-0.478741	0.306482	-1.034035
13D	1.567492	0.321174	-1.039825
14D	-0.475293	0.323254	1.030829
15D	1.575892	0.323911	1.030535
16D	-0.477375	1.075904	-0.023304
17D	0.553664	-1.484969	1.057341
18D	0.550786	-1.488337	-1.059487
19D	1.575234	1.079442	-0.015993
20D	0.537387	0.506191	-1.753131
21D	-1.175087	-0.010386	-0.000423
22D	2.274310	-0.005028	-0.006949
23D	0.550627	0.489339	1.768668
24D	-0.083872	-1.929270	0.002499
25D	1.191533	-1.925529	-0.001691
26D	-0.092808	-0.634591	-1.818744
27D	1.184347	-0.627472	-1.822167
28D	1.193627	-0.634021	1.814376
29D	-0.088926	-0.634697	1.815926
30D	0.545720	1.830029	-0.096692
31D	-0.083921	1.510212	-1.186270

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.102396	0.000000	0.000000
3A	0.551198	-0.939907	0.000000
4A	0.551198	-0.305726	-0.888795
5A	0.551198	-0.296079	0.886057
6A	0.551198	0.741567	-0.568189
7B	0.551198	0.805100	0.574462
8D	-0.472444	-0.885576	-0.631884
9D	1.574841	-0.885576	-0.631884
10D	-0.473858	-0.879579	0.629624
11D	1.576255	-0.879578	0.629625
12D	-0.473859	0.309282	-1.036547
13D	1.576255	0.309282	-1.036547
14D	1.576757	1.079067	-0.024665
15D	1.576757	0.327667	1.028411
16D	-0.474361	0.327668	1.028410
17D	-0.474361	1.079067	-0.024665
18D	0.551198	-1.481535	1.058375
19D	0.551198	0.518916	-1.745230
20D	0.551199	-1.486439	-1.060617
21D	-1.173967	-0.006013	-0.004290
22D	2.276364	-0.006013	-0.004290
23D	0.551198	0.494636	1.765940
24D	0.551198	1.830800	-0.106675
25D	1.188617	-1.926169	0.001582
26D	-0.086220	-1.926169	0.001581
27D	1.188617	-0.625036	-1.821938
28D	-0.086220	-0.625036	-1.821938
29D	-0.090176	-0.629092	1.814806
30D	1.192571	-0.629092	1.814807
31D	1.192571	1.511491	-1.185190
32D	-0.090176	1.511491	-1.185190

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.108754	0.000000	0.000000
3A	0.555131	-0.934225	0.000000
4A	0.555132	-0.292602	0.887221
5A	0.551720	-0.289769	-0.885994
6A	0.551720	0.750660	0.552686
7A	0.561708	0.761299	-0.550558
8D	-0.468667	-0.877889	0.634875
9D	-0.471990	0.325160	1.029249
10D	-0.471991	-0.875622	-0.631163
11D	1.581937	-0.873990	0.632054
12D	1.579310	-0.871292	-0.636097
13D	1.579311	0.331201	1.026681
14D	-0.473483	1.076194	0.003422
15D	-0.473484	0.333817	-1.023118
16D	1.573112	0.338348	-1.030525
17D	1.573112	1.084647	0.001439
18D	0.553666	-1.469975	-1.064009
19D	0.553668	0.550073	1.729265
20D	0.558360	-1.471658	1.064277
21D	0.541599	0.542443	-1.733905
22D	0.541600	1.816561	0.027914
23D	-1.174584	-0.004549	0.003290
24D	2.280921	0.003890	-0.002814
25D	-0.080216	-1.918816	0.000261
26D	-0.080215	-0.601228	1.822191
27D	1.194870	-1.915777	-0.002364
28D	1.194871	-0.597783	1.820127
29D	-0.090269	-0.601892	-1.817172
30D	-0.090268	1.537229	1.140753
31D	1.186764	-0.599430	-1.821341
32D	1.186766	1.541959	1.139719
33D	-0.062171	1.553368	-1.123370

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.111188	0.000000	0.000000
3A	0.555595	-0.932413	0.000000
4A	0.555595	-0.288132	-0.886778
5A	0.555593	0.754338	0.548059
6A	0.555594	-0.288132	0.886778
7A	0.555594	0.754338	-0.548059
8D	-0.469954	-0.873174	-0.634398
9D	1.581143	0.333524	1.026477
10D	1.581143	1.079302	0.000001
11D	-0.469955	-0.873174	0.634396
12D	-0.469955	0.333521	-1.026477
13D	1.581145	-0.873172	0.634398
14D	1.581145	0.333523	-1.026476
15D	1.581146	-0.873172	-0.634396
16D	-0.469957	0.333521	1.026476
17D	-0.469957	1.079300	-0.000001
18D	0.555592	0.560324	1.724500
19D	0.555592	1.813246	0.000000
20D	0.555595	-1.466947	1.065799
21D	0.555595	0.560323	-1.724500
22D	0.555597	-1.466948	-1.065799
23D	-1.173273	-0.000002	-0.000002
24D	2.284462	0.000002	0.000002
25D	-0.081744	1.549323	1.125649
26D	-0.081740	-0.591790	1.821339
27D	1.192931	-0.591789	-1.821339
28D	-0.081741	1.549323	-1.125651
29D	1.192931	-1.915069	0.000001
30D	1.192925	1.549325	1.125650
31D	1.192928	-0.591789	1.821340
32D	1.192928	1.549324	-1.125650
33D	-0.081738	-0.591791	-1.821340
34D	-0.081738	-1.915071	0.000000

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092910	0.000000	0.000000
3A	0.552232	-0.943129	0.000000
4A	0.552231	-0.316584	-0.888407
5A	0.533796	-0.306016	0.883290
6A	-0.359647	-0.829155	-0.584757
7A	0.533795	0.729318	-0.584757
8C	-0.454254	-0.873037	0.587563
9C	0.523859	0.833132	0.587564
10C	-0.454256	0.260415	-1.019609
11D	1.566035	-0.897778	-0.633155
12D	1.558193	-0.893283	0.629576
13D	1.558191	0.293197	-1.052786
14D	0.534318	-1.492793	-1.052786
15D	-0.517354	0.296588	1.007112
16D	-1.165988	-0.083207	-0.058679
17D	-0.517356	1.048233	-0.058679
18D	0.513386	0.472443	-1.761061
19D	-0.148287	-1.887728	-0.051049
20D	0.513389	-1.500296	1.036173
21D	-0.148289	-0.681748	-1.761061
22D	1.554090	0.315047	1.036174
23D	1.554089	1.081807	-0.051048
24D	1.147157	-1.945196	-0.004981
25D	2.258252	-0.007061	-0.004980
26D	1.147154	-0.657642	-1.830661
27D	0.504539	1.828353	-0.166432
28D	-1.322846	-0.613038	-1.224501
29D	-0.139392	-0.666289	1.778137
30D	-0.139395	1.451310	-1.224500
31D	0.504540	0.456952	1.778138
32D	-1.322844	-1.359237	-0.166433
33D	1.152116	-0.660488	1.812285
34D	-0.699703	-1.744785	-1.230501
35D	1.152113	1.485426	-1.230500

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.104229	0.000000	0.000000
3A	0.554209	-0.931235	0.000000
4A	0.554209	-0.288716	0.885348
5A	0.542620	-0.291827	-0.884013
6A	0.542620	0.749976	0.551522
7A	0.538135	0.751916	-0.545684
8A	-0.360688	-0.820921	0.595762
9C	-0.450104	0.304898	1.001358
10C	-0.450105	-0.857486	-0.600331
11D	-0.499142	1.057284	0.013165
12D	-0.499143	0.315279	-1.009268
13D	1.565938	-0.881582	0.639785
14D	1.564853	-0.882421	-0.633615
15D	1.564854	0.328811	1.035382
16D	1.561452	0.330929	-1.028972
17D	1.561453	1.080869	0.004394
18D	0.522166	-1.464820	1.063055
19D	-1.162216	-0.062251	0.045178
20D	0.522490	0.541141	1.727462
21D	0.522488	-1.474568	-1.050051
22D	0.522267	1.804466	0.009565
23D	0.522266	0.550354	-1.718517
24D	-0.142328	-1.871389	0.036352
25D	-0.142327	-0.614759	1.767906
26D	2.269698	-0.002615	0.001897
27D	-0.118227	-0.613073	-1.793101
28D	-0.118226	1.514671	1.138789
29D	1.150431	-0.605052	1.830553
30D	1.150429	-1.927941	0.007700
31D	-0.116262	1.534976	-1.113970
32D	1.162379	1.543212	1.137727
33D	1.162377	-0.603216	-1.819907
34D	1.163039	1.548241	-1.123598
35D	-1.319895	-1.335443	0.162183
36D	-1.319895	-0.568226	1.219357

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.102720	0.000000	0.000000
3A	0.555936	-0.933152	0.000000
4A	0.555936	-0.293010	-0.885956

5A	0.539416	0.746410	-0.555636
6A	0.539415	-0.293161	0.883129
7A	0.533794	0.752003	0.543355
8A	-0.356006	-0.814630	-0.588606
9C	-0.451012	-0.863972	0.594475
10C	-0.451011	0.293121	-1.006940
11D	-0.505482	0.310669	1.004640
12D	-0.505482	1.051378	-0.020501
13D	1.572169	-0.879889	-0.635758
14D	1.563490	0.327530	-1.036303
15D	1.563490	-0.881046	0.636364
16D	1.555528	0.333678	1.029820
17D	1.555528	1.082510	-0.006562
18D	0.539862	-1.467380	-1.060246
19D	-1.163812	-0.071166	-0.051421
20D	-0.143622	-0.642752	-1.760090
21D	-0.143622	-1.872894	-0.057575
22D	0.519816	0.529911	-1.731781
23D	0.519816	-1.477801	1.046889
24D	0.513448	0.550228	1.715842
25D	0.513449	1.801831	-0.016374
26D	2.268026	0.002527	0.001826
27D	1.151455	-1.929463	-0.005563
28D	1.151455	-0.611133	-1.830129
29D	-0.124250	-0.617144	1.788566
30D	-0.124250	1.504323	-1.147540
31D	-1.317149	-0.585126	-1.222988
32D	-1.317149	-1.344863	-0.171514
33D	-0.126462	1.532248	1.107116
34D	1.156310	-0.602506	1.820620
35D	1.156311	1.539352	-1.143707
36D	1.153600	1.551047	1.120700
37D	-0.694566	-1.720091	-1.242841

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099718	0.000000	0.000000
3A	0.569462	-0.934886	0.000000
4A	0.542269	-0.299350	-0.885358
5A	0.536539	-0.296779	0.882933
6A	0.532045	0.745166	-0.554319
7A	0.529137	0.748209	0.548617
8A	-0.359818	-0.830494	-0.559756
9A	-0.367440	-0.847166	0.557129
10D	-0.495807	0.290631	-1.016398
11D	-0.507384	0.294143	1.004571
12D	-0.512419	1.049570	-0.007522
13D	1.569048	-0.881773	-0.637827
14D	1.563901	-0.880236	0.643631
15D	1.552951	0.322522	-1.037483
16D	1.546775	0.327569	1.037972
17D	1.549575	1.079986	-0.001141
18D	-1.159695	-0.090010	-0.007818
19D	0.529811	-1.484784	-1.041423
20D	0.516600	-1.481191	1.044574
21D	-0.128111	-1.875152	-0.008132
22D	0.507703	1.798222	-0.005705
23D	0.498532	0.534337	1.722608
24D	-0.177783	-0.690000	-1.734863
25D	0.510144	0.526443	-1.730039
26D	-1.284438	-1.343898	-0.033700
27D	-0.178019	-0.661644	1.740130
28D	2.262976	0.002289	0.003588
29D	1.165407	-1.932189	0.003525
30D	1.124620	-0.625430	-1.828830
31D	-0.126799	1.514617	-1.135261
32D	-0.134866	1.518899	1.120910
33D	-1.353799	-0.649301	-1.148297
34D	1.120862	-0.615287	1.829634
35D	1.152660	1.537272	-1.138237
36D	1.145581	1.543221	1.131918
37D	-0.716630	-1.762742	-1.156523
38D	-1.360205	-0.667331	1.124821

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.097702	0.000000	0.000000
3A	0.572487	-0.936593	0.000000
4A	0.537284	-0.301293	-0.884696
5A	0.537284	-0.301293	0.884696
6A	-0.360851	-0.837710	0.552634
7A	-0.360851	-0.837710	-0.552634
8A	0.526565	0.744782	-0.552634
9A	0.526565	0.744782	0.552634
10D	-0.505215	0.283310	-1.011731
11D	-0.505215	0.283310	1.011731
12D	-1.160661	-0.100579	0.000000
13D	-0.519506	1.042768	0.000000
14D	1.567842	-0.879200	0.641369
15D	1.567842	-0.879200	-0.641369
16D	0.528457	-1.488085	-1.039189
17D	0.528457	-1.488085	1.039189
18D	1.545289	0.325189	1.039189
19D	1.545289	0.325189	-1.039189
20D	1.543315	1.081291	0.000000
21D	-0.117702	-1.880734	0.000000
22D	-1.271861	-1.361262	0.000000
23D	0.498154	1.795134	0.000000
24D	0.498542	0.525523	1.727425
25D	0.498542	0.525523	-1.727425
26D	-0.188387	-0.699449	-1.727425
27D	-0.188387	-0.699449	1.727425
28D	2.260503	0.006674	0.000000
29D	1.173232	-1.932212	0.000000
30D	1.115133	-0.625334	1.830391
31D	1.115133	-0.625334	-1.830391
32D	-1.361195	-0.668423	1.128808
33D	-0.139589	1.510019	-1.128808
34D	-1.361195	-0.668423	-1.128808
35D	-0.139589	1.510019	1.128808
36D	-0.718767	-1.776726	1.136404
37D	1.141097	1.539895	-1.136404
38D	1.141097	1.539895	1.136404
39D	-0.718767	-1.776726	-1.136404

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.090700	0.000000	0.000000
3A	0.557162	-0.937654	0.000000
4A	0.548360	-0.312023	0.882079
5A	0.521087	-0.296505	-0.884356
6A	0.514081	0.735460	0.565902
7A	-0.369653	-0.817641	0.565902
8A	0.515969	0.752436	-0.540305
9A	-0.383283	-0.827935	-0.540305
10A	-0.401713	0.228580	0.966798
11D	-0.519730	0.295734	-0.999736
12D	-0.531126	1.029294	0.028191
13D	-1.156180	-0.069194	0.028191
14D	1.560387	-0.887880	0.634727
15D	1.546678	-0.880079	-0.647563
16D	1.535067	0.323787	1.047741
17D	0.505804	-1.485069	1.047741
18D	1.524084	1.087897	0.022741
19D	-0.156698	-1.865957	0.022741
20D	0.493625	-1.486125	-1.034100
21D	1.529753	0.334798	-1.034100
22D	0.471294	0.489476	1.735870
23D	-0.180042	-0.655201	1.735870
24D	0.469073	1.792482	0.038798
25D	-1.301348	-1.318906	0.038798
26D	0.481337	0.543719	-1.715024
27D	-0.221543	-0.691544	-1.715024
28D	-0.225391	1.408196	1.178578
29D	-1.325736	-0.525582	1.178578
30D	2.248651	0.008779	0.000384
31D	1.141131	-1.937608	0.000384
32D	1.122897	-0.638942	1.830447
33D	-1.390460	-0.641039	-1.095440
34D	-0.159198	1.522816	-1.095439
35D	1.086321	-0.618129	-1.833157
36D	1.079536	1.530617	1.177487
37D	-0.764385	-1.709941	1.177487
38D	1.123899	1.556866	-1.110451
39D	-0.764288	-1.761489	-1.110452
40D	-1.406602	0.800375	0.943424

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.087614	0.000000	0.000000
3A	0.551073	-0.937669	0.000000
4A	0.551072	-0.315328	0.883058
5A	0.512940	-0.293508	-0.884274
6A	-0.372969	-0.814162	0.573785
7A	0.512939	0.734069	0.573786
8A	-0.393008	-0.824915	-0.533356
9A	0.512058	0.756794	-0.533355
10A	-0.393009	0.224881	0.956232
11D	-0.530152	0.303358	-0.987722
12D	-1.158522	-0.065939	0.046470
13D	-0.530153	1.032211	0.046471
14D	1.558648	-0.891871	0.628552
15D	1.536733	-0.879330	-0.653455
16D	1.536732	0.319687	1.047867
17D	0.503019	-1.486850	1.047866
18D	1.521001	0.338588	-1.034523
19D	1.521000	1.088135	0.029033
20D	-0.167457	-0.653729	1.744396
21D	0.478753	0.475600	1.744397
22D	0.478754	-1.482861	-1.034524
23D	-0.167456	-1.862643	0.029031
24D	-0.238997	-0.683511	-1.707829
25D	0.468184	0.552371	-1.707828
26D	-1.309552	-0.492415	1.218026
27D	-0.238999	1.378504	1.218028
28D	-1.309551	-1.312682	0.054124
29D	0.468183	1.794118	0.054126
30D	1.131214	-1.938937	-0.005049
31D	2.244787	0.007164	-0.005048
32D	1.131213	-0.647290	1.827709
33D	-1.403648	0.803176	0.957691
34D	-1.403646	-0.631813	-1.078461
35D	-0.166492	1.530259	-1.078459
36D	1.070343	-0.612457	-1.836938
37D	-0.771562	-1.694956	1.194529
38D	1.070341	1.523989	1.194532
39D	-0.781351	-1.755425	-1.101585
40D	1.117516	1.563070	-1.101583
41D	-0.781353	0.447093	2.023638

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.065151	0.000000	0.000000
3A	0.505565	-0.937524	0.000000
4A	0.505565	-0.301760	-0.887633
5A	0.489469	-0.292153	0.885885
6A	-0.423153	-0.784290	-0.561745
7A	0.489469	0.744707	-0.561745
8A	-0.436516	-0.781794	0.540969
9A	0.480930	0.755284	0.540969
10A	-0.436516	0.260546	-0.914311
11A	-0.472027	0.281741	0.909377
12A	-1.061682	-0.036234	-0.025952
13A	-0.472027	0.951668	-0.025952
14D	1.499831	-0.895215	-0.641195
15D	0.412521	-1.468976	-1.052149
16D	1.488762	-0.888607	0.655017
17D	1.488761	0.334145	-1.052149
18D	-0.271982	-1.822697	-0.008677
19D	0.394511	-1.463287	1.048536
20D	-0.271983	-0.594884	-1.722908
21D	0.394510	0.521750	-1.722908
22D	1.475206	1.104521	-0.008677
23D	1.475206	0.347297	1.048536
24D	-1.391257	-0.406596	-1.108653
25D	-1.391257	-1.180526	-0.028118
26D	0.378725	1.784882	-0.028118
27D	-0.302471	-0.593392	1.698948
28D	-0.302472	1.417543	-1.108653
29D	0.378725	0.547877	1.698948
30D	-1.425642	-0.413056	1.039183
31D	-0.313107	1.450874	1.039183
32D	-1.425643	0.850933	-0.725555
33D	-1.451831	0.866563	0.620674
34D	1.042360	-1.949121	0.005494
35D	2.210322	0.007670	0.005494
36D	1.042359	-0.622160	-1.847165
37D	-0.887747	-1.633819	-1.170218
38D	1.016692	-0.606840	1.850662
39D	1.016692	1.556854	-1.170218
40D	-0.912258	-1.637017	1.131631
41D	1.007872	1.579947	1.131631
42D	-0.912260	0.544506	-1.914138

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.060662	0.000000	0.000000
3A	0.495634	-0.937737	0.000000
4A	0.490764	-0.295708	-0.888203
5A	0.490764	-0.295707	0.888203
6A	-0.440926	-0.776391	-0.551574
7A	0.480372	0.752622	-0.551575

8A	-0.440926	-0.776391	0.551574
9A	0.480372	0.752623	0.551573
10A	-0.453310	0.273138	-0.898545
11A	-0.453310	0.273139	0.898544
12A	-1.066749	-0.024391	-0.000001
13A	-0.476915	0.954516	-0.000001
14D	1.483369	-0.893795	0.649412
15D	1.483369	-0.893796	-0.649411
16D	0.386599	-1.461717	-1.052779
17D	0.386599	-1.461716	1.052779
18D	1.472964	0.341247	-1.052779
19D	1.472964	0.341248	1.052779
20D	-0.290891	-1.815534	0.000000
21D	1.469193	1.105554	-0.000001
22D	-0.301571	-0.578893	-1.712109
23D	0.370881	0.537128	-1.712109
24D	-0.301572	-0.578891	1.712108
25D	0.370880	0.537130	1.712108
26D	0.370483	1.786519	-0.000001
27D	-1.406349	-1.162365	0.000000
28D	-0.317587	1.430909	-1.080872
29D	-1.413479	-0.387867	-1.080872
30D	-0.317587	1.430911	1.080870
31D	-1.413480	-0.387867	1.080870
32D	-1.438221	0.866591	-0.685307
33D	-1.438222	0.866591	0.685304
34D	1.025004	-1.951347	0.000001
35D	2.204167	0.005627	0.000000
36D	1.015270	-0.611746	-1.853448
37D	1.015268	-0.611744	1.853448
38D	-0.919742	-1.619799	-1.154696
39D	1.002289	1.570059	-1.154697
40D	-0.919742	-1.619798	1.154696
41D	1.002288	1.570061	1.154695
42D	-0.941278	0.567161	-1.888092
43D	-0.941281	0.567162	1.888090

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.056723	0.000000	0.000000
3A	0.481528	-0.936485	0.000000
4A	0.481527	-0.289390	0.890650
5A	0.481527	-0.289390	-0.890650
6A	0.481526	0.757632	0.550452
7A	0.481526	0.757632	-0.550452
8A	-0.457485	-0.761246	0.553077
9A	-0.457486	-0.761246	-0.553076
10A	-0.457487	0.290768	0.894897
11A	-0.457488	0.290768	-0.894896
12A	-0.457488	0.940949	0.000000
13A	-1.071375	-0.000003	0.000001
14D	1.467676	-0.896307	0.651205
15D	1.467675	-0.896307	-0.651206
16D	1.467674	0.342360	1.053672
17D	1.467673	0.342360	-1.053673
18D	1.467673	1.107898	-0.000001
19D	0.362469	-1.452681	1.055434
20D	0.362468	-1.452681	-1.055434
21D	0.362466	0.554874	1.707728
22D	0.362465	0.554874	-1.707729
23D	0.362464	1.795612	0.000000
24D	-0.319000	-1.800491	0.000000
25D	-0.319000	-0.556383	1.712368
26D	-0.319002	-0.556383	-1.712367
27D	-0.319004	1.456626	1.058302
28D	-0.319005	1.456625	-1.058301
29D	-1.427324	-1.132606	0.000001
30D	-1.427326	-0.349997	-1.077169
31D	-1.427325	-0.349997	1.077171
32D	-1.427328	0.916292	-0.665726
33D	-1.427327	0.916292	0.665728
34D	2.198618	0.000001	-0.000001
35D	0.999012	-1.953882	0.000000
36D	0.999011	-0.603782	1.858252
37D	0.999010	-0.603782	-1.858253
38D	0.999008	1.580724	1.148463
39D	0.999007	1.580724	-1.148464
40D	-0.949341	-1.593852	1.158000
41D	-0.949341	-1.593852	-1.157999
42D	-0.949344	0.608794	1.873684
43D	-0.949346	0.608794	-1.873683
44D	-0.949348	1.970105	0.000000

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.049821	0.000000	0.000000
3A	0.469495	-0.938988	0.000000
4A	0.469495	0.759657	0.551923
5A	0.469494	-0.290163	-0.893031
6A	0.469494	0.759657	-0.551923
7A	0.469495	-0.290163	0.893031
8A	-0.469493	0.938988	0.000000
9A	-0.469493	-0.759657	-0.551923
10A	-1.049820	0.000000	0.000000
11A	-0.469493	0.290163	0.893031
12A	-0.469493	-0.759657	0.551923
13A	-0.469494	0.290163	-0.893031
14D	1.453409	-0.898256	-0.652621
15D	1.453409	1.110305	0.000000
16D	0.343104	-1.453408	-1.055963
17D	0.343104	1.796512	0.000000
18D	1.453409	0.343103	-1.055963
19D	1.453409	-0.898256	0.652621
20D	1.453409	0.343103	1.055963
21D	-0.343103	-0.555153	-1.708584
22D	-0.343103	1.453408	-1.055963
23D	0.343104	-1.453408	1.055963
24D	0.343104	0.555153	1.708584
25D	-1.453408	-0.343103	-1.055963
26D	-1.453408	0.898256	-0.652621
27D	-1.453408	-0.343103	1.055964
28D	-0.343102	-1.796512	0.000000
29D	-0.343102	1.453409	1.055963
30D	-1.453408	-1.110305	0.000000
31D	-1.453408	0.898256	0.652622
32D	-0.343102	-0.555153	1.708584
33D	0.343103	0.555153	-1.708584
34D	2.189748	0.000000	0.000000
35D	0.979286	-0.605231	1.862711
36D	0.979286	-1.958570	0.000000
37D	0.979286	1.584516	1.151218
38D	0.979286	-0.605231	-1.862711
39D	0.979286	1.584516	-1.151219
40D	-0.979285	0.605231	-1.862711
41D	-0.979284	-1.584517	-1.151219
42D	-0.979284	1.958570	0.000000
43D	-0.979284	-1.584517	1.151219
44D	-0.979284	0.605232	1.862711
45D	-2.189748	0.000000	0.000001

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.050956	0.000000	0.000000
3A	0.475331	-0.937320	0.000000
4A	-0.472141	0.938131	0.000000
5A	-1.050236	-0.003210	0.000000
6A	0.467684	0.761050	0.551467
7A	0.467685	0.761050	-0.551467
8A	-0.467234	-0.761326	0.551467
9A	-0.467234	-0.761326	-0.551467
10A	-0.472944	0.290444	-0.892257
11A	-0.472944	0.290444	0.892257
12A	0.463483	-0.284633	-0.896702
13A	0.463483	-0.284633	0.896702
14D	1.438808	-0.883598	-0.681471
15D	1.438807	-0.883598	0.681471
16D	0.346283	-1.451916	1.057058
17D	1.451545	0.347837	1.057058
18D	0.346284	-1.451916	-1.057058
19D	1.451545	0.347837	-1.057058
20D	0.337341	0.561100	-1.709172
21D	0.337341	0.561100	1.709172
22D	-0.347857	-0.554641	-1.709172
23D	-0.347857	-0.554641	1.709172
24D	-0.347453	1.454081	1.054531
25D	-0.347453	1.454081	-1.054531
26D	-1.454004	-0.347773	1.054531
27D	-1.454004	-0.347773	-1.054531
28D	-1.457451	0.895048	0.651460
29D	-1.457451	0.895048	-0.651460
30D	0.341435	1.796653	0.000000
31D	-1.447963	-1.117113	0.000000
32D	-0.326322	-1.798677	0.000000
33D	1.456604	1.104551	0.000000
34D	1.054890	-1.922240	0.000000
35D	2.191506	-0.071431	0.000000
36D	0.966714	-0.593677	1.873859
37D	0.966715	-0.593677	-1.873859
38D	-0.984704	0.604725	1.861178
39D	-0.984704	0.604725	-1.861178
40D	-0.983552	1.956944	0.000000
41D	-2.190192	-0.007889	0.000000
42D	0.976501	1.587351	1.149469
43D	0.976502	1.587351	-1.149469
44D	-0.974062	-1.588849	1.149469
45D	-0.974061	-1.588849	-1.149469
46D	2.332506	-1.432436	0.000000

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.051030	0.000000	0.000000
3A	0.464599	-0.942768	0.000000
4A	0.454483	-0.282703	-0.896692
5A	0.487960	-0.303525	0.888370
6A	0.488533	0.746931	0.561478
7A	-0.454040	-0.768384	0.561479
8A	-0.444268	0.276350	0.912097
9A	0.472561	0.760331	-0.543716
10A	-0.473121	-0.759983	-0.543715
11A	-0.458705	0.938140	0.026004
12A	-1.044273	-0.003240	0.026005
13A	-0.490497	0.305104	-0.905092
14A	1.335334	-0.830619	-0.613817
15D	1.465081	-0.911325	0.623110
16D	1.453045	0.329408	-1.053320
17D	0.346829	-1.448986	-1.053319
18D	0.386720	0.527963	1.717551
19D	-0.302632	-0.580264	1.717552
20D	-0.307791	1.436135	1.090485
21D	-1.424261	-0.358741	1.090487
22D	1.487108	0.315581	1.040841
23D	0.374290	-1.473426	1.040842
24D	1.476156	1.090462	-0.000885
25D	-0.325616	-1.806133	-0.000883
26D	0.368837	1.789423	0.030250
27D	-1.442061	-1.121843	0.030252
28D	-1.428288	0.888442	0.705970
29D	-1.461610	0.909167	-0.587960
30D	-0.330667	1.475840	-1.014021
31D	-1.469989	-0.355776	-1.014020
32D	0.362511	0.557368	-1.701254
33D	-0.339713	-0.571551	-1.701253
34D	2.186855	-0.113870	-0.088887
35D	1.068822	-1.911261	-0.088886
36D	1.058363	-0.658335	-1.793405
37D	1.020936	-0.635052	1.841447
38D	2.269933	-1.411968	-0.237725
39D	1.572811	-1.748102	-1.286336
40D	2.263285	-0.638069	-1.286337
41D	-0.929580	0.578230	1.899020
42D	1.021256	1.555658	1.163407
43D	-0.943979	-1.603724	1.163410
44D	0.999383	1.582173	-1.132304
45D	-0.977433	-1.595828	-1.132302
46D	-0.956820	1.962657	0.062707
47D	-2.183446	-0.009311	0.062709

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.047982	0.000000	0.000000
3A	0.455820	-0.943661	0.000000
4A	0.455820	-0.286035	-0.899266
5A	0.474286	-0.297623	0.889297
6A	0.474286	0.757247	-0.553177
7A	-0.475576	-0.756438	-0.553177
8A	0.480529	0.754637	0.551861
9A	-0.470511	-0.760924	0.551861
10A	-0.470511	0.295253	-0.892401
11A	-0.460402	0.288910	0.896405
12A	-1.048305	0.004933	0.003608
13A	-0.460402	0.941805	0.003608
14A	1.330197	-0.834720	-0.610424
15D	0.339262	-1.447325	-1.058417
16D	1.450812	0.324024	-1.058417
17D	1.450812	-0.910409	0.629599
18D	-0.332141	1.455835	-1.054218
19D	0.362799	1.791515	0.001128
20D	-1.455378	-0.334137	-1.054218
21D	-0.332141	-0.563342	1.706892
22D	0.362800	0.544103	1.706891
23D	-1.455378	-1.105904	0.001128
24D	-1.440686	0.904054	0.661128
25D	-1.447220	0.908154	-0.645649

26D	-1.447220	-0.340003	1.061134
27D	-0.323310	1.451040	1.061134
28D	-0.342617	-0.553858	-1.712713
29D	0.349702	0.549412	-1.712713
30D	-0.342617	-1.800020	-0.008658
31D	0.349703	-1.465606	1.042708
32D	1.471815	1.091430	-0.008658
33D	1.471815	0.322574	1.042708
34D	1.056390	-0.662902	-1.796546
35D	1.056390	-1.912961	-0.087163
36D	2.182011	-0.119189	-0.087162
37D	2.259468	-0.647132	-1.282012
38D	1.565469	-1.753078	-1.282013
39D	2.259468	-1.417853	-0.228095
40D	0.995218	1.571999	-1.155360
41D	-0.982644	-1.579889	-1.155360
42D	0.995218	-0.624516	1.848247
43D	-0.960586	1.965113	0.007488
44D	-0.960585	0.602784	1.870396
45D	-2.187302	0.010239	0.007488
46D	1.006610	1.569899	1.148055
47D	-0.975799	0.612330	-1.862457
48D	-0.975799	-1.589233	1.148056

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.063099	0.000000	0.000000
3A	-0.448636	-0.950693	0.000000
4A	0.476929	-0.739404	-0.562472
5A	0.476928	-0.739404	0.562473
6A	0.488448	0.287732	0.892626
7A	0.488449	0.287732	-0.892626
8A	0.489812	0.931157	0.000000
9A	-0.453661	-0.300025	-0.897174
10A	-0.453662	-0.300024	0.897174
11A	-0.453995	0.754884	-0.555970
12A	-0.453995	0.754884	0.555969
13A	1.330941	-1.046494	0.000001
14A	0.388262	-1.640714	0.000001
15A	-1.070596	-0.018274	-0.000001
16D	1.473063	-0.374936	1.045097
17D	1.473064	-0.374937	-1.045096
18D	-0.274867	-1.479055	-1.048847
19D	-0.274868	-1.479054	1.048847
20D	0.376685	-0.568755	1.710872
21D	0.376687	-0.568757	-1.710871
22D	0.373364	1.444737	-1.056480
23D	0.373362	1.444737	1.056479
24D	-0.310377	0.543202	-1.715181
25D	-0.310379	0.543203	1.715181
26D	-0.311948	1.791661	-0.000001
27D	1.027944	-1.605643	-1.056860
28D	1.027943	-1.605641	1.056862
29D	1.485788	0.873406	0.651135
30D	1.485789	0.873406	-0.651134
31D	-1.422365	1.118663	-0.000001
32D	-1.421574	0.332368	-1.079666
33D	-1.421575	0.332369	1.079663
34D	-1.402047	-0.955612	-0.668296
35D	-1.402048	-0.955611	0.668295
36D	1.413592	-2.218874	0.000002
37D	2.196997	-0.205993	0.000001
38D	-0.735512	-2.066852	0.000000
39D	2.228772	-1.360590	0.651133
40D	2.228773	-1.360590	-0.651131
41D	0.292208	-2.585997	0.652367
42D	0.292208	-2.585998	-0.652364
43D	1.017585	0.582890	-1.857590
44D	1.017583	0.582891	1.857590
45D	1.017932	1.940418	0.000000
46D	-0.929788	-0.640291	-1.873917
47D	-0.929791	-0.640290	1.873916
48D	-0.944070	1.584341	-1.162972
49D	-0.944071	1.584341	1.162970

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.055744	0.000000	0.000000
3A	-0.463925	-0.948350	0.000000
4A	0.462786	-0.741584	0.565050
5A	0.462787	-0.741584	-0.565049
6A	0.474444	0.288251	-0.895291
7A	-0.467413	-0.299515	-0.895291
8A	0.474443	0.288252	0.895290
9A	-0.467414	-0.299514	0.895290
10A	0.475107	0.934157	-0.000001
11A	-1.047908	-0.016281	-0.000001
12A	-0.469232	0.751914	-0.554276
13A	-0.469233	0.751915	0.554274
14A	1.312842	-1.050694	0.000001
15A	0.366913	-1.641002	0.000001
16D	1.457309	-0.376789	-1.047228
17D	-0.301923	-1.474639	-1.047228
18D	-0.301924	-1.474638	1.047229
19D	1.457308	-0.376788	1.047229
20D	0.354703	-0.568387	-1.712574
21D	0.354701	-0.568385	1.712575
22D	-0.338072	0.541739	1.710983
23D	-0.338070	0.541736	-1.710985
24D	-1.454474	1.091913	-0.000002
25D	-0.341701	1.786341	-0.000002
26D	-1.451643	0.321797	1.056981
27D	0.348833	1.445384	1.056981
28D	0.348834	1.445383	-1.056983
29D	-1.451641	0.321795	-1.056983
30D	1.005420	-1.611119	-1.058812
31D	1.005420	-1.611118	1.058813
32D	-1.433117	-0.932415	-0.653451
33D	-1.433117	-0.932414	0.653450
34D	1.467322	0.877605	-0.653450
35D	1.467321	0.877606	0.653450
36D	1.387968	-2.224126	0.000001
37D	-0.763317	-2.060502	0.000001
38D	2.186327	-0.219774	0.000000
39D	0.261649	-2.584719	-0.652567
40D	2.206818	-1.370834	-0.652567
41D	0.261649	-2.584718	0.652569
42D	2.206818	-1.370833	0.652568
43D	0.995077	0.584750	-1.862683
44D	-0.962533	-0.636898	-1.862683
45D	-0.962535	-0.636894	1.862683
46D	0.995075	0.584753	1.862683
47D	-0.980913	1.571850	-1.155077
48D	-0.980914	1.571852	1.155072
49D	0.992616	1.947266	-0.000001
50D	-2.185369	-0.035958	-0.000001

QLJ (S_D = 1.3)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124044	0.000000	0.000000
3A	0.562022	-0.973450	0.000000
4D	0.562022	-0.324483	-1.111850
5D	0.562022	-0.324483	1.111850

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.512772	0.000000	0.000000
3D	0.756386	-1.033689	0.000000
4D	0.756386	0.000000	-1.033689
5D	0.756386	1.033689	0.000000
6D	0.756386	0.000000	1.033689

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.239074	0.000000	0.000000
3D	0.496788	-1.188846	0.000000
4D	0.497208	0.942111	-0.724966
5D	0.497208	0.942111	0.724966
6A	0.513102	-0.320942	0.943512
7A	0.513102	-0.320942	-0.943512

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.122610	0.000000	0.000000
3D	0.561305	-1.153397	0.000000
4D	0.561305	0.663861	-0.943193
5D	-0.163109	-0.582635	-1.122566
6D	1.285719	-0.582635	-1.122566
7D	0.561305	-0.235587	1.128993
8D	0.561305	1.058833	0.457163

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.281503	0.000000	0.000000
3D	0.443369	-1.202361	0.000000
4B	0.481226	-0.335450	-1.020024
5A	0.494768	-0.344890	0.950099
6D	0.428923	0.919068	0.760236
7D	-0.713913	-0.720409	0.760236
8D	0.435785	0.964352	-0.700511
9D	-0.754026	-0.742514	-0.700510

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.255488	0.000000	0.000000
3D	-0.098441	-1.251622	0.000000
4D	0.387706	0.938717	-0.738068
5D	-0.966227	-0.312909	-0.738068
6D	0.387706	0.938717	0.738068
7D	-0.966227	-0.312909	0.738068
8D	-0.864817	0.935506	0.000000
9D	0.432408	-0.467753	1.103319
10D	0.432408	-0.467753	-1.103319

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.254360	0.000000	0.000000
3D	0.411930	-1.184793	0.000000
4D	0.411929	-0.151397	-1.175080
5D	0.278276	-0.339365	1.175080
6D	0.278274	1.122082	-0.486740
7D	-0.968467	-0.631327	0.486739
8D	-0.968468	0.402074	-0.688349
9D	-0.697819	0.782720	0.688344
10A	0.562818	0.791549	0.696107
11A	-0.562821	-0.791548	-0.696107

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.237327	0.000000	0.000000
3D	0.333637	-1.206010	0.000000
4D	-0.803366	0.585732	0.780174
5A	-0.229069	-0.552422	0.944349
6A	0.445644	0.326371	0.968718
7D	0.321118	1.229349	0.093569
8D	-0.810867	0.677823	-0.673451
9D	-1.086118	-0.627954	0.000278
10D	-0.222718	-0.563936	-1.151606
11A	0.456784	0.470000	-0.907574
12D	1.007326	-0.788197	1.199760

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.127281	0.000000	0.000000
3D	-0.557138	-1.170355	0.000000
4D	-0.557138	-0.285910	-1.134894
5A	0.574282	0.963459	0.046541
6A	0.574282	0.280497	0.922898
7D	-1.286395	0.078018	0.060801
8C	-0.467259	0.987945	-0.590589
9C	-0.467259	-0.331346	1.102289
10B	0.586597	0.369928	-0.960091
11B	0.586597	-0.840630	0.593263
12B	-0.404299	0.871982	0.679552
13B	0.565559	-0.809979	-0.631232

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.126692	0.000000	0.000000
3A	0.581174	-0.961073	0.000000
4A	0.546226	-0.300066	-0.911708
5D	-0.472563	-1.031975	-0.689178
6C	0.609875	0.888541	-0.638877
7A	0.577999	-0.326031	0.907696
8D	-0.552727	0.329103	-1.127182
9B	0.582530	0.809130	0.635457
10B	-0.396674	-0.909709	0.634300
11D	-0.564557	1.160196	0.053197
12C	-0.469720	0.269911	1.115091
13D	-1.282675	-0.095049	0.049929
14D	1.635407	-0.927266	-0.717256

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ

1A	0.000000	0.000000	0.000000
2A	1.130766	0.000000	0.000000
3A	0.575449	-0.953038	0.000000
4A	0.559077	-0.293314	0.911896
5A	0.559077	-0.293314	-0.911896
6D	-0.469684	-1.004743	-0.717251
7D	-0.469684	-1.004743	0.717251
8B	0.594373	0.827084	0.611250
9B	0.594373	0.827084	-0.611250
10C	-0.482491	0.327807	-1.086036
11C	-0.482491	0.327807	1.086036
12D	-0.531551	1.187669	0.000000
13D	-1.279657	-0.045551	0.000000
14D	1.631168	-0.937720	0.724003
15D	1.631168	-0.937720	-0.724003

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.054977	0.000000	0.000000
3D	0.527489	-1.203548	0.000000
4D	0.527488	1.156827	0.000000
5A	0.527489	-0.370189	-0.921289
6A	0.527489	-0.370189	0.921289
7D	-0.224177	0.618543	-1.093748
8D	-0.224177	0.618543	1.093748
9D	1.279154	0.618544	-1.093748
10D	1.279154	0.618544	1.093748
11D	1.735770	-0.748602	0.732949
12D	1.735770	-0.748602	-0.732949
13D	-0.680792	-0.748604	0.732949
14D	-0.680792	-0.748604	-0.732949
15D	2.223075	0.439406	0.000000
16D	-1.168098	0.439403	0.000000

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.057933	0.000000	0.000000
3D	0.528966	-1.170259	0.000000
4D	0.528966	0.585130	1.013474
5D	0.528966	0.585130	-1.013474
6B	1.143854	1.168680	0.000000
7B	1.143854	-0.584339	-1.012106
8B	-0.085922	-0.584339	-1.012106
9B	-0.085922	1.168680	0.000000
10B	1.143854	-0.584339	1.012106
11B	-0.085922	-0.584339	1.012106
12D	-0.921162	0.425866	0.737620
13D	-0.921162	0.425866	-0.737620
14D	1.979094	0.425866	0.737621
15D	1.979095	-0.851730	0.000000
16D	1.979094	0.425866	-0.737621
17D	-0.921163	-0.851730	0.000000

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.150346	0.000000	0.000000
3A	0.570382	-0.948112	0.000000
4A	0.570382	-0.292983	-0.901708
5A	0.570382	0.767039	0.557286
6A	0.570382	0.767039	-0.557287
7A	0.570382	-0.292982	0.901708
8D	-0.475032	-0.986759	0.716922
9D	-0.475031	0.376908	-1.160006
10D	-0.475033	0.376909	1.160004
11D	-0.475032	1.219701	-0.000001
12D	-0.475032	-0.986759	-0.716923
13D	-1.266964	0.000000	-0.000001
14D	1.617651	-0.985641	-0.716110
15D	1.617651	1.218319	0.000000
16D	1.617651	0.376481	1.158689
17D	1.617651	0.376481	-1.158690
18D	1.617651	-0.985640	0.716110

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.141477	0.000000	0.000000
3A	0.570739	-0.948804	0.000000
4A	0.570739	-0.293196	0.902366
5A	0.570739	0.767599	0.557693
6A	0.570739	0.767599	-0.557693
7A	0.570739	-0.293196	-0.902366
8D	1.615692	-0.986751	-0.716917
9D	1.615692	0.376906	-1.159997
10D	-0.474215	-0.986751	-0.716918
11D	1.615692	0.376906	1.159997
12D	-0.474214	0.376907	-1.159997
13D	1.615692	-0.986751	0.716917
14D	-0.474215	-0.986751	0.716917
15D	-0.474215	0.376907	1.159997
16D	1.615692	1.219693	0.000000
17D	-0.474214	1.219694	0.000000
18D	-1.266465	0.000002	-0.000001
19D	2.407943	0.000001	0.000000

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.128443	0.000000	0.000000
3A	0.564221	-0.956534	0.000000
4A	0.564221	-0.328351	0.898411
5A	0.564221	-0.291869	-0.901652
6A	0.564221	0.746674	0.583645
7A	0.564222	0.776065	-0.542637
8B	-0.436436	-0.879909	0.615246
9B	1.564878	-0.879910	0.615246
10D	1.605780	0.323148	1.175034
11D	-0.477338	0.323149	1.175033
12D	1.605780	-0.992708	-0.706868
13D	-0.477338	-0.992707	-0.706869
14D	-0.483032	1.203867	0.035669
15D	1.611476	1.203866	0.035670
16D	-0.483032	0.379750	-1.142961
17D	1.611476	0.379749	-1.142960
18D	-1.270239	-0.017880	0.012501
19D	2.398681	-0.017882	0.012502
20D	0.564220	-1.589145	1.111155

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.116718	0.000000	0.000000
3A	0.558360	-0.963024	0.000000
4A	0.558359	-0.328297	-0.897624
5A	0.558359	-0.328297	0.897624
6A	0.558359	0.755851	0.569199
7A	0.558359	0.755851	-0.569199
8B	-0.439131	-0.884135	0.608997
9B	1.555851	-0.884134	-0.608997
10B	-0.439131	-0.884135	-0.608997
11B	1.555851	-0.884134	0.608997
12D	-0.484763	0.328239	1.158553
13D	1.601480	0.328240	-1.158553
14D	1.601480	0.328240	1.158553
15D	-0.484763	0.328239	-1.158553
16D	1.607614	1.190539	0.000000
17D	-0.490898	1.190538	0.000000
18D	2.390114	-0.034899	0.000000
19D	-1.273395	-0.034903	0.000000
20D	0.558361	-1.594992	1.105518
21D	0.558361	-1.594992	-1.105518

N = 22

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.115266	0.000000	0.000000
3A	0.556229	-0.972151	0.000000
4A	0.554413	-0.321363	-0.892600
5A	0.554413	-0.321363	0.892600
6A	0.536479	0.759557	-0.568596
7A	0.536479	0.759557	0.568596
8A	-0.393371	-0.842294	-0.568212
9A	-0.393371	-0.842294	0.568212
10C	1.590510	-0.926827	-0.656859
11C	1.590510	-0.926827	0.656859
12D	-0.503555	0.292792	1.155480
13D	-0.503555	0.292792	-1.155480
14D	1.585058	0.358040	-1.160257
15D	1.585058	0.358040	1.160257
16D	-0.533430	1.158041	0.000000
17D	-1.269994	-0.109474	0.000000
18D	1.576059	1.212041	0.000000
19D	2.386428	0.009191	0.000000
20D	0.476006	-1.554279	-1.160912
21D	0.476006	-1.554279	1.160912
22D	-0.260180	-1.971653	0.000000

N = 23

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.111662	0.000000	0.000000
3A	0.554111	-0.963720	0.000000
4A	0.554565	-0.320839	-0.892744
5A	0.554564	-0.320839	0.892744
6B	1.539429	-0.890623	-0.613717
7B	1.539429	-0.890623	0.613717
8A	-0.386034	-0.850248	-0.570447
9A	-0.386035	-0.850248	0.570446
10A	0.544673	0.758468	-0.570447
11A	0.544673	0.758468	0.570447
12D	-0.502330	0.290617	1.153954
13D	-0.502328	0.290617	-1.153956
14D	1.596317	0.326353	-1.156920
15D	1.596317	0.326353	1.156920
16D	0.512768	-1.546547	1.156919
17D	0.512769	-1.546547	-1.156920
18D	1.600470	1.184709	0.000000
19D	-0.229284	-1.977997	0.000000
20D	-1.265145	-0.118984	-0.000001
21D	-0.527467	1.156082	-0.000001
22D	2.379706	-0.053031	0.000000
23D	1.232147	-2.036574	0.000000

N = 24

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.117459	0.000000	0.000000
3A	0.556250	-0.965622	0.000000
4A	0.559182	-0.325429	0.886944
5A	0.553954	-0.321920	-0.892707
6C	0.557767	0.864552	0.679925
7C	0.554810	0.878424	-0.644217
8A	-0.366107	-0.878253	0.575878
9A	1.485060	-0.882943	0.564019
10A	1.478918	-0.881766	-0.572954
11A	-0.372178	-0.880415	-0.563406
12D	1.682982	0.216533	1.151001
13C	-0.526273	0.208385	1.087782
14D	0.562499	-1.537358	1.166016
15D	0.549321	-1.547790	-1.151838
16D	-0.551950	0.232758	-1.150326
17D	1.655759	0.232198	-1.160877
18D	-1.281960	-0.208266	0.008943
19D	1.286697	-2.007374	0.002630
20D	-0.177388	-2.004456	0.011973
21D	2.397875	-0.212540	-0.013712
22D	-0.644077	1.095129	0.020307
23D	1.758709	1.095435	0.007322
24D	0.517100	0.295907	1.982901

N = 25

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099429	0.000000	0.000000
3A	0.539470	-0.957975	0.000000
4A	0.541173	-0.316329	-0.910802
5A	0.528143	-0.308711	0.897368
6A	0.541792	0.745405	-0.589407
7A	-0.383653	-0.837841	-0.589406
8B	1.531557	-0.895232	-0.592985
9B	1.510849	-0.883126	0.635846
10A	-0.415088	-0.838430	0.553334
11A	0.526881	0.773085	0.553333
12A	-0.422861	0.247171	-0.961296
13D	0.534352	-1.560949	-1.141558
14D	1.622311	0.300327	-1.141559
15D	-1.267140	-0.104220	-0.067063
16D	-0.530952	1.155246	-0.067064
17D	-0.538665	0.314863	1.113121
18D	1.565399	0.344574	1.160625
19D	0.467873	-1.533068	1.160626
20D	1.589267	1.182869	-0.012978
21D	-0.250855	-1.965202	-0.012976
22D	1.215241	-2.035197	0.033217
23D	2.369643	-0.060252	0.033216
24D	0.415968	0.589393	-1.842089
25D	-0.309454	-0.651655	-1.842089

N = 26

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.106795	0.000000	0.000000
3A	0.550055	-0.960434	0.000000
4A	0.550547	-0.319138	-0.902072
5B	0.540314	-0.313206	0.971160

6B	1.523309	-0.883023	-0.639480
7A	0.544865	0.738352	-0.604170
8A	-0.369927	-0.839758	-0.604170
9C	1.600513	-0.927777	0.629556
10B	0.534184	0.846624	0.570220
11B	0.524508	-1.460320	-1.057954
12B	1.527880	0.270603	-1.057954
13B	-0.469189	-0.884299	0.570220
14A	-0.394748	0.228826	-0.997366
15D	-0.550324	1.155287	-0.136902
16D	-1.276014	-0.096603	-0.136902
17D	-0.230182	-0.702846	-1.850500
18D	0.495507	0.549044	-1.850500
19D	1.619210	1.185994	-0.106850
20D	-0.224444	-1.994504	-0.106851
21D	-0.601484	0.348666	1.068085
22D	1.219313	-0.706805	-1.915295
23D	1.221789	-2.049982	-0.091220
24D	1.663452	0.377481	1.092843
25D	2.386102	-0.041421	-0.091220
26D	0.499140	-1.631081	1.092842

N = 27

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.104997	0.000000	0.000000
3A	0.552498	-0.957688	0.000000
4A	0.552499	-0.322969	0.897880
5A	0.552499	0.731162	0.602990
6B	0.552499	-0.306472	-0.970251
7A	1.463017	-0.854652	0.612341
8A	-0.358020	-0.854651	0.612342
9C	0.552499	0.916954	-0.597969
10B	1.557609	-0.898019	-0.570644
11B	-0.452612	-0.898019	-0.570644
12B	0.552498	-1.461432	1.055658
13A	-0.384573	0.219153	1.009778
14A	1.489571	0.219152	1.009778
15D	1.691966	1.127419	0.154411
16D	-0.586967	1.127421	0.154412
17D	0.552500	0.547685	1.834521
18D	2.377858	-0.132112	0.149576
19D	-1.272860	-0.132111	0.149576
20D	1.285588	-0.704668	1.863929
21D	-0.180589	-0.704667	1.863930
22D	1.282720	-2.007277	0.100363
23D	-0.177724	-2.007276	0.100363
24D	-0.614153	0.330396	-1.061690
25D	1.719151	0.330395	-1.061690
26D	0.552498	-1.619198	-1.089130
27D	0.552500	1.970561	0.353390

N = 28

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.100025	0.000000	0.000000
3A	0.548873	-0.953307	0.000000
4A	0.540047	-0.312227	-0.906217
5A	0.556023	-0.321464	0.908744
6B	-0.433226	-0.888593	-0.610369
7B	0.553910	0.818819	-0.610369
8A	1.460443	-0.844352	-0.603346
9B	0.569884	0.812545	0.613989
10B	-0.419818	-0.899306	0.613988
11C	-0.514558	0.297490	-1.064381
12A	1.499466	-0.866913	0.535082
13B	1.556244	0.251389	-1.029163
14B	0.558650	-1.474112	-1.029163
15B	-0.455393	0.263284	1.021481
16D	0.626684	-1.571727	1.119629
17D	1.674787	0.241138	1.119628
18D	1.328331	-1.977830	-0.070024
19D	2.376822	-0.164295	-0.070025
20D	-1.281027	-0.091345	0.028537
21D	-0.560025	1.155745	0.028537
22D	-0.124194	-2.033793	-0.024829
23D	1.700561	1.122419	-0.024829
24D	1.300723	-0.752011	-1.855208
25D	0.578043	0.502344	-1.895369
26D	-0.146921	-0.751599	-1.895368
27D	0.512006	0.527917	1.898551
28D	-0.202036	-0.707129	1.898550

N = 29

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.098121	0.000000	0.000000
3A	0.544237	-0.948200	0.000000
4A	0.537065	-0.322030	0.903948
5A	0.537064	-0.322028	-0.903948
6B	0.530302	0.813129	0.615010
7B	1.513834	-0.900434	-0.615010
8B	1.513835	-0.900434	0.615008
9B	0.530302	0.813131	-0.615008
10A	-0.384839	-0.851173	0.572543
11A	-0.384839	-0.851172	-0.572543
12C	1.588362	0.281384	-1.081783
13C	1.588363	0.281383	1.081783
14B	-0.487003	0.242388	1.008311
15B	0.507892	-1.490973	-1.008311
16B	0.507892	-1.490974	1.008310
17B	-0.487004	0.242389	-1.008310
18D	-1.272989	-0.157477	0.000001
19D	-0.233828	-1.967962	0.000000
20D	-0.603231	1.120750	0.000001
21D	1.207710	-2.034373	-0.000001
22D	2.374171	-0.101799	-0.000001
23D	1.653851	1.153183	0.000001
24D	-0.244751	-0.770768	1.827885
25D	-0.244752	-0.770766	-1.827885
26D	1.201961	-0.777058	1.895570
27D	0.479528	0.481606	-1.895570
28D	1.201960	-0.777055	-1.895571
29D	0.479530	0.481603	1.895571

N = 30

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.096269	0.000000	0.000000
3A	0.553303	-0.952247	0.000000
4A	0.550477	-0.306023	0.906799
5A	0.555740	-0.309579	-0.904841
6A	0.547993	0.752477	0.572109
7B	-0.436161	-0.864869	0.616118
8B	-0.428968	-0.872399	-0.618562
9B	1.542583	-0.863853	0.609464
10B	1.544518	-0.862569	-0.614248
11A	0.552062	0.752062	-0.577306
12C	-0.497449	0.343879	1.047662
13B	1.552659	0.299654	1.005622
14C	0.557125	-1.521853	1.075954
15C	0.561829	-1.521839	-1.081442
16B	-0.442481	0.284853	-1.023756
17B	1.552431	0.304793	-1.006496
18D	-0.501532	1.180866	-0.052858
19D	0.588788	0.567578	1.854148
20D	1.582772	1.189152	0.006333
21D	-1.273698	-0.046505	-0.028150
22D	2.370310	-0.025125	-0.000827
23D	-0.166627	-2.011112	-0.000704
24D	1.282320	-2.009022	-0.001896
25D	0.557111	0.589481	-1.833293
26D	-0.154178	-0.677570	1.906610
27D	1.298462	-0.676927	1.887879
28D	1.288604	-0.657061	-1.893882
29D	-0.160869	-0.670009	-1.902514
30D	-0.035507	1.678630	1.204198

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.089953	0.000000	0.000000
3A	0.544977	-0.958752	0.000000
4A	0.544976	-0.316033	-0.897122
5A	0.544977	-0.306025	0.904131
6A	0.544976	0.760570	-0.579186
7B	-0.443361	-0.866773	-0.617728
8B	1.533315	-0.866773	-0.617729
9B	-0.443057	-0.862287	0.615327
10B	1.533011	-0.862287	0.615327
11A	0.544977	0.756234	0.572464
12B	-0.446537	0.301728	-1.004993
13B	1.536489	0.301729	-1.004994
14D	0.544977	-1.577945	-1.133376
15C	0.544977	-1.514309	1.088789
16B	1.544302	0.299388	1.010259
17B	-0.454349	0.299388	1.010259
18B	0.544976	0.491990	-1.716101
19D	1.587407	1.181526	0.015454
20D	-0.497454	1.181526	0.015455
21D	-1.271278	-0.031754	-0.004531
22D	2.361232	-0.031754	-0.004532
23D	-0.181356	-0.614402	-1.908837
24D	1.271309	-0.614401	-1.908837
25D	0.544977	0.597640	1.827240
26D	1.274641	-2.011869	0.020494
27D	-0.184687	-2.011870	0.020494
28D	1.270961	-0.653683	1.898143
29D	-0.181007	-0.653684	1.898143
30D	-0.169146	1.548583	-1.327330
31D	1.259098	1.548583	-1.327331

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.084059	0.000000	0.000000
3A	0.542029	-0.949741	0.000000
4A	0.542029	-0.294889	0.902800
5A	0.542029	-0.286924	-0.905354
6A	0.542029	0.771520	0.553849
7A	0.542030	0.770900	-0.559178
8B	1.532810	-0.852036	0.618030
9B	-0.448751	-0.852036	0.618030
10B	1.533124	-0.845533	-0.619988
11B	-0.449065	-0.845533	-0.619988
12B	1.533124	0.326813	0.996245
13B	-0.449065	0.326813	0.996245
14B	-0.453887	0.330595	-0.998097
15B	1.537946	1.051414	-0.004354
16B	-0.453887	1.051414	-0.004354
17B	1.537946	0.330595	-0.998097
18D	0.542029	-1.560577	1.131974
19C	0.542029	0.578302	1.757934
20C	0.542029	-1.491490	-1.095547
21D	2.354746	-0.005414	0.003927
22D	-1.270687	-0.005413	0.003927
23D	0.542030	1.921635	-0.040700
24D	0.542030	0.635342	-1.814023
25D	1.271902	-0.595528	1.905058
26D	-0.187843	-1.995809	-0.025415
27D	-0.187843	-0.595528	1.905058
28D	1.271902	-1.995809	-0.025415
29D	1.268478	1.612711	1.175815
30D	-0.184419	-0.616966	-1.898087
31D	-0.184419	1.612711	1.175815
32D	1.268478	-0.616966	-1.898087

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.084180	0.000000	0.000000
3A	0.534780	-0.953088	0.000000
4A	0.537421	-0.301553	-0.902307
5A	0.538817	-0.290901	0.904247
6A	0.541775	0.769459	-0.559884
7A	0.540638	0.776694	0.558561
8B	-0.455749	-0.854228	-0.614880
9B	-0.454965	-0.846249	0.618716
10B	1.521316	-0.862936	-0.618944
11B	-0.453367	0.315153	-0.998224
12B	1.522169	-0.859110	0.617737
13B	1.530404	0.316544	-1.001792
14B	-0.453041	0.323197	0.997505
15B	-0.456685	1.045757	-0.009841
16C	1.590007	1.095685	0.015732
17B	1.539382	0.307423	1.004822
18D	0.529756	-1.569784	-1.130068
19C	0.533423	0.558549	-1.765397
20C	0.528871	-1.499284	1.093150
21D	0.552546	0.610794	1.821590
22D	0.522091	1.935524	-0.008639
23D	-1.273656	-0.002556	-0.000110
24D	2.358699	-0.043624	-0.006473
25D	1.264192	-0.611467	-1.905644
26D	1.257629	-2.007028	0.024742
27D	-0.201968	-1.998927	0.025778
28D	-0.197558	-0.610182	-1.904314
29D	-0.191609	-0.623336	1.896909
30D	-0.203005	1.593292	-1.200839
31D	1.262893	-0.642921	1.898304
32D	1.250172	1.603746	-1.220301
33D	-0.230068	1.616458	1.166060

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.083195	0.000000	0.000000
3A	0.541597	-0.946916	0.000000

4A	0.541598	-0.293261	0.905123
5A	0.541597	-0.293261	-0.905122
6A	0.541598	0.766203	0.561264
7A	0.541598	0.766203	-0.561263
8B	-0.449806	-0.851182	0.615068
9B	1.533000	-0.851183	0.615067
10B	-0.449806	-0.851182	-0.615067
11B	1.533000	-0.851183	-0.615068
12B	-0.450318	0.322573	1.001446
13B	1.533514	0.322571	1.001446
14B	-0.450318	0.322573	-1.001445
15B	1.533514	0.322572	-1.001446
16B	-0.449823	1.046969	0.000001
17B	1.533020	1.046968	0.000000
18D	0.541598	0.592437	-1.835271
19D	0.541599	0.592437	1.835272
20C	0.541599	1.849942	0.000001
21C	0.541597	-1.503711	1.082002
22C	0.541597	-1.503711	-1.082002
23D	-1.269013	-0.000850	0.000000
24D	2.352209	-0.000852	0.000000
25D	1.266414	-1.996075	0.000000
26D	-0.183221	-1.996075	0.000000
27D	1.272269	1.625289	-1.158843
28D	-0.189071	1.625289	1.158845
29D	-0.189071	1.625290	-1.158843
30D	1.272270	1.625288	1.158844
31D	-0.188317	-0.641808	1.892096
32D	1.271510	-0.641809	-1.892096
33D	-0.188317	-0.641807	-1.892095
34D	1.271511	-0.641809	1.892096

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.083186	0.000000	0.000000
3A	0.542658	-0.950138	0.000000
4A	0.541657	-0.298463	-0.903347
5A	0.541615	-0.286872	0.905411
6A	0.541772	0.763667	-0.559696
7A	0.541698	0.771059	0.557141
8B	-0.446651	-0.845046	0.617267
9B	-0.447011	-0.851620	-0.616577
10B	-0.450113	0.322644	-0.998759
11B	-0.450629	0.330423	0.998185
12B	-0.447308	1.052012	-0.006732
13B	1.533825	-0.851238	-0.617867
14B	1.532696	0.322942	-0.999694
15B	1.533584	-0.843646	0.619232
16B	1.533029	1.049955	-0.006713
17B	1.533212	0.331275	0.999020
18D	0.541756	-1.563064	-1.129822
19C	0.542902	-1.492877	1.093009
20D	0.540023	0.604862	1.830871
21C	0.540185	0.572457	-1.761608
22C	0.542958	1.852805	-0.015518
23D	-1.267532	0.012011	-0.000347
24D	-0.173963	-2.002923	0.026851
25D	2.352207	0.001147	-0.000613
26D	-0.192173	-0.629050	1.892666
27D	-0.191489	-0.602601	-1.903173
28D	-0.183048	1.609920	-1.179779
29D	1.279632	-1.994113	0.025242
30D	1.266216	1.609490	-1.180200
31D	1.270627	-0.626997	1.895929
32D	1.269443	-0.601015	-1.906161
33D	-0.188211	1.635171	1.147729
34D	1.271208	1.634785	1.148170
35D	-1.484423	-1.409959	0.002480

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.083146	0.000000	0.000000
3A	0.546018	-0.952605	0.000000
4A	0.545852	-0.296835	0.903374
5A	0.539215	-0.294863	-0.899287
6A	0.538988	0.768372	0.557218
7A	0.540953	0.769562	-0.558017
8B	-0.425458	-0.852734	0.616132
9B	-0.454737	-0.850938	-0.611059
10B	-0.455099	0.314017	0.996140
11B	-0.447796	0.320878	-1.001098
12B	-0.448492	1.053020	-0.001241
13B	1.536334	-0.852014	0.615650
14B	1.533089	-0.847986	-0.620930
15B	1.532897	0.324812	0.996322
16B	1.530667	0.321041	-1.000463
17B	1.531018	1.052696	-0.001068
18D	-1.266890	0.020134	-0.015713
19D	0.549410	-1.565827	1.132726
20C	0.536371	0.567166	1.760367
21C	0.536817	-1.495812	-1.092027
22D	0.539261	1.928168	-0.000358
23C	0.539581	0.561820	-1.764837
24D	-0.181331	-0.608076	1.906585
25D	-0.180812	-2.002657	-0.019454
26D	2.351500	0.001853	-0.002172
27D	-0.190822	-0.622467	-1.891599
28D	-0.197528	1.595661	1.190184
29D	1.276885	-0.599438	1.904026
30D	1.259990	-0.620415	-1.898210
31D	1.276244	-1.997895	-0.026501
32D	-0.189476	1.600292	-1.193854
33D	1.265251	1.602862	1.191830
34D	1.268906	1.600580	-1.193886
35D	-1.490253	-0.509398	1.294755
36D	-1.490061	-1.390442	0.078349

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.089097	0.000000	0.000000
3A	0.535117	-0.944610	0.000000
4A	0.542340	-0.289974	-0.897424
5A	0.529116	-0.310472	0.899974
6A	0.537371	0.762831	0.561920
7A	0.539358	0.770191	-0.563451
8A	-0.397477	-0.818011	-0.593138
9B	-0.462494	-0.861022	0.590597
10B	-0.458995	0.295857	-0.994460
11C	1.588942	0.319402	-1.055053
12B	-0.460536	0.305285	0.995268
13B	-0.458408	1.040219	0.005197
14C	1.590307	1.091451	0.010069
15B	1.518209	-0.868926	-0.618066
16B	1.510317	-0.880089	0.617887
17B	0.506843	-1.437457	-1.037748
18B	1.518751	0.301240	1.015029
19D	-1.269851	0.000398	0.001973
20D	0.505153	-1.589667	1.104165
21D	0.502486	0.556744	-1.850559
22C	-0.166049	-0.656123	-1.798979
23C	-0.165574	-1.919439	-0.063998
24D	0.512704	1.927594	0.015695
25C	0.516989	0.539587	1.769840
26D	2.359786	-0.057657	0.034271
27D	1.222186	-2.016212	-0.060940
28D	1.213322	-0.710198	-1.899284
29D	-0.220811	-0.634326	1.885113
30D	-0.236148	1.589842	-1.174461
31D	-0.215800	1.580202	1.202724
32D	1.238571	-0.641359	1.902667
33D	1.233860	1.592223	1.236844
34D	-1.440693	-1.410934	-0.126146
35D	-1.440211	-0.555003	-1.300568
36D	1.214155	1.639713	-1.209619
37D	-0.732728	-1.820998	-1.320744

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069379	0.000000	0.000000
3A	0.489986	-0.955376	0.000000
4A	0.493470	-0.303548	-0.903764
5A	0.495276	-0.296296	0.902199
6A	0.487410	0.772608	-0.559750
7A	0.488091	0.774408	0.560040
8A	-0.463990	-0.786366	-0.564166
9A	-0.466133	-0.782627	0.573601
10A	-0.455713	0.286807	-0.928274
11A	-0.451511	0.291275	0.929237
12B	-0.536913	0.997142	0.000335
13C	1.522243	-0.916768	-0.657929
14C	1.521309	-0.911620	0.664141
15D	0.403584	-1.560293	-1.122493
16C	1.520675	0.344731	-1.067347
17C	1.520131	0.346625	1.071586
18C	1.515663	1.129919	0.001284
19A	-1.068194	-0.020040	-0.000142
20D	-0.337550	-1.928280	0.029152
21D	-0.333730	-0.585590	-1.840217
22C	0.406359	-1.490562	1.091650
23C	0.416110	0.558527	-1.759634
24C	0.412999	0.554798	1.763387
25D	0.393986	1.925115	0.000411
26D	-0.334638	-0.602583	1.830034
27D	-1.547053	-1.192748	0.021578
28D	-1.542145	-0.329671	-1.126321
29D	-0.350367	1.533414	-1.180421
30D	-0.349747	1.535052	1.181847
31D	2.335232	0.001493	0.001930
32D	1.107388	-2.063494	0.027758
33D	1.114312	-0.630028	-1.961179
34D	1.106352	-0.641669	1.956987
35D	1.102532	1.652997	-1.228621
36D	1.100732	1.652938	1.232094
37D	-1.031988	-1.697539	-1.231409
38D	-1.545267	-0.293343	1.135510

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.076275	0.000000	0.000000
3A	0.516091	-0.944467	0.000000
4A	0.512794	-0.304150	0.905232
5A	0.512794	-0.304150	-0.905232
6A	0.513166	0.766536	0.567493
7A	-0.426589	-0.817887	0.567493
8A	0.513166	0.766536	-0.567493
9A	-0.426589	-0.817887	-0.567493
10B	-0.488093	0.289498	0.980647
11B	-0.488093	0.289498	-0.980647
12B	-1.132126	-0.045533	0.000000
13B	-0.502918	1.015311	0.000000
14C	0.467961	-1.515999	1.061284
15C	1.554733	0.316296	1.061284
16C	0.467961	-1.515999	-1.061284
17C	1.554733	0.316296	-1.061284
18B	1.489557	-0.883488	0.619865
19B	1.489557	-0.883488	-0.619865
20C	1.559981	1.100533	0.000000
21C	-0.217717	-1.896660	0.000000
22D	0.465949	0.555652	-1.850776
23D	-0.264173	-0.675331	-1.850776
24D	0.465949	0.555652	1.850776
25D	-0.264173	-0.675331	1.850776
26D	-1.463595	-1.325242	0.000000
27D	0.461123	1.919828	0.000000
28D	1.184027	-2.024851	0.000000
29D	2.344633	-0.068072	0.000000
30D	1.185796	-0.703321	-1.910946
31D	1.185796	-0.703321	1.910946
32D	-1.519882	-0.510967	-1.178965
33D	-1.519882	-0.510967	1.178965
34D	-0.280419	1.578762	-1.178965
35D	-0.280419	1.578762	1.178965
36D	-0.875525	-1.817457	-1.219373
37D	-0.875525	-1.817457	1.219373
38D	1.175048	1.639802	1.219374
39D	1.175048	1.639802	-1.219374

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069921	0.000000	0.000000
3A	0.491871	-0.949822	0.000000
4A	0.493550	-0.293270	-0.903043
5A	0.490791	0.767595	-0.564127
6A	0.489009	-0.294804	0.906026
7A	0.488531	0.768148	0.561119
8A	-0.459125	-0.780943	-0.565573
9A	-0.463033	0.297708	-0.922510
10A	-0.468139	-0.785469	0.562063
11A	-0.464508	0.962295	-0.005235
12A	-0.467585	0.293735	0.917721
13A	-1.067189	-0.006629	-0.011337
14C	1.517842	-0.913965	-0.663966
15C	1.519738	-0.912642	0.659434
16C	1.517686	1.123672	-0.001728
17C	1.517280	0.344450	-1.078323
18C	1.516432	0.347736	1.073969
19C	0.397992	-1.495690	-1.078708
20D	0.389124	0.584062	-1.829124
21D	-0.327387	-1.927633	0.009151
22D	0.389269	0.589741	1.824202
23C	0.407828	-1.497907	1.078182
24C	-0.298823	-0.596511	-1.763653

25C	0.403892	1.842724	-0.002512
26D	-0.351747	1.564378	1.107180
27D	-0.342684	-0.624966	1.818465
28D	-0.339750	1.568803	-1.117914
29D	-1.512666	-0.370256	-1.171101
30D	-1.538700	-1.197544	-0.020114
31D	-1.546679	-0.359194	1.121144
32D	-1.544751	0.961423	-0.691733
33D	2.333244	-0.000439	-0.002253
34C	-1.481778	0.928406	0.671873
35D	1.104247	-2.057887	-0.004768
36D	1.089116	-0.666340	-1.954723
37D	1.105832	1.672847	-1.200934
38D	1.104483	-0.658553	1.951950
39D	1.099601	1.677090	1.195245
40D	-0.966797	-1.708875	-1.263614

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069325	0.000000	0.000000
3A	0.498567	-0.945985	0.000000
4A	0.490574	-0.295987	-0.907795
5A	0.490572	-0.295985	0.907796
6A	0.485001	0.765694	-0.563585
7A	-0.451247	-0.786060	-0.563584
8A	0.485000	0.765696	0.563582
9A	-0.451248	-0.786059	0.563583
10A	-0.472478	0.285068	-0.922272
11A	-0.472481	0.285071	0.922269
12A	-0.476832	0.955182	-0.000003
13A	-1.067327	-0.023516	-0.000002
14C	1.519147	-0.916574	0.660813
15C	1.519149	-0.916576	-0.660809
16C	1.513256	1.123299	-0.000001
17C	-0.288186	-1.862444	0.000001
18C	1.516227	0.345157	1.074670
19C	0.401589	-1.502266	1.074670
20C	1.516230	0.345154	-1.074669
21C	0.401591	-1.502269	-1.074668
22D	0.392984	0.587589	1.826627
23D	-0.336586	-0.621615	1.826628
24D	-0.336582	-0.621620	-1.826629
25D	0.392989	0.587584	-1.826630
26C	-1.441809	-1.207058	-0.000002
27C	0.395595	1.838289	-0.000003
28D	-1.543137	-0.419228	1.113675
29D	-0.348607	1.560608	1.113674
30D	-1.543134	-0.419231	-1.113680
31D	-0.348603	1.560605	-1.113682
32D	-1.550242	0.935336	0.706817
33D	-1.550240	0.935334	-0.706827
34D	2.332280	-0.000862	0.000002
35D	1.088177	-2.062863	0.000003
36D	1.104182	-0.666207	-1.951166
37D	1.104177	-0.666202	1.951168
38D	1.099821	1.675474	-1.195754
39D	-0.969433	-1.754145	-1.195752
40D	1.099817	1.675478	1.195750
41D	-0.969436	-1.754142	1.195752

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.074152	0.000000	0.000000
3A	0.486688	-0.949894	0.000000
4A	0.486688	-0.305689	0.899363
5A	-0.465864	-0.783955	0.561539
6A	0.488128	-0.293719	-0.903418
7A	0.488127	0.760837	0.568825
8A	-0.467522	-0.781199	-0.555255
9A	-0.467524	0.274317	0.918328
10A	0.488763	0.773417	-0.553992
11A	-1.074832	-0.012643	0.009054
12A	-0.475827	0.289727	-0.909523
13A	-0.475828	0.954377	0.018379
14C	1.502655	-0.932860	0.668200
15D	1.564792	0.357128	-1.125633
16D	1.564791	1.180682	0.024114
17C	0.382147	-1.503798	1.077158
18C	1.505005	0.325841	1.094868
19C	1.505006	-0.931764	-0.660849
20C	0.379320	0.528696	1.766619
21C	0.379323	-1.502500	-1.069093
22C	-0.316368	-1.859934	0.004086
23C	-0.316370	-0.602420	1.759675
24D	0.348472	1.915763	0.037181
25D	0.348473	0.581313	-1.825817
26D	-1.530799	-0.395432	1.151716
27D	-1.530798	-1.217706	0.003758
28C	-0.326068	1.461092	1.137983
29C	-0.326065	-0.607249	-1.749586
30D	-1.531262	0.956993	0.729475
31D	-1.531260	-0.382701	-1.140842
32C	-0.340888	1.497110	-1.072369
33D	-1.538985	0.961808	-0.688938
34D	1.060499	-2.073319	0.002679
35D	1.060497	-0.669757	1.962163
36D	2.337563	-0.040330	0.028889
37D	-0.969128	-1.726882	1.236950
38D	1.049534	-0.690339	-1.965176
39D	1.049531	1.638475	1.286035
40D	-0.974634	-1.727517	-1.225236
41D	-0.974638	0.604120	2.029912
42D	1.035438	1.701517	-1.218783

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.066630	0.000000	0.000000
3A	0.492634	-0.946050	0.000000
4A	0.487700	-0.295902	-0.908787
5A	0.485473	-0.294550	0.908799
6A	0.482629	0.766513	-0.564480
7A	-0.456953	-0.782091	-0.564480
8A	0.481771	0.766935	0.563749
9A	-0.457724	-0.781524	0.563749
10A	-0.467643	0.283732	-0.918415
11A	-0.475321	0.288391	0.914931
12A	-0.475475	0.955259	-0.001687
13A	-1.066873	-0.019472	-0.001687
14C	1.512129	-0.917452	0.661439
15C	1.513000	-0.917980	-0.661011
16D	-0.341389	-0.620171	-1.826459
17D	0.392388	0.589229	-1.826459
18D	0.391425	0.589428	1.825103
19D	-0.342011	-0.619408	1.825103
20C	1.509174	1.124209	-0.000468
21C	-0.300092	-1.857793	-0.000467
22C	1.513143	0.345307	-1.074730
23C	0.392591	-1.501570	-1.074730
24C	0.392074	-1.501000	1.074353
25C	1.512399	0.345502	1.074353
26D	-1.548897	-0.400280	-1.109594
27D	-0.360344	1.558673	-1.109594
28D	-1.548911	-0.404733	1.110323
29D	-0.356401	1.560742	1.110323
30C	-1.450732	-1.196193	-0.000726
31C	0.390931	1.839205	-0.000726
32D	-1.558460	0.945563	0.672156
33C	-1.489157	0.903515	-0.689939
34D	1.077439	-2.063598	0.000193
35D	2.327941	-0.002542	0.000193
36D	1.097669	-0.665987	-1.951989
37D	1.096599	-0.665338	1.951813
38D	1.092587	1.677190	1.195512
39D	-0.982965	-1.743699	1.195512
40D	-0.983843	-1.742190	-1.196664
41D	1.090841	1.677271	-1.196664
42D	-1.045503	0.634337	-1.988571
43D	-1.044390	0.633662	1.991439

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.070522	0.000000	0.000000
3A	0.496426	-0.947931	0.000000
4A	0.492084	-0.297060	-0.897271
5A	0.492084	-0.297060	0.897271
6A	0.485117	0.769539	-0.559212
7A	0.485117	0.769539	0.559212
8A	-0.456660	-0.784796	-0.559785
9A	-0.456660	-0.784796	0.559785
10A	-0.467798	0.285172	-0.912041
11A	-0.467798	0.285172	0.912041
12A	-0.474076	0.956024	0.000000
13A	-1.071426	-0.020163	0.000000
14D	0.398978	1.913948	0.000000
15D	-0.341372	1.538740	1.145485
16D	-0.341372	1.538740	-1.145485
17C	1.512125	0.339041	-1.076531
18C	1.512125	0.339041	1.076531
19C	1.517902	-0.918920	-0.663455
20C	1.517902	-0.918920	0.663455
21C	0.400293	-1.495752	1.076764
22C	0.400293	-1.495752	-1.076764
23C	0.386734	0.547140	1.754988
24C	0.386734	0.547140	-1.754988
25C	1.515413	1.123956	0.000000
26C	-0.305153	-0.593643	-1.755168
27C	-0.305153	-0.593643	1.755168
28C	-0.295507	-1.861384	0.000000
29D	-1.522242	-0.407299	1.145191
30D	-1.522242	-0.407299	-1.145191
31D	-1.514034	-1.233478	0.000000
32D	-1.546566	0.935652	0.709615
33D	-1.546566	0.935652	-0.709615
34D	2.330739	-0.003197	0.000000
35D	1.073363	-0.649261	-1.956809
36D	1.073363	-0.649261	1.956809
37D	1.081638	-2.063508	0.000000
38D	1.096781	1.642790	-1.236233
39D	1.096781	1.642790	1.236233
40D	-0.947228	-1.731332	-1.236670
41D	-0.947228	-1.731332	1.236670
42D	-0.980842	0.596972	-2.023858
43D	-0.980842	0.596972	2.023858
44D	-1.035021	2.091313	0.000000

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.068505	0.000000	0.000000
3A	0.494238	-0.947328	0.000000
4A	0.494238	-0.299605	-0.898703
5A	0.485546	-0.294335	0.905838
6A	0.485546	0.766256	-0.565711
7A	-0.454767	-0.784913	-0.565711
8A	0.481513	0.773618	0.557570
9A	-0.463160	-0.784742	0.557571
10A	-0.463160	0.280766	-0.920802
11A	-0.475921	0.288503	0.910537
12A	-0.475921	0.955043	-0.014275
13A	-1.066872	-0.019806	-0.014275
14D	-1.553306	0.941610	0.678647
15D	-1.514018	-1.236267	-0.021584
16D	-1.514019	-0.411463	-1.165984
17D	-0.335510	1.532641	-1.165985
18D	-0.335508	-0.621418	1.822731
19D	0.395757	0.584899	1.822731
20D	0.395756	1.914155	-0.021586
21D	-1.540931	-0.405121	1.119706
22D	-1.540931	0.934107	-0.738449
23D	-0.353579	1.553569	1.119705
24C	0.404643	-1.497437	-1.079249
25C	1.514786	-0.918257	0.658076
26C	1.514785	0.333888	-1.079249
27C	1.518765	-0.920669	-0.663555
28C	-0.295468	-0.599275	-1.762751
29C	0.394645	0.539156	-1.762752
30C	0.394645	-1.501757	1.068975
31C	1.513991	1.123138	-0.011023
32C	-0.295468	-1.861801	-0.011022
33C	1.513992	0.344751	1.068975
34D	2.330924	-0.003837	-0.002766
35D	1.081573	-0.655645	-1.957947
36D	1.081573	-2.064805	-0.002766
37D	1.101701	1.635886	-1.249344
38D	1.101702	-0.667846	1.947039
39D	-0.940772	-1.733440	-1.249343
40D	1.103942	1.669300	1.203115
41D	-0.969359	-1.750881	1.203117
42D	-0.969360	0.587623	-2.041512
43D	-1.039457	0.630117	1.994783
44D	-1.039458	2.091676	-0.033103
45D	-2.335267	-0.045929	-0.033101

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.063836	0.000000	0.000000
3A	0.489554	-0.944502	0.000000
4A	0.490658	-0.298333	-0.905075
5A	0.490658	-0.298333	0.905075
6A	0.491489	0.766372	-0.564497
7A	0.491489	0.766372	0.564497
8A	-0.454233	-0.789024	-0.564497
9A	-0.454233	-0.789024	0.564497

10A	-0.462457	0.281187	-0.922133
11A	-0.462457	0.281187	0.922133
12A	-0.468291	0.954157	0.000000
13A	-1.062623	-0.023319	0.000000
14B	1.455625	-0.885058	0.624327
15B	1.455625	-0.885058	-0.624327
16C	1.529280	0.322226	1.063715
17C	1.529280	0.322226	-1.063715
18C	0.417659	-1.506016	-1.063716
19C	0.417659	-1.506016	1.063716
20D	-1.538446	0.935418	0.707728
21D	-1.538446	0.935418	-0.707728
22D	0.409312	1.907905	0.000000
23D	-1.505533	-1.241371	0.000000
24D	-0.307259	-0.636252	1.831941
25D	-0.307259	-0.636252	-1.831941
26D	0.423489	0.565582	-1.831941
27D	0.423489	0.565582	1.831941
28D	-1.522180	-0.413698	1.142708
29D	-1.522180	-0.413698	-1.142708
30D	-0.333179	1.541808	-1.142708
31D	-0.333179	1.541808	1.142708
32C	-0.280806	-1.868754	0.000000
33C	1.529910	1.109266	0.000000
34D	1.119197	-2.031493	0.000000
35D	2.318644	-0.058804	0.000000
36D	1.144086	-0.695634	-1.913296
37D	1.144086	-0.695634	1.913296
38D	1.127326	1.650088	-1.215652
39D	1.127326	1.650088	1.215652
40D	-0.946223	-1.760202	1.215652
41D	-0.946223	-1.760202	-1.215652
42D	-1.010170	0.614212	-2.017557
43D	-1.010170	0.614212	2.017557
44D	-1.028068	2.090629	0.000000
45D	-2.329210	-0.049311	0.000000
46D	2.457499	-1.494224	0.000000

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.065823	0.000000	0.000000
3A	0.478248	-0.952330	0.000000
4A	0.478247	-0.278774	-0.910614
5A	0.493274	-0.305188	0.903778
6A	0.493274	0.774851	-0.556381
7A	0.498478	0.757912	0.560607
8A	-0.456089	0.290228	0.918712
9A	-0.456089	0.963426	0.008582
10A	-0.471431	-0.769138	-0.568911
11A	-0.465128	-0.782086	0.567258
12A	-0.465129	0.313471	-0.913879
13A	-1.064063	0.008840	0.006539
14B	1.423720	-0.869257	-0.642966
15C	1.517922	0.348183	-1.063502
16C	1.517923	-0.914993	0.644247
17C	0.389163	-1.477092	-1.092565
18D	0.421322	0.608833	-1.823941
19D	0.421323	-1.565822	1.116082
20C	1.527697	1.119843	0.011532
21C	1.527697	0.338837	1.067413
22D	-0.325981	-0.582280	-1.839146
23D	-0.325981	-1.929033	-0.018404
24D	-0.314769	1.582982	-1.109244
25D	-0.314768	-0.597270	1.838347
26D	-1.536322	-0.348782	-1.136415
27D	-1.536322	-1.188734	-0.000843
28D	-1.511680	0.983832	0.727714
29D	-1.526750	0.995923	-0.683650
30D	-1.526750	-0.362169	1.152422
31C	0.408552	0.563615	1.751618
32C	0.408551	1.839875	0.026178
33C	-0.290573	1.490943	1.102809
34D	2.325582	-0.034909	-0.025822
35D	1.130513	-0.658544	-1.926231
36D	1.130513	-2.034628	-0.065837
37D	1.091038	1.653015	1.222689
38D	1.122430	-0.627400	1.956283
39D	1.122429	1.686933	-1.172577
40D	-0.955839	0.675438	2.016096
41D	-0.955840	2.125501	0.055683
42D	-1.001183	-1.695735	-1.254289
43D	-1.010771	0.682370	-1.999038
44D	-1.010771	-1.711722	1.237654
45D	-2.331051	0.021524	0.015921
46D	2.484714	-1.476967	-0.176788
47D	2.484713	-0.601391	-1.360521

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.065330	0.000000	0.000000
3A	0.461462	-0.960198	0.000000
4A	0.473488	-0.297776	-0.906179
5A	0.495199	0.761616	-0.573412
6A	-0.471953	-0.776235	-0.573413
7A	-0.454475	0.285819	-0.922112
8A	0.477306	-0.300178	0.905698
9A	-0.462462	0.959687	-0.025604
10A	-1.065303	0.001122	-0.025604
11A	0.491956	0.778844	0.549032
12A	-0.488887	-0.780775	0.549031
13A	-0.483525	0.304088	0.897374
14B	1.401382	-0.881327	-0.639969
15C	0.369668	-1.487532	-1.100951
16C	1.500862	0.311159	-1.100950
17C	1.495052	-0.940236	0.638412
18D	0.375183	-1.573069	1.102528
19D	1.580346	0.343238	1.102529
20D	-0.356841	-1.935883	-0.042488
21D	1.590270	1.160181	-0.042487
22C	-0.315021	-0.577778	-1.777471
23C	0.384305	0.534208	-1.777470
24D	-0.375021	-0.598179	1.809437
25D	0.376701	0.597120	1.809437
26D	-1.556551	-1.186675	-0.057276
27D	0.395327	1.916968	-0.057275
28D	-1.555086	0.977991	0.635538
29D	-0.357867	1.573934	1.087361
30D	-1.573626	-0.359222	1.087360
31C	-0.318406	1.468029	-1.138123
32C	-1.461078	-0.348912	-1.138124
33C	-1.462032	0.919470	-0.734888
34D	1.080431	-0.679481	-1.945745
35D	2.324652	-0.093318	-0.069786
36D	1.091064	-2.054822	-0.069787
37D	-0.986759	0.620573	-2.014361
38D	1.066665	1.627611	-1.301224
39D	-1.004949	-1.666423	-1.301226
40D	1.070357	-0.673147	1.963017
41D	-1.029476	2.087764	-0.110592
42D	-2.327666	0.023538	-0.110593
43D	1.080102	1.698307	1.196578
44D	-1.062849	-1.709159	1.196576
45D	-1.061508	0.667580	1.964313
46D	2.440645	-0.671145	-1.403041
47D	1.662113	-1.909074	-1.403041
48D	2.442879	-1.536324	-0.208854

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.061936	0.000000	0.000000
3A	0.494623	-0.950968	0.000000
4A	0.480325	-0.303551	0.896443
5A	0.490606	0.761926	0.572540
6A	0.495020	-0.292121	-0.904227
7A	0.495608	0.778857	-0.544627
8A	-0.455228	-0.787269	0.567960
9A	-0.456202	0.284341	0.927161
10A	-0.456621	-0.787623	-0.559064
11A	-0.459362	0.964078	0.026743
12A	-0.463298	0.302639	-0.905737
13A	-1.061192	-0.008671	0.020082
14A	1.406744	-0.832282	0.625335
15B	1.435256	0.285065	1.035687
16C	1.528531	-0.901905	-0.633276
17C	0.422128	-1.479560	1.091843
18C	1.534176	1.106943	0.040131
19C	0.412484	0.529097	1.768277
20C	1.533910	0.353470	-1.048923
21D	-0.296199	-1.940997	0.025766
22D	0.434880	-1.560102	-1.110959
23D	0.432691	1.915018	0.052769
24C	-0.285533	-0.594504	1.774232
25D	0.416992	0.605614	-1.806996
26D	-1.506751	-0.396262	1.173664
27D	-1.530719	-0.376869	-1.114519
28D	-1.532729	0.967618	-0.665086
29D	-0.302582	1.534894	1.187351
30D	-0.323161	-0.597190	-1.823817
31D	-0.324998	1.573716	-1.096560
32D	-1.520353	0.952396	0.752406
33D	-1.517012	-1.219226	0.026556
34D	2.311227	-0.015804	0.047402
35D	1.111672	-0.638869	1.927233
36D	1.161616	-2.014098	0.072943
37D	1.163389	1.573272	1.274662
38D	2.423822	-0.514540	1.368081
39D	1.137551	-0.630693	-1.943772
40D	-0.941383	-1.713941	1.282804
41D	1.135939	1.676344	-1.170911
42D	-0.950914	0.593735	2.053101
43D	-0.998311	-1.722410	-1.222025
44D	-1.003159	2.108405	0.058949
45D	-1.018818	0.662700	-1.983707
46D	-2.325874	-0.017842	0.040977
47D	2.474354	-1.423263	0.225226
48D	1.731821	-1.807547	1.388310
49D	2.513808	0.996591	1.054719

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.057327	0.000000	0.000000
3A	0.484341	-0.939867	0.000000
4A	0.498888	-0.304144	0.901247
5A	0.498888	-0.304144	-0.901247
6A	0.499550	0.762152	-0.564969
7A	0.499550	0.762152	0.564969
8A	-0.448652	-0.793179	-0.564969
9A	-0.448652	-0.793179	0.564969
10A	-0.452119	0.275635	-0.925361
11A	-0.452119	0.275635	0.925361
12A	-0.459715	0.953297	0.000000
13A	-1.057981	-0.028034	0.000000
14A	1.405809	-0.857044	0.575600
15A	1.405809	-0.857044	-0.575600
16C	1.538933	0.307259	1.049548
17C	1.538933	0.307259	-1.049548
18C	0.431825	-1.508722	1.049548
19C	0.431825	-1.508722	-1.049548
20C	-0.265752	-1.877422	0.000000
21C	1.547132	1.096238	0.000000
22D	-0.285422	-0.648237	1.831353
23D	-0.285422	-0.648237	-1.831353
24D	0.445483	0.550661	1.831352
25D	0.445483	0.550661	-1.831352
26D	0.425244	1.900553	0.000000
27D	-1.494630	-1.248600	0.000000
28D	-1.526034	0.930345	0.709782
29D	-1.526034	0.930345	-0.709782
30D	-1.509536	-0.420481	1.146250
31D	-1.509536	-0.420481	-1.146250
32D	-0.317710	1.534461	1.146250
33D	-0.317710	1.534461	-1.146250
34C	2.234189	-0.091589	0.000000
35C	1.104847	-1.944041	0.000000
36D	1.182574	-0.720951	1.871737
37D	1.182574	-0.720951	-1.871737
38D	2.382737	-1.452627	0.000000
39D	1.145725	1.636543	1.215017
40D	1.145725	1.636543	-1.215017
41D	-0.929912	-1.768108	1.215017
42D	-0.929912	-1.768108	-1.215017
43D	-0.990477	0.603845	2.021603
44D	-0.990477	0.603845	-2.021603
45D	-1.013204	2.086816	0.000000
46D	-2.319121	-0.055268	0.000000
47D	1.739242	-1.902258	-1.226758
48D	1.739242	-1.902258	1.226758
49D	2.487650	-0.674650	-1.226759
50D	2.487650	-0.674650	1.226759

QLJ (S_D = 1.45)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.124011	0.000000	0.000000
3A	0.562005	-0.973421	0.000000
4D	0.562005	-0.324474	1.207635
5D	0.562005	-0.324474	-1.207635

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.205682	0.000000	0.000000

3D	0.602841	-1.205765	0.000000
4D	0.602841	0.000000	-1.205765
5D	0.602841	0.000000	1.205765
6D	0.602841	1.205765	0.000000

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.288871	0.000000	0.000000
3D	0.451701	-1.300489	0.000000
4D	0.453187	1.019740	0.805834
5D	0.453187	1.019740	-0.805834
6A	0.487785	-0.332186	0.955506
7A	0.487785	-0.332186	-0.955506

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.348260	0.000000	0.000000
3D	0.255477	-1.323264	0.000000
4D	0.255477	0.890189	-0.979077
5A	0.517681	-0.428501	-0.968735
6D	0.382074	-0.325837	1.267109
7D	0.382074	1.156726	0.611326
8D	-0.832189	-0.423783	-0.958069

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.344044	0.000000	0.000000
3D	0.353927	-1.296606	0.000000
4D	0.353931	0.756070	1.053350
5D	0.346187	-0.264356	-1.271504
6D	0.346190	1.187107	-0.526673
7D	-0.636186	-0.540534	1.053349
8D	-1.054047	-0.646570	-0.526673
9D	-1.054044	0.804892	0.218158

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.345310	0.000000	0.000000
3D	0.256514	-1.320628	0.000000
4D	0.256512	0.897661	0.968640
5D	-0.832283	-0.422968	0.968639
6D	-1.054608	0.869472	0.017692
7D	0.391812	-0.323031	-1.269104
8D	-1.054606	-0.603979	-0.625707
9D	0.391811	1.150420	-0.625706
10A	0.510838	-0.421162	0.964507

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.361691	0.000000	0.000000
3D	0.369107	-1.310711	0.000000
4D	-0.623481	-0.559039	-1.073754
5D	0.369103	0.751673	-1.073755
6D	0.400847	1.203587	0.472016
7D	0.400849	-0.303557	1.256692
8D	-1.049869	-0.712091	0.472018
9D	-1.049873	0.795053	-0.312659
10A	-0.631663	0.478351	0.918782
11A	0.725752	-0.549603	-1.055635

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.349580	0.000000	0.000000
3D	0.381674	-1.294486	0.000000
4D	-0.878490	0.656857	0.800996
5D	-1.153419	-0.727637	-0.007217
6D	0.371732	1.312115	-0.007213
7A	0.445130	0.360516	0.956719
8A	-0.219914	-0.528918	0.956718
9D	-0.868099	0.649090	-0.818518
10A	-0.200781	-0.538746	-0.961747
11A	0.459969	0.344951	-0.961747
12D	1.045712	-0.781897	1.379496

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.376011	0.000000	0.000000
3A	-1.155223	0.000000	0.000000
4C	0.460619	-1.030665	-0.658336
5C	0.460619	0.446865	1.138415
6C	0.460619	1.220786	-0.073205
7C	0.460619	0.307622	-1.183658
8C	0.460619	-0.944608	0.776784
9A	-0.592605	0.801590	0.512015
10A	-0.592606	-0.239250	0.920578
11A	-0.592606	0.734660	-0.604136
12A	-0.592606	-0.347545	-0.885391
13A	-0.592606	-0.949454	0.056934

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.082404	0.000000	0.000000
3D	0.541202	-1.224336	0.000000
4D	0.541203	0.018324	-1.224199
5A	0.541202	-0.198949	0.943228
6A	0.541202	0.946100	-0.184810
7D	1.349456	0.912327	0.926086
8D	-0.267053	0.912328	0.926085
9D	-0.740216	-0.667680	0.879316
10D	1.822619	-0.667681	0.879317
11D	-0.740215	0.889211	-0.654446
12D	1.822620	0.889212	-0.654444
13D	-0.818544	-0.743604	-0.754817
14D	1.900949	-0.743603	-0.754816

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.106365	0.000000	0.000000
3D	0.589950	-1.221957	0.000000
4D	0.589950	-0.071349	-1.219872
5A	0.571655	0.929261	-0.210554
6A	0.571655	-0.155935	0.939969
7D	-0.240537	0.944112	0.890505
8D	1.383381	0.946225	0.892497
9D	-0.618058	0.902163	-0.825933
10D	-0.618058	-0.771847	0.948851
11D	-0.799272	-0.770997	-0.727220
12D	1.840545	-0.639687	0.911450
13D	1.840546	0.872543	-0.691814
14D	1.972803	-0.749922	-0.707341
15A	-1.121343	0.192775	0.181829

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069973	0.000000	0.000000
3D	0.466722	-1.326467	0.000000
4D	0.500717	1.253289	0.000000
5A	0.516015	-0.370812	-0.911009
6A	0.516015	-0.370812	0.911009
7D	1.295464	0.660040	-1.230771
8D	1.295464	0.660040	1.230770
9D	-0.808847	-0.696141	0.810185
10D	-0.808847	-0.696141	-0.810185
11D	1.792375	-0.819202	0.803843
12D	1.792374	-0.819202	-0.803844
13B	-0.161078	0.576772	-1.065639
14B	-0.161078	0.576771	1.065639
15D	-1.122389	0.715508	0.000000
16D	2.308669	0.513963	-0.000001

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.342227	0.000000	0.000000
3A	0.435857	-0.989984	0.000000
4A	0.414050	-0.408646	0.910254
5D	-0.808994	-0.947112	0.558571
6D	-0.591072	0.497770	1.142028
7D	0.403861	-1.762071	1.142027
8C	-0.481579	-0.802963	-0.889923
9D	0.965112	0.703720	1.433115
10D	1.606611	-0.753351	1.433117
11D	0.973469	-1.038119	-1.233068
12D	0.327530	0.429029	-1.233069
13D	1.603145	-1.641352	0.094782
14D	0.307807	1.300805	0.094781
15D	-1.133919	0.517323	-0.400170
16D	0.051718	-2.175662	-0.400171
17D	0.124611	-0.536076	2.186240

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1B	0.000000	0.000000	0.000000
2A	1.160283	0.000000	0.000000
3A	0.656528	-0.956496	0.000000
4D	0.836458	-0.461571	-1.229832
5A	0.659750	-0.347348	0.927842
6D	0.833469	1.001417	0.810429
7D	-0.354882	-1.231828	0.835534
8D	2.013036	-0.991132	-0.281510
9D	0.723048	1.046109	-0.764515
10D	-0.470182	-1.202417	-0.736621
11D	1.977217	-0.126640	1.072430
12D	-0.476311	0.271741	1.351915
13D	1.237032	-1.586943	1.006593
14D	-0.622277	0.313392	-1.243479
15D	-0.629272	1.268423	0.089803
16D	-1.402380	-0.185293	0.107866
17D	0.876949	-2.109020	-0.586170
18D	2.243185	0.661708	-0.335459

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099478	0.000000	0.000000
3A	0.549739	-0.916057	0.000000
4D	0.549740	0.548908	1.123109
5D	0.549738	0.548908	-1.123109
6D	1.858577	-1.229584	-0.000002
7D	-0.759097	-1.229586	0.000002
8A	1.095174	-0.660576	0.927729
9A	0.004304	-0.660576	-0.927729
10A	1.095172	-0.660576	-0.927730
11A	0.004307	-0.660576	0.927730
12D	1.363104	1.337100	-0.000001
13D	-0.263627	1.337099	0.000001
14D	2.146423	0.176454	-0.816272
15D	-1.046945	0.176452	0.816272
16D	-1.046947	0.176452	-0.816268
17D	2.146425	0.176454	0.816268
18D	0.549739	-1.926436	-0.831020
19D	0.549741	-1.926436	0.831020

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.191513	0.000000	0.000000
3A	0.595757	-0.906081	0.000000
4A	0.595757	-0.296641	-0.897375
5A	0.595757	-0.296642	0.897375
6A	0.595756	0.752443	0.556693
7A	0.595756	0.752444	-0.556692
8D	1.617007	-1.163843	-0.801386
9D	-0.425491	-1.163847	-0.801387
10D	1.617007	-1.163844	0.801385
11D	-0.425492	-1.163847	0.801385
12D	-0.485129	0.371662	1.283973
13D	1.676640	0.371666	-1.283973
14D	1.676640	0.371665	1.283974
15D	-0.485127	0.371664	-1.283974
16D	-0.497701	1.309416	0.000001
17D	1.689212	1.309419	0.000001
18D	-1.341311	-0.093271	-0.000001
19D	2.532825	-0.093266	0.000000
20D	0.595760	-2.217198	-0.000001

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1B	0.000000	0.000000	0.000000
2A	1.202011	0.000000	0.000000
3A	0.707001	-0.972098	0.000000
4A	0.639229	-0.325505	-0.892455
5D	0.756152	1.002353	-0.817140
6D	-0.365878	-1.201084	-0.817141
7D	-0.377839	-1.214024	0.770117
8D	0.759581	1.019637	0.770118
9A	0.628478	-0.320031	0.913511
10D	2.052589	-1.045215	-0.019190
11D	1.890993	-0.052032	-1.248529
12D	1.154326	-1.498693	-1.248533
13D	-0.570216	0.290366	-1.294770
14D	1.895094	-0.048247	1.212097
15D	1.153675	-1.504240	1.212098
16D	-0.548291	0.279201	1.299574
17D	-0.647353	1.258352	-0.002005
18D	-1.398427	-0.216601	-0.002006
19D	0.530387	-2.305343	-0.023101
20D	2.176364	0.927024	-0.023098

21D	0.600258	-0.305654	-2.212723

N = 22

atom	*X*/σ	*Y*/σ	*Z*/σ
1B	0.000000	0.000000	0.000000
2A	1.209048	0.000000	0.000000
3A	0.713814	-0.975841	0.000000
4A	0.641635	-0.325626	-0.889459
5A	0.641634	-0.325626	0.889459
6D	0.759652	1.004233	0.798218
7D	0.759652	1.004233	-0.798218
8D	-0.362038	-1.206021	-0.798218
9D	-0.362039	-1.206021	0.798217
10D	2.057986	-1.044419	0.000001
11D	1.897002	-0.050771	-1.231671
12D	1.897001	-0.050771	1.231672
13D	1.160953	-1.501124	1.231675
14D	1.160955	-1.501124	-1.231675
15D	-0.561109	0.284759	-1.293731
16D	-0.561110	0.284759	1.293730
17D	-0.642875	1.258709	0.000000
18D	-1.395472	-0.224260	-0.000001
19D	0.535862	-2.305710	0.000000
20D	2.177341	0.928779	0.000001
21D	0.615320	-0.312268	-2.209195
22D	0.615319	-0.312267	2.209195

N = 23

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.145780	0.000000	0.000000
3A	0.572890	-0.992275	0.000000
4A	0.572890	-0.330758	0.867225
5A	0.572890	-0.330759	-0.867225
6A	1.505102	-0.868971	-0.571679
7A	1.505102	-0.868971	0.571678
8A	0.572890	0.745667	-0.571679
9A	0.572890	0.745668	0.571678
10A	-0.359322	-0.868971	-0.571679
11A	-0.359322	-0.868971	0.571678
12D	-0.507871	0.293220	1.280404
13D	-0.507870	0.293219	-1.280407
14D	0.572890	-1.578713	-1.280406
15D	0.572890	-1.578713	1.280405
16D	1.653650	0.293219	-1.280407
17D	1.653651	0.293220	1.280404
18D	-1.358254	-0.159880	-0.000001
19D	-0.540668	1.256222	-0.000001
20D	-0.244697	-2.088618	0.000000
21D	1.390477	-2.088618	0.000000
22D	1.686448	1.256222	-0.000001
23D	2.504034	-0.159880	-0.000001

N = 24

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.145007	0.000000	0.000000
3A	0.572502	-0.991605	0.000000
4A	0.572503	-0.330535	-0.869410
5A	0.572503	-0.330535	0.867306
6A	-0.358618	-0.868117	-0.573732
7A	1.503623	-0.868118	-0.573732
8A	0.572503	0.744630	-0.573732
9A	1.502344	-0.867380	0.574426
10A	-0.357339	-0.867379	0.574426
11A	0.572504	0.743154	0.574426
12D	1.670930	0.303641	-1.258079
13D	0.572502	-1.598890	-1.258079
14D	-0.525924	0.303643	-1.258079
15D	0.572502	-1.574247	1.288967
16D	-0.504583	0.291322	1.288967
17D	1.649591	0.291321	1.288966
18D	2.504694	-0.164043	0.014187
19D	-1.359688	-0.164041	0.014188
20D	1.682787	1.259544	0.014187
21D	-0.249406	-2.087108	0.014188
22D	-0.537779	1.259545	0.014187
23D	1.394409	-2.087109	0.014188
24D	0.572502	-0.330536	-2.224932

N = 25

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.146727	0.000000	0.000000
3A	0.577241	-0.997509	0.000000
4A	0.576776	-0.329426	0.864212
5A	0.562299	-0.331035	-0.870963
6A	-0.324474	-0.873825	0.574960
7B	0.567594	0.823567	0.670532
8D	0.576134	-1.562674	1.319171
9B	-0.461957	0.199561	1.086079
10A	1.496189	-0.883652	0.574671
11B	0.558363	0.842574	-0.612658
12A	-0.365126	-0.889672	-0.545490
13A	1.495544	-0.887437	-0.568924
14D	1.708066	0.226370	1.299468
15D	-1.385121	-0.260527	0.088558
16D	-0.253442	-2.096991	0.055119
17D	0.551605	-1.597921	-1.253418
18D	-0.590367	0.238951	-1.236306
19D	1.686561	0.250120	-1.275750
20D	1.374661	-2.103359	0.026927
21D	2.523934	-0.237358	0.001562
22D	-0.673137	1.187476	0.058368
23D	1.794095	1.201551	0.023322
24D	0.403241	-0.172643	2.166997
25D	-0.925901	-1.009943	1.731954

N = 26

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.114524	0.000000	0.000000
3A	0.554650	-0.966709	0.000000
4A	0.554900	-0.321372	0.908683
5A	0.558665	-0.323554	-0.886870
6A	1.465194	-0.848574	0.597626
7A	0.548528	0.723522	0.601521
8A	-0.354586	-0.835843	0.601522
9B	1.574609	-0.911942	-0.603483
10A	-0.391856	0.226947	1.000156
11A	0.549500	0.775755	-0.535033
12A	0.541813	-1.407793	1.006275
13A	-0.399409	-0.862681	-0.535032
14A	1.490721	0.230643	1.006275
15D	-0.553882	0.320783	-1.208185
16D	1.354329	-0.784365	1.916626
17D	-0.257021	-0.779462	1.920249
18D	-1.364511	-0.138055	0.106666
19D	0.548179	0.610840	1.920248
20D	-0.559311	1.252247	0.106665
21D	1.645478	1.275176	0.126755
22D	-0.287173	-2.061844	0.126757
23D	0.495608	-1.628546	-1.202262
24D	1.314380	-2.102741	0.138526
25D	2.477973	-0.093619	0.138526
26D	1.659202	0.380576	-1.202262

N = 27

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.118452	0.000000	0.000000
3A	0.556249	-0.970321	0.000000
4A	0.557187	-0.322834	-0.905741
5A	0.560203	-0.324582	0.871419
6A	1.468183	-0.850664	-0.592120
7A	0.550299	0.723035	-0.598174
8A	-0.353590	-0.837008	-0.598174
9B	1.571127	-0.910310	0.615615
10A	0.551679	0.769970	0.542623
11A	-0.393622	-0.861549	0.542622
12A	-0.391155	0.226635	-0.997658
13A	0.544087	-1.410755	-1.003572
14A	1.494505	0.229596	-1.003571
15D	-0.544758	0.315632	1.220536
16D	0.494972	-1.628159	1.209235
17D	1.658689	0.380328	1.209236
18D	-0.555753	1.249589	-0.095380
19D	-1.360486	-0.139320	-0.095382
20D	1.357658	-0.786626	-1.911673
21D	1.646088	1.273261	-0.119420
22D	-0.285963	-2.061316	-0.119422
23D	0.551157	0.608885	-1.916855
24D	-0.254131	-0.780981	-1.916855
25D	1.316054	-2.102233	-0.128383
26D	2.478330	-0.096230	-0.128383
27D	0.591269	-0.342582	2.194031

N = 28

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.097271	0.000000	0.000000
3A	0.542437	-0.953818	0.000000
4A	0.514432	-0.299244	-0.915222
5A	0.539725	-0.313958	0.913806
6A	-0.391082	-0.829549	-0.578839
7A	0.527762	0.750042	-0.578838
8A	1.426696	-0.829906	-0.624150
9A	-0.370455	-0.856880	0.578866
10A	0.561718	0.745622	0.578867
11B	-0.513364	0.298623	-1.011963
12A	0.512597	-1.391905	-1.002571
13A	1.463332	0.242511	-1.002570
14A	1.509828	-0.878265	0.501654
15A	-0.424343	0.246838	0.950872
16D	0.623258	-1.623445	1.185809
17D	1.719307	0.260777	1.185809
18D	-0.552171	1.258753	0.056441
19D	-1.367153	-0.142287	0.056440
20D	-0.265052	-2.050096	-0.079213
21D	1.651039	1.243868	-0.079211
22D	2.463354	-0.149673	-0.166549
23D	1.347869	-2.067308	-0.166549
24D	1.319709	-0.767671	-1.932804
25D	-0.283091	-0.783853	-1.917251
26D	0.541427	0.633581	-1.917250
27D	0.385752	0.700939	1.909749
28D	-0.418607	-0.681833	1.909747

N = 29

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094259	0.000000	0.000000
3A	0.544468	-0.946115	0.000000
4A	0.536172	-0.313299	0.913377
5A	0.542974	-0.325120	-0.913377
6A	0.537184	0.746036	0.588896
7A	1.459400	-0.856489	-0.588897
8A	-0.382448	-0.837783	0.573873
9A	-0.372048	-0.855857	-0.573871
10A	0.547522	0.735873	-0.586264
11A	1.455809	-0.842443	0.586263
12B	0.531456	-1.520890	-1.018012
13B	-0.503496	0.277536	1.018013
14B	1.567187	0.274645	-1.038027
15B	1.569338	0.270912	1.038025
16A	0.534859	-1.416968	0.973794
17A	-0.411937	0.228262	-0.973793
18D	-0.553734	1.244843	-0.050866
19D	1.342567	-2.050331	0.050866
20D	-1.363632	-0.143446	-0.056325
21D	-0.264690	-2.053062	0.056328
22D	2.454926	-0.163038	-0.002936
23D	1.636936	1.258370	0.002934
24D	-0.312648	-0.763135	-1.901890
25D	-0.272432	-0.833010	1.901891
26D	0.487173	0.621202	-1.915209
27D	1.326344	-0.837007	1.915208
28D	0.526140	0.582533	1.947472
29D	1.312482	-0.783889	-1.947473

N = 30

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.101806	0.000000	0.000000
3A	0.543764	-0.948822	0.000000
4A	0.526133	-0.302977	-0.912873
5A	0.551859	-0.310444	0.919825
6A	0.555916	0.730573	0.570814
7B	1.556490	-0.883290	0.623446
8A	0.524519	0.750967	-0.569693
9A	-0.392938	-0.825155	-0.587058
10A	1.448452	-0.846952	-0.599190
11A	-0.372018	-0.834980	0.578346
12C	1.655937	0.382371	1.081470
13B	-0.504569	0.316452	-1.005270
14B	0.516461	-1.501943	1.040725
15A	-0.410126	0.246553	0.965016
16B	0.515361	-1.481898	-1.049796
17D	-0.542069	1.273312	0.076073
18A	1.467186	0.253467	-0.990944
19D	1.628704	1.289220	-0.112048
20D	0.435178	0.668042	1.912384
21D	-1.362408	-0.120653	0.057791
22D	-0.312630	-2.034598	-0.010823
23D	2.461100	-0.088257	-0.142657
24D	1.301697	-2.095140	-0.041109
25D	0.558069	0.671278	-1.900818
26D	-0.353361	-0.729878	1.900236

27D	1.355479	-0.719863	-1.927673
28D	-0.274585	-0.720547	-1.946077
29D	1.246432	-0.735001	2.016967
30D	0.653128	1.978825	0.978737

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.101498	0.000000	0.000000
3A	0.550749	-0.940743	0.000000
4A	0.544133	-0.294055	0.914040
5A	0.557365	-0.294054	-0.914040
6A	0.558791	0.746095	-0.554332
7A	0.542708	0.746094	0.554333
8A	1.474400	-0.827955	-0.597407
9A	-0.372902	-0.827955	0.597407
10A	1.460262	-0.833694	0.594476
11A	-0.358765	-0.833693	-0.594476
12D	1.672564	1.253005	0.067378
13D	-0.571065	1.253005	-0.067376
14B	-0.482471	0.324209	1.012789
15B	1.583969	0.324210	-1.012789
16B	0.550547	-1.478302	-1.047064
17B	0.550949	-1.478304	1.047063
18A	1.500921	0.256915	0.970631
19A	-0.399423	0.256917	-0.970630
20D	0.596853	0.711434	1.874724
21D	0.504645	0.711437	-1.874723
22D	-1.350766	-0.143290	-0.046913
23D	2.452264	-0.143291	0.046913
24D	-0.265937	-2.032960	0.002611
25D	1.367433	-2.032961	-0.002613
26D	-0.282600	-0.694551	-1.923562
27D	1.384097	-0.694554	1.923562
28D	-0.232619	-0.704428	1.953936
29D	1.334116	-0.704426	-1.953936
30D	0.496192	2.033156	0.841408
31D	0.605307	2.033158	-0.841403

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.084154	0.000000	0.000000
3A	0.525762	-0.949486	0.000000
4A	0.558392	-0.299319	0.901072
5A	0.525176	-0.290595	-0.917277
6A	0.558978	0.778898	0.564942
7A	0.542077	0.764411	-0.551560
8B	-0.497558	-0.850778	-0.615990
9B	1.581712	0.316380	1.001583
10A	-0.379161	-0.822004	0.606936
11A	1.463314	-0.835120	0.588759
12A	1.437760	-0.841849	-0.583370
13A	-0.353607	0.288239	0.982826
14C	-0.567581	0.432711	-1.048047
15C	1.651736	1.131016	-0.080260
16B	0.542077	-1.469589	1.060380
17B	0.555012	0.524564	1.738564
18B	0.529142	-1.484554	-1.045886
19A	-0.419829	0.987565	0.083740
20A	1.503983	0.231850	-0.963609
21D	-1.361942	-0.006341	0.167951
22D	2.446096	-0.161389	-0.046928
23D	1.354929	-2.040338	0.007436
24D	-0.270775	-0.650258	1.933958
25D	0.655831	0.703902	-1.884722
26D	0.428324	2.010521	-0.073868
27D	1.341046	-0.696142	1.949518
28D	-0.256893	-2.069568	0.046078
29D	-0.321149	1.582414	1.290293
30D	1.405304	-0.725661	-1.908484
31D	1.277356	1.689352	1.279180
32D	-0.193201	-0.681402	-2.006466

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.071172	0.000000	0.000000
3A	0.505281	-0.957228	0.000000
4A	0.505281	-0.300099	0.908970
5A	0.509227	-0.282538	-0.919460
6A	0.509228	0.784528	0.556553
7A	0.500828	0.776942	-0.561681
8B	1.505170	-0.892122	0.644948
9B	1.506349	-0.879668	-0.642431
10B	1.506350	0.334259	1.036728
11A	-0.436825	-0.797692	0.576682
12A	-0.430039	-0.788431	-0.581197
13A	-0.430039	0.304716	0.930893
14A	-0.435598	0.295093	-0.935870
15A	-0.435598	0.981203	0.013188
16B	1.516885	1.092390	-0.002387
17B	1.516884	0.344740	-1.036570
18C	0.430266	-1.558747	1.126877
19B	0.442424	0.560620	1.720536
20B	0.442423	-1.458036	-1.071759
21D	-1.361085	0.002748	-0.001987
22D	0.440346	0.719992	-1.891866
23D	0.440346	2.022211	-0.090577
24D	2.441671	-0.011111	0.008031
25D	-0.411400	-0.585904	1.915437
26D	-0.411400	-2.002557	-0.044140
27D	-0.401440	-0.640293	-1.905377
28D	-0.401439	1.608580	1.205365
29D	1.202392	-0.627616	2.037635
30D	1.202391	-2.131672	-0.042841
31D	1.210321	1.703532	1.279322
32D	1.210320	-0.680754	-2.018728
33D	-0.673349	1.587817	-1.147893

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.072735	0.000000	0.000000
3A	0.507258	-0.959864	0.000000
4A	0.507258	0.777109	-0.563419
5A	0.510383	-0.293954	-0.906236
6A	0.507071	-0.302525	0.907968
7A	0.507071	0.777883	0.557519
8B	1.509422	1.098042	-0.003614
9B	1.509422	-0.891099	0.641600
10B	1.509463	0.335448	-1.040703
11B	1.509463	-0.882449	-0.645657
12B	1.507287	0.335721	1.034998
13A	-0.434108	-0.800779	0.575432
14A	-0.434108	0.986079	-0.004168
15A	-0.429859	0.297888	-0.935729
16A	-0.429858	-0.790423	-0.582716
17A	-0.430928	0.301398	0.929183
18C	0.435220	1.924411	-0.005078
19C	0.435220	-1.560990	1.125475
20B	0.441873	0.558004	1.720281
21B	0.443402	0.549096	-1.729064
22B	0.443403	-1.459471	-1.077549
23D	-1.358645	-0.000701	-0.002160
24D	2.438739	-0.000064	-0.000200
25D	-0.394071	-0.618855	-1.907880
26D	-0.408784	1.600971	1.203219
27D	-0.408784	-0.589889	1.913864
28D	-0.407402	-2.004831	-0.046049
29D	-0.407402	1.596089	-1.214072
30D	1.200962	-0.656251	-2.023170
31D	1.206081	-0.628000	2.035029
32D	1.206081	1.702948	1.278944
33D	1.205090	-2.132636	-0.046051
34D	1.205090	1.699559	-1.289093

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.141417	0.000000	0.000000
3B	-1.236021	-0.004786	0.000000
4A	0.551817	-0.934575	0.000695
5A	0.549446	-0.279461	-0.897473
6A	0.549444	-0.278127	0.897888
7D	0.021311	-1.497237	1.103157
8D	0.021315	-1.498875	-1.100932
9A	-0.528553	-0.947356	0.000702
10A	-0.528873	-0.284493	-0.906688
11A	-0.528877	-0.283145	0.907107
12A	0.552529	0.762233	-0.546463
13A	0.552527	0.763045	0.545330
14A	-0.536538	0.768400	-0.552331
15A	-0.536540	0.769221	0.551185
16D	1.607257	-1.086643	-0.801797
17D	1.607255	-1.085450	0.803415
18D	0.016085	0.642641	-1.755120
19D	0.016079	0.645249	1.754161
20D	-1.570749	-1.128212	0.828824
21D	-1.570746	-1.129443	-0.827154
22D	1.609172	0.438130	-1.289409
23D	1.609168	0.440046	1.288760
24D	-1.583499	0.442301	1.323674
25D	-1.583494	0.440333	-1.324338
26D	0.013629	1.866035	-0.001388
27D	1.605148	1.375119	-0.001020
28D	0.852868	-2.267625	0.001686
29D	-1.584115	1.400357	-0.001045
30D	-0.795908	-2.284635	0.001696
31D	0.838826	-0.664010	-2.168679
32D	0.838819	-0.660786	2.169664
33D	-0.791152	-0.670949	-2.180094
34D	-0.791160	-0.667708	2.181085
35D	2.482107	0.009064	-0.000004

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.132148	0.000000	0.000000
3A	-1.132124	-0.007215	0.000000
4A	0.543038	-0.936325	-0.000082
5A	-0.537060	-0.939767	-0.000082
6A	0.540066	-0.279372	-0.898819
7A	0.540066	-0.279530	0.898770
8A	-0.538273	-0.282966	0.898770
9A	-0.538273	-0.282809	-0.898819
10D	0.004771	-1.496923	-1.100432
11D	0.004771	-1.497116	1.100169
12A	0.542891	0.764109	0.547075
13A	0.542891	0.764204	-0.546941
14A	-0.547750	0.760729	-0.546942
15A	-0.547749	0.760633	0.547075
16D	1.595269	-1.088919	-0.804000
17D	1.595269	-1.089060	0.803809
18D	-1.588295	-1.099204	0.803808
19D	-1.588296	-1.099063	-0.804001
20D	-0.002049	0.643300	-1.751682
21D	-0.002049	0.642993	1.751795
22D	-1.600990	0.426837	1.290470
23D	1.598238	0.437031	1.290471
24D	1.598238	0.437258	-1.290394
25D	-1.600990	0.427063	-1.290395
26D	-0.005934	1.862269	0.000162
27D	-1.603987	1.363691	0.000119
28D	1.595264	1.373886	0.000120
29D	0.834830	-2.269256	-0.000199
30D	-0.820351	-2.274530	-0.000199
31D	0.819502	-0.662693	2.169730
32D	-0.815262	-0.667522	-2.169847
33D	-0.815261	-0.667902	2.169730
34D	0.819502	-0.662312	-2.169846
35D	-2.471169	-0.009826	-0.000001
36D	2.471182	0.005924	0.000000

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.140243	0.000000	0.000000
3B	-1.234790	-0.001141	0.000000
4A	0.550420	-0.753677	-0.555262
5A	0.550420	-0.753623	0.555336
6A	0.548314	0.301526	-0.894124
7A	0.548314	0.301613	0.894095
8D	0.019084	-1.857209	0.000091
9A	-0.530485	-0.762924	-0.561033
10A	-0.530485	-0.762869	0.561107
11D	0.017465	-0.561278	-1.777411
12D	0.017464	-0.561105	1.777466
13A	-0.529444	0.304141	-0.902631
14A	-0.529444	0.304228	0.902602
15A	0.554928	0.932609	-0.000045
16A	-0.536833	0.942591	-0.000046
17D	1.607908	-1.348385	0.000066
18D	1.605516	-0.404556	1.294803
19D	1.605516	-0.404681	-1.294763
20D	0.016229	1.554609	-1.040271
21D	0.016229	1.554710	1.040121
22D	-1.576304	-1.393247	0.000068
23D	-1.574532	-0.420168	1.333451
24D	-1.574532	-0.420298	-1.333410
25D	1.608592	1.113530	-0.793673
26D	1.608591	1.113606	0.793567
27D	-1.583686	1.137827	0.813438
28D	-1.583686	1.137748	-0.813549
29D	0.849780	-1.831351	-1.342474
30D	0.849780	-1.831221	1.342652
31D	2.480679	0.007460	0.000001
32D	-0.802186	-1.843138	-1.349527

33D	-0.802186	-1.843006	1.349707
34D	0.834401	0.742227	2.148516
35D	0.834402	0.742019	-2.148587
36D	-0.793334	0.745349	2.158284
37D	-0.793333	0.745139	-2.158356

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.131116	0.000000	0.000000
3A	-1.131114	-0.002993	0.000000
4A	-0.539466	-0.756515	-0.555994
5A	-0.539466	-0.756497	0.556018
6A	0.541464	-0.755085	-0.555994
7A	0.541464	-0.755067	0.556019
8D	0.002453	-1.855062	0.000031
9A	-0.539428	0.300400	-0.895095
10A	-0.539428	0.300429	0.895085
11A	0.538630	0.301826	-0.895095
12A	0.538630	0.301856	0.895085
13D	0.000741	-0.561217	1.774872
14D	0.000742	-0.561276	-1.774854
15A	-0.548033	0.933105	-0.000016
16A	0.545560	0.934552	-0.000016
17D	-1.592940	-1.354952	0.000022
18D	1.596518	-1.350733	0.000022
19D	1.593703	-0.405874	-1.296700
20D	1.593703	-0.405830	1.296713
21D	-1.592626	-0.410089	-1.296700
22D	-1.592626	-0.410046	1.296713
23D	-0.002055	1.552563	-1.037582
24D	-0.002056	1.552597	1.037530
25D	-1.600792	1.108701	-0.794830
26D	-1.600792	1.108728	0.794793
27D	1.597850	1.112934	-0.794830
28D	1.597850	1.112960	0.794793
29D	-0.827031	-1.834581	-1.342660
30D	-0.827031	-1.834537	1.342720
31D	0.831880	-1.832387	-1.342660
32D	0.831880	-1.832342	1.342720
33D	2.469669	0.005739	-0.000001
34D	-2.469678	-0.000797	0.000000
35D	-0.817170	0.740529	-2.148281
36D	-0.817171	0.740600	2.148256
37D	0.815206	0.742689	-2.148281
38D	0.815205	0.742760	2.148256

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.137724	0.000000	0.000000
3B	-1.230979	0.000000	0.000000
4A	0.550035	0.519446	-0.783498
5A	0.550035	0.905668	0.251908
6A	0.550035	-0.584633	-0.736137
7A	0.550035	0.040288	0.939185
8A	0.550035	-0.880769	0.328540
9D	0.016793	-1.796560	-0.499707
10D	0.016792	-0.079918	-1.863048
11D	0.016793	1.747168	-0.651720
12D	0.016793	1.159727	1.460263
13D	0.016794	-1.030417	1.554212
14A	-0.530580	-0.590940	-0.744078
15A	-0.530580	-0.890271	0.332085
16A	-0.530580	0.525050	-0.791950
17A	-0.530580	0.040722	0.949318
18A	-0.530580	0.915439	0.254626
19D	1.607189	-0.750682	1.132278
20D	1.607189	0.844888	1.063834
21D	1.607188	-1.308835	-0.364049
22D	1.607188	1.272852	-0.474794
23D	1.607188	-0.058222	-1.357274
24D	-1.579097	-1.344635	-0.374005
25D	-1.579098	1.307667	-0.487779
26D	-1.579098	-0.059815	-1.394397
27D	-1.579097	0.867997	1.092934
28D	-1.579097	-0.771215	1.163250
29D	2.478704	0.000000	-0.000002
30D	0.848495	2.195707	0.610728
31D	0.848495	-2.135342	0.796514
32D	0.848496	0.097674	2.276967
33D	0.848494	-1.417387	-1.784695
34D	0.848494	1.259348	-1.899517
35D	-0.806497	-2.145902	0.800454
36D	-0.806499	-1.424397	-1.793520
37D	-0.806497	0.098156	2.288228
38D	-0.806499	1.265576	-1.908910
39D	-0.806498	2.206566	0.613749

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.128706	0.000000	0.000000
3A	-1.128706	-0.000004	0.000000
4A	0.540575	-0.761627	-0.553271
5A	0.540575	-0.761548	0.553380
6A	-0.540570	-0.761630	-0.553271
7A	-0.540570	-0.761551	0.553380
8A	-0.540574	0.290834	-0.895321
9A	-0.540574	0.290962	0.895279
10A	0.540573	0.290837	-0.895321
11A	0.540573	0.290965	0.895279
12A	-0.540576	0.941372	-0.000068
13A	0.540571	0.941374	-0.000067
14D	0.000002	-0.575510	-1.770801
15D	0.000002	-0.575257	1.770883
16D	-0.000004	1.506289	-1.094549
17D	-0.000004	1.506446	1.094333
18D	0.000006	-1.861976	0.000133
19D	1.595772	-1.359973	0.000097
20D	1.595769	-0.420160	1.293444
21D	1.595769	-0.420345	-1.293385
22D	-1.595770	1.100295	0.799295
23D	-1.595770	1.100181	-0.799453
24D	-1.595766	-0.420170	1.293445
25D	-1.595766	-0.420355	-1.293385
26D	-1.595763	-1.359983	0.000097
27D	1.595764	1.100305	0.799295
28D	1.595764	1.100191	-0.799453
29D	2.467657	0.000007	0.000000
30D	-2.467657	-0.000009	0.000000
31D	0.830873	2.279252	-0.000163
32D	-0.830874	-1.843861	1.339841
33D	-0.830874	-1.844053	-1.339578
34D	-0.830886	2.279247	-0.000164
35D	0.830886	-1.843856	1.339841
36D	0.830887	-1.844048	-1.339578
37D	0.830878	0.704483	2.167646
38D	0.830878	0.704173	-2.167747
39D	-0.830882	0.704478	2.167646
40D	-0.830882	0.704168	-2.167747

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069511	0.000000	0.000000
3A	0.471740	-0.949392	0.000000
4A	0.471740	-0.306206	-0.898656
5A	-0.482292	-0.779886	-0.558180
6A	0.486482	-0.294176	0.904565
7A	0.486481	0.761345	-0.570203
8A	-0.484249	-0.774533	0.560524
9A	-0.484249	0.280760	-0.913927
10A	0.480536	0.785818	0.562425
11A	-1.073265	-0.007088	-0.005073
12A	-0.466025	0.287723	0.907082
13A	-0.466025	0.951406	-0.020213
14C	1.559549	1.172647	-0.033137
15C	1.559549	0.346846	1.120668
16B	1.449099	-0.921047	-0.659212
17B	1.462165	0.307252	-1.079259
18B	1.462165	-0.922486	0.638924
19B	0.355682	-1.469862	-1.052009
20B	-0.327939	-1.816189	0.000075
21B	-0.327939	-0.585703	-1.719155
22B	0.357188	-1.471029	1.039769
23B	0.357187	0.509754	-1.727773
24C	0.340765	1.918959	-0.052107
25C	0.340766	0.569597	1.833215
26C	-1.544626	-0.382148	-1.142367
27C	-1.544626	-1.204572	0.006721
28B	-0.320402	-0.598909	1.715814
29B	-0.320402	1.430955	-1.120302
30D	-1.625409	-0.274220	1.193454
31D	-1.625409	1.041231	-0.644490
32D	-0.544720	1.592289	1.139633
33D	1.075862	-2.152754	-0.007197
34D	1.075862	-0.701137	-2.035389
35D	2.421483	-0.078886	-0.056461
36D	-1.004927	-1.798038	-1.286890
37D	1.082640	-0.758107	2.034061
38D	1.082640	1.680849	-1.373637
39D	-1.009458	0.643908	-2.110316
40D	-1.009458	-1.789860	1.290135
41D	1.065144	1.781742	1.275228

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.086579	0.000000	0.000000
3A	0.494627	-0.935075	0.000000
4A	0.512087	0.751815	0.565004
5A	0.512085	0.751818	-0.565000
6A	0.499642	-0.286675	0.910772
7A	0.499639	-0.286671	-0.910772
8A	-0.472955	-0.778887	0.567830
9A	-0.472958	-0.778885	-0.567829
10A	-0.437108	0.972338	0.000005
11B	-1.157695	0.031771	0.000004
12A	-0.457627	0.308163	0.919923
13A	-0.457632	0.308169	-0.919917
14C	1.568497	0.377962	1.134369
15C	1.568492	0.377968	-1.134370
16B	1.487847	-0.900605	-0.648207
17B	1.487850	-0.900609	0.648200
18B	-0.286277	-1.813191	-0.000003
19B	1.498556	1.106863	0.000001
20B	0.401634	-1.461832	-1.037817
21B	0.401639	-1.461838	1.037812
22A	0.415841	1.675422	0.000005
23D	0.317768	0.666237	1.922986
24D	0.317761	0.666248	-1.922981
25D	-1.623191	-1.297462	0.000001
26B	-0.274674	-0.614074	-1.725979
27B	-0.274667	-0.614084	1.725980
28A	-0.211567	1.462054	-0.949696
29A	-0.211563	1.462049	0.949708
30D	-1.512902	1.154760	-0.812018
31D	-1.512898	1.154755	0.812034
32D	-1.588863	-0.361842	1.293499
33D	-1.588869	-0.361835	-1.293492
34D	1.124108	-2.135620	-0.000006
35D	1.079794	1.842742	1.152436
36D	1.079789	1.842749	-1.152427
37D	-0.742856	2.305986	0.000009
38D	2.448157	-0.037615	-0.000004
39D	1.120680	-0.742235	-2.038760
40D	1.120689	-0.742245	2.038755
41D	-0.927823	-1.838058	-1.316197
42D	-0.927817	-1.838065	1.316193

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.070680	0.000000	0.000000
3A	0.479175	-0.957469	0.000000
4A	0.490627	-0.303100	-0.891777
5A	0.488121	-0.301550	0.891354
6A	0.490572	0.773632	-0.558166
7A	-0.472279	-0.784934	-0.558165
8A	0.489070	0.774389	0.556986
9A	-0.473627	-0.783927	0.556988
10A	-0.463720	0.286478	0.911096
11A	-0.454586	0.280834	-0.914860
12A	-0.478364	0.957133	-0.003258
13A	-1.070016	-0.000574	-0.003257
14C	-0.350490	-1.921912	-0.000194
15C	1.561836	1.173567	-0.000196
16B	1.469677	-0.907936	0.649875
17B	1.471010	-0.908760	-0.648625
18B	0.375332	-1.466443	1.058689
19B	1.479364	0.320651	1.058688
20B	1.480766	0.320292	-1.058830
21B	0.376280	-1.467539	-1.058829
22B	0.384252	0.518680	1.718468
23B	-0.291865	-0.575750	1.718469
24B	-0.290395	-0.577061	-1.720983
25B	0.386079	0.517947	-1.720984
26D	-1.669708	-1.189886	-0.000010
27D	0.316807	2.025683	-0.000013
28B	-0.314568	1.426562	-1.127495
29B	-1.416504	-0.357141	-1.127494
30B	-1.417079	-0.361039	1.129789
31B	-0.311338	1.428824	1.129788
32D	-1.617331	0.999157	0.733434
33C	-1.520741	0.939484	-0.750592
34D	1.110706	-0.686170	2.025076
35D	1.113194	-0.687710	-2.024594

36D	2.420522	-0.058581	0.000798
37D	1.135673	-2.138364	0.000799
38D	-0.982146	0.606749	-2.126767
39D	1.105006	1.687167	1.355411
40D	-1.014232	-1.743242	1.355414
41D	-1.015083	-1.741669	-1.355769
42D	1.103217	1.687221	-1.355773
43D	-0.977724	0.604021	2.134041

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.074860	0.000000	0.000000
3A	0.492639	-0.948810	0.000000
4A	-0.458688	-0.788612	0.559684
5A	0.494633	-0.303816	0.892006
6A	-0.462745	-0.785510	-0.556568
7A	0.491243	-0.303256	-0.891572
8A	0.493276	0.769122	-0.558496
9A	0.492129	0.769392	0.558433
10A	-0.470123	0.281007	-0.913420
11A	-0.462923	0.270341	0.917212
12A	-1.074408	-0.012265	0.003736
13A	-0.475057	0.952513	0.002359
14C	1.564389	1.171592	0.000719
15C	-1.507201	-1.237088	0.004241
16C	-1.517020	-0.395899	-1.145087
17C	-1.506932	-0.409767	1.161647
18B	1.479222	-0.910094	-0.648388
19B	1.481587	-0.909547	0.646814
20B	-0.294924	-0.593243	-1.714544
21B	0.389690	-1.468811	-1.048501
22B	0.396075	-1.469405	1.049083
23B	1.485101	0.314651	-1.059008
24B	-0.288300	-1.826412	-0.000278
25B	-0.286814	-0.596774	1.720918
26B	1.484808	0.318543	1.058984
27B	0.390132	0.507842	-1.719908
28B	0.387074	0.510411	1.719620
29D	0.320098	2.020907	-0.003411
30D	-1.588637	1.054526	-0.742279
31C	-1.514067	0.954048	0.744353
32B	-0.309293	1.420781	1.124915
33B	-0.288040	1.425630	-1.141540
34D	1.116224	-2.144330	-0.001373
35D	1.112507	-0.695099	-2.023699
36D	1.119474	-0.690887	2.023147
37D	2.426957	-0.055989	-0.000703
38D	-0.967039	-1.808420	-1.290904
39D	-0.956020	-1.817622	1.293584
40D	-0.968831	0.616827	2.133148
41D	1.119502	1.677856	-1.358799
42D	1.103873	1.682842	1.356600
43D	-0.961158	0.610430	-2.144159
44D	-2.440109	-0.044841	0.028180

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.071639	0.000000	0.000000
3A	0.504346	-0.945539	0.000000
4A	0.488681	0.768476	-0.559130
5A	-0.448061	-0.792846	-0.559130
6A	0.488681	0.768476	0.559130
7A	-0.448061	-0.792846	0.559130
8A	0.497209	-0.298309	-0.893204
9A	0.497209	-0.298309	0.893204
10A	-0.465064	0.279023	-0.915633
11A	-0.465064	0.279023	0.915633
12A	-0.475115	0.957074	0.000000
13A	-1.068059	-0.031220	0.000000
14C	-1.503949	-0.428245	1.150339
15C	-0.329951	1.528526	1.150339
16C	-1.503949	-0.428245	-1.150339
17C	-0.329951	1.528525	-1.150339
18C	-1.538660	0.923146	0.716733
19C	-1.538660	0.923146	-0.716733
20C	-1.488909	-1.260195	0.000000
21C	0.411181	1.906796	0.000000
22B	1.495224	-0.897085	0.646564
23B	1.495224	-0.897085	-0.646564
24B	-0.280810	-0.593317	-1.717606
25B	0.391343	0.527000	-1.717606
26B	-0.280810	-0.593316	1.717606
27B	0.391343	0.527001	1.717606
28B	1.486824	0.323966	1.050084
29B	1.486824	0.323965	-1.050084
30B	0.413901	-1.464338	-1.050084
31B	0.413901	-1.464337	1.050085
32B	1.491113	1.095121	0.000000
33B	-0.264494	-1.831051	0.000000
34D	1.125582	-0.675313	-2.023561
35D	1.125583	-0.675312	2.023561
36D	2.420625	-0.002386	0.000000
37D	1.141327	-2.134667	0.000001
38D	1.171830	1.683228	-1.294440
39D	-0.933663	-1.826120	-1.294439
40D	1.171830	1.683228	1.294439
41D	-0.933663	-1.826120	1.294440
42D	-0.988254	0.592920	-2.130730
43D	-0.988254	0.592920	2.130729
44D	-2.434425	-0.072766	0.000000
45D	-1.081512	2.182213	-0.000001

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.071807	0.000000	0.000000
3A	0.495990	-0.942512	0.000000
4A	0.504338	-0.300001	-0.896350
5A	0.488529	-0.287347	0.905673
6A	0.488529	0.773536	0.552020
7A	-0.449136	-0.780443	-0.575204
8A	0.496862	0.752462	-0.566219
9A	-0.447819	0.279497	-0.929366
10A	-0.466184	-0.779084	0.554901
11A	-0.464835	0.957101	-0.025372
12A	-0.474892	0.303463	0.907957
13A	-1.068233	-0.008695	-0.029649
14B	1.493598	-0.897833	-0.643686
15B	1.484625	-0.893676	0.638030
16C	-0.329403	-0.606896	1.814449
17C	-0.329204	1.575220	1.085917
18C	-1.506891	-1.223988	-0.041981
19C	0.412164	0.602682	1.808935
20C	-1.539020	-0.385727	1.103066
21C	-1.503377	0.956645	-0.770841
22C	-1.538121	0.973482	0.648840
23C	-1.489133	-0.397565	-1.195931
24B	1.495061	0.328301	-1.055350
25B	0.412669	-1.459937	-1.055971
26B	0.389813	-1.462155	1.043960
27B	1.490833	0.345849	1.038760
28B	1.483106	1.101880	-0.025520
29B	-0.287966	-1.814737	-0.018763
30B	0.414914	0.530674	-1.721876
31B	-0.263611	-0.579995	-1.736996
32B	0.390754	1.796422	-0.044306
33B	-0.280400	1.441366	-1.107157
34D	1.104494	-2.142882	0.000698
35D	2.419397	0.018818	-0.002304
36D	1.144780	-0.679415	-2.021148
37D	1.125383	1.704724	-1.282758
38D	1.174642	-0.697639	2.003469
39D	-0.935414	-1.804703	-1.322595
40D	1.171962	1.760284	1.187950
41D	-0.932502	0.649838	-2.142517
42D	-0.990729	-1.831408	1.237849
43D	-0.987804	2.209392	-0.112222
44D	-1.080493	0.691677	2.070323
45D	-2.434869	-0.019981	-0.069158
46D	2.594842	-1.568664	0.009031

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.065355	0.000000	0.000000
3A	0.496644	-0.948660	0.000000
4A	0.496643	-0.305184	0.898231
5A	0.483424	-0.301098	-0.904391
6A	0.483423	0.759452	0.576033
7A	-0.436538	-0.789674	0.565708
8A	-0.456781	-0.793406	-0.552104
9A	-0.456782	0.267517	0.928840
10A	0.472621	0.774700	-0.554983
11A	-1.063382	-0.033725	0.024158
12A	-0.488359	0.277870	-0.908706
13A	-0.488360	0.949791	0.029228
14B	1.473180	-0.901526	0.645838
15B	1.489129	0.307196	1.055913
16B	1.489131	-0.900958	-0.630551
17B	0.400487	-1.475977	1.057364
18C	0.383742	1.902872	0.042768
19C	0.383743	0.571654	-1.815480
20C	-0.373406	1.540922	-1.103892
21C	-0.338816	1.503556	1.195572
22C	-0.338814	-0.648329	-1.808246
23C	-1.546015	0.887146	0.769017
24C	-1.546013	-0.442747	-1.087383
25C	-1.575900	0.908296	-0.650691
26B	1.471350	1.099932	0.019259
27B	1.471350	0.335610	-1.047658
28B	0.391128	-1.483246	-1.035611
29B	0.391126	0.503402	1.737553
30B	-0.283319	-0.613034	1.721243
31B	-0.283317	-1.826959	0.026724
32B	-1.408509	-0.420855	1.105371
33B	-1.408508	-1.182002	0.042884
34D	2.410481	0.033479	-0.023983
35D	1.117718	-0.699575	2.029425
36D	1.117719	-2.146597	0.009525
37D	-0.989334	-1.788889	1.281528
38D	1.167848	-0.719271	-1.998294
39D	1.167846	1.660681	1.323883
40D	-1.010298	-1.858338	-1.187099
41D	-1.010301	0.526170	2.141438
42D	1.159748	1.728669	-1.238390
43D	-2.415141	-0.152513	0.109254
44D	-1.113445	0.632174	-2.071588
45D	-1.113447	2.164833	0.067853
46D	2.605253	-1.542306	0.076838
47D	2.605252	-0.568910	1.435603

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069386	0.000000	0.000000
3A	0.497242	-0.946751	0.000000
4A	0.497241	-0.300495	0.897798
5A	0.494356	-0.298750	-0.902838
6A	0.494354	0.761333	0.569860
7A	-0.444160	-0.791667	0.569860
8A	0.489707	0.772449	-0.556026
9A	-0.456161	-0.792721	-0.556028
10A	-0.456163	0.275669	0.928212
11A	-0.470392	0.284270	-0.915287
12A	-0.470393	0.958186	0.020937
13A	-1.067026	-0.029087	0.020936
14B	1.473268	-0.890331	0.640882
15B	1.497985	0.305741	1.056963
16B	1.497987	-0.905268	-0.625407
17B	0.425853	-1.468362	1.056962
18C	-1.542431	0.932127	-0.670968
19C	-0.315193	1.522144	1.178819
20C	-1.494146	-0.428720	1.178817
21C	-1.494145	-1.253940	0.032396
22C	0.415395	0.574189	-1.817592
23C	0.415394	1.905855	0.032399
24C	-0.315190	-0.634742	-1.817593
25C	-0.336407	1.549567	-1.115414
26C	-1.528288	0.923580	0.754858
27C	-1.528286	-0.422687	-1.115416
28B	1.492652	1.091160	0.019893
29B	0.404140	-1.473742	-1.041054
30B	-0.271978	-0.599332	1.727966
31B	-0.271975	-1.828844	0.019891
32B	1.492653	0.327468	-1.041052
33B	0.404137	0.519463	1.727966
34D	1.114792	-2.150888	-0.009479
35D	1.114789	-0.673694	2.042682
36D	2.422582	0.013170	-0.009478
37D	-0.919109	-1.828228	1.316000
38D	1.191205	-0.719871	-1.995457
39D	1.191202	1.663794	1.316001
40D	1.198486	1.721265	-1.239006
41D	-0.966604	0.584140	2.158405
42D	-0.966600	-1.861396	-1.239009
43D	-1.077117	0.650929	-2.089180
44D	-2.437705	-0.063666	0.045825
45D	-1.077119	2.187756	0.045828
46D	2.596953	-0.604562	1.452628
47D	2.596955	-1.569401	0.112249
48D	1.742761	-2.018030	1.452628

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.063962	0.000000	0.000000

3A	0.482794	-0.955864	0.000000
4A	0.484580	-0.291742	-0.909461
5A	0.504790	-0.295802	0.897091
6A	0.499979	0.773213	-0.551418
7A	0.511549	0.754606	0.564552
8A	-0.434518	0.297914	0.931948
9A	-0.455226	-0.772642	0.584093
10A	-0.443783	0.971563	0.028792
11A	-0.475434	-0.780142	-0.553429
12A	-0.469072	0.319206	-0.903561
13A	-1.064675	0.017241	0.038693
14B	1.473101	-0.876681	-0.627367
15B	1.480868	-0.889626	0.639247
16C	0.410046	-1.554427	-1.110673
17B	1.501053	0.338490	-1.034775
18B	1.509420	0.321869	1.048835
19C	0.419225	0.613939	-1.804071
20C	-0.325612	-1.924673	0.040194
21B	1.504481	1.089818	0.022401
22C	-0.343746	-0.581357	-1.817707
23B	0.405200	-1.449561	1.077285
24C	2.314989	0.016049	0.002765
25C	-1.545811	-0.340037	-1.088594
26C	-0.302793	1.593401	-1.080277
27C	-1.532125	-1.182481	0.061692
28C	-1.485400	-0.350449	1.209226
29C	-1.518740	1.013732	-0.637637
30C	-1.477467	0.997831	0.779859
31B	0.438344	0.540555	1.720583
32B	-0.256656	-0.551029	1.747279
33B	0.425266	1.799810	0.043874
34B	-0.246059	1.459122	1.108723
35D	1.169863	-2.137106	0.057646
36D	1.180527	-0.658867	-2.028576
37D	1.153596	-0.673038	2.023188
38D	2.627271	-1.463023	-0.018131
39D	1.164433	1.699493	1.277869
40D	1.202492	1.752264	-1.188630
41D	-0.903926	0.687114	2.149532
42D	-0.966543	-1.750860	1.389220
43D	-0.943246	2.238980	0.118707
44D	-1.085944	-1.779818	-1.263144
45D	-1.073895	0.727230	-2.061783
46D	-2.432315	0.040218	0.086248
47D	2.634479	-0.531149	-1.369544
48D	1.872901	-1.987091	-1.393370
49D	2.638460	-0.544089	1.372468

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069473	0.000000	0.000000
3A	0.471236	-0.952725	0.000000
4A	0.479760	-0.310109	-0.907627
5A	0.479760	-0.310109	0.907627
6A	-0.455941	-0.798260	-0.552645
7A	-0.455941	-0.798260	0.552645
8A	-1.068274	-0.050008	0.000000
9A	-0.487821	0.257187	-0.915994
10A	-0.487821	0.257187	0.915994
11A	0.472229	0.764664	-0.577318
12A	0.472229	0.764664	0.577318
13A	-0.513439	0.933166	0.000000
14B	1.437975	-0.930381	0.631625
15B	1.437975	-0.930381	-0.631625
16C	1.556943	0.316323	1.137705
17C	1.556943	0.316323	-1.137705
18B	0.365256	-1.498743	1.038018
19B	0.365256	-1.498743	-1.038018
20C	1.552555	1.165383	0.000000
21D	2.435606	-0.086578	0.000000
22C	1.015213	-2.079995	0.000000
23B	-0.309494	-1.841228	0.000000
24C	0.350391	0.525037	1.846120
25C	0.350391	0.525037	-1.846120
26C	0.327831	1.893181	0.000000
27C	-0.413379	1.497989	1.153027
28C	-0.413379	1.497989	-1.153027
29C	-1.596713	0.856088	0.707986
30C	-1.596713	0.856088	-0.707986
31B	-0.333407	-0.635832	-1.706065
32B	-0.333407	-0.635832	1.706065
33B	-1.416257	-1.197802	0.000000
34B	-1.450542	-0.446069	-1.055536
35B	-1.450542	-0.446069	1.055536
36D	1.074422	-0.789547	-2.038538
37D	1.074422	-0.789547	2.038538
38D	2.480015	-1.681698	0.000000
39D	-1.023620	-1.809338	-1.246363
40D	-1.023620	-1.809338	1.246363
41D	-2.421636	-0.200710	0.000000
42D	-1.132710	0.497454	-2.094448
43D	-1.132710	0.497454	2.094448
44D	1.076940	1.746634	-1.316011
45D	1.076940	1.746634	1.316011
46D	-1.172655	2.132256	0.000000
47D	1.650271	-2.130485	1.363302
48D	1.650271	-2.130485	-1.363302
49D	2.591384	-0.806358	1.427927
50D	2.591384	-0.806358	-1.427927

QLJ (S_D = 1.6)

N = 5

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.123972	0.000000	0.000000
3A	0.561985	-0.973388	0.000000
4D	0.561986	-0.324462	-1.301696
5D	0.561986	-0.324462	1.301696

N = 6

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.161602	0.000000	0.000000
3D	0.580800	-1.312441	0.000000
4D	0.580800	0.000000	-1.312441
5D	0.580800	0.000000	1.312441
6D	0.580800	1.312441	0.000000

N = 7

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.462464	0.000000	0.000000
3D	0.351120	-1.413250	0.000000
4D	0.354329	1.096111	-0.891534
5D	0.354329	1.096111	0.891534
6A	0.435898	-0.346080	-0.973719
7A	0.435898	-0.346080	0.973719

N = 8

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.422607	0.000000	0.000000
3D	0.210332	-1.439661	0.000000
4D	0.210327	0.964520	1.068797
5A	0.454392	-0.431816	0.971339
6D	-0.989289	-0.415745	0.935180
7D	0.313550	-0.351683	-1.381999
8D	0.313550	1.261605	-0.664799

N = 9

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.411875	0.000000	0.000000
3D	0.113789	-1.407282	0.000000
4D	0.210699	1.063726	-0.906118
5D	0.210699	1.063726	0.906118
6D	-1.043284	-0.295740	-0.906120
7D	-1.043286	-0.295740	0.906117
8A	0.405250	-0.373806	0.974336
9A	0.405252	-0.373806	-0.974336

N = 10

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.418215	0.000000	0.000000
3D	0.240118	-1.397740	0.000000
4D	0.152583	1.066750	0.922007
5D	-1.025514	-0.330992	0.922008
6D	-1.025516	0.864364	-0.461002
7D	0.240118	-0.202386	-1.383010
8A	-0.835834	-0.567628	-0.490608
9A	0.417917	0.919872	-0.490608
10A	0.417918	-0.352246	0.981215

N = 11

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.335580	0.000000	0.000000
3C	0.429565	-1.264614	0.000000
4D	-1.061083	0.760199	0.605627
5B	-0.361830	-0.573136	1.007063
6B	0.426308	0.526945	1.007062
7D	0.398582	1.328864	-0.345653
8D	-1.130059	-0.804809	-0.345648
9D	0.368133	-0.263746	-1.346359
10A	-0.692947	0.496450	-0.755370
11D	1.110840	-0.795844	1.447178

N = 12

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2C	1.327227	0.000000	0.000000
3A	0.429304	-1.005012	0.000000
4A	0.429304	-0.358438	0.938921
5D	-0.982332	-0.979878	-0.395695
6D	-0.982332	0.020200	1.056563
7D	0.375359	-0.376603	-1.328554
8D	0.375359	1.106870	0.825664
9D	-0.975529	0.826399	-0.569090
10D	-0.279350	-1.606727	1.106450
11A	0.468146	0.844073	-0.581260
12D	1.474414	-1.360531	0.936911

N = 13

atom	*X*/σ	*Y*/σ	*Z*/σ
1B	0.000000	0.000000	0.000000
2A	1.222237	0.000000	0.000000
3B	0.739257	-1.129614	0.000000
4B	0.739258	0.913876	-0.663970
5B	0.739258	0.913876	0.663970
6B	0.739257	-0.349070	-1.074326
7B	0.739258	-0.349070	1.074326
8D	-0.544282	1.494407	0.000001
9D	-0.544283	-1.209000	-0.878390
10D	-0.544281	0.461797	1.421266
11D	-0.544282	-1.209000	0.878390
12D	-0.544282	0.461798	-1.421265
13D	-1.539271	0.000001	0.000001

N = 14

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069407	0.000000	0.000000
3A	0.534704	-0.972693	0.000000
4A	0.534704	0.333353	0.913787
5A	0.534704	-0.333352	-0.913788
6A	0.534704	0.972693	-0.000002
7D	-0.368818	-0.778883	1.113232
8D	1.438226	-0.778883	1.113231
9D	-0.368819	0.778883	-1.113232
10D	1.438226	0.778882	-1.113232
11D	-0.754619	-0.966558	-0.676261
12D	1.824026	-0.966558	-0.676261
13D	-0.754619	0.966558	0.676260
14D	1.824026	0.966558	0.676260

N = 15

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.150793	0.000000	0.000000
3D	0.575397	-1.315325	0.000000
4D	0.575397	-0.042742	-1.302121
5A	0.575396	-0.155420	0.897577
6D	-0.300235	0.989924	1.010309
7D	1.451026	0.989924	1.010310
8A	0.575397	0.925001	-0.148998
9D	-0.711678	-0.718680	1.070073
10D	1.862470	-0.718680	1.070074
11D	1.901240	0.997973	-0.710124
12D	-0.750447	0.997972	-0.710125
13D	-0.965179	-0.774524	-0.710306
14D	2.115973	-0.774524	-0.710305
15D	0.575395	-0.000199	2.278691

N = 16

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.092840	0.000000	0.000000
3A	0.540056	-0.950074	0.000000
4D	0.476564	-0.277281	1.288451
5D	0.480135	1.303233	0.183257
6D	-0.895709	-1.061437	0.183260
7D	1.380717	-0.803348	-1.168291
8A	-0.023567	-0.632433	-0.903159
9A	0.538168	0.333021	-0.903160
10D	1.875397	-1.091167	0.504612

11D	-0.898209	0.522610	-0.937410
12D	1.890490	0.856723	-0.820910
13D	0.189430	-2.066892	-0.820911
14D	1.956972	0.640611	0.948802
15D	0.410169	-2.017893	0.948801
16D	-1.009680	0.587467	0.845460

N = 17

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2D	1.426512	0.000000	0.000000
3D	-0.921180	-1.152173	0.000000
4A	0.415335	-0.846297	0.544280
5A	0.415336	-0.846297	-0.544280
6B	-0.475690	-0.217531	-1.113319
7B	0.373873	-1.948622	0.000000
8B	-0.475691	-0.217531	1.113319
9D	0.932313	-0.245279	-1.745821
10D	1.596797	-1.599247	0.875041
11D	1.596797	-1.599247	-0.875041
12D	0.932312	-0.245278	1.745820
13D	0.264575	1.115316	0.870780
14D	0.264577	1.115316	-0.870779
15D	-1.257743	0.614535	-0.000001
16D	-0.111630	-1.720812	-1.501934
17D	-0.111629	-1.720812	1.501935

N = 18

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.093196	0.000000	0.000000
3A	0.546599	-0.936196	0.000000
4A	0.546599	0.301579	0.886291
5D	0.546598	-0.294840	-1.274867
6D	0.546598	1.301887	-0.131556
7A	1.108508	-0.644819	0.900541
8A	-0.015309	-0.644820	0.900541
9D	-0.848071	-1.113101	-0.173369
10D	-0.848073	0.522692	0.997919
11D	1.941270	-1.113099	-0.173370
12D	1.941270	0.522696	0.997916
13D	0.546601	-1.958604	0.963004
14D	0.546600	-0.280738	2.164415
15D	-0.972928	0.587369	-0.820308
16D	2.066123	0.587370	-0.820310
17D	0.546600	-2.051610	-0.856304
18D	0.546598	1.471551	1.666401

N = 19

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094865	0.000000	0.000000
3A	0.543811	-0.950263	0.000000
4A	0.543810	0.319555	-0.894922
5A	-0.007245	-0.630708	-0.894921
6D	1.401248	-0.812580	-1.152983
7D	0.475302	-0.275626	1.286097
8D	0.475301	1.303885	0.172916
9D	-0.895600	0.519355	-0.940265
10D	-0.895598	-1.060157	0.172917
11D	1.874830	-1.087207	0.521263
12D	1.874829	0.856513	-0.848600
13D	0.187819	-0.108917	-2.218464
14D	0.187820	-2.052639	-0.848599
15D	-1.013066	0.587472	0.833578
16D	-1.149663	-1.122647	-1.592940
17D	1.956359	0.654846	0.929171
18D	0.403351	-2.023234	0.929171
19D	0.403349	1.555432	-1.592941

N = 20

atom	*X*/σ	*Y*/σ	*Z*/σ
1B	0.000000	0.000000	0.000000
2A	1.199485	0.000000	0.000000
3A	0.702454	-0.972277	0.000000
4A	0.702454	-0.359097	0.903533
5D	1.950250	-0.996974	0.676593
6B	0.705854	0.854782	0.728010
7B	0.705853	-0.360834	-1.063226
8B	-0.279499	-1.072737	0.728009
9D	-0.411991	-1.368658	-0.770590
10D	-0.411991	0.210610	1.556496
11D	0.868131	1.135479	-0.770588
12D	2.228896	0.837002	0.492618
13D	0.626850	-1.306104	1.952531
14D	1.425801	-1.719640	-0.959767
15D	1.425802	0.256780	1.952532
16D	2.228895	-0.148651	-0.959766
17D	0.626852	-2.296870	0.492617
18D	-0.661879	1.355384	0.174583
19D	-0.661879	0.338356	-1.324032
20D	-1.486261	-0.257250	0.174582

N = 21

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.222575	0.000000	0.000000
3A	0.611288	-0.913426	0.000000
4A	0.611288	-0.302417	-0.861912
5A	0.611288	0.751757	0.532920
6A	0.611288	-0.300443	0.885291
7A	0.611288	0.735892	-0.576602
8B	-0.358965	-0.998218	-0.707638
9B	1.581541	-0.998218	-0.707637
10D	-0.437172	0.350830	-1.485566
11D	1.659747	0.350831	-1.485566
12D	-0.437173	-1.285629	0.822884
13D	1.659749	-1.285628	0.822884
14D	1.723973	1.425870	-0.067050
15D	-0.501399	0.408810	1.367651
16D	-0.501398	1.425869	-0.067050
17D	1.723974	0.408810	1.367651
18D	-1.429011	-0.092653	-0.065684
19D	2.651587	-0.092652	-0.065683
20D	0.611289	-1.168638	-1.940393
21D	0.611289	-2.217872	-0.460308

N = 22

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.088774	0.000000	0.000000
3A	0.535888	-0.947762	0.000000
4A	-0.016999	-0.625230	-0.891193
5A	0.535887	0.322532	-0.891193
6D	0.677110	-0.394999	-2.193084
7D	2.011362	0.359418	-1.117750
8D	0.677111	-1.927765	-1.117751
9D	2.011363	-1.173349	-0.042417
10A	1.068554	-0.623352	-0.888516
11D	-0.436693	-0.783687	1.091649
12D	0.467251	0.765861	1.091649
13D	-1.340640	-0.256362	-0.365412
14D	-0.436695	1.293187	-0.365412
15B	1.092428	1.196648	-0.244651
16B	-0.503980	0.294001	-1.531269
17B	-0.503978	-1.539926	-0.244651
18B	1.092430	-0.637280	1.041967
19D	-0.871571	-1.255161	-1.789087
20D	0.663621	-2.150730	0.685471
21D	0.663618	1.376472	-1.789087
22D	2.198810	0.480903	0.685472

N = 23

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.210252	0.000000	0.000000
3A	0.605127	-1.048109	0.000000
4A	0.605127	-0.349370	-0.825998
5A	0.605126	-0.349370	0.825998
6A	1.536857	-0.887304	-0.567183
7A	-0.326602	-0.887304	-0.567185
8A	1.536856	-0.887303	0.567186
9A	-0.326603	-0.887304	0.567184
10A	0.605126	0.726499	-0.567185
11A	0.605126	0.726499	0.567184
12D	-0.480634	0.277493	1.413656
13D	1.690884	0.277495	1.413658
14D	0.605125	-1.603096	1.413657
15D	1.690887	0.277494	-1.413655
16D	0.605129	-1.603097	-1.413656
17D	-0.480632	0.277493	-1.413657
18D	-0.545625	1.349941	0.000000
19D	1.755876	1.349942	0.000001
20D	-1.441895	-0.202447	-0.000001
21D	2.652148	-0.202445	0.000003
22D	-0.291144	-2.195604	-0.000001
23D	1.501398	-2.195604	0.000002

N = 24

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.075037	0.000000	0.000000
3A	0.466160	-0.968709	0.000000
4A	-0.018959	-0.631345	0.917028
5A	0.560683	0.290853	0.917026
6D	0.379680	1.375713	-0.022768
7D	-1.075010	-0.938667	-0.022761
8A	1.067559	-0.671006	0.859549
9D	-0.874286	0.549529	0.949691
10D	1.399716	-0.879785	-1.067724
11D	2.380794	-0.444241	0.370374
12D	1.432670	-1.952687	0.370378
13D	1.628573	0.018258	1.957332
14D	0.689740	-1.475407	1.957337
15B	0.090462	-0.056853	1.984573
16B	-0.075372	-1.826045	0.697790
17B	1.612758	0.859736	0.697783
18A	0.555911	0.293639	-0.930169
19A	-0.023544	-0.628260	-0.930168
20D	1.893525	0.823146	-0.826755
21D	0.079340	-2.063184	-0.826748
22D	-0.884186	0.555747	-0.945642
23D	-1.052929	-1.100157	1.745126
24D	0.534776	1.425850	1.745119

N = 25

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.115344	0.000000	0.000000
3A	0.597977	-0.947160	0.000000
4A	0.517367	0.322884	-0.890425
5A	1.105108	-0.570703	-0.916241
6A	0.010237	-0.666807	-0.848862
7D	0.706872	-1.895056	-1.141096
8D	0.408473	-0.426725	-2.170539
9D	-0.886078	0.369082	-1.238309
10D	2.001423	-1.289955	-0.075162
11D	-0.373198	-0.843808	1.083226
12D	1.488543	1.305993	-0.423994
13D	0.557672	0.746203	1.064337
14A	-0.905718	-0.615320	-0.223422
15A	2.021062	-0.000279	-0.654626
16A	-0.308470	-1.532930	-0.197004
17A	1.423816	0.337368	-1.508265
18B	-0.025511	1.215112	-0.296274
19B	1.140856	-0.692757	1.041329
20D	2.116116	-0.902236	-1.821351
21D	-1.000771	-1.404683	-1.469087
22D	-1.188180	0.609188	0.509776
23D	2.303524	0.271569	0.746480
24D	0.674519	-2.200024	0.646640
25D	0.440826	1.357889	-1.847804

N = 26

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.129285	0.000000	0.000000
3A	0.564641	-0.977990	0.000000
4A	0.564642	-0.325996	0.922058
5A	0.564642	-0.325997	-0.869185
6A	1.462542	-0.844400	0.597081
7A	-0.333259	-0.844399	0.597081
8A	0.564642	0.710810	0.597081
9A	-0.381528	-0.872267	-0.542029
10A	0.564641	-1.418538	1.003058
11A	-0.381527	0.220275	1.003058
12A	1.510811	-0.872268	-0.542029
13A	0.564642	0.766546	-0.542029
14A	1.510811	0.220274	1.003059
15D	-1.462795	-0.178738	0.126388
16D	-0.321549	-2.155437	0.126388
17D	1.705890	0.332902	-1.320753
18D	0.564642	0.697286	1.990037
19D	2.592079	-0.178740	0.126389
20D	1.450830	-2.155438	0.126389
21D	1.705891	1.356186	0.126388
22D	1.450831	-0.837640	1.990037
23D	-0.576606	0.332904	-1.320754
24D	-0.576605	1.356187	0.126388
25D	-0.321549	-0.837639	1.990037
26D	0.564641	-1.643796	-1.320753

N = 27

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.126458	0.000000	0.000000
3A	0.560489	-0.977118	0.000000
4A	0.570967	-0.330717	0.922478

5A	-0.332679	-0.845784	0.599911
6A	0.568125	0.709409	0.599911
7A	1.462523	-0.847126	0.599264
8A	0.552726	-0.320151	-0.870640
9A	-0.355743	0.206054	0.991281
10A	1.506105	0.226076	1.008134
11A	-0.398352	-0.867712	-0.529368
12A	0.553285	-1.418921	1.008134
13A	0.554468	0.777286	-0.529368
14A	1.503249	-0.870716	-0.545375
15D	-0.588080	1.361623	0.187107
16D	-0.358134	-0.813553	1.989484
17D	-1.473716	-0.167384	0.187106
18D	0.527501	0.715453	1.989484
19D	-0.607710	0.352000	-1.276118
20D	1.419666	-0.822303	1.999392
21D	-0.334363	-2.155503	0.131406
22D	1.703370	1.362544	0.131406
23D	1.436799	-2.155988	0.124137
24D	2.585063	-0.173566	0.124137
25D	1.693125	0.343065	-1.316912
26D	0.544860	-1.639357	-1.316912
27D	-1.328676	0.769598	1.795513

N = 28

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.120126	0.000000	0.000000
3A	0.555720	-0.980368	0.000000
4A	0.531927	-0.321755	0.919253
5A	0.558713	-0.325540	-0.874596
6A	-0.354369	-0.850506	0.579909
7A	-0.357292	-0.864087	-0.550580
8A	0.544160	0.728265	0.580119
9A	1.428953	-0.852633	0.616429
10D	0.575723	-1.641372	-1.334039
11B	0.552403	0.860472	-0.665790
12B	-0.542129	0.237483	-1.048369
13A	1.504559	-0.891419	-0.517692
14A	0.519852	-1.422621	0.999079
15A	1.478892	0.208368	1.017133
16A	-0.432433	0.195860	0.982647
17D	-1.496058	-0.266572	0.046588
18D	1.797660	0.250919	-1.300655
19D	-0.364698	-2.144791	0.071518
20D	1.410051	-2.168299	0.142482
21D	-0.678398	1.296850	0.117315
22D	0.500578	0.691510	1.974155
23D	1.389582	-0.843873	2.007140
24D	2.593706	-0.237402	0.192996
25D	-0.379441	-0.850063	1.973997
26D	1.760553	1.316598	0.157067
27D	0.335677	-0.116422	-2.248381
28D	-1.113227	-1.062141	-1.695768

N = 29

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.097921	0.000000	0.000000
3A	0.549143	-0.950722	0.000000
4A	0.538076	-0.310590	0.925736
5A	0.557728	-0.321933	-0.925057
6A	1.472517	-0.849970	-0.583250
7A	0.533737	0.737004	0.585201
8A	-0.371237	-0.830804	0.585200
9A	0.563301	0.736100	-0.577108
10A	-0.355667	-0.855950	-0.577109
11A	1.446732	-0.835087	0.584636
12B	-0.521417	0.300973	1.042607
13B	0.544952	-1.551780	-1.032988
14B	1.616300	0.304258	-1.032987
15A	1.500147	0.225516	0.982339
16A	0.555041	-1.411818	0.982338
17A	-0.399191	0.230423	-0.974053
18D	-1.466410	-0.177720	-0.077489
19D	-0.579554	1.358699	-0.077488
20D	1.678509	1.356862	0.087678
21D	-0.335415	-2.132126	0.087677
22D	1.440443	-2.130436	0.076522
23D	2.565269	-0.181750	0.076523
24D	1.468051	-0.847393	1.969042
25D	0.610450	0.693271	1.999272
26D	-0.294999	-0.875359	1.999271
27D	-0.395479	-0.787599	-1.981378
28D	0.484201	0.736389	-1.981378
29D	1.397577	-0.806712	-2.037361

N = 30

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.099894	0.000000	0.000000
3A	0.549947	-0.949571	0.000000
4A	0.549945	-0.307954	0.926856
5A	0.549949	-0.327062	-0.924405
6A	0.549946	0.741860	0.580163
7A	0.549947	0.723385	-0.577843
8A	-0.355649	-0.856080	-0.585652
9A	1.455545	-0.856080	-0.585649
10A	1.468175	-0.828204	0.578533
11A	-0.368283	-0.828205	0.578529
12B	1.612079	0.308362	1.036182
13B	-0.512190	0.308362	1.036178
14D	1.688613	1.355453	-0.089798
15D	-0.588721	1.355452	-0.089802
16B	0.549949	-1.551141	-1.042349
17A	-0.396641	0.233271	-0.981997
18A	1.496538	0.233272	-0.981995
19A	0.549945	-1.412320	0.973038
20D	0.549942	0.626951	2.065525
21D	-1.463903	-0.178699	-0.077906
22D	2.563797	-0.178697	-0.077899
23D	1.437788	-2.129511	0.078122
24D	-0.337893	-2.129513	0.078118
25D	0.549950	0.749089	-1.961730
26D	1.434785	-0.908798	1.977832
27D	-0.334900	-0.908799	1.977828
28D	-0.353918	-0.766850	-2.000541
29D	1.453819	-0.766849	-2.000539
30D	0.549943	2.072126	1.062157

N = 31

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.111655	0.000000	0.000000
3A	0.549158	-0.966542	0.000000
4A	0.573622	0.950853	0.000000
5A	-0.543361	-0.968463	0.000000
6D	1.345602	0.766207	1.249307
7D	1.345602	0.766207	-1.249307
8D	-0.001459	-1.548456	-1.249306
9D	-0.001459	-1.548456	1.249306
10A	-1.110490	-0.004732	0.000000
11A	-0.544465	0.967868	0.000000
12A	0.537142	-0.312599	-0.883861
13A	0.537142	-0.312599	0.883861
14A	-0.002247	0.627667	0.882948
15A	-0.546843	-0.308113	0.882948
16A	-0.002247	0.627667	-0.882948
17A	-0.546843	-0.308113	-0.882948
18D	1.731068	-1.007427	-0.878622
19D	1.731068	-1.007427	0.878622
20D	-1.384140	0.805529	-1.146671
21D	-1.384140	0.805529	1.146671
22D	0.026027	2.006569	-0.877599
23D	0.026027	2.006569	0.877599
24D	-1.731778	-1.013872	-0.877598
25D	-1.731778	-1.013872	0.877598
26D	-0.034040	0.019811	-2.161164
27D	-0.034040	0.019811	2.161164
28D	2.496928	0.358898	0.000000
29D	0.921437	-2.348278	0.000000
30D	1.593942	1.958899	0.000000
31D	-0.915781	-2.353566	0.000000

N = 32

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.109419	0.000000	0.000000
3A	-0.546421	-0.969311	0.000000
4A	0.573326	-0.953146	0.000001
5A	-1.111540	-0.033928	-0.000002
6A	0.546822	0.970668	-0.000001
7A	-0.571171	0.951841	-0.000002
8D	1.348078	-0.760760	1.248371
9D	1.348081	-0.760761	-1.248368
10D	-1.328875	-0.801606	-1.249086
11D	-1.328879	-0.801603	1.249082
12A	0.008756	-0.623298	-0.882506
13A	0.008753	-0.623296	0.882506
14A	0.534475	0.326490	0.881747
15A	0.534477	0.326488	-0.881747
16A	-0.549214	0.303553	0.881233
17A	-0.549212	0.303551	-0.881235
18D	-0.042729	1.582391	-1.178324
19D	-0.042732	1.582394	1.178319
20D	0.027600	-2.004222	-0.878581
21D	0.027598	-2.004221	0.878583
22D	1.741784	0.991785	0.883207
23D	1.741786	0.991784	-0.883207
24D	-1.762324	0.959531	0.876619
25D	-1.762321	0.959529	-0.876629
26D	-0.001360	0.028461	-2.160625
27D	-0.001365	0.028465	2.160624
28D	1.591473	-1.959543	0.000002
29D	-1.537640	-2.003477	-0.000001
30D	2.500100	-0.368697	0.000003
31D	-2.489402	-0.431091	-0.000004
32D	1.012483	2.343454	-0.000002

N = 33

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.110416	0.000000	0.000000
3A	0.569313	-0.953366	0.000000
4A	-0.555208	-0.961649	0.000000
5A	-0.555209	0.961648	0.000000
6A	-1.110296	-0.016358	0.000000
7A	0.540982	0.969723	0.000000
8D	1.349258	-0.765799	-1.245128
9D	1.349258	-0.765799	1.245128
10D	-1.337831	-0.785593	1.245128
11D	-1.337831	-0.785593	-1.245128
12D	-0.011428	1.551392	1.245128
13D	-0.011428	1.551392	-1.245128
14A	0.004606	-0.625383	-0.881185
15A	0.004606	-0.625383	0.881185
16A	0.539294	0.316681	0.881186
17A	0.539294	0.316681	-0.881186
18A	-0.543901	0.308702	0.881185
19A	-0.543901	0.308702	-0.881185
20D	0.014761	-2.004046	0.877168
21D	0.014761	-2.004046	-0.877168
22D	1.728173	1.014807	0.877167
23D	1.728173	1.014807	-0.877167
24D	-1.742935	0.989238	-0.877168
25D	-1.742935	0.989238	0.877168
26D	0.000000	-0.000001	-2.163217
27D	0.000000	-0.000001	2.163217
28D	1.583853	-1.963750	0.000000
29D	-1.554753	-1.986869	0.000000
30D	2.498055	-0.353020	0.000000
31D	-2.492584	-0.389782	0.000000
32D	-0.943303	2.339890	0.000000
33D	0.908729	2.353532	0.000000

N = 34

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.060246	0.000000	0.000000
3A	0.530123	-0.956651	0.000000
4A	0.530123	-0.295622	-0.909828
5A	0.530123	0.773946	-0.562306
6A	0.530123	-0.295621	0.909829
7A	0.530122	0.773946	0.562305
8A	-0.396506	-0.808926	-0.587718
9A	1.456751	-0.808926	-0.587718
10A	-0.396506	-0.808926	0.587719
11A	1.456751	0.308981	-0.950949
12A	-0.396506	0.308981	-0.950949
13A	1.456751	-0.808926	0.587719
14A	1.456751	0.999887	0.000000
15A	1.456751	0.308982	0.950949
16A	-0.396506	0.308982	0.950949
17A	-0.396506	0.999887	-0.000001
18D	-1.424605	0.000000	0.000000
19D	2.484850	0.000000	0.000000
20B	0.530122	0.568449	1.749505
21B	0.530122	1.839539	-0.000001
22B	0.530123	-1.488218	1.081254
23B	0.530123	0.568447	-1.749506
24B	0.530123	-1.488219	-1.081253
25D	1.436068	1.702128	-1.236670
26D	1.436068	1.702129	1.236668
27D	-0.375823	-0.650156	2.000972
28D	1.436069	-0.650155	2.000972
29D	-0.375823	1.702128	-1.236670
30D	-0.375823	1.702129	1.236668
31D	-0.375823	-2.103948	0.000001
32D	-0.375823	-0.650157	-2.000972

33D	1.436069	-2.103947	0.000000
34D	1.436068	-0.650157	-2.000972

N = 35

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2B	1.176731	0.000000	0.000000
3A	0.447602	-0.998913	0.000000
4B	0.454106	0.912453	-0.619313
5A	-0.526310	-0.749431	0.625910
6B	0.433375	-0.344573	-1.057870
7A	0.462205	0.782443	0.597974
8A	0.460122	-0.319927	0.894233
9A	-0.470467	0.294430	0.948171
10A	-0.590450	0.319654	-0.852488
11A	-0.530190	-0.766475	-0.491597
12A	-1.085214	0.009735	0.091854
13A	-0.504355	0.935952	0.059119
14D	-1.773349	-1.234013	-0.145323
15C	1.521770	-1.092922	0.860478
16D	-0.154597	-0.520885	2.103702
17D	1.689379	1.443566	0.135059
18D	1.663734	-1.223088	-0.778925
19D	1.470422	0.404241	1.536126
20D	0.116159	2.162634	0.338062
21D	-0.848457	1.730679	-1.048867
22D	1.724527	0.476269	-1.353740
23D	-1.720083	-0.283920	1.332242
24A	0.250441	-1.398344	1.015687
25A	-0.405003	-1.693360	0.103807
26D	0.060635	-1.818869	-1.234168
27D	0.090302	0.697743	-2.101269
28D	-1.558582	1.362576	0.797045
29D	-1.096712	-0.609638	-1.772141
30D	-0.061101	1.267275	1.847373
31D	-2.053716	0.492603	-0.750637
32D	-1.030582	-1.905724	1.356226
33D	0.806089	-2.433834	0.227404
34D	2.665317	-0.054402	0.178840
35D	0.901343	2.147193	-1.334338

N = 36

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2B	1.183495	0.000000	0.000000
3B	0.431415	-1.096552	0.000000
4A	0.448982	-0.307388	0.950719
5B	0.455076	-0.318290	-1.060822
6A	-0.529744	0.359127	0.902491
7A	-0.583810	-0.727765	-0.560982
8A	-0.533709	-0.703196	0.576295
9A	0.466868	0.749338	0.579285
10A	0.456807	0.801678	-0.570961
11A	-1.092817	0.081259	0.009737
12A	-0.473469	0.981372	0.012151
13A	-0.500192	0.336003	-0.874998
14D	1.651889	-1.135964	0.924293
15D	1.705595	-1.182031	-0.859554
16D	1.626303	0.558135	1.382897
17C	0.105202	-1.596026	1.298075
18D	-0.151261	1.835633	1.136649
19D	-1.774204	-0.525171	1.134401
20D	0.093936	-1.788228	-1.328237
21D	1.688877	0.542144	-1.347132
22D	-0.945376	-1.945360	0.081936
23D	-0.868558	-0.476749	-1.957676
24D	0.115687	0.962113	-1.969000
25D	1.437999	1.615166	0.024745
26A	-0.413189	-0.431873	1.637798
27D	-1.718366	1.176461	0.682558
28A	0.239815	0.522123	1.647019
29D	-1.623782	1.069928	-1.048731
30D	-2.020954	-0.704280	-0.648808
31D	-0.131767	2.125290	-0.672890
32D	0.773442	-0.573723	2.393445
33D	-1.035084	0.697496	2.231476
34D	0.843277	-2.534792	0.108994
35D	0.889254	-0.630231	-2.459302
36D	2.687808	0.078980	0.042995

N = 37

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.149568	0.000000	0.000000
3A	-1.151157	-0.063380	0.000000
4A	0.534695	0.867190	-0.333723
5A	-0.571677	0.577492	0.719139
6A	0.535249	0.607738	0.720316
7A	-0.583771	0.837597	-0.332743
8D	-0.033960	1.142803	-1.586405
9A	-0.543038	-0.079986	-0.939369
10A	0.548712	-0.050870	-0.948185
11A	-0.529412	-0.499983	0.808220
12A	0.552082	-0.470578	0.809263
13D	-0.010700	0.232221	1.970787
14A	0.562378	-0.892092	-0.207448
15A	-0.515181	-0.922058	-0.207012
16C	0.030385	-1.196939	-1.376961
17D	-1.705589	0.717637	-1.193320
18D	1.666598	0.812302	-1.185273
19A	-0.041092	1.467384	0.379693
20D	-1.597629	-1.053747	-1.086266
21D	1.655789	-0.969256	-1.075101
22D	-1.657478	0.043947	1.482399
23D	1.645236	0.134635	1.488582
24B	1.556976	1.104058	0.301768
25B	-1.619899	1.016527	0.296001
26D	-1.507635	-1.490886	0.617871
27D	1.581249	-1.407301	0.625328
28D	0.829646	2.245315	-0.422798
29D	-0.953535	2.197156	-0.422823
30D	-0.933626	1.724780	1.460313
31D	0.830238	1.772686	1.464725
32D	0.059423	-2.194474	-0.028701
33D	0.037357	-1.519353	1.597003
34D	0.835232	-0.158791	-2.387852
35D	2.600348	-0.028435	0.049799
36D	-2.597897	-0.171238	0.039534
37C	-0.796097	-0.187785	-2.238600

N = 38

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.048667	0.000000	0.000000
3A	0.464624	-0.968416	0.000000
4A	0.464625	-0.330322	-0.910338
5A	0.496222	-0.279467	0.919802
6A	0.496223	0.769316	-0.576446
7A	0.509071	0.801165	0.561571
8B	-0.613559	-0.849266	-0.595286
9A	-0.417684	0.312575	0.931302
10A	-0.417684	0.982069	-0.023831
11A	-0.455618	-0.758231	0.585311
12A	-0.455616	0.291582	-0.912406
13A	-1.066594	0.094350	0.066134
14B	1.541034	0.328306	1.042689
15B	1.541034	1.092141	-0.047036
16A	1.372331	-0.858203	-0.601549
17A	1.393738	-0.819482	0.596948
18A	1.393738	0.281628	-0.973952
19D	-0.538172	1.698072	1.190251
20C	0.422617	0.582902	1.911498
21C	0.422618	1.995688	-0.104053
22D	-0.498707	-0.766250	1.951861
23D	-0.498707	1.573443	-1.386064
24C	0.427378	-1.639317	-1.149065
25D	-0.416629	-2.137957	0.205266
26D	-0.416628	-0.536289	-2.079757
27A	0.447132	0.486098	-1.624790
28A	0.447131	-1.361545	1.011154
29D	2.471628	-0.142926	-0.100183
30D	-1.821196	-0.036132	-1.133438
31D	-1.821197	-1.077789	0.352640
32D	1.349245	-2.122726	0.128511
33D	1.349246	-0.603247	-2.039257
34D	-1.744585	0.369024	1.336145
35D	-1.744585	1.381888	-0.108855
36D	1.292032	-0.832890	2.018040
37D	1.292032	1.612923	-1.471280
38D	1.268234	1.829449	1.282340

N = 39

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.051055	0.000000	0.000000
3A	0.459662	-0.977643	0.000000
4A	0.459663	-0.337596	0.917505
5A	0.487191	-0.275585	-0.919433
6A	0.487191	0.767711	0.576128
7A	0.495136	0.804799	-0.561424
8B	-0.606406	-0.835951	0.583155
9A	-0.429204	0.980336	0.024694
10A	-0.429204	0.315351	-0.928559
11A	-0.470830	-0.749793	-0.590074
12A	-0.470829	0.294861	0.907433
13A	-1.072660	0.092770	-0.064716
14D	0.378197	-1.780606	1.242142
15B	1.515782	0.340530	-1.056299
16B	1.515782	1.108912	0.045174
17B	1.476842	-0.925802	0.645835
18A	1.391077	0.283410	0.978318
19A	1.391077	-0.820272	-0.603805
20D	-0.475222	-0.511551	2.086396
21D	-0.475224	-2.134700	-0.240383
22D	-0.562117	1.699565	-1.185609
23C	0.397511	2.000182	0.109998
24C	0.397512	0.587464	-1.915128
25D	-0.527090	1.575651	1.387540
26D	-0.527090	-0.758089	-1.957867
27D	-1.844216	-0.057527	1.121876
28D	-1.844218	-1.072729	-0.333412
29A	0.405139	0.493313	1.619105
30A	0.405138	-1.349159	-1.022071
31D	2.507851	-0.044699	0.031182
32D	-1.760475	0.364738	-1.327038
33D	-1.760475	1.371357	0.115947
34D	1.265823	-0.832972	-2.021184
35D	1.265822	1.609216	1.479680
36D	1.285068	-2.173649	-0.243456
37D	1.285069	-0.522118	2.124008
38D	1.237467	1.841029	-1.284293
39D	-1.453537	-1.843864	1.286272

N = 40

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.059659	0.000000	0.000000
3A	0.450993	-0.958896	0.000000
4A	0.465201	-0.295289	-0.912851
5A	0.465201	-0.295289	0.912851
6A	0.465608	0.785757	-0.568963
7A	0.465608	0.785757	0.568963
8A	-0.512878	-0.755750	0.568963
9A	-0.512878	-0.755750	-0.568963
10A	-0.474489	0.301187	0.905016
11A	-0.474489	0.301187	-0.905016
12A	-0.472181	0.955117	0.000000
13A	-1.065256	0.020787	0.000000
14B	1.465425	-0.930189	-0.666961
15B	1.465425	-0.930189	0.666961
16B	0.314092	-1.483593	-1.083659
17B	0.314092	-1.483593	1.083659
18B	1.476200	0.347193	1.083659
19B	1.476200	0.347193	-1.083659
20B	-0.399268	-1.820903	0.000000
21B	1.477829	1.136280	0.000000
22B	0.338612	0.571951	-1.760537
23B	0.338612	0.571951	1.760537
24B	-0.373451	-0.549834	1.760537
25B	-0.373451	-0.549834	-1.760537
26D	-0.631774	1.653935	-1.211822
27D	-0.631774	1.653935	1.211822
28D	-1.765547	-0.132211	1.211822
29D	-1.765547	-0.132211	-1.211822
30B	0.334817	1.853784	0.000000
31B	-1.535013	-1.091946	0.000000
32D	-1.862806	1.182435	0.000000
33D	2.511897	-0.011851	0.000000
34D	1.079787	-2.267999	0.000000
35D	1.115245	-0.707910	-2.148987
36D	1.115245	-0.707910	2.148987
37D	-1.174034	-1.801102	-1.328288
38D	-1.174034	-1.801102	1.328288
39D	1.130173	1.828947	1.328288
40D	1.130173	1.828947	-1.328288

N = 41

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.059709	0.000000	0.000000
3A	0.479917	-0.947575	0.000000
4A	0.479915	-0.259466	0.911359
5A	-0.472817	-0.758425	0.572636
6A	0.464493	-0.296131	-0.926355
7A	0.464491	0.809864	0.538467
8A	-0.493464	-0.768060	-0.577413
9A	-0.493467	0.345034	0.896811
10A	0.492558	0.747370	-0.564292

11A	-0.469427	0.295059	-0.915516
12A	-0.469429	0.961318	-0.033097
13A	-1.053200	-0.002026	0.001527
14B	1.493376	0.386514	1.049247
15B	1.493379	-0.903309	-0.659045
16B	0.371611	-1.451640	1.096041
17B	1.509752	-0.885652	0.668701
18D	0.365418	2.094072	-0.350927
19D	0.365422	0.910913	-1.917949
20B	-0.344261	-0.514948	1.749912
21B	-0.344257	-1.824037	0.016104
22B	0.356103	0.642443	1.723033
23B	0.356107	-1.481267	-1.089691
24A	1.379879	1.046191	-0.001298
25A	1.379881	0.287718	-1.005850
26C	-0.393260	1.685290	1.053751
27C	-0.393255	-0.552014	-1.909419
28B	-1.493665	-0.332612	1.079388
29B	-1.493663	-1.129214	0.024337
30D	-1.801598	-0.164761	-1.151267
31D	-1.801600	1.062148	0.473698
32D	2.478316	0.144807	-0.109332
33D	-1.138584	1.510572	-1.140541
34D	1.137830	-0.626195	2.150368
35D	1.137833	-2.239647	0.013449
36D	1.231562	1.866771	1.172554
37D	1.231567	-0.616581	-2.116492
38D	-1.102677	-1.802769	1.361153
39D	-1.152079	0.727762	2.135684
40D	-1.152073	-1.854788	-1.284744
41D	1.848144	1.595879	-1.204945

N = 42

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.067047	0.000000	0.000000
3A	0.430033	-0.976556	0.000000
4A	0.468582	-0.305660	0.889509
5A	0.468582	-0.305660	-0.889509
6A	0.473677	0.801903	0.556948
7A	-0.543001	-0.756683	0.556948
8A	0.473676	0.801903	-0.556949
9A	-0.543001	-0.756683	-0.556948
10A	-0.454443	0.296436	0.893260
11A	-0.454444	0.296437	-0.893259
12A	-0.473117	0.967935	0.000000
13A	-1.076521	0.042905	0.000001
14C	-0.494559	-1.958108	0.000000
15C	1.592738	1.241758	-0.000001
16B	0.297583	-1.475701	-1.094257
17B	1.470484	0.322378	1.094257
18B	0.297583	-1.475702	1.094257
19B	1.470483	0.322378	-1.094257
20B	1.449740	-0.945676	0.682956
21B	1.449739	-0.945676	-0.682956
22D	-0.695951	1.566434	1.326912
23D	-1.714069	0.005640	1.326912
24D	-0.695953	1.566434	-1.326911
25D	-1.714070	0.005640	-1.326910
26A	-0.324378	-0.513062	1.604184
27A	-0.324379	-0.513062	-1.604183
28A	0.338824	0.503639	1.604183
29A	0.338823	0.503639	-1.604184
30D	0.260244	2.164668	0.000000
31D	-1.876212	-1.110561	0.000001
32D	0.968679	-0.631877	2.191775
33D	0.968677	-0.631876	-2.191775
34D	-1.856222	1.210827	0.000001
35D	-1.157871	-1.660795	-1.517128
36D	1.053315	1.728996	-1.517128
37D	1.053317	1.728997	1.517127
38D	-1.157870	-1.660796	1.517128
39D	1.101521	-2.269706	0.000000
40D	2.521149	-0.093389	-0.000001
41D	-0.581688	0.379438	-2.657939
42D	-0.581684	0.379438	2.657940

N = 43

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.052825	0.000000	0.000000
3A	0.521904	-0.961925	0.000000
4A	0.479353	0.787389	-0.559363
5A	0.479351	0.787389	0.559364
6A	0.494430	-0.296062	-0.915283
7A	0.494428	-0.296063	0.915283
8B	-0.559756	1.048777	-0.000001
9A	-0.416578	-0.794011	-0.580884
10A	-0.416580	-0.794011	0.580883
11A	-1.069289	-0.039348	-0.000001
12A	-0.473539	0.287356	0.914372
13A	-0.473537	0.287356	-0.914373
14C	0.423684	-1.573904	-1.223267
15C	0.423681	-1.573904	1.223267
16D	-0.458711	-0.474014	-2.055820
17D	-0.458716	-0.474015	2.055819
18B	1.544450	-0.871522	0.663807
19B	1.544451	-0.871522	-0.663805
20C	0.463960	2.010822	0.000001
21B	-0.275614	-1.860120	-0.000001
22D	-0.351168	1.651233	-1.400828
23D	-0.351172	1.651232	1.400828
24A	-1.266630	-1.123252	-0.000002
25D	-1.803284	0.879916	-0.880426
26D	-1.803287	0.879915	0.880422
27A	1.385479	1.040482	0.000002
28A	1.405304	0.317278	0.959290
29A	1.405306	0.317278	-0.959288
30A	-1.381359	-0.463523	0.949001
31A	-1.381357	-0.463523	-0.949005
32D	2.480687	0.165246	0.000002
33A	0.480374	0.535962	-1.613391
34A	0.480370	0.535962	1.613391
35D	1.400689	1.655988	1.311058
36D	1.400693	1.655989	-1.311052
37D	-1.219880	-1.849926	1.214039
38D	-1.219877	-1.849926	-1.214043
39D	-2.490543	-0.481576	-0.000003
40D	1.314710	-0.490602	2.127285
41D	1.314714	-0.490602	-2.127284
42D	1.259017	-2.237937	0.000001
43D	-1.224798	2.387719	-0.000001

N = 44

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.068540	0.000000	0.000000
3A	0.477013	-0.956429	0.000000
4A	0.477012	-0.295553	-0.909618
5A	0.477011	-0.295553	0.909618
6A	0.477009	0.773768	-0.562175
7A	0.477009	0.773767	0.562175
8A	-0.479640	-0.773709	-0.562131
9A	-0.479641	-0.773709	0.562130
10A	-0.479643	0.295527	-0.909548
11A	-0.479644	0.295527	0.909547
12A	-0.479645	0.956352	0.000000
13A	-1.067656	-0.000004	-0.000001
14B	1.488610	1.138185	0.000001
15B	1.488611	0.351720	1.082478
16B	1.488613	0.351720	-1.082476
17B	1.488615	-0.920808	0.669008
18B	1.488615	-0.920808	-0.669007
19B	0.350566	0.568985	-1.751156
20B	0.350562	1.841274	0.000000
21B	0.350564	0.568984	1.751156
22B	0.350570	-1.489623	1.082274
23B	0.350571	-1.489623	-1.082274
24B	-0.355071	-0.568668	1.750173
25B	-0.355066	-1.840244	-0.000001
26B	-0.355074	1.488784	-1.081667
27B	-0.355075	1.488784	1.081667
28B	-0.355069	-0.568668	-1.750174
29B	-1.498590	-1.131318	-0.000001
30B	-1.498592	-0.349600	-1.075943
31B	-1.498593	-0.349600	1.075940
32B	-1.498595	0.915245	-0.664970
33B	-1.498596	0.915245	0.664967
34D	2.527680	0.000004	0.000001
35D	1.128375	-0.698995	-2.151290
36D	1.128377	-2.262000	0.000001
37D	1.128367	1.829998	1.329572
38D	1.128373	-0.698996	2.151291
39D	1.128368	1.829998	-1.329570
40D	-1.130775	2.262391	-0.000001
41D	-1.130773	0.699114	2.151665
42D	-1.130770	0.699114	-2.151667
43D	-1.130765	-1.830322	1.329802
44D	-1.130764	-1.830321	-1.329804

N = 45

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.069032	0.000000	0.000000
3A	0.478086	-0.956171	0.000000
4A	0.478086	-0.295473	0.909373
5A	0.478086	-0.295473	-0.909373
6A	0.478086	0.773559	0.562023
7A	0.478086	0.773559	-0.562023
8A	-0.478085	-0.773559	-0.562023
9A	-0.478085	-0.773559	0.562023
10A	-0.478086	0.295473	-0.909373
11A	-0.478085	0.295473	0.909373
12A	-0.478086	0.956171	0.000000
13A	-1.069032	-0.000001	0.000000
14B	-1.489652	-0.351661	1.082296
15B	-1.489652	-1.137995	0.000000
16B	-0.351660	1.489652	-1.082296
17B	-1.489653	0.920655	0.668896
18B	-0.351659	1.489652	1.082296
19B	1.489653	-0.920656	0.668896
20B	0.351659	0.568997	-1.751192
21B	-0.351659	-0.568997	-1.751192
22B	0.351660	-1.489653	1.082296
23B	-1.489652	-0.351661	-1.082296
24B	1.489653	0.351659	1.082296
25B	0.351659	1.841312	0.000000
26B	1.489653	-0.920656	-0.668896
27B	0.351660	0.568997	1.751192
28B	1.489653	0.351659	-1.082296
29B	1.489653	1.137993	0.000000
30B	-1.489653	0.920655	-0.668896
31B	0.351660	-1.489653	-1.082296
32B	-0.351658	-1.841312	0.000000
33B	-0.351658	-0.568997	1.751192
34D	1.130859	1.829768	-1.329404
35D	-1.130860	2.261717	0.000000
36D	-2.528677	-0.000002	0.000000
37D	-1.130858	-1.829769	-1.329404
38D	-1.130857	-1.829769	1.329404
39D	1.130859	1.829768	1.329404
40D	-1.130858	0.698908	2.151022
41D	-1.130859	0.698908	-2.151021
42D	1.130859	-0.698909	-2.151022
43D	2.528678	0.000000	0.000000
44D	1.130860	-2.261718	0.000000
45D	1.130860	-0.698909	2.151021

N = 46

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.065570	0.000000	0.000000
3A	0.471228	-0.955711	0.000000
4A	0.471228	-0.293049	0.909673
5A	0.485115	0.769662	0.564898
6A	0.485114	-0.301685	-0.905801
7A	-0.475778	-0.775468	0.564899
8A	0.489539	0.769045	-0.560219
9A	-0.473267	0.294318	0.913410
10A	-0.473268	-0.779164	-0.560219
11A	-0.469440	0.956404	0.001391
12A	-0.469441	0.291938	-0.910759
13A	-1.065401	-0.001910	0.001392
14A	1.360188	-0.845880	0.616191
15B	0.364318	-1.482085	1.079642
16B	1.490397	-0.926855	-0.643885
17B	1.490397	0.328668	1.079641
18B	-0.337905	-0.573673	1.758817
19B	-0.337906	-1.849998	0.006734
20B	1.509833	1.121195	0.006732
21B	0.365096	-1.503372	-1.069250
22B	0.365096	0.556766	1.758816
23B	1.509832	0.337383	-1.069251
24B	0.369758	1.834962	0.003530
25B	-0.338113	-0.578973	-1.747652
26B	-0.338112	1.485936	1.086965
27B	-1.482261	-1.143113	0.003531
28B	-1.482260	-0.353872	1.086966
29B	0.369757	0.559294	-1.747652
30B	-1.478688	0.919573	-0.669873
31B	-1.480816	-0.355914	-1.082159
32B	-0.335643	1.485542	-1.082159
33B	-1.480815	0.920897	0.670591
34D	2.515890	-0.077302	0.056311
35D	1.181938	-0.735027	2.098001
36D	1.181937	-2.222319	0.056312
37D	-1.116825	-1.832058	1.334584
38D	1.149280	-0.714720	-2.133818

39D	1.149281	1.811876	1.334582
40D	-1.112938	0.692118	-2.151504
41D	-2.519250	-0.001286	0.000938
42D	-1.112937	2.260088	0.000937
43D	-1.119597	-1.836735	-1.323197
44D	-1.119596	0.696261	2.153989
45D	1.152249	1.816429	-1.323199
46D	2.463033	-1.531721	1.115799

N = 47

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.047715	0.000000	0.000000
3A	0.523858	-0.907348	0.000000
4A	0.523858	-0.302449	-0.938841
5A	0.523858	-0.302449	0.938841
6A	1.442952	-0.833089	-0.601572
7A	1.442952	-0.833089	0.601572
8A	0.523858	0.758829	-0.601572
9A	0.523858	0.758829	0.601572
10A	-0.395236	-0.833088	-0.601572
11A	-0.395236	-0.833088	0.601572
12B	1.611625	0.325572	0.992687
13B	-0.563908	0.325573	-0.992687
14B	0.523858	-1.558493	-0.992687
15B	0.523858	-1.558493	0.992687
16B	-0.563908	0.325573	0.992687
17B	1.611625	0.325572	-0.992687
18A	-1.038734	-0.185747	0.000000
19A	-0.358505	0.992444	0.000000
20A	1.204086	-1.714045	0.000000
21A	-0.156371	-1.714045	0.000000
22A	2.086450	-0.185748	0.000000
23A	1.406222	0.992444	0.000000
24D	1.395828	-0.805881	2.021456
25D	0.523859	0.704414	2.021456
26D	-0.348110	-0.805880	2.021456
27D	1.395828	-0.805881	-2.021456
28D	-0.348110	-0.805880	-2.021456
29D	0.523859	0.704414	-2.021456
30A	-1.189952	-1.291918	0.000000
31A	0.523859	1.676488	0.000000
32A	2.237667	-1.291919	0.000000
33D	1.440057	1.868365	1.074021
34D	2.861938	-0.594407	1.074021
35D	-0.898023	-2.181307	1.074022
36D	-0.392339	1.868365	-1.074022
37D	-0.898023	-2.181307	-1.074022
38D	-0.392339	1.868365	1.074022
39D	-1.814221	-0.594406	-1.074022
40D	-1.814221	-0.594406	1.074022
41D	1.945739	-2.181308	1.074021
42D	1.945739	-2.181308	-1.074021
43D	1.440057	1.868365	-1.074021
44D	2.861938	-0.594407	-1.074021
45D	2.788904	1.005274	0.000000
46D	0.523858	-2.917898	0.000000
47D	-1.741187	1.005275	0.000000

N = 48

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.046930	0.000000	0.000000
3A	0.522467	-0.907244	0.000000
4A	0.533968	-0.308677	-0.940867
5A	0.515972	-0.298277	0.937524
6A	-0.392149	-0.833957	-0.607579
7A	0.526987	0.756012	-0.607577
8B	-0.528054	0.305262	-0.999614
9A	0.515316	0.763769	0.592043
10A	-0.404698	-0.827717	0.592041
11A	1.447053	-0.836518	-0.595512
12A	1.437051	-0.830738	0.607493
13B	0.528139	-1.559827	-0.991817
14B	1.615276	0.320755	-0.991815
15B	1.602242	0.331101	0.994335
16B	0.512666	-1.553701	0.994332
17B	-0.573125	0.331313	0.982368
18D	-0.335209	-0.808751	-2.036015
19D	0.533562	0.694092	-2.036012
20A	-0.372906	0.990659	-0.016594
21A	-1.044578	-0.171232	-0.016596
22A	-0.159863	-1.712278	-0.002875
23A	1.404039	0.993040	-0.002871
24A	1.201694	-1.714242	0.007504
25A	2.085221	-0.185873	0.007507
26D	1.407416	-0.813602	-2.017550
27D	-0.369981	1.859211	-1.109220
28D	-1.795783	-0.607212	-1.109224
29D	1.378320	-0.796789	2.026822
30D	0.508333	0.714753	2.013312
31D	-0.365710	-0.797209	2.013309
32A	0.518704	1.675650	-0.015181
33A	-1.193220	-1.285722	-0.015186
34A	2.236307	-1.292775	0.013947
35D	-1.741414	1.006686	-0.295557
36D	-0.889889	-2.181733	-1.083913
37D	1.446542	1.859944	-1.083907
38D	1.949897	-2.184968	-1.060237
39D	2.866529	-0.599332	-1.060234
40D	-0.912250	-2.173836	1.064815
41D	1.428537	1.875375	1.064823
42D	2.851396	-0.589661	1.089821
43D	1.933961	-2.176686	1.089818
44D	-0.400659	1.875240	1.051020
45D	-1.824986	-0.588632	1.051016
46D	0.519155	-2.916657	0.003821
47D	2.786586	1.005657	0.003830
48D	-1.308330	0.756329	-2.186431

N = 49

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.104543	0.000000	0.000000
3A	0.567342	-0.947701	0.000000
4A	0.544068	0.994643	0.000000
5A	-0.573950	-0.977704	0.000000
6A	1.707622	-0.967960	0.000000
7A	0.018343	-0.638755	0.868337
8A	0.018344	-0.638756	-0.868337
9A	0.557476	0.312354	0.868337
10A	0.557477	0.312354	-0.868337
11A	1.112200	-0.630447	0.871128
12A	1.112201	-0.630447	-0.871128
13D	-1.666965	0.944913	0.000000
14D	-0.324287	0.183821	1.939863
15D	-0.324286	0.183820	-1.939863
16A	-0.371674	0.838706	0.595469
17A	-0.910521	-0.111899	0.595469
18A	-0.371674	0.838706	-0.595470
19A	-0.910521	-0.111899	-0.595469
20D	-1.090990	-1.325026	1.389456
21D	0.576497	1.616665	1.389455
22D	-1.090990	-1.325027	-1.389456
23D	0.576498	1.616665	-1.389456
24A	0.028368	-1.701005	0.571646
25A	0.028368	-1.701005	-0.571645
26A	1.474040	0.849371	-0.571646
27A	1.474040	0.849371	0.571646
28D	-0.343051	2.143455	-0.000001
29D	-2.015298	-0.806634	0.000000
30A	2.029140	-0.093223	0.574702
31A	1.122241	-1.693126	0.574702
32A	2.029141	-0.093224	-0.574701
33A	1.122241	-1.693126	-0.574701
34D	0.580606	-1.416885	1.900730
35D	0.580607	-1.416886	-1.900729
36D	1.513918	0.229612	1.900730
37D	1.513918	0.229611	-1.900730
38D	2.253906	-1.277619	1.382516
39D	2.253906	-1.277620	-1.382514
40D	1.453523	2.163182	-0.000001
41D	-1.109425	-2.358233	0.000001
42D	3.164016	-0.753475	0.000001
43D	2.271660	-2.327721	0.000001
44D	0.585428	-2.885426	0.000001
45D	2.776407	0.979781	0.000000
46D	-1.163046	1.673172	-1.501668
47D	-1.163046	1.673173	1.501667
48D	-2.032979	0.138483	-1.501668
49D	-2.032980	0.138484	1.501668

N = 50

atom	*X*/σ	*Y*/σ	*Z*/σ
1A	0.000000	0.000000	0.000000
2A	1.102589	0.000000	0.000000
3A	-0.457247	-1.017188	0.000000
4A	0.493467	-0.756722	0.521580
5A	0.493466	-0.756722	-0.521580
6A	0.477544	0.253362	0.958938
7A	0.477543	0.253361	-0.958938
8A	1.384795	-1.137890	0.000000
9B	1.469366	-0.493111	1.062426
10B	1.469365	-0.493112	-1.062427
11B	0.464203	1.048284	-0.000001
12A	-0.447763	-0.393996	-0.895169
13A	-0.447762	-0.393995	0.895169
14A	0.399158	-1.692730	0.000000
15D	2.551139	-0.249978	-0.000001
16D	1.731272	1.007271	0.866574
17D	1.731271	1.007270	-0.866576
18A	-1.064132	-0.104518	0.000000
19A	-0.166142	-1.481569	-0.949149
20A	-0.166141	-1.481568	0.949150
21A	0.364238	-0.684803	1.571196
22A	-0.518556	0.668941	-0.638111
23A	-0.518555	0.668941	0.638110
24A	0.967955	-1.610590	0.933086
25A	0.364237	-0.684804	-1.571196
26A	0.967954	-1.610591	-0.933086
27D	-1.597226	-1.148891	-0.887456
28D	-1.597226	-1.148890	0.887459
29D	-0.757602	-2.436437	0.000002
30D	-0.656993	0.278042	-2.068133
31D	-0.656992	0.278044	2.068132
32D	1.299669	-2.722456	0.000001
33D	1.060868	0.312984	2.309892
34D	0.201648	1.630576	-1.401725
35D	2.387040	-1.720673	0.908168
36D	2.387039	-1.720674	-0.908169
37D	1.060867	0.312981	-2.309894
38D	0.201648	1.630578	1.401723
39D	-0.866262	1.876789	-0.000001
40D	1.302970	-1.449678	2.292811
41D	1.302968	-1.449680	-2.292811
42D	0.287655	-2.733083	-1.430023
43D	-1.899842	0.621399	-0.882096
44D	-1.899842	0.621400	0.882096
45D	-0.546894	-1.453314	2.312122
46D	0.287658	-2.733082	1.430027
47D	-0.546896	-1.453317	-2.312120
48D	2.717126	-0.210210	1.832492
49D	2.717125	-0.210211	-1.832493
50D	0.983400	2.448418	-0.000002