Binary Lennard-Jones Atomic Clusters: Structural Features Induced by Large-Sized Atoms

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Abstract

Global-minimum geometries of binary Lennard-Jones clusters (BLJ_N where N is the number of atoms) are previously elucidated when the size ratio of the large B atom to the small A atom is 1.05 to 1.3. In the present study, BLJ clusters for larger size ratios (1.4 to 2.0) are investigated to clarify the structural features. The heuristic method combined with geometrical perturbations and atom-type conversion is developed to search for the global minima of the BLJ clusters. In the lowest-energy geometries of the BLJ clusters ($N \leq 50$), A and B atoms form cores and outer shells, respectively. The existence of fairly large sized atoms induces complicated structural growth sequence patterns (including icosahedron, triangular orthobicupola, cuboctahedron, etc.). New global minima of BLJ_{59} for $s = 1.15$, BLJ_{68} for $s = 1.15$ and BLJ_{70} for $s = 1.2$ are also reported.

Keyword: Binary clusters; Lennard-Jones potential; Global optimization; Structural growth sequence

1. Introduction

Global optimization plays an important role in a field of computational chemistry including prediction of the lowest-energy structures of biomolecules, clusters, and crystals. However, it is a difficult problem since the optimal geometry of a system must be searched from enormous number of stable geometries. Hence a strategy to efficiently move from a local minimum to the global minimum on the potential energy surface of the system is indispensable.

For atomic and molecular clusters, many investigations on the structures and properties have been performed due to their importance. However, global optimization of the clusters is still challenging. In the field of atomic clusters, Lennard-Jones (LJ) clusters are well elucidated and putative global minima of the LJ clusters up to 1610 atoms are tabulated [1 – 9]. Accordingly the LJ clusters are considered as a test problem for investigating performance of global optimization algorithms. Previously the present author developed an efficient method for geometry optimization of Lennard-Jones clusters [10]. The method optimizes cluster geometries with two types of geometrical perturbations and yielded the global minima of LJ clusters with 10 to 561 atoms reported previously and the new minima for 6 LJ clusters. Then the method is improved to apply it to complicated clusters, molecular homoclusters where molecular orientations are further required as optimized parameters [11, 12]. The first purpose of the present study is to improve the above optimization method for application to another type of complicated clusters, atomic heteroclusters.

For the heteroclusters, the composition of different atoms makes global optimization more difficult [13 – 23]. Since one of the simplest heteroclusters is the binary Lennard-Jones (BLJ) cluster, the putative global minima of the BLJ clusters have been examined [13 – 19]. For the *N*-atom BLJ clusters (BLJ_N), the potential energy is calculated using the atom-atom interaction potential $V(i, j)$:

$$E_N = \sum_{i<j}^{N} V(i,j) = 4\sum_{i<j}^{N} \varepsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r_{ij}}\right)^{6}\right] \quad (1)$$

Here r_{ij} represents the distance between atoms *i* and *j*, and α and β mean the atom types of atoms *i* and *j* (represented by A and B). The relation of $\varepsilon_{\mathrm{AA}} = \varepsilon_{\mathrm{BB}} = \varepsilon_{\mathrm{AB}} = \varepsilon$ is used throughout the present

study as adopted in the previous studies [13 – 19]. The values of σ_{AA} and σ_{BB} are set to be σ and $s\sigma$, respectively, and the σ_{AB} value is equal to $(\sigma_{AA} + \sigma_{BB})/2$ where the parameter s is a predefined constant of the system representing the size ratio of the B atom to the A atom. The BLJ clusters have been considered as an important model to study performance of optimization methods and structural properties of binary clusters.

The original investigation on the BLJ clusters was performed by Doye and Meyer [13] with basin-hopping (BH) algorithm. The study was aimed at finding the effect of the size of the B atom (s = 1.05, 1.1, 1.15, 1.2, 1.25, 1.3) on the global minima of the BLJ clusters with 5 to 100 atoms. The lowest energies and the corresponding geometries are tabulated in the CCD (Cambridge Cluster Database[7]). Cassioli et al. [14] confirmed a lot of the global minima with the population-based BH method and found 95 new minima. Marques and Pereira [15] proposed an evolutionary algorithm to search for global minima of the BLJ clusters and applied it to the BLJ clusters with 10 to 50 atoms. A new minimum was located for BLJ_{38} for s = 1.05 (E_{38}/ε = -177.260697). Kolossváry and Bowers [16] developed the hidden-force Monte Carlo (HFMC) algorithm. The results obtained for the geometries of BLJ_{90} to BLJ_{100} show that the HFMC method improved 17 global minima. In the study of Sicher et al., [17] the minima hopping method was applied to the clusters with N = 5 to 100 and yielded 17 new global minima. Most of the new minima were independently obtained with the HFMC algorithm [16]. Tao et al. [18] optimizes the geometries of the BLJ clusters with N = 5 to 100. Although 12 new global minima of the BLJ clusters were located, 15 global minima reported previously were missing. After the publication, Wenqi and Tao deposited following new minima in the CCD [7]; BLJ_{66} for s = 1.15 (E_{66}/ε = -359.49937), BLJ_{89} for s = 1.15 (E_{89}/ε = -510.052009), BLJ_{72} for s = 1.2 (E_{72}/ε = -404.850951), BLJ_{65} for s = 1.25 (E_{65}/ε = -363.528091) and BLJ_{99} for s = 1.3 (E_{99}/ε = -597.679071). Recently Rondina and Da Silva [19] developed a global optimization method based on the BH algorithm and applied it to several cases including the BLJ clusters with N = 5 – 100. Comparison of the results with the data taken from the above-mentioned studies shows that 2 new global minima are

located with the method: BLJ_{38} for s = 1.05 (E_{38}/ε = -177.260679) and BLJ_{66} for s = 1.15 (E_{66}/ε = -359.749940). However, the global minima of BLJ_{99} and BLJ_{100} for s = 1.3 were not found with the method. To enhance the reliability of the global minima, it would be necessary to search for the global minima of the BLJ clusters with different methods.

In the previous study on the LJ clusters by the present author [10], two geometrical perturbations followed by local optimizations efficiently explore geometrical space. For the BLJ clusters, the atom types must be taken into account in the optimization algorithm. A simple way to optimize the type of the atom is to convert A into B or vice versa in the algorithm as performed in the literature [18]. In the present study, an optimization method was developed by combination of the two perturbations [10] with the atom-type conversion [18] algorithm. To evaluate the combined method, geometry optimization was performed for the BLJ_5 to BLJ_{100} for s = 1.05, 1.1, 1.15, 1.2, 1.25, 1.3. Since these s-values were rather limited, the global-minima of BLJ_5 to BLJ_{50} for s = 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0 were also calculated. The second purpose of the present study is to examine the structures, relative stability and growth sequence patterns of the BLJ clusters. The results of the present study complement the previous data of the BLJ clusters.

2. Calculation

The optimization procedure proposed in the present study starts with a cluster configuration randomly generated. The number of the A atoms N_A is randomly selected from zero to N. The atoms are placed within a sphere with the volume of $N_A\left(\sqrt[6]{2}\sigma_{AA}\right)^3 + (N - N_A)\left(\sqrt[6]{2}\sigma_{BB}\right)^3$. The geometry of the cluster is locally optimized with a limited memory quasi-Newton method (L-BFGS [24]). Then the type of an atom is converted from A to B or from B to A. After the conversion, the geometry of the cluster is optimized by the L-BFGS [24] method. If the potential energy of the cluster is improved, the cluster geometry and the type of the atom are updated. This procedure is repeated for every atom and thus the atom-type conversion is N times carried out.

After performing the above conversion operator, an atom or some atoms with the highest potential energy are moved to positions which are expected to decrease the potential energy of the cluster. The positions are selected from the surface of the cluster or neighborhood of the center of mass of the cluster. The above geometrical perturbations are called the surface and interior operations. By applying local optimization (the L-BFGS [24] method) to geometries created with these operators, new minima are repeatedly searched. The details of the operators are described below.

An atom or *M* atoms with the highest potential energy are selected as follows: (i) create a list of atoms on the outer shell of the cluster. (ii) the potential energy of an atom *i* in the list, *E*(*i*), is calculated by using the following equation:

$$E_{\mathrm{select}}(i) = \sum_{j\neq i}^{N} V(i,j) \qquad (2)$$

For all combinations of *M* atoms (numbering of *M* atoms is represented by k_1, k_2,…, k_M), the contribution of *M* atoms to the potential energy of the cluster $E_{\mathrm{select}}(k_1, k_2,\ldots, k_M)$ is calculated by the formula:

$$E_{\mathrm{select}}(k_1, k_2, \cdots, k_M) = \sum_{i=1}^{M} E_{\mathrm{select}}(k_i) - \sum_{i=1}^{M-1}\sum_{j=i+1}^{M} V(k_i, k_j) \qquad (3)$$

(iii) select the atoms with the highest energy contribution from all the combinations.

Many methods ignore the second term in the right-side of eq 3. This is mainly because the computation of the second term is time-consuming for large *M* values. The neglect of the second terms is a good approximation if the atoms are far from each other. According to our experience on the LJ clusters [10], the second term is often crucial to efficiently search for new minima. The following conditions are used for the BLJ clusters [10]: $M \leq 4$ for the surface operator and $M \leq 5$ for the interior operator, respectively.

The interior operator moves the selected atoms to the surface of the sphere whose center is coincident with the center of mass of the cluster. It takes the radius of $r_e/2$ where $r_e = \sqrt[6]{2}\sigma_{AA}$ for the A atoms and $r_e = \sqrt[6]{2}\sigma_{BB}$ for the B atoms. The number of atoms surrounding the atoms moved by using the interior operator usually increases compared with that surrounding the atoms at the original surface

positions. Consequently the potential energy of the atoms obtained after local optimization is expected to be lower than that at the original positions. This leads to a probability that the potential energy of the cluster is improved with the interior operator. This is theoretical background on the development of the operator.

In the geometries created with the interior operator, some atoms are very close to each other. Hence displacement of them caused by local optimization (Δx, Δy, and Δz) is large, leading to the possibility of the evaporation. To avoid it, if the absolute values of Δx, Δy, and Δz are larger than σ, these are reduced to 0.1σ.

If the potential energy of the cluster is not improved during the last ten interior operations followed by local optimizations, the surface operator is carried out. In the operator, stable positions on the surface of the cluster are first examined and the best positions are chosen from them as the positions of the moved atoms as follows: (i) remove the moved atoms from the cluster and prepare the template cluster composed of the ($N - M$) atoms; (ii) add an atom on the surface of the template at random and optimize the position of the added atom. The surface is constructed by the spheres which have radii of $r_e/2$ and centers coincident with the positions of the template atoms. A vector generated randomly is used to show the direction from the center of mass of the cluster to the added atom; (iii) the obtained position P of the atom and the potential energy between the atom and the template $E_{\mathrm{template}}(P)$ are stored; (iv) This is repeated $2N$ times to create a set of stable positions on the surface. The set of stable positions is separately created for the A and B atoms; (v) calculate the potential energy E_{surface} for all combinations of M independent positions by

$$E_{\mathrm{surface}}(P_1, P_2, \cdots, P_M) = \sum_{i=1}^{M} E_{\mathrm{template}}(P_i) + \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} V(P_i, P_j) \qquad (4)$$

where numbering of M positions is represented by P_1, P_2,…, P_M and $E_{\mathrm{template}}(P_i)$ is obtained in (iii). If the positions P_1, P_2,…, P_M are similar to the coordinates of the atoms removed in the step (i), the positions are excluded in the calculation of E_{surface}; and (vi) select the positions with the lowest potential

energy $E_{\mathrm{surface}}^{\mathrm{min}}$ from all the combinations. This operator does not change the number of the A and B atoms in the cluster.

The cases with $M \geq 2$ must be carefully treated by the following reason. If the distances between the selected positions are close to the equilibrium distance, slight changes of the positions introduce a large energy difference because of the term $V(P_i, P_j)$. Therefore, when $M \geq 2$, the following step is carried out instead of (vi): for all the configurations with the potential energy less than $E_{\mathrm{surface}}^{\mathrm{min}} + 0.2\varepsilon$, positions of M atoms are simultaneously optimized and the positions giving the lowest energy are selected.

Stable positions on the surface of the cluster are also used in the previous optimization methods [18, 25]. However, the interactions between $P_1, P_2, \ldots, P_M$ are ignored in the methods and thus the number of the moved atoms (N_{move} = 10 to 40) is larger than that in the surface operator. However, the experience on the LJ clusters [10] suggests that the interactions should be taken into account since the efficiency of the optimization method is often enhanced.

The value of M is initially 1 and increases up to 4 at an interval of 1 if the energy of the cluster is not improved. When energy-lowering is observed, the M-value is initialized and the cluster geometry is updated. It was found that moving the second or third highest-energy atom by the surface operator improves performance of the method [10]. Hence, if the energy of the cluster is not improved by moving the highest-energy atom, the second highest-energy atom and the third highest-energy atom are separately moved by the surface operator. If the surface operator with 4 moved atoms does not improve the energy of the cluster, optimization algorithm returns to the atom-type conversion operator. In the present algorithm, a series of the atom-type conversion, the interior operator, and the surface operator is repeated. The termination condition of the algorithm is that the lowest energy obtained before the atom-type conversion operator is invariant compared with that obtained after the surface operator.

A lot of initial geometries were prepared randomly and were optimized with the above algorithm. The computations were performed on dual core 3 GHz Intel Xeon 5160 processors. No parallel computation was carried out. A geometry of the 50-atom BLJ cluster was optimized in 3 s and the corresponding time needed for the 100-atom BLJ cluster was 40 s.

The global minima of the BLJ clusters for s = 1.0 to 1.3 ($N \leq 100$) and those for s = 1.4 to 2.0 ($N \leq 50$) were searched with the present method (the heuristic method combined with geometrical perturbations and atom-type conversion, HMGPAC). The potential energies of the putative global minima of these clusters are tabulated in supplementary data.

3. Discussion

3.1. Efficiency of the optimization method

The global minima of the BLJ clusters (s = 1.05 to 1.3 and $N \leq 100$) reported in the previous studies [7, 13 – 19] were confirmed by HMGPAC except for 7 clusters (3 new minima and 4 missing minima). Three potential energies obtained in the present study (E_{59}/ε = -315.027359 for s = 1.15, E_{68}/ε = -372.247969 for s = 1.15 and E_{70}/ε = -391.735161 for s = 1.2) are lower than the corresponding energies given previously, -315.023963ε [19], -371.831801ε [7], and -391.581513ε [7]. The significant energy differences between the present and previous potential energies indicates that the present method locate new global minima; the geometrical data are deposited in supplementary data. The potential energy of the 72-atom BLJ cluster for s = 1.2, -404.850956ε, was slightly lower than the value of Tao et al. [18], -404.850951ε. Since the geometries obtained in the present and previous studies are the same, the present potential energy would be obtained with the tighter convergence criterion in the local optimization compared with the criterion in [18].

The global minima of BLJ_{93} and BLJ_{94} for s = 1.2, and BLJ_{99} and BLJ_{100} for s = 1.25 could not be found under the condition that the number of initial geometries was 1×10^5 for each of the clusters. Although HMGPAC is efficient for searching for global minima as shown in the above results of the

clusters with N = 59, 68, 70, any improvement on the optimization algorithm might be necessary to locate the missing global minima.

The number of local optimizations required for searching for the global minimum N_{opt} is a useful parameter to evaluate the efficiency of the present algorithm. It can be derived from the total number of local optimizations divided by the number of times that the global minimum is located. The results obtained for s = 1.1, 1.2, 1.3 are shown in Figure 1 except for the unsuccessful clusters. For the clusters with $N \geq 90$, the N_{opt} values of the clusters for s = 1.1 are smaller than the corresponding values of the clusters for s = 1.2 and 1.3. This trend is observed in the study of Tao et al. [18], suggesting that the difficulty for searching for the global minima for $N \geq 90$ and s = 1.2, 1.3 is due to the complicated potential energy surfaces. For s = 1.1, the global-minimum geometries with $N \geq 90$ include a lot of Ino decahedra (the notation (10/5) is used for it as described later) whereas the other geometries are based on icosahedra. For s = 1.2, 1.3, the global-minimum geometries take icosahedra as building units. The geometries based on Ino decahedra must reduce the ruggedness of the potential energy surfaces compared with the icosahedron-based geometries.

Figure 2 shows the performance of HMGPAC for the BLJ clusters for s = 1.4, 1.6, 1.8, 2.0. Compared with the results for the BLJ clusters for $s \leq 1.3$ (Figure 1), computational costs increase for $s \geq 1.4$. Hence the efficiency of HMGPAC is affected by the difference between the sizes of the A and B atoms.

According to the study of Tao et al. [18], the shapes of the global-minimum geometries affect the efficiency of their optimization method. Among the minima missed by them, the global minima of BLJ_{88} and BLJ_{89} for s = 1.3 take oblate structures whereas those of BLJ_{99} and BLJ_{100} for s = 1.3 are prolate. They mention that the method disfavors oblate or prolate structures because a variant of the interior operator used in the study favors spherical shapes. Rondina and Da Silva [19] could not find the minima of BLJ_{99} and BLJ_{100} for s = 1.3 because their geometrical operators did not favor very pronounced prolate structures. In the present study, however, these minima were located by

HMGPAC. The shapes of the global-minimum structures would not influence the efficiency of HMGPAC.

Most of the clusters show core-shell structures where the core is constructed by small sized A atoms and the shell consists of the B atoms [13]. In the present algorithm, the atom-type conversion operator is first carried out. Consequently core-shell structures would be generated after the conversion operator. Hence the interior operator may move the B atom present in the outer shell to the core region formed by A atoms. This movement cannot lower the potential energy of the cluster since it destroys the A-atom core. The following modification on the interior operator must improve the optimization algorithm: the highest-energy atom in the core is moved to the vicinity of the center of the mass of the cluster.

3.2. Global minima of BLJ_5 to BLJ_{50} for s = 1.4 to 2.0.

The global optimization of the BLJ clusters with s = 1.4 to 2.0 has been never performed. The optimized geometries are deposited in supplementary data. To clarify relative positions of the A and B atoms, distances between the atoms and the center of mass of the cluster are plotted in Figure 3. The distances for the A atoms are usually shorter than those for the B atoms. Hence the A atoms construct cores of the clusters whereas the B atoms form shells of them. The overlaps of the distributions of the A and B atoms are found for a few clusters. In this case, A atoms may occupy positions in the outer shell. The distribution patterns of the A atoms in the s = 2.0 clusters are considerably different from the corresponding ones in the s = 1.4 clusters and the distribution patterns gradually change depending on the parameter s. This is also the case for the distribution patterns of the B atoms. This suggests that the structures of the BLJ clusters are sensitive to the s parameter.

The geometries of the BLJ clusters with $N \leq 12$ are shown in supplementary data. The configurations of the N = 5, 6 clusters are independent of the s value. However the structures of clusters with $N \geq 7$ are sensitive to the size ratio and thus no common growth sequence is observed for the BLJ clusters.

For the BLJ clusters with $N \geq 13$, the number of the A atoms in BLJ_N, $N_A(N)$, is shown in Figure 4. In this figure, structural properties of the clusters are also shown by symbols. The number $N_A(N)$ tends to increase with increasing cluster size. The curves for s = 1.4, 1.5 are more rugged than those for larger s values. This indicates that the growth sequence patterns of the clusters for $s \leq 1.5$ are considerably different from those for $s \geq 1.6$.

The number of atoms surrounding a core atom (coordination number for an A atom) was analyzed for the global-minimum structures. In the analysis, the surrounding atom must satisfy the following condition: the distance between it and a core atom is shorter than a tentative cutoff distance which is 1.2 times as long as the equilibrium interatomic distance. The value of N_{max} is 12 for a lot of the BLJ clusters (closed symbols in Figure 4).

Figure 5 shows the geometries of the coordination atoms and the core atom in the BLJ clusters with N_{max} = 12. The polyhedron constructed by the coordination atoms is characterized with the numbers of triangular and square faces (r and q) in the surface and the notation (r/q) is used to represent it. The icosahedra are denoted by (20/0). The BLJ clusters for s = 1.4, 1.5 shows both the icosahedral and (10/5) structures. The (8/6) structures are not found for the BLJ clusters with $s \leq 1.5$. These structures are divided into two types I and II, triangular orthobicupola and cuboctahedron, which are included in the hexagonal close-packed and cubic close-packed structures, respectively. The triangular orthobicupolas appear in the clusters for $s \geq 1.6$ whereas the cuboctahedra are found for $s \geq 1.7$. The large sized atoms of $s \geq 1.7$ induce complicated structural transitions in the growth sequence patterns of the BLJ clusters. Hence it is interesting to determine structures of clusters such as a mixture of CH_4 and SiF_4 molecules (ε/k = 140.42 K and σ = 4.015 Å for CH_4 [26] and ε/k = 140.14 K and σ = 6.692 Å for SiF_4 [26] where k is Boltzmann constant). Bimetallic clusters with a significant size difference between constituent metal atoms might display novel structures and properties.

The relative stability of the BLJ clusters is calculated using

$$S_N = E_{N+1} + E_{N-1} - 2E_N \qquad (5)$$

The results are shown in Figure 6 where a positive value of S_N means that BLJ_N is relatively stable compared with $BLJ_{N\pm1}$. The magic numbers of 13, 19, 23, 26, and 29 are observed for the BLJ clusters for s = 1.4. The BLJ clusters with the magic numbers are stabilized because 1, 2, 3, 4, and 5 icosahedra are constructed in them. A few BLJ clusters for s = 1.5, 1.6 are relatively stable because of the formation of the icosahedral structures. For $s \geq 1.6$, the magic numbers considerably depend on the size ratio, s.

The structural analysis based on the coordination atoms is not useful for understanding stability of non-icosahedral clusters. An example is drawn by using the s = 1.4 cluster with N = 40. Each of the s = 1.4 clusters with N = 36 – 40 includes one (20/0) structure and two (10/5) structures. Since the number of these structures is constant, these structures are not responsible for the relative stability of the cluster with N = 40. We can see another example relating to (8/6) structures, the s = 1.7, 1.8 clusters with N = 44 – 50. The clusters with 44 to 50 atoms include 2, 3, 3, 3, 4, 4, and 4 (8/6) structures, respectively. However, the cluster sizes at which the number of the (8/6) structures increases (N = 45, 48) are different from the magic number of 47.

Stability of the BLJ cluster is related to the structure of the outer shell. In the 40-atom cluster for s = 1.4, 13 A atoms form the (10/5) core structure. It is covered with many triangles formed by 27 B atoms as shown in Figure 7. The lengths of the sides of them range from 1.54σ to 1.65σ. This indicates that no more atoms can be embedded in the shell. Hence the core is fully surrounded by the B atoms. This covering due to the B atoms results in the relative stability of the cluster.

In the 47-atom clusters for s = 1.7, 1.8, the outer shells formed by the B atoms fully cover the cores of the 25 A atoms. The outer shell consists of triangles and 4-membered rings. This is usually found for many clusters corresponding to the magic numbers. The stability of the BLJ clusters can be explained by the existence of the icosahedra and the stable outer shells formed by the 3-membered and 4-membered rings.

4. Conclusions

The heuristic method combined with the atom-type conversion, interior, and surface operators was applied to the BLJ clusters for s = 1.05 to 1.3. It reproduced most of the global minima reported previously and located three new global minima. Moreover the method was used to examine the BLJ clusters for s = 1.4 to 2.0. Hence the structural data of the BLJ clusters with $N \leq 50$ are extended. For s = 1.4, 1.5, icosahedral structures are often observed whereas two close-packed structures appear for $s \geq 1.6$. The clusters for $s \geq 1.6$ show complicated growth sequence patterns including two close-packed structures. The complicated patterns have never been obtained experimentally. It would be interesting to determine structures of clusters with significant differences between atomic sizes.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.comptc.2014.xx.xxx.

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Figure Captions

Figure 1. The number of local optimizations N_{opt} required for searching for the global minimum of the binary Lennard-Jones cluster: circles, s = 1.1; squares, s = 1.2; triangles, s = 1.3. For clarity the data for s = 1.2, 1.3 are offset vertically by 10^2 and 10^4, respectively.

Figure 2. The number of local optimizations N_{opt} required for searching for the global minimum of the binary Lennard-Jones cluster: circles, s = 1.4; squares, s = 1.6; triangles, s = 1.8; diamonds, s = 2.0. For clarity the data for s = 1.6, 1.8, 2.0 are offset vertically by 10^2, 10^4 and 10^6, respectively.

Figure 3. Distribution patterns of distances r(X-COM) (X = A or B) between the center of mass (COM) of the binary Lennard-Jones cluster and the A (or B) atoms: (a), s = 1.4; (b), s = 1.6; (c), s = 1.8; (d), s = 2.0. Bars and dots represent distances obtained for the A and B atoms, respectively.

Figure 4. The number of the A atoms $N_A(N)$ in the global-minimum geometry of the binary Lennard-Jones cluster for s = 1.4 to 2.0. The data for s = 1.5 to 2.0 are offset vertically by 100(s – 1.4) for clarity. The maximum coordination number (N_{max}) obtained for the cluster is also shown in this figure using symbols (see text for the definition of N_{max}): □, $N_{max} < 12$; ○, $N_{max} > 12$; closed symbols, $N_{max} = 12$. For $N_{max} = 12$, five symbols are used to distinguish the geometries formed by 12 coordination atoms: ●, (20/0); ♦, mixture of (20/0) and (10/5); ■; (10/5), ▲, (8/6)-I; ▼, (8/6)-II (see the text for the definitions of (20/0), (10/5), and (8/6)).

Figure 5. Stereographic views of typical geometries constructed by the 12 coordination atoms and the core atom in the binary Lennard-Jones clusters with $N \geq 13$. These views are drawn using only the A atoms. In the (20/0) configurations, however, the number of the A atoms ranges from 4 to 12. The (10/5) configurations include 10 to 12 A atoms. The (8/6) configurations consist of only the A atoms.

Figure 6. Relative stability S_N of the global-minimum geometries of the binary Lennard-Jones clusters. The data for s = 1.5 to 2.0 are offset vertically by 50(s – 1.4) for clarity. The sizes of the clusters with $S_N \geq \varepsilon$ are also described.

Figure 7. The stereographic views of the s = 1.4 cluster with N = 40. The A atoms are shown by spheres and the outer shell is shown by small spheres (the positions of the B atoms) and connectors between them. The connectors with the lengths of 1.54σ to 1.65σ are drawn to understand the shape of the shell.

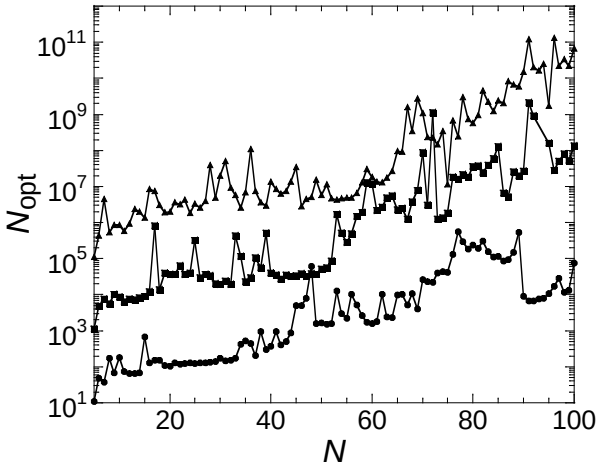
10^{11}
10^{9}
10^{7}
10^{5}
10^{3}
10^{1}
N_{opt}
20
40
60
80
100
N

Fig. 1

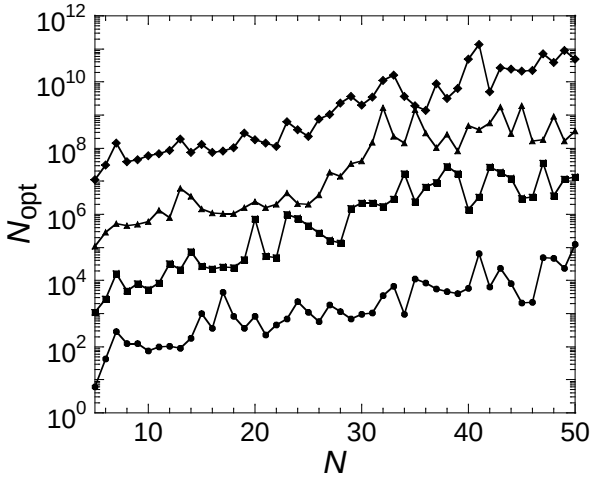
10^{12}
10^{10}
10^{8}
10^{6}
10^{4}
10^{2}
10^{0}
N_{opt}
10
20
30
40
50
N

Fig. 2

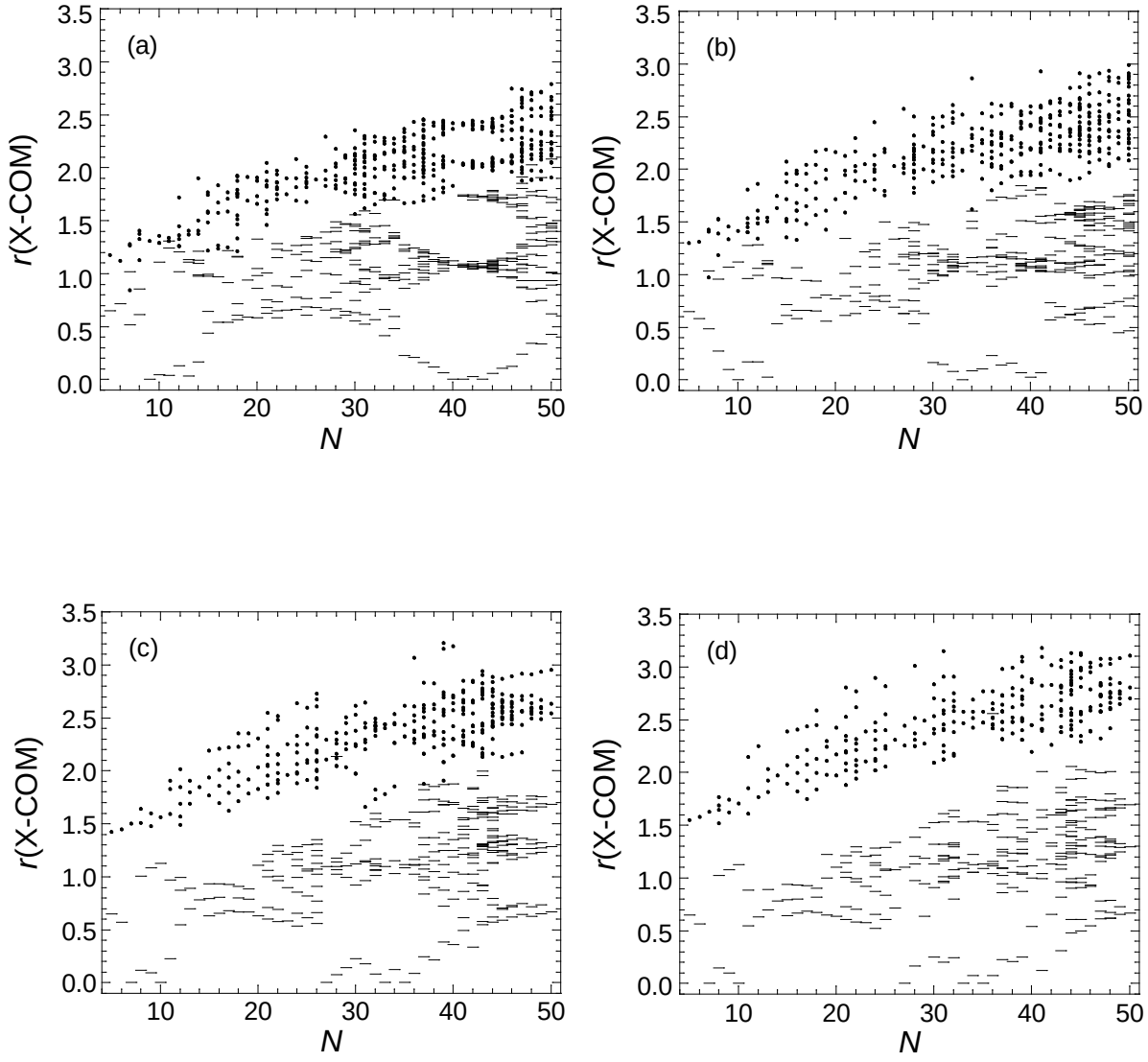

Fig. 3

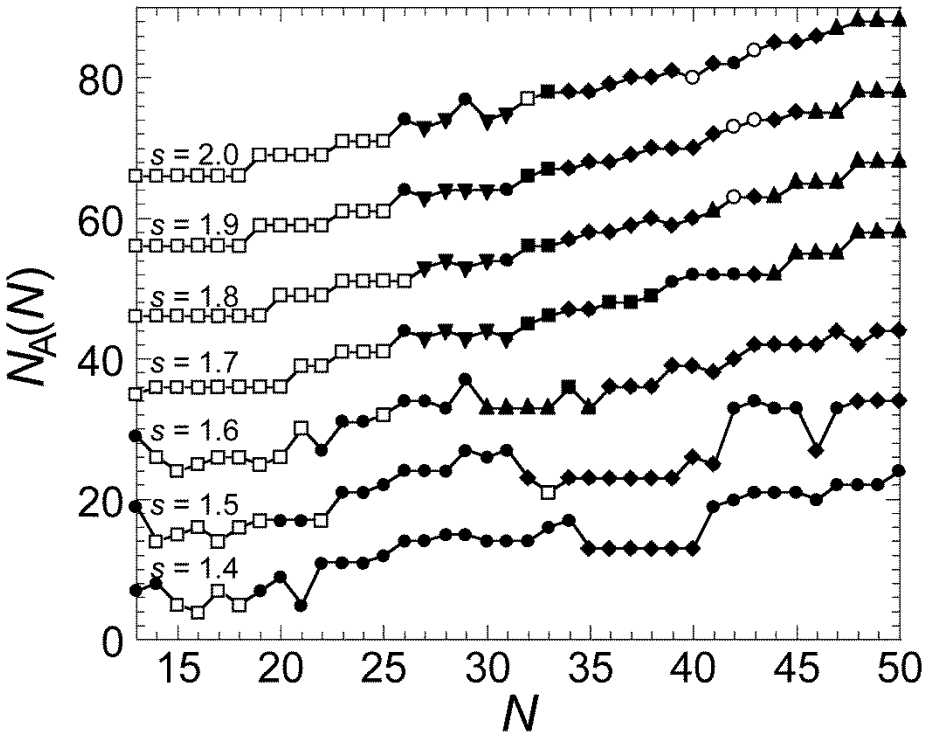
80
60
40
20
0
$N_A(N)$
s = 2.0
s = 1.9
s = 1.8
s = 1.7
s = 1.6
s = 1.5
s = 1.4
15
20
25
30
35
40
45
50
N

Fig. 4

(20/0)

(10/5)

(8/6)-I

(8/6)-II

Fig. 5

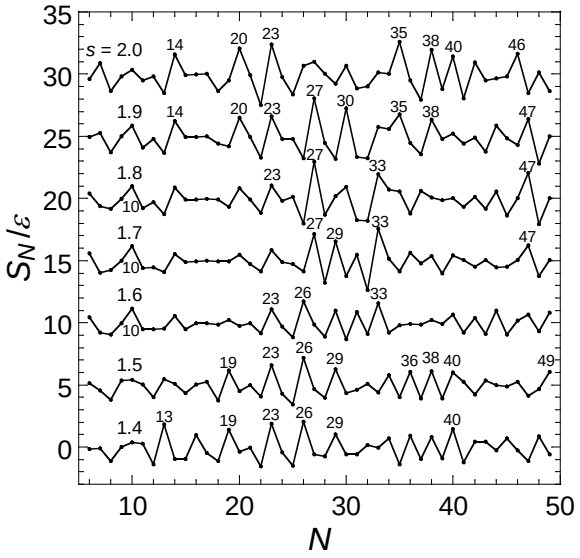

Fig. 6

Fig. 7

Binary Lennard-Jones Atomic Clusters: Structural Features Induced by Large-Sized Atoms

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Supplementary data

Table S1. The lowest energies of the binary Lennard-Jones clusters for s = 1.05 to 1.3 obtained in the present study (E_N/ε).

Table S2. The lowest energies of the binary Lennard-Jones clusters for s = 1.4 to 2.0 obtained in the present study (E_N/ε).

Table S3. The Cartesian coordinates of new global minima of BLJ_{59}(s = 1.15), BLJ_{68}(s = 1.15), and BLJ_{70}(s = 1.2).

Table S4. The Cartesian coordinates of the lowest energies of the binary Lennard-Jones clusters for s = 1.4 to 2.0.

Figure S1. Configurations of the binary Lennard-Jones clusters with N = 5 – 12. The configurations of the s = 1.8 clusters are similar to the corresponding ones of the s = 1.9 clusters. The configurations of the N = 5, 6 clusters are independent of the s value.

Table S1. The lowest energies of the binary Lennard-Jones clusters for s = 1.05 to 1.3 obtained in the present study (E_N/ε).

	E_N/ε					
N	s = 1.05	s = 1.1	s = 1.15	s = 1.2	s = 1.25	s = 1.3
5	-9.111507	-9.119302	-9.127219	-9.135241	-9.143350	-9.151532
6	-12.712962	-12.715734	-12.720554	-12.727718	-12.737707	-12.751325
7	-16.547241	-16.557098	-16.562111	-16.565375	-16.572175	-16.576776
8	-19.887476	-19.948687	-20.102320	-20.233378	-20.333773	-20.400814
9	-24.234145	-24.300649	-24.364017	-24.442494	-24.533074	-24.644760
10	-28.641948	-28.771585	-28.863192	-28.963939	-29.502679	-29.896713
11	-33.127634	-33.371304	-33.571031	-33.966602	-34.345763	-34.749685
12	-38.629544	-38.954245	-39.016600	-39.055815	-39.087588	-39.203335
13	-45.166580	-45.543272	-45.577215	-45.553927	-45.592206	-45.601094
14	-48.678921	-49.049816	-49.252081	-49.327774	-49.361851	-49.421887
15	-53.167589	-53.599281	-53.874698	-54.064278	-54.163210	-54.222875
16	-57.758981	-58.279990	-58.561496	-58.855874	-59.067444	-59.470682
17	-62.419138	-63.059172	-63.367529	-63.715344	-64.365365	-64.790023
18	-68.022619	-68.792764	-69.162203	-69.601233	-69.915015	-70.151377
19	-74.524048	-75.433396	-75.742422	-76.235787	-76.589260	-76.859376
20	-79.067291	-80.143826	-80.606044	-81.049244	-81.465579	-81.777835
21	-83.735808	-84.978975	-85.558493	-85.958319	-86.397935	-86.806107
22	-89.272798	-90.682088	-91.377400	-91.867225	-92.368564	-92.720013
23	-95.813706	-97.429591	-98.124846	-98.645805	-99.186042	-99.606519
24	-100.407430	-102.241482	-103.094695	-103.594194	-104.215802	-104.674634
25	-105.878653	-108.045220	-108.973915	-109.567066	-110.182559	-110.621882
26	-112.438253	-114.892839	-115.856394	-116.459773	-117.119402	-117.480017
27	-116.926080	-119.543605	-120.824602	-121.413505	-122.140725	-122.587527
28	-122.322287	-125.296607	-126.686572	-127.341138	-128.036984	-128.415202
29	-128.795218	-132.108090	-133.610721	-134.246055	-134.974912	-135.341699
30	-133.409767	-136.742249	-138.632308	-139.296381	-139.997093	-140.582023
31	-138.662748	-142.433255	-144.488697	-145.238298	-145.962936	-146.516926
32	-145.044787	-149.212031	-151.384854	-152.149159	-152.905938	-153.348422
33	-150.010109	-154.633546	-157.272375	-158.185112	-159.258976	-159.598157
34	-156.228179	-161.360048	-164.222021	-165.168631	-166.318301	-166.653616
35	-161.190333	-166.185706	-168.882563	-170.282025	-171.344302	-171.853006
36	-166.111652	-171.524014	-174.798837	-176.347917	-177.367846	-177.844845
37	-172.189967	-178.167061	-181.675233	-183.248506	-184.345543	-184.724505
38	-177.260697	-183.371989	-187.367687	-189.280007	-190.778073	-191.184019
39	-183.003251	-189.903875	-194.229977	-196.261792	-197.847765	-198.228135
40	-188.146744	-195.024681	-199.703534	-203.169138	-204.897420	-204.963823
41	-193.743072	-201.346753	-206.479560	-210.149549	-212.023029	-212.073757

42	-199.257511	-207.024045	-212.864370	-217.116931	-219.151586	-219.163369
43	-205.003305	-213.011525	-219.440909	-224.072028	-226.283209	-226.239574
44	-210.978612	-218.600859	-226.066862	-231.099052	-233.490683	-233.385520
45	-216.856331	-224.652192	-232.763363	-238.202225	-240.774604	-240.676356
46	-223.210589	-229.387288	-237.126607	-242.531934	-245.105004	-245.364214
47	-228.725544	-234.934267	-242.723641	-248.218022	-251.068364	-251.181462
48	-235.079224	-240.845542	-249.375588	-255.212873	-258.051347	-258.057115
49	-242.011604	-247.555272	-254.328385	-260.339254	-263.648530	-264.146588
50	-247.882695	-254.363907	-260.903328	-267.329407	-270.658086	-271.250575
51	-254.916947	-261.263002	-265.962776	-272.214736	-276.007398	-277.913411
52	-261.953177	-266.585540	-272.093082	-279.115531	-282.974620	-285.100422
53	-268.991573	-271.915714	-277.756061	-284.687258	-289.573568	-292.286192
54	-276.058231	-278.194041	-283.532817	-291.129765	-296.605354	-299.477866
55	-283.154531	-284.159496	-289.358203	-297.413420	-303.663061	-306.733764
56	-287.691892	-290.398039	-296.263148	-304.064330	-310.691065	-313.981977
57	-292.490914	-296.039531	-302.288570	-308.603733	-315.238733	-318.655257
58	-298.295002	-302.562491	-309.171713	-314.892908	-321.914589	-325.589970
59	-303.893779	-309.038480	-315.027359	-320.706313	-327.501569	-331.286991
60	-310.001341	-315.474426	-321.988253	-326.165572	-333.705967	-338.396340
61	-316.112220	-321.775834	-327.728804	-332.499319	-339.574283	-345.440684
62	-321.789205	-326.823952	-334.662475	-339.138840	-346.177037	-352.541258
63	-327.901806	-333.289735	-340.639075	-345.885361	-351.339146	-357.469508
64	-334.013197	-339.577727	-347.239596	-352.249726	-358.040393	-363.997742
65	-339.910437	-345.702127	-352.920771	-358.785658	-363.528091	-369.664027
66	-346.360633	-352.051080	-359.749940	-365.735817	-370.103112	-376.666635
67	-352.827543	-358.106731	-365.780253	-372.494895	-376.843606	-383.146334
68	-359.272795	-364.666125	-372.247969	-378.825463	-383.252132	-388.025204
69	-365.744424	-371.201139	-378.279505	-384.981542	-389.872707	-393.796485
70	-372.669868	-377.921655	-385.326178	-391.735161	-396.944371	-400.540009
71	-379.710375	-384.295723	-391.564061	-398.156558	-403.529486	-407.410007
72	-385.168824	-390.588771	-397.654760	-404.850956	-410.107263	-414.312666
73	-391.559518	-396.776526	-404.095588	-411.255891	-416.498169	-420.923993
74	-397.664635	-402.397866	-410.534023	-418.261933	-423.659482	-427.714840
75	-403.509173	-408.569903	-417.299214	-425.265743	-430.250717	-434.557994
76	-409.836259	-414.633801	-423.812270	-431.281457	-436.538490	-441.662589
77	-416.441050	-420.873025	-430.684586	-437.832462	-443.347693	-448.595192
78	-422.800176	-427.333481	-436.990405	-444.864069	-450.147772	-455.747811
79	-429.291308	-433.956776	-443.855667	-451.921407	-457.300970	-462.413785
80	-436.214492	-440.436405	-450.392713	-457.933230	-464.399834	-469.652236
81	-443.191273	-446.783469	-456.626482	-464.450846	-471.122664	-476.399256
82	-448.772200	-453.113837	-463.282074	-471.263190	-477.619634	-483.437070
83	-455.072951	-459.576481	-470.064073	-477.723147	-484.474951	-490.324955

84	-461.542943	-466.338378	-476.669838	-484.538812	-491.591546	-497.524938
85	-468.086930	-472.943379	-483.671543	-491.066290	-498.453301	-504.660242
86	-474.634175	-479.520778	-490.630031	-497.860282	-504.842168	-511.844354
87	-481.551013	-485.876908	-497.578761	-504.764331	-511.400044	-518.785356
88	-488.468369	-492.216494	-503.728759	-511.443323	-518.256499	-525.996499
89	-494.056891	-498.342007	-510.052009	-517.829589	-525.381891	-530.791989
90	-500.273073	-504.977129	-516.704386	-524.617913	-531.763926	-537.327668
91	-506.729133	-511.845979	-522.859880	-531.680233	-538.411196	-542.989912
92	-513.205038	-518.431759	-529.190149	-538.316013	-544.507909	-549.757224
93	-519.775813	-524.964281	-535.594853	-544.573272[a]	-551.431854	-556.443498
94	-526.614509	-531.583051	-542.476905	-550.802667[a]	-558.070885	-562.801205
95	-533.465067	-538.741277	-548.732770	-557.785086	-564.709518	-569.480421
96	-539.063361	-544.671597	-555.145507	-564.674461	-571.389275	-576.517002
97	-545.436537	-551.416081	-561.876490	-571.392434	-578.201634	-583.871531
98	-551.683813	-558.264685	-568.603054	-578.000233	-584.953816	-590.787413
99	-558.310074	-564.964519	-575.609709	-585.066165	-592.008931[a]	-597.679071
100	-564.909753	-571.812888	-582.701043	-591.768143	-599.043884[a]	-604.796307

[a] The global minima reported previously are not obtained in the present study: the reported lowest energies of the four clusters are -544.766420ε, -551.033813ε, -592.138846ε, and -599.264624ε.

Table S2. The lowest energies of the binary Lennard-Jones clusters for s = 1.4 to 2.0 obtained in the present study (E_N/ε).

	E_N						
N	s = 1.4	1.5	1.6	1.7	1.8	1.9	2.0
5	-9.168058	-9.184718	-9.201428	-9.218112	-9.234711	-9.251172	-9.267450
6	-12.797426	-12.968869	-13.138655	-13.273980	-13.373777	-13.439465	-13.473670
7	-16.584984	-16.609636	-16.634759	-16.781371	-17.140302	-17.672694	-18.073130
8	-20.491743	-20.714043	-20.902561	-21.283208	-21.521513	-21.634684	-21.814930
9	-25.532740	-25.991730	-26.148194	-26.529040	-26.756037	-26.868864	-26.901093
10	-30.595637	-30.931901	-31.451692	-31.799676	-32.012806	-32.132430	-32.187970
11	-35.274878	-35.487787	-35.603591	-35.917049	-36.270022	-36.549295	-37.111833
12	-39.688603	-40.000211	-40.269325	-40.619462	-41.305141	-41.889065	-42.523248
13	-45.511459	-45.475297	-45.438215	-45.844938	-46.632565	-47.448527	-48.110134
14	-49.508949	-50.489724	-51.095901	-51.987964	-53.222502	-54.331902	-55.233067
15	-54.477032	-55.390724	-56.181783	-57.624738	-58.931166	-59.981696	-60.758081
16	-60.382227	-60.928253	-61.799365	-63.402124	-64.728570	-65.711712	-66.356133
17	-65.332397	-66.446027	-67.449039	-69.267007	-70.600218	-71.481302	-71.965936
18	-70.757536	-71.703520	-73.165711	-75.146699	-76.485964	-77.246409	-77.549442
19	-77.314533	-78.191386	-79.045725	-81.113225	-82.446070	-83.597114	-84.509377
20	-82.495693	-83.514565	-84.683290	-87.167631	-89.054680	-90.753192	-91.988951
21	-88.025471	-89.330178	-90.570373	-92.763166	-94.850253	-96.404037	-97.424715
22	-93.601467	-95.143253	-96.512158	-98.657162	-100.718586	-102.128446	-102.921119
23	-100.740941	-101.901346	-103.276147	-105.416880	-107.744490	-109.579428	-110.903815
24	-106.012643	-107.064064	-108.932853	-111.349064	-113.721598	-115.433419	-116.521863
25	-111.721202	-112.963841	-114.879107	-117.418348	-119.874315	-121.508101	-122.388638
26	-118.914648	-120.425633	-122.006208	-123.754916	-125.890569	-127.784324	-129.869161
27	-124.066931	-125.697620	-127.430425	-130.980905	-133.907416	-135.837752	-136.658297
28	-129.778684	-131.301741	-133.017782	-136.064944	-138.966341	-140.858567	-142.460916
29	-136.240883	-137.929835	-139.739463	-142.945508	-145.342393	-146.434540	-148.254717
30	-141.678730	-143.322385	-145.480894	-148.313123	-151.524277	-153.819680	-154.825577
31	-147.678325	-149.398191	-152.530780	-154.937882	-156.759040	-158.954495	-160.752462
32	-154.290081	-155.872192	-158.700621	-161.073978	-163.768277	-165.730628	-167.803356
33	-160.737338	-162.262866	-165.783355	-169.571951	-172.578008	-174.297678	-175.843136
34	-167.225215	-169.250795	-171.326596	-175.526184	-179.450528	-182.112852	-183.740999
35	-173.011973	-175.447948	-177.660242	-181.357766	-185.635002	-189.341608	-191.637722
36	-180.176688	-182.632268	-184.177344	-188.040054	-191.280568	-194.828824	-196.965963
37	-186.439022	-188.761434	-190.811208	-194.081783	-198.154921	-200.863152	-202.799137
38	-193.649484	-195.963276	-197.608976	-200.368418	-204.430886	-208.347221	-210.677219
39	-200.030446	-202.040051	-204.172478	-206.281050	-210.627234	-214.480766	-216.589951
40	-207.322597	-209.230681	-210.847376	-213.220313	-216.945765	-220.807300	-223.700145
41	-213.170471	-215.407179	-216.848113	-219.743606	-223.258093	-226.951993	-229.365627

42	-220.223427	-221.319539	-223.652390	-226.250732	-230.236470	-233.679219	-236.995833
43	-226.823468	-227.979704	-230.062836	-233.255889	-237.073585	-240.538283	-243.686941
44	-232.998720	-234.297422	-237.368902	-240.201249	-244.756631	-248.636081	-250.867906
45	-239.434596	-240.654799	-243.724171	-247.677700	-251.897352	-255.883412	-258.409108
46	-245.176668	-247.137015	-251.048217	-255.625219	-260.391381	-263.282585	-266.121423
47	-251.178900	-253.365117	-258.224693	-263.555682	-268.881577	-271.372063	-272.215887
48	-258.325633	-260.451080	-264.768267	-270.247871	-275.324355	-278.085201	-279.832502
49	-264.629464	-267.906522	-271.973689	-278.200778	-283.859545	-286.985560	-287.340181
50	-271.536410	-274.312888	-278.361820	-286.133713	-292.387819	-295.883575	-296.237038

Table S3. The Cartesian coordinates of new global minima of BLJ_{59}(s = 1.15), BLJ_{68}(s = 1.15), and BLJ_{70}(s = 1.2).

s = 1.15, $E59/\varepsilon$ = -315.027359

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.140175	0.000000	0.000000
3B	-1.137834	-0.057027	0.000000
4A	0.494187	-0.979074	0.261753
5A	-0.443904	-0.999367	-0.269042
6A	0.491238	-0.724123	-0.753911
7A	-0.453420	-0.757523	0.749344
8A	0.329392	-1.754730	-0.467342
9A	-0.240578	-1.774761	0.451201
10A	-0.454998	-0.288714	-1.040820
11A	0.444840	1.002915	-0.269773
12A	0.469900	-0.283722	1.045810
13A	0.453347	0.725873	0.756281
14A	-0.485194	0.726546	-0.750983
15A	-0.257030	-1.330716	-1.274224
16A	0.460516	0.283724	-1.046651
17A	0.323572	-1.333161	1.263963
18A	-0.472350	0.248359	1.047400
19A	-0.493856	0.983287	0.282673
20B	0.936278	-2.037827	0.510308
21B	-0.833277	-2.075499	-0.529333
22B	-0.332862	-0.571121	1.904278
23B	0.361440	-0.534588	-1.906511
24B	1.453960	-1.255739	-0.345379
25B	-1.388775	-1.330603	0.334954
26B	-1.401959	-0.989578	-0.917156
27B	1.450746	-0.930534	0.911088
28B	-0.847727	-1.616480	1.455926
29B	0.928114	-1.555597	-1.469166
30B	0.333868	0.482580	1.924487
31B	-0.361441	0.478854	-1.923385
32B	0.295385	1.402377	-1.381990
33B	-0.364885	1.385079	1.373319
34B	-0.387379	1.883489	-0.443870
35B	1.460348	-0.328179	-1.245316
36B	-1.439191	-0.418115	1.248239
37B	1.431138	1.217419	0.339671
38B	1.430818	0.918431	-0.904357
39B	1.441542	0.311080	1.259047
40B	-1.454125	0.255687	-1.252327
41B	-0.895490	-0.695612	-2.050873
42B	0.929582	-0.672499	2.049860
43B	0.070335	-2.812766	-0.014254
44A	0.326650	1.777139	0.496090
45B	0.045420	-2.482042	-1.341051
46B	0.078924	-2.497485	1.317160
47B	-1.489342	1.153296	-0.326527
48B	-1.479030	0.823218	0.911139
49B	0.922867	2.052260	-0.495873
50B	0.965160	0.564896	-2.063933
51B	0.938886	1.505524	1.486566
52B	1.177358	-2.517976	-0.656181
53B	-1.049795	-2.580724	0.631567
54B	-0.983047	0.503541	2.066233
55B	-1.014318	1.471749	-1.482597
56B	-1.117291	-1.946052	-1.759617
57B	1.213697	-1.908147	1.743174
58B	-0.016431	-1.662660	-2.361797
59B	0.099777	-1.685507	2.348008

s = 1.15, $E68/\varepsilon$ = -372.247969

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.142436	0.000000	0.000000
3B	-1.140848	-0.060190	0.000000
4A	0.478257	-0.271482	0.984821
5A	-0.463264	-0.296999	-0.984632
6A	0.469029	0.268552	-1.005925
7A	-0.482541	0.244179	1.005732
8A	-0.451447	-0.761115	0.727938
9A	0.490939	-0.736787	-0.727420
10A	-0.478833	0.726060	-0.750603
11A	0.439906	0.750810	0.750068
12A	0.499931	-1.012039	0.264663
13A	-0.445905	-1.037160	-0.263950
14A	0.328880	-1.775100	-0.467316
15A	-0.234902	-1.789632	0.468565
16A	-0.253727	-1.326826	-1.270476
17A	0.323263	-1.310716	1.271396
18A	-0.497638	1.002681	0.271389
19A	0.444129	1.027315	-0.272120
20A	0.291367	-0.516383	-1.747674
21A	-0.263782	-0.529780	1.748032
22A	-0.297823	0.397142	-1.775600
23A	0.276459	0.413538	1.775300
24B	0.914881	-1.518425	-1.482884
25B	-0.833630	-1.563470	1.483962
26B	-0.877050	-0.645366	-2.018622
27B	0.909804	-0.596832	2.019049
28B	0.940297	-2.052033	0.537475
29B	-0.830859	-2.099104	-0.536019
30B	0.321871	1.352686	-1.417456
31B	-0.392713	1.334852	1.416492
32B	-1.402969	-1.003798	-0.915025
33B	1.453896	-0.927837	0.915694
34B	1.458018	-1.267968	-0.345225
35B	-1.389188	-1.342781	0.346136
36B	1.432659	-0.354576	-1.278537
37B	-1.412006	-0.428661	1.278801
38B	-1.435426	0.250199	-1.270118
39B	1.420233	0.326378	1.269898
40B	-0.388823	1.875813	-0.533820
41B	0.289449	1.894071	0.532472
42B	0.876321	0.454114	-2.094426
43B	-0.899063	0.408794	2.094109
44B	1.435361	0.895681	-0.911482
45B	-1.480570	0.819457	0.910860
46B	-1.480160	1.162607	-0.357253
47B	1.416849	1.239227	0.356388
48B	-0.942579	1.381160	-1.603456
49B	0.868478	1.430037	1.602447
50B	-0.021687	-0.136440	-2.805580
51B	0.028801	-0.133123	2.805663
52B	0.024429	-1.464707	-2.399932
53B	0.052738	-1.462262	2.400955
54B	0.073267	-2.455767	1.384798
55B	0.056254	-2.457195	-1.383073
56B	0.074415	-2.822696	0.000992
57B	0.936756	2.047055	-0.551376
58B	-1.043311	1.995248	0.549933
59B	1.179281	-1.855787	1.806634
60B	-1.079826	-1.916620	-1.805313
61B	1.126025	-0.748735	-2.504677
62B	-1.085053	-0.805249	2.505214
63B	1.182878	-2.511194	-0.668360
64B	-1.048933	-2.569555	0.670144
65B	-1.178482	0.484521	-2.526527
66B	1.151279	0.547726	2.526147
67B	-0.085172	1.165687	-2.616060
68B	0.023597	1.170407	2.615220

s = 1.2, $E70/\varepsilon$ = -391.735161

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.165837	0.000000	0.000000
3B	-1.163824	-0.046742	0.000000
4A	0.474046	-0.006897	1.029543
5A	0.474083	-0.008769	-1.029535
6A	-0.459050	-0.546907	0.897761
7A	-0.459015	-0.548539	-0.896807
8A	-0.481452	0.508523	0.909942
9A	-0.481417	0.506866	-0.910907
10A	0.492439	-0.919819	0.520140
11A	0.492458	-0.920764	-0.518473
12A	-0.450684	-1.077743	0.000959
13A	0.448779	0.932190	0.532520
14A	0.448799	0.931220	-0.534222
15A	0.308969	-0.950669	-1.575933
16A	0.308909	-0.947801	1.577645
17A	-0.253128	-1.622866	-0.910143
18A	-0.253162	-1.621208	0.913058
19A	0.320543	-1.857887	0.001683
20A	-0.276607	-0.057271	-1.835432
21A	-0.276676	-0.053933	1.835498
22A	-0.495301	1.063379	-0.000989
23A	0.282675	0.868498	-1.624883
24A	0.282613	0.871452	1.623286
25B	-0.874401	-1.142043	-1.852699
26B	-0.874472	-1.138672	1.854714
27B	0.941537	-1.883275	1.068007
28B	0.941577	-1.885215	-1.064571
29B	-0.863524	-2.198720	0.001970
30B	0.919355	-0.062496	-2.141127
31B	0.919276	-0.058602	2.141246
32B	-0.385280	1.703274	1.027979
33B	-0.385240	1.701401	-1.031115
34B	-1.436581	-1.213570	-0.664544
35B	-1.436607	-1.212359	0.666668
36B	1.481177	-0.680203	-1.141719
37B	1.481135	-0.678124	1.142981
38B	1.489703	-1.343942	0.001237
39B	-1.454793	-0.072068	-1.346076
40B	-1.454845	-0.069620	1.346121
41B	1.456927	0.648915	-1.153722
42B	1.456885	0.651012	1.152565
43B	0.326467	2.021953	-0.001845
44B	-0.926728	0.968446	-1.942844
45B	-0.926803	0.971978	1.941019
46B	-1.509043	1.072714	-0.675484
47B	-1.509069	1.073939	0.673445
48B	1.454506	1.327627	-0.001194
49B	0.909086	1.838947	-1.194889
50B	0.909040	1.841117	1.191552
51B	0.015841	0.610375	2.799768
52B	0.015947	0.605282	-2.800899
53B	0.030744	-0.810787	2.747730
54B	0.030847	-0.815783	-2.746276
55B	0.044182	-2.059222	2.006425
56B	0.044257	-2.062869	-2.002700
57B	0.050737	-2.786654	0.736713
58B	0.050764	-2.787989	-0.731667
59B	1.180371	-1.367742	-2.274432
60B	1.180286	-1.363602	2.276933
61B	-1.055891	2.146483	-0.001985
62B	1.191670	-2.665752	0.002434
63B	-1.098037	-2.353508	-1.314892
64B	-1.098086	-2.351112	1.319103
65B	-1.128779	-0.124609	-2.672217
66B	-1.128881	-0.119750	2.672369
67B	1.185912	1.205338	-2.351734
68B	1.185823	1.209613	2.349555
69B	0.032919	1.854078	-2.271260
70B	0.032832	1.858205	2.267860

Table S4. The Cartesian coordinates of the lowest energies of the binary Lennard-Jones clusters for s = 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0.

s = 1.4

$E5/\varepsilon$ = -9.168058

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
4B	0.562011	-0.324478	-1.175919
5B	0.562011	-0.324478	1.175919

$E6/\varepsilon$ = -12.797426

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.428479	0.000000	0.000000
3B	0.714240	-1.123439	0.000000
4B	0.714240	0.000000	-1.123439
5B	0.714240	0.000000	1.123439
6B	0.714240	1.123439	0.000000

$E7/\varepsilon$ = -16.584984

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.357580	0.000000	0.000000
3B	0.435909	-1.268000	0.000000
4B	0.436723	0.997830	0.782784
5B	0.436723	0.997830	-0.782784
6A	0.475301	-0.330713	0.957995
7A	0.475301	-0.330713	-0.957995

$E8/\varepsilon$ = -20.491743

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.129529	0.000000	0.000000
3B	0.564764	-1.207598	0.000000
4A	0.564764	0.485415	-0.828600
5B	1.343739	-0.545947	-1.190464
6B	-0.214212	-0.545946	-1.190464
7B	0.564763	1.157968	0.339096
8B	0.564763	-0.174674	1.194419

$E9/\varepsilon$ = -25.532740

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.307282	0.000000	0.000000
3B	0.341600	-1.261862	0.000000
4B	0.341600	0.739019	1.022813
5B	-0.624083	-0.522842	1.022812
6B	0.341240	-0.261144	-1.234644
7B	0.341241	1.153693	-0.511405
8B	-1.024440	-0.630850	-0.511407
9B	-1.024440	0.783988	0.211831

$E10/\varepsilon$ = -30.595637

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.309426	0.000000	0.000000
3B	0.245227	-1.286259	0.000000
4B	-0.818971	-0.405785	0.937669
5B	0.245230	0.880476	0.937668
6B	-1.022484	-0.587101	-0.609167
7B	0.385225	1.114343	-0.609168
8B	-1.022483	0.845962	0.011004
9B	0.385226	-0.318722	-1.229335
10A	0.500593	-0.414170	0.957050

$E11/\varepsilon$ = -35.274878

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

$E12/\varepsilon$ = -39.688603

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.311588	0.000000	0.000000
3B	0.364072	-1.260046	0.000000
4B	-0.857166	0.644562	-0.772968
5A	0.441371	0.363806	-0.954437
6A	-0.226993	-0.525013	-0.954437
7B	0.358811	1.277244	0.008300
8B	-1.127452	-0.699250	0.008301
9B	-0.845320	0.635655	0.793882
10A	-0.205900	-0.536056	0.959506
11A	0.457837	0.346609	0.959506
12B	1.027664	-0.772772	-1.322644

$E13/\varepsilon$ = -45.511459

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.162625	0.000000	0.000000
3B	-1.334847	-0.000001	0.000000
4A	0.599099	0.216006	0.924718
5A	0.599099	0.946209	0.080320
6A	0.599099	0.368784	-0.875078
7A	0.599099	-0.812710	0.491187
8A	0.599099	-0.718288	-0.621148
9B	-0.481013	1.117323	-0.675291
10B	-0.481013	0.987511	0.853962
11B	-0.481013	-0.296968	-1.271314
12B	-0.481012	-0.507009	1.203068
13B	-0.481012	-1.300861	-0.110425

$E14/\varepsilon$ = -49.508949

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.127352	0.000000	0.000000
3A	0.592266	-0.959242	0.000000
4A	0.521580	-0.290949	-0.914384
5B	0.673056	1.015971	-0.678662
6B	-0.510872	-1.106442	-0.678662
7A	0.609418	-0.339947	0.913923
8B	-0.645716	0.360193	-1.120994
9B	-0.592637	1.211545	0.188371
10B	-1.342227	-0.132237	0.188371
11A	-0.324398	-0.858651	0.628930
12A	0.560182	0.727125	0.628930
13A	-0.352689	0.196737	1.029165
14B	1.670547	-0.931868	-0.780079

$E15/\varepsilon$ = -54.477032

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.079526	0.000000	0.000000
3B	0.556964	-1.240618	0.000000
4A	0.558971	-0.302088	-0.927172
5A	0.558972	-0.302088	0.927172
6A	0.523314	0.964169	0.000000
7B	-0.213255	0.746781	1.084870
8B	-0.213255	0.746781	-1.084870
9B	-0.692887	-0.762093	0.807401
10B	-0.692887	-0.762094	-0.807400
11B	1.359862	0.766280	-1.018760
12B	1.359862	0.766281	1.018760
13B	-1.266295	0.443607	0.000000
14B	1.817039	-0.738623	-0.793370
15B	1.817040	-0.738623	0.793369

$E16/\varepsilon$ = -60.382227

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.078297	0.000000	0.000000
3B	0.539149	-1.288155	0.000000
4B	0.539150	1.212605	0.000000
5A	0.539149	-0.361462	0.908853
6A	0.539149	-0.361462	-0.908853
7B	-0.248183	0.646524	1.187849
8B	-0.248183	0.646524	-1.187849
9B	1.326481	0.646524	1.187850
10B	1.326481	0.646524	-1.187850
11B	1.800066	-0.787221	-0.781957
12B	1.800066	-0.787221	0.781957
13B	-0.721767	-0.787222	-0.781958
14B	-0.721767	-0.787222	0.781958
15B	2.300474	0.491473	0.000000
16B	-1.222177	0.491471	0.000000

$E17/\varepsilon$ = -65.332397

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.077076	0.000000	0.000000
3B	0.538537	-1.224158	0.000000
4B	0.538537	0.712228	0.995637
5A	0.538537	0.440928	-0.857548
6B	-0.236599	-0.608287	1.183039
7B	1.313673	-0.608287	1.183039
8A	1.085593	1.106981	-0.139731
9A	-0.008519	1.106981	-0.139731
10A	-0.008519	-0.530406	-0.981632
11A	1.085593	-0.530407	-0.981631
12B	1.899563	0.495209	-0.963118
13B	-0.822488	0.495209	-0.963118
14B	-1.007667	-0.829216	-0.144188
15B	2.084742	-0.829216	-0.144188
16B	2.084742	0.599718	0.590531
17B	-1.007667	0.599717	0.590531

$E/18$ ε= -70.757536

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.068583	0.000000	0.000000
3B	0.472375	-1.290041	0.000000
4A	0.539432	-0.354732	0.886332
5B	-0.716191	-0.673692	0.892452
6B	0.509702	1.215967	0.025333
7B	1.274938	0.641774	1.219719
8B	1.755298	-0.813443	0.806258
9A	0.501198	-0.371929	-0.911803
10A	-0.085764	0.535832	0.977633
11B	1.307560	0.637842	-1.157045
12B	-0.272188	0.653714	-1.168568
13B	1.762089	-0.811401	-0.759516
14B	-0.818082	-0.727974	-0.687868
15B	-1.109768	0.658640	0.137896
16B	2.284609	0.467289	0.044596
17B	0.170159	-0.088561	2.114292

18B	0.507957	-1.495441	1.532933

*E*19/ε = -77.314533

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	0.586945	0.761546	-0.553295
5A	0.586944	-0.290884	-0.895250
6A	0.586945	-0.290884	0.895251
7A	0.586946	0.761546	0.553295
8B	-0.473978	0.404933	-1.246251
9B	-0.473978	-1.060124	-0.770225
10B	1.647868	0.404931	1.246251
11B	1.647868	1.310386	0.000000
12B	1.647866	-1.060126	0.770226
13B	1.647867	0.404932	-1.246252
14B	1.647866	-1.060125	-0.770227
15B	-0.473976	1.310388	0.000001
16B	-0.473977	-1.060124	0.770227
17B	-0.473976	0.404933	1.246253
18B	-1.324398	0.000001	0.000002
19B	2.498288	-0.000002	-0.000001

*E*20/ε = -82.495693

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	0.574751	-0.340219	0.889804
5A	0.574753	-0.297721	-0.893889
6A	0.574752	0.728611	0.597329
7A	0.574753	0.772526	-0.531691
8A	1.522972	-0.851866	0.586298
9A	-0.373470	-0.851865	0.586297
10B	-0.482852	0.296434	1.276761
11B	1.632355	-1.086694	-0.732863
12B	-0.482852	-1.086693	-0.732864
13B	1.632355	0.296431	1.276764
14B	1.650150	0.390721	-1.205832
15B	1.650150	1.265852	0.065698
16B	-0.500643	1.265853	0.065696
17B	-0.500643	0.390722	-1.205834
18B	-1.329483	-0.061373	0.042240
19B	2.478987	-0.061376	0.042244
20B	0.574750	-1.634602	1.125019

*E*21/ε = -88.025471

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.143552	0.000000	0.000000
3A	0.631350	-0.953471	0.000000
4A	0.565963	-0.304034	-0.870382
5B	-0.408481	-1.163658	-0.797102
6B	0.744716	0.983034	-0.797103
7A	0.558151	-0.299836	0.889909
8B	-0.426612	-1.162470	0.743274
9B	0.733717	0.997497	0.743273
10B	1.948323	-1.046633	-0.010071
11B	1.064478	-1.464406	-1.196799
12B	1.808688	-0.079050	-1.196799
13B	-0.542524	0.291441	-1.267745
14B	1.056713	-1.470330	1.172724
15B	1.809341	-0.069303	1.172724
16B	-0.559582	0.300607	1.225481
17B	-1.330967	-0.173858	-0.029460
18B	-0.589860	1.205722	-0.029461
19B	2.111990	0.881298	-0.018003
20B	0.431210	-2.247497	-0.018002
21B	0.580801	-0.312001	-2.162446

*E*22/ε = -93.601467

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.128779	0.000000	0.000000
3A	0.559560	-0.984600	0.000000
4A	0.565306	-0.333589	0.878954
5A	0.565306	-0.333589	-0.878954
6A	0.564288	0.748104	0.573595
7A	0.564288	0.748105	-0.573594
8A	-0.371480	-0.858593	-0.576428
9A	-0.371481	-0.858593	0.576427
10A	1.502321	-0.868461	-0.563396
11A	1.502321	-0.868461	0.563396
12B	-0.506606	0.298133	1.238203
13B	-0.506604	0.298135	-1.238203
14B	1.636613	0.293979	-1.236513
15B	1.636613	0.293977	1.236514
16B	-1.327696	-0.141408	-0.000001
17B	-0.532614	1.226211	0.000000
18B	1.658320	1.229384	0.000001
19B	2.459303	-0.128964	0.000000
20B	0.580000	-1.597472	1.190838
21B	0.580001	-1.597472	-1.190838
22B	-0.296640	-2.043755	0.000000

*E*23/ε =-100.740941

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	1.498873	-0.865374	-0.572054
7A	-0.366534	-0.865374	0.572054
8A	1.498873	-0.865374	0.572054
9A	-0.366534	-0.865374	-0.572054
10A	0.566169	0.750115	-0.572054
11A	0.566169	0.750115	0.572054
12B	0.566170	-1.566992	1.236889
13B	-0.507801	0.293180	1.236889
14B	1.640140	0.293180	-1.236889
15B	-0.507801	0.293180	-1.236889
16B	0.566170	-1.566992	-1.236889
17B	1.640140	0.293180	1.236889
18B	1.667041	1.223017	0.000000
19B	-0.534702	1.223018	0.000000
20B	2.458853	-0.148441	0.000000
21B	-0.225643	-2.055208	0.000000
22B	1.357982	-2.055207	0.000000
23B	-1.326514	-0.148441	0.000000

*E*24/ε =-106.012643

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.135260	0.000000	0.000000
3A	0.567630	-0.983164	0.000000
4A	0.567630	-0.327721	0.866998
5A	0.567631	-0.327721	-0.874624
6A	1.497924	-0.864827	0.578368
7A	-0.362664	-0.864827	0.578367
8A	0.567630	0.746490	0.578366
9A	-0.365453	-0.866438	-0.569122
10A	0.567631	0.749711	-0.569123
11A	1.500715	-0.866438	-0.569121
12B	-0.508718	0.293709	1.236024
13B	0.567630	-1.570581	1.236025
14B	1.643977	0.293709	1.236026
15B	1.642303	0.292740	-1.233753
16B	0.567631	-1.568645	-1.233754
17B	-0.507041	0.292740	-1.233755
18B	2.460307	-0.151212	0.003326
19B	-0.531570	1.223130	0.003322
20B	-1.325047	-0.151212	0.003323
21B	1.361107	-2.055082	0.003324
22B	1.666830	1.223130	0.003324
23B	-0.225847	-2.055083	0.003324
24B	0.567628	-0.327721	2.174920

*E*25/ε =-111.721202

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.112432	0.000000	0.000000
3A	0.548334	-0.967902	0.000000
4A	0.544591	-0.317390	0.911073
5A	0.532271	-0.310210	-0.885358
6A	0.561764	0.736317	0.594129
7A	-0.363752	-0.851719	0.594128
8A	1.494042	-0.870735	0.537747
9A	1.461146	-0.851563	-0.606317
10A	-0.401833	-0.851094	-0.551301
11A	0.542449	0.769142	-0.551300
12A	-0.415775	0.242316	0.961442
13B	1.683082	0.247249	1.209860
14B	0.614488	-1.586283	1.209860
15B	-1.332692	-0.133543	0.083200
16B	-0.540709	1.225372	0.083200
17B	-0.558078	0.325251	-1.182124
18B	1.595473	0.325609	-1.246980
19B	0.503128	-1.548683	-1.246980
20B	-0.246432	-2.039275	0.017186
21B	1.652857	1.219604	0.017187
22B	2.446137	-0.158309	-0.058210
23B	1.343478	-2.050296	-0.058209
24B	0.390557	0.666372	1.899665
25B	-0.387291	-0.668281	1.899663

*E*26/ε =-118.914648

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	1.462844	-0.844574	0.597204
6A	-0.356180	-0.844573	0.597204
7A	0.553333	0.730748	0.597204
8A	0.553332	-0.319467	-0.888023
9A	0.553331	-1.410964	0.997703
10A	0.553333	0.772031	-0.545909
11A	-0.391933	-0.865216	-0.545908
12A	1.498598	-0.865217	-0.545908
13A	1.498598	0.226282	0.997703
14A	-0.391933	0.226283	0.997703
15B	-1.323784	-0.134588	0.095168
16B	-0.545335	0.314849	-1.176034
17B	1.331780	-2.037537	0.095170
18B	-0.545335	1.213725	0.095167
19B	2.430449	-0.134589	0.095169
20B	0.553332	-1.588100	-1.176033
21B	1.652001	1.213724	0.095168
22B	-0.225118	-2.037536	0.095169
23B	1.652000	0.314848	-1.176033
24B	-0.225117	-0.768903	1.889285
25B	0.553332	0.579410	1.889285
26B	1.331781	-0.768904	1.889286

*E*27/ε =-124.066931

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.111020	0.000000	0.000000
3A	0.555510	-0.962171	0.000000
4A	0.555510	-0.320723	0.900102
5A	0.555510	-0.320723	-0.869063
6A	-0.355416	-0.846646	0.592316
7A	1.466436	-0.846646	0.592316
8A	0.555510	0.731123	0.592315

9A	-0.385584	-0.864064	-0.555223
10A	1.496604	-0.864064	-0.555223
11A	0.555510	0.765958	-0.555223
12A	0.555510	-1.414571	0.993957
13A	-0.391790	0.226202	0.993957
14A	1.502810	0.226201	0.993957
15B	-0.532771	0.307596	-1.192687
16B	0.555510	-1.577361	-1.192688
17B	1.643791	0.307596	-1.192687
18B	-1.319406	-0.136112	0.080691
19B	1.333090	-2.036753	0.080691
20B	-0.541826	1.210696	0.080691
21B	-0.222070	-2.036753	0.080691
22B	1.652846	1.210696	0.080691
23B	2.430426	-0.136112	0.080691
24B	-0.223030	-0.770213	1.884415
25B	1.334050	-0.770213	1.884415
26B	0.555510	0.578259	1.884414
27B	0.555510	-0.320721	-2.159459

$E28/\varepsilon$ =-129.778684

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.092188	0.000000	0.000000
3A	0.537566	-0.950736	0.000000
4A	0.515886	-0.300947	-0.906316
5A	0.529280	-0.308763	0.910651
6A	-0.391414	-0.829252	-0.578692
7A	0.529204	0.748873	-0.578689
8A	1.427452	-0.832720	-0.625472
9A	0.548145	0.755306	0.569288
10A	-0.387693	-0.848910	0.569285
11A	0.502928	-1.390372	-1.005262
12A	1.457839	0.246539	-1.005260
13A	1.498945	-0.874428	0.511091
14A	-0.435265	0.253919	-0.962297
15A	-0.442180	0.257949	0.938308
16B	1.684580	0.267993	1.156217
17B	0.595850	-1.598312	1.156214
18B	-0.549716	1.212296	-0.002783
19B	-1.325853	-0.118161	-0.002786
20B	-0.249808	-2.019758	-0.074406
21B	1.635219	1.211562	-0.074400
22B	2.415802	-0.136864	-0.147896
23B	1.308176	-2.035560	-0.147899
24B	1.266382	-0.738755	-1.911490
25B	-0.291298	-0.731308	-1.872568
26B	0.493223	0.613520	-1.872566
27B	0.390605	0.665318	1.872817
28B	-0.386902	-0.667486	1.872815

$E29/\varepsilon$ =-136.240883

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.089984	0.000000	0.000000
3A	0.530452	-0.952200	0.000000
4A	0.537085	-0.292453	0.911197
5A	0.516862	-0.326867	-0.911197
6A	0.548506	0.762374	0.572722
7A	-0.399067	-0.850187	-0.572722
8A	-0.390741	-0.817888	0.576109
9A	0.524342	0.739382	-0.576108
10A	1.430292	-0.867735	-0.598452
11A	1.454113	-0.827198	0.598452
12B	0.504200	-1.671104	-1.122281
13B	1.705237	0.372796	1.122281
14A	0.501028	-1.388028	0.993919
15A	1.456399	0.237806	-0.993919
16A	-0.436214	0.247387	0.955473
17A	-0.428403	0.260681	-0.955473
18B	-1.326245	-0.110689	-0.009649
19B	-0.548733	1.212465	0.009650
20B	2.404010	-0.153217	-0.130100
21B	1.303785	-2.025557	0.130099
22B	1.629747	1.232776	-0.127173
23B	-0.283809	-2.023676	0.127174
24B	0.506309	0.646108	-1.860755
25B	-0.318033	-0.756742	1.860756
26B	0.417445	0.597201	1.898308
27B	-0.318557	-0.655310	-1.898308
28B	1.311249	-0.671631	-1.929039
29B	1.224865	-0.818639	1.929039

$E30/\varepsilon$ =-141.678730

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.104550	0.000000	0.000000
3A	0.534062	-0.955024	0.000000
4A	0.509082	-0.289117	0.906197
5A	0.531027	-0.315117	-0.917908
6A	0.542789	0.732120	-0.556608
7B	1.696238	-0.979322	-0.673101
8A	0.510401	0.752461	0.576535
9A	-0.407868	-0.833984	-0.555511
10A	1.429483	-0.831965	0.630524
11A	-0.409063	-0.796452	0.589526
12B	1.686132	0.464380	-1.122880
13B	0.441874	-1.676378	-1.122955
14A	-0.442221	0.283553	0.953179
15A	-0.439146	0.272113	-0.932280
16A	1.428967	0.272689	1.020769
17A	0.465681	-1.364048	1.026732
18B	-0.529193	1.249533	-0.026723
19B	1.582156	1.293624	0.143286
20B	0.366423	0.708850	-1.860546
21B	-1.330665	-0.073302	0.001640
22B	-0.341958	-1.997926	0.145613
23B	1.245752	-0.716062	1.917201
24B	0.472324	0.643818	1.872259
25B	-0.315710	-0.688948	1.881295
26B	2.426138	-0.003800	0.223549
27B	1.201361	-2.096249	0.225927
28B	-0.415602	-0.640769	-1.863874
29B	1.123556	-0.635715	-2.066949
30B	0.634713	1.956799	-0.923526

$E31/\varepsilon$ =-147.678325

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.110516	0.000000	0.000000
3A	0.535483	-0.950830	0.000000
4A	0.513076	-0.281858	0.907278
5A	0.533021	-0.300790	-0.915679
6A	0.520808	0.746439	0.560672
7A	0.545134	0.745356	-0.542368
8B	1.696495	-0.975712	-0.675868
9A	1.428916	-0.831394	0.634827
10A	-0.405310	-0.828351	-0.560339
11A	-0.403796	-0.792609	0.597032
12B	-0.556158	1.231918	-0.009506
13B	1.692507	0.472799	-1.109458
14B	1.617140	1.283186	0.163844
15A	-0.435286	0.294402	0.952421
16B	0.442061	-1.661372	-1.133347
17A	1.433644	0.277769	1.021112
18A	-0.441306	0.281882	-0.926188
19A	0.469106	-1.356243	1.032234
20B	0.478781	0.690341	1.850071
21B	0.370313	0.759157	-1.831357
22B	-1.333700	-0.089411	0.007864
23B	1.247260	-0.690552	1.922890
24B	-0.339472	-1.989039	0.139639
25B	-0.305511	-0.657820	1.888334
26B	2.434576	-0.022157	0.235311
27B	1.199573	-2.091356	0.223584
28B	-0.407562	-0.610941	-1.869212
29B	1.124057	-0.601019	-2.066929
30B	0.587449	2.011009	-0.745468
31B	0.446408	1.998283	0.887277

$E32/\varepsilon$ =-154.290081

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.097810	0.000000	0.000000
3A	0.584491	-0.953899	0.000000
4A	0.513318	-0.270704	-0.914682
5A	0.511222	0.793380	-0.563917
6A	0.586588	-0.315582	0.920794
7A	0.548905	0.748379	0.558979
8B	1.774583	-0.934088	0.653622
9B	-0.676773	0.361669	-1.081174
10A	-0.321742	-0.877000	0.582555
11A	1.419551	0.309722	-1.006266
12A	-0.372441	-0.828999	-0.582138
13A	1.470249	-0.793464	-0.629714
14B	1.715390	0.507797	1.095196
15B	-0.617580	1.194277	0.176117
16B	0.532732	0.597019	-1.938767
17B	0.565077	-1.689632	1.122672
18A	0.548903	-1.356949	-1.013534
19A	-0.396500	0.192316	0.976362
20A	1.494310	0.990797	-0.092670
21B	-1.342970	-0.217070	0.149250
22B	2.440779	0.081511	-0.250502
23B	1.334813	-0.705317	-1.903969
24B	-0.237007	-2.025850	-0.135996
25B	0.694690	1.985452	0.137233
26B	0.403121	0.695038	1.864879
27B	1.310208	-2.071709	-0.231199
28B	-0.212402	-0.809618	-1.920924
29B	1.413610	1.623067	-1.219406
30B	-0.315800	-0.708665	1.902391
31B	1.221520	-0.615601	2.054798
32B	-0.123710	1.795620	-1.173418

$E33/\varepsilon$ =-160.737338

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.077876	0.000000	0.000000
3A	-0.462312	-0.973696	0.000000
4A	-0.445028	-0.318459	0.936062
5A	0.478556	0.265424	0.936062
6A	0.500436	-0.791588	-0.566681
7A	0.494201	-0.781725	0.541610
8A	-0.474808	0.751049	0.636624
9A	-0.488169	-0.331230	-0.898236
10A	0.508596	0.298918	-0.898236
11A	0.476352	0.947960	0.051508
12A	-1.060649	-0.023721	0.051508
13B	0.488872	-0.773296	1.824870
14B	0.384203	-2.013686	0.097223
15B	1.654268	-1.210760	0.097223
16B	-0.328639	0.519840	1.958989
17B	-0.423140	-1.639120	-1.139392
18B	1.662183	-0.320794	-1.139392
19A	1.416318	-0.287760	1.000267
20A	-0.347527	-1.402850	1.000268
21A	1.388280	0.815907	0.676087
22A	-1.332495	-0.904147	0.676087
23B	-0.614317	0.971724	-0.679313
24B	0.414657	1.605432	1.162534
25B	-1.628113	0.314008	1.162534
26B	1.549775	1.118696	-0.633198
27B	-1.675286	-0.920164	-0.633198
28B	0.342672	-0.542038	-1.896621
29B	-1.056197	-0.873158	1.980097
30B	1.241778	0.579606	1.980097
31B	-1.140524	-2.114591	0.192412
32B	2.399393	0.123318	0.192412

33B	1.110502	-1.756588	-1.255554

*E*34/ε =-167.225215

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.075288	0.000000	0.000000
3A	0.514226	-0.953485	0.000000
4A	0.514225	0.785195	-0.540928
5A	0.494457	-0.285582	0.913768
6A	0.494457	0.753571	0.590474
7A	0.518553	-0.285264	-0.916913
8B	1.686729	-0.985091	-0.653501
9B	1.686728	0.440482	-1.097016
10A	-0.444732	0.298867	0.960638
11A	-0.433902	-0.778047	0.587465
12A	-0.433902	0.974000	0.042380
13A	-0.433048	-0.809588	-0.553924
14A	-0.433048	0.352445	-0.915448
15A	1.413758	-0.820699	0.630394
16A	1.413758	1.033478	0.053534
17A	1.395361	0.317553	1.020703
18B	0.454515	0.596444	1.917132
19B	0.413965	-1.650877	-1.124120
20B	0.413964	0.721766	-1.862282
21A	0.441102	1.700413	0.073207
22A	0.441102	-1.358761	1.024956
23B	-1.325594	0.000251	0.000807
24B	2.379995	0.071238	0.228975
25B	1.238871	1.679703	1.163427
26B	1.238870	-0.723209	1.911005
27B	-0.343709	-0.703068	1.877768
28B	-0.343708	1.644262	1.147483
29B	-0.372133	-1.980284	0.142209
30B	-0.372133	1.711441	-1.006336
31B	-0.427510	-0.574514	-1.846635
32B	1.170951	-2.097349	0.231397
33B	1.170949	1.858443	-0.999304
34B	1.120712	-0.639753	-2.056332

*E*35/ε =-173.011973

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.127618	0.000000	0.000000
3A	-1.143657	-0.027534	0.000000
4A	0.547053	-0.935553	0.000008
5A	-0.523156	-0.946944	0.000008
6A	0.540803	-0.287492	-0.890212
7A	0.540802	-0.287478	0.890216
8B	0.020230	-1.483990	-1.076166
9B	0.020229	-1.483972	1.076189
10A	-0.531549	-0.299824	-0.889422
11A	-0.531550	-0.299809	0.889427
12A	0.538518	0.761864	0.551444
13A	0.538518	0.761855	-0.551456
14A	-0.553647	0.747971	0.551020
15A	-0.553647	0.747962	-0.551033
16B	1.574497	-1.076670	0.783048
17B	1.574497	-1.076683	-0.783030
18B	-0.003598	0.591461	1.726298
19B	-0.003598	0.591433	-1.726307
20B	-1.546365	-1.112229	-0.784120
21B	-1.546365	-1.112217	0.784138
22B	1.580266	0.402001	1.256926
23B	1.580267	0.401981	-1.256932
24B	-1.582704	0.367244	-1.263120
25B	-1.582705	0.367264	1.263114
26B	1.586463	1.309896	-0.000010
27B	-0.019462	1.817562	-0.000016
28B	0.829951	-2.222095	0.000018
29B	-0.770711	-2.240837	0.000018
30B	0.810614	-0.670250	-2.113983
31B	0.810613	-0.670217	2.113994
32B	-1.613299	1.273190	-0.000011
33B	-0.783872	-0.689485	-2.115799
34B	-0.783872	-0.689450	2.115810
35B	2.429289	-0.020407	0.000001

*E*36/ε =-180.176688

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.126202	0.000000	0.000000
3A	-1.125875	-0.027117	0.000000
4A	0.546086	-0.935893	0.000152
5A	-0.523393	-0.948770	0.000153
6A	-0.532399	-0.300917	-0.890255
7A	0.539490	-0.288010	-0.890255
8A	0.539488	-0.287720	0.890349
9A	-0.532402	-0.300627	0.890349
10B	0.017877	-1.484728	-1.076101
11B	0.017875	-1.484377	1.076583
12A	-0.555099	0.748701	-0.551985
13A	0.536910	0.761849	-0.551986
14A	-0.555101	0.748880	0.551737
15A	0.536909	0.762029	0.551736
16B	-1.546296	-1.115096	-0.783302
17B	1.572695	-1.077285	0.783657
18B	1.572696	-1.077540	-0.783306
19B	-1.546297	-1.114841	0.783660
20B	-0.007109	0.590295	-1.726549
21B	-0.007113	0.590857	1.726354
22B	-1.587666	0.363027	-1.257431
23B	1.578462	0.401150	-1.257435
24B	1.578460	0.401560	1.257303
25B	-1.587669	0.363436	1.257307
26B	-1.616067	1.270584	-0.000210
27B	1.585005	1.309128	-0.000214
28B	-0.021883	1.817376	-0.000297
29B	0.827246	-2.222451	0.000362
30B	-0.773492	-2.241726	0.000363
31B	0.806417	-0.670913	-2.114245
32B	-0.790034	-0.690136	-2.114243
33B	-0.790038	-0.689448	2.114464
34B	0.806415	-0.670225	2.114462
35B	2.427570	-0.021351	0.000004
36B	-2.426352	-0.079797	0.000010

*E*37/ε =-186.439022

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.127757	0.000000	0.000000
3A	-1.123774	-0.022392	0.000000
4A	0.546169	-0.928218	-0.110752
5A	-0.523987	-0.940288	-0.111940
6A	0.540748	-0.390886	0.850502
7A	-0.531132	-0.402989	0.848909
8A	0.539702	-0.178723	-0.917748
9A	-0.532687	-0.190434	-0.918803
10B	0.018938	-1.600419	0.892643
11B	0.016724	-1.343928	-1.244492
12A	0.537033	0.685639	0.633930
13A	-0.548972	0.682823	0.640432
14B	-0.010892	0.372962	1.787240
15A	0.538857	0.822475	-0.456969
16A	-0.552638	0.810581	-0.456845
17B	1.573924	-1.160101	0.650373
18B	1.573709	-0.974312	-0.904579
19B	-1.547268	-1.195338	0.646773
20B	-1.548396	-1.008561	-0.907841
21B	1.577707	0.252356	1.297728
22B	-0.006307	0.794274	-1.642388
23B	-1.581544	0.216750	1.295667
24B	1.579647	0.549033	-1.199942
25B	-1.586587	0.515951	-1.201401
26B	1.585596	1.301205	0.154730
27B	-0.019236	1.807482	0.208212
28B	-1.608748	1.268393	0.156198
29B	0.827311	-2.204841	-0.264251
30B	-0.775210	-2.222851	-0.265237
31B	0.809047	-0.915544	2.020164
32B	-0.791322	-0.940343	2.017188
33B	0.805938	-0.412610	-2.178254
34B	-0.791402	-0.429683	-2.179667
35B	2.428264	-0.016811	0.001058
36B	-2.424044	-0.070121	-0.004108
37B	0.844799	1.628427	1.494076

*E*38/ε =-193.649484

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.124935	0.000000	0.000000
3A	-1.124842	-0.014460	0.000000
4A	-0.531146	-0.763093	-0.550332
5A	0.540910	-0.756203	-0.550332
6A	-0.531146	-0.763081	0.550348
7A	0.540910	-0.756191	0.550348
8A	-0.538764	0.285201	0.889357
9A	-0.538763	0.285182	-0.889364
10A	0.535053	0.292102	0.889357
11A	0.535053	0.292083	-0.889364
12B	0.011763	-1.830324	0.000019
13B	0.003625	-0.564005	-1.738717
14B	0.003625	-0.563967	1.738729
15A	-0.551529	0.932054	-0.000010
16A	0.539503	0.939067	-0.000010
17B	-1.555807	-1.346106	0.000014
18B	1.572980	-1.325997	0.000014
19B	1.569079	-0.408228	-1.264774
20B	1.569080	-0.408201	1.264781
21B	-1.563703	-0.428335	1.264782
22B	-1.563703	-0.428362	-1.264774
23B	-0.009623	1.497206	1.042924
24B	-0.009622	1.497183	-1.042957
25B	1.577881	1.064124	-0.778356
26B	-1.591429	1.043755	-0.778356
27B	1.577881	1.064141	0.778332
28B	-1.591429	1.043772	0.778333
29B	-0.793159	-1.804763	-1.306745
30B	-0.793159	-1.804735	1.306782
31B	0.816290	-1.794392	1.306782
32B	0.816290	-1.794420	-1.306744
33B	-0.805357	0.692647	-2.102470
34B	-0.805358	0.692692	2.102455
35B	0.796388	0.702941	-2.102470
36B	0.796388	0.702987	2.102454
37B	-2.423376	-0.042342	-0.000001
38B	2.423720	-0.011190	-0.000001

*E*39/ε =-200.030446

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.126000	0.000000	0.000000
3A	-1.123254	-0.011001	0.000000
4A	0.540971	-0.755697	0.550106
5A	0.540971	-0.755557	-0.550298
6A	-0.531426	-0.762236	0.550267
7A	-0.531427	-0.762097	-0.550459
8A	0.536080	0.292675	0.889191
9A	0.536079	0.292900	-0.889117
10A	-0.537818	0.285257	0.889508
11A	-0.537819	0.285482	-0.889434
12B	0.010779	-1.829406	-0.000231
13B	0.005191	-0.563591	1.738343
14B	0.005189	-0.563150	-1.738485
15A	0.539505	0.934695	0.000118
16A	-0.546864	0.935883	0.000119
17B	-0.014554	1.491942	1.051102
18B	-0.014555	1.492208	-1.050723
19B	1.573153	-1.325387	-0.000168
20B	-1.557099	-1.343120	-0.000169

21B	1.569444	-0.408775	1.264531
22B	1.569443	-0.408454	-1.264636
23B	-1.564273	-0.425973	1.263751
24B	-1.564274	-0.425653	-1.263857
25B	1.580249	1.061363	0.778920
26B	1.580248	1.061561	-0.778652
27B	-1.586491	1.048091	0.778563
28B	-1.586492	1.048288	-0.778295
29B	0.816007	-1.794633	1.305860
30B	0.816005	-1.794302	-1.306315
31B	-0.794116	-1.803018	1.306761
32B	-0.794117	-1.802687	-1.307217
33B	0.798887	0.703545	2.101891
34B	0.798885	0.704077	-2.101713
35B	2.424544	-0.010449	-0.000002
36B	-0.807006	0.687863	2.105824
37B	-0.807008	0.688397	-2.105648
38B	-2.421674	-0.035829	-0.000003
39B	0.865048	2.211801	0.000280

$E40/\varepsilon$ =-207.322597

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	-0.935832	-0.000288
5A	-0.537061	-0.935832	-0.000288
6A	0.537062	-0.289461	0.889940
7A	0.537062	-0.288914	-0.890118
8A	-0.537061	-0.289462	0.889940
9A	-0.537061	-0.288914	-0.890118
10A	0.537061	0.756935	0.550301
11A	0.537061	0.757273	-0.549835
12A	-0.537062	0.756934	0.550301
13A	-0.537062	0.757273	-0.549835
14B	0.000000	1.826899	0.000562
15B	0.000000	0.564009	1.737658
16B	0.000000	0.565077	-1.737311
17B	0.000000	-1.478323	1.073370
18B	0.000000	-1.477662	-1.074279
19B	1.570538	1.325050	0.000408
20B	1.570538	0.409076	1.260324
21B	1.570538	0.409851	-1.260071
22B	-1.570537	-1.071749	-0.779174
23B	1.570538	-1.072228	0.778516
24B	1.570538	-1.071749	-0.779174
25B	-1.570538	0.409850	-1.260071
26B	-1.570537	-1.072228	0.778516
27B	-1.570538	1.325050	0.000408
28B	-1.570538	0.409075	1.260324
29B	-0.808693	-0.686528	2.110708
30B	-0.808693	-0.685230	-2.111129
31B	0.808693	-0.685230	-2.111129
32B	0.808693	-0.686528	2.110708
33B	0.808693	1.796056	-1.304067
34B	0.808693	1.795254	1.305171
35B	-0.808694	1.795253	1.305172
36B	-0.808693	1.796056	-1.304067
37B	0.808693	-2.219551	-0.000682
38B	-0.808693	-2.219551	-0.000682
39B	2.420332	0.000000	0.000000
40B	-2.420332	-0.000001	0.000000

$E41/\varepsilon$ =-213.170471

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.068072	0.000000	0.000000
3A	-0.444792	-0.971050	0.000000
4A	0.444793	0.971049	0.000000
5A	-1.068071	-0.000001	0.000000
6A	0.501927	-0.781985	0.548298
7A	-0.501926	0.781984	-0.548299
8A	0.496979	-0.774277	-0.587465
9A	-0.496978	0.774276	0.587465
10A	0.468693	0.301249	-0.902770
11A	0.469069	0.300664	0.902770
12A	-0.469069	-0.300665	-0.902770
13A	-0.468693	-0.301250	0.902770
14B	-1.660579	1.167383	-0.008813
15B	0.369803	-1.995884	0.008813
16B	-0.369802	1.995883	-0.008813
17B	1.660579	-1.167384	0.008812
18B	-1.588215	0.238449	-1.235068
19B	0.444613	1.543244	-1.235068
20B	1.588216	-0.238450	1.235067
21B	-0.444612	-1.543245	1.235068
22B	-1.612681	0.245824	1.209008
23B	1.612681	-0.245825	-1.209008
24B	-0.448097	-1.568561	-1.209007
25B	0.448097	1.568559	1.209008
26A	1.378621	0.882021	-0.568073
27A	1.376019	0.886077	0.568072
28A	-1.378620	-0.882022	0.568073
29A	-1.376018	-0.886077	-0.568072
30B	-0.315579	0.491662	1.951783
31B	0.315579	-0.491663	-1.951783
32A	-0.364405	0.567731	-1.608659
33A	0.364406	-0.567732	1.608659
34B	-2.389618	-0.241451	-0.015918
35B	-1.214658	-2.071999	0.015919
36B	2.389619	0.241450	0.015917
37B	1.214659	2.071998	-0.015919
38B	-1.079161	1.681297	-1.354217
39B	1.079162	-1.681297	1.354216
40B	1.090929	-1.699633	-1.334517
41B	-1.090929	1.699631	1.334518

$E42/\varepsilon$ =-220.223427

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.068792	0.000000	0.000000
3A	0.466512	-0.961605	0.000000
4A	0.453264	-0.283893	-0.914885
5A	-0.487641	0.951227	0.001232
6A	-1.068678	0.023540	0.001232
7A	0.505004	0.761620	0.551669
8A	-0.464812	-0.786794	0.551669
9A	0.495760	-0.310509	0.920831
10A	-0.497820	0.311799	-0.927650
11A	0.458726	0.765653	-0.577477
12A	-0.488640	-0.746917	-0.577476
13A	-0.448574	0.280955	0.914741
14B	1.622663	-1.016321	0.665756
15B	-1.633958	1.023394	-0.646816
16B	1.647682	0.430279	1.112664
17B	0.332060	-1.670250	1.112664
18A	1.357577	-0.850290	-0.625824
19B	-1.532256	0.959696	0.884662
20B	-0.459857	-1.955447	-0.165824
21B	1.558618	1.267261	-0.165823
22B	-1.634024	-0.430952	-1.129218
23B	-0.325495	1.658253	-1.129219
24B	-0.455305	-0.606378	1.880012
25B	0.346831	0.674318	1.880012
26B	0.463754	0.612783	-1.887419
27B	-0.348907	-0.684717	-1.887419
28A	-1.400260	-1.016692	0.027800
29A	0.303537	1.703601	0.027799
30A	-1.378724	-0.366186	0.975403
31A	-0.272331	1.400289	0.975402
32A	1.385807	0.251871	-1.020682
33A	0.378272	-1.356765	-1.020681
34B	1.201016	-0.752231	-1.909299
35B	1.084142	-2.119558	-0.226879
36B	2.380202	-0.050261	-0.226879
37B	0.978342	1.860701	1.144306
38B	-1.247063	-1.692394	1.144306
39B	-0.939413	2.195153	0.165932
40B	-2.385044	-0.112951	0.165933
41B	1.080020	-0.676448	2.061764
42B	-1.081616	0.677445	-2.062147

$E43/\varepsilon$ =-226.823468

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.056172	0.000000	0.000000
3A	0.451932	-0.954598	0.000000
4A	-0.451932	0.954598	-0.000001
5A	-1.056172	0.000000	0.000001
6A	0.481482	-0.267142	-0.917061
7A	0.447474	-0.320868	0.917062
8A	-0.481481	0.267142	0.917062
9A	-0.447474	0.320867	-0.917062
10A	0.507020	0.801005	-0.552306
11A	-0.507019	-0.801005	0.552306
12A	0.480128	0.758522	0.567410
13A	-0.480129	-0.758522	-0.567410
14B	0.395892	-1.648834	1.119233
15B	1.659664	0.347710	-1.119232
16B	-0.395892	1.648834	-1.119234
17B	-1.659663	-0.347710	1.119234
18B	0.383423	0.605742	-1.905221
19B	-0.383422	-0.605742	1.905221
20B	0.434072	0.685762	1.837822
21B	-0.434072	-0.685761	-1.837822
22A	-1.346711	0.878300	-0.608759
23A	-1.370085	0.841374	0.608758
24A	1.346711	-0.878301	0.608759
25A	1.370086	-0.841374	-0.608757
26B	-0.364042	-1.996890	-0.150584
27B	-1.649072	-1.183493	-0.150583
28B	1.649072	1.183493	0.150585
29B	0.364042	1.996890	0.150584
30A	-1.394787	-0.220713	-1.004932
31A	-0.397337	1.355090	1.004932
32A	1.394786	0.220713	1.004934
33A	0.397337	-1.355090	-1.004933
34B	-1.201015	2.031190	0.132083
35B	-2.349756	0.216372	-0.132083
36B	1.201015	-2.031190	-0.132083
37B	2.349756	-0.216372	0.132086
38B	1.118413	-0.807677	-1.948028
39B	1.208563	-0.665250	1.948030
40B	-1.118412	0.807677	1.948029
41B	-1.208563	0.665249	-1.948030
42B	-1.132580	-1.789285	1.189849
43B	1.132580	1.789285	-1.189848

$E44/\varepsilon$ =-232.998720

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.060415	0.000000	0.000000
3A	0.454311	-0.967622	0.000000
4A	-0.447160	0.324442	-0.906437
5A	0.487269	-0.282752	-0.904941
6A	0.462757	-0.314572	0.901838
7A	0.494332	0.771195	0.572929
8A	-1.062930	0.009857	-0.005240
9A	-0.433809	0.975443	0.020071
10A	0.514740	0.798058	-0.528295
11A	-0.491163	-0.771156	-0.557424
12A	-0.501432	-0.781566	0.575769
13A	-0.464146	0.282748	0.912568
14B	-0.398751	1.592375	-1.173572
15B	0.466752	-1.534203	-1.218356
16B	1.633277	0.264986	-1.176328
17B	-1.574061	-0.220721	-1.231255
18B	1.672433	1.172448	0.039524
19B	0.399194	1.999924	0.071958

20B	-1.658687	-1.159976	-0.036087
21B	0.411699	-1.596198	1.193571
22B	-0.374157	-1.993586	-0.035741
23B	-0.397511	1.503135	1.284641
24A	1.359493	-0.856792	0.626860
25A	1.390828	0.289152	0.990698
26B	-1.620782	-0.254626	1.193752
27B	-0.337683	-0.518766	1.948648
28A	-0.329579	-0.526043	-1.601792
29A	0.394638	0.588833	-1.578335
30A	-1.350478	0.907389	-0.569368
31A	1.402545	-0.867414	-0.548500
32A	-1.360977	0.883524	0.585895
33A	0.426018	0.492804	1.625065
34B	2.358309	-0.196079	0.136628
35B	1.227319	-0.549790	1.959246
36B	1.241754	-2.046628	0.007288
37B	-1.175149	2.076673	0.062516
38B	1.152203	1.560613	1.413301
39B	-2.376341	0.272518	-0.024793
40B	-1.048855	-1.644421	-1.395643
41B	1.112040	1.699261	-1.305645
42B	-0.717594	0.539279	-2.248310
43B	0.797299	-0.448830	-2.250780
44B	-1.118289	-1.712568	1.305170

$E45/\varepsilon$ =-239.434596

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.089679	0.000000	0.000000
3A	-0.409841	-1.009668	0.000000
4A	0.512288	0.264418	0.914231
5A	-0.437680	-0.375221	0.914231
6A	0.512288	0.264418	-0.914231
7A	-0.437680	-0.375221	-0.914231
8A	0.511547	-0.759729	0.533373
9A	0.511547	-0.759729	-0.533373
10A	0.513777	0.944192	0.000000
11A	-1.068101	-0.120929	0.000000
12A	-0.485356	0.720835	0.606184
13A	-0.485356	0.720835	-0.606184
14B	-0.382023	1.919667	0.000000
15B	-1.635028	1.075985	0.000000
16B	-0.299901	0.445404	-1.949129
17B	-0.299901	0.445404	1.949129
18B	-1.457822	-1.243898	-0.751179
19B	-1.457822	-1.243898	0.751179
20B	1.700871	0.882934	-0.751179
21B	1.700871	0.882934	0.751179
22B	0.432027	1.536912	1.226325
23B	-1.586551	0.177749	-1.226326
24B	-1.586551	0.177749	1.226326
25B	0.432027	1.536912	-1.226325
26A	0.474018	-1.704546	0.000000
27A	1.401104	-1.080314	0.000000
28A	1.431241	-0.406181	0.964921
29A	-0.161951	-1.478919	-0.964922
30A	1.431241	-0.406181	-0.964921
31A	-0.161951	-1.478919	0.964922
32A	0.425878	-0.632497	-1.586262
33A	0.425878	-0.632497	1.586262
34B	1.139963	-1.693030	-1.167785
35B	1.139963	-1.693030	1.167785
36B	2.396037	-0.265178	0.000000
37B	-0.655473	-2.319841	0.000000
38B	-0.747529	-1.000613	2.063637
39B	1.208298	0.316298	2.063637
40B	-0.747529	-1.000613	-2.063637
41B	1.208298	0.316298	-2.063637
42B	-2.403770	-0.274229	0.000000
43B	1.158184	2.124130	0.000000
44B	-1.104798	1.640807	1.347343
45B	-1.104798	1.640807	-1.347343

$E46/\varepsilon$ =-245.176668

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.094799	0.000000	0.000000
3A	-0.417732	-1.011972	0.000000
4A	0.491261	0.298070	0.911173
5A	-0.462964	-0.340363	0.911173
6A	0.526295	-0.786621	-0.527297
7A	0.518756	0.274389	-0.890711
8A	-0.451568	-0.374814	-0.890710
9A	0.493319	-0.737334	0.555445
10A	-0.491346	0.734383	-0.583238
11A	-1.075805	-0.096974	-0.003154
12A	0.500120	0.957412	-0.003155
13A	-0.499039	0.745882	0.581453
14B	1.614909	-0.546744	-1.155050
15B	-0.110807	-1.701348	-1.155049
16B	0.396844	1.522522	-1.244381
17B	-1.558757	0.214112	-1.244380
18B	-0.398227	1.949089	-0.029810
19B	-1.649683	1.111792	-0.029809
20B	1.666981	0.923740	0.740246
21B	-1.489906	-1.188402	0.740248
22B	-0.336323	0.502682	1.933287
23B	1.686420	0.899819	-0.771230
24B	-1.475215	-1.215498	-0.771228
25B	0.404405	1.581274	1.204039
26B	-1.615946	0.229541	1.204040
27A	0.450177	-1.703545	0.086490
28A	1.402891	-1.066123	0.086489
29A	-0.284540	0.425281	-1.631620
30A	1.397460	-0.364539	1.002670
31A	-0.196256	-1.430828	1.002670
32A	0.358974	-0.536540	-1.579180
33A	0.385925	-0.576818	1.605114
34B	1.102687	-1.648118	1.249138
35B	-0.780216	-0.733834	-2.149378
36B	0.976010	0.441184	-2.149379
37B	2.411302	-0.238006	0.117567
38B	-0.700058	-2.319687	0.117569
39B	1.340958	-2.004249	-0.826419
40B	-0.804722	-0.932651	2.068999
41B	1.169140	0.387979	2.068998
42B	-2.415951	-0.229563	-0.038615
43B	1.134025	2.145578	-0.038618
44B	-1.128709	1.687011	1.310153
45B	-1.090342	1.629665	-1.396976
46B	0.965353	-1.442858	-2.261084

$E47/\varepsilon$ =-251.178900

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.073779	0.000000	0.000000
3A	0.484381	-0.931986	0.000000
4A	0.542583	-0.270697	0.898067
5A	0.484491	0.761944	-0.561859
6A	0.505054	-0.299264	-0.904195
7A	-0.414492	-0.781214	0.609545
8A	0.520864	0.757510	0.555779
9A	-0.449957	0.963899	0.020238
10A	-0.474741	0.299426	-0.909377
11A	-0.463007	-0.808485	-0.535662
12A	-1.062970	-0.004180	0.076064
13A	1.419883	-0.862988	0.587806
14A	-0.410893	0.297330	0.936140
15B	1.665004	0.391539	1.117849
16A	0.470672	-1.350307	1.002248
17A	1.416521	-0.862348	-0.548383
18B	-0.214345	-2.036562	0.118398
19B	0.531653	-1.637465	-1.117539
20B	-1.602521	-0.404649	-1.081037
21B	0.494323	0.622252	-1.871843
22B	-0.300504	1.657867	-1.126220
23B	-1.530302	-1.283975	0.165175
24B	-1.585379	1.044000	-0.618876
25B	-0.312077	-0.647255	-1.872219
26B	0.382051	0.638314	1.894269
27A	0.395122	1.689620	0.000082
28A	1.424251	0.369252	-0.953543
29A	1.417213	1.032451	-0.004978
30B	2.367032	-0.057727	-0.136751
31B	-1.433001	-0.377258	1.381041
32B	-1.464212	1.058024	0.897308
33B	1.132116	-0.752945	1.964675
34A	-0.153841	-0.557109	1.661630
35A	-0.195637	1.429033	0.991381
36A	1.090118	-1.803740	0.072178
37B	1.092161	1.811313	1.090451
38B	1.236389	1.722949	-1.079414
39B	1.397700	-0.611030	-1.840484
40B	-0.711083	-1.731311	1.510436
41B	1.577268	-2.037771	1.252234
42B	2.373380	-1.608101	-0.052558
43B	-0.818556	2.243844	0.168667
44B	-1.012745	-1.837902	-1.187207
45B	-1.062973	0.687270	-2.043130
46B	-2.383765	0.006417	0.207387
47B	2.558041	-0.829127	1.264520

$E48/\varepsilon$ =-258.325633

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.073996	0.000000	0.000000
3A	0.466208	-0.930545	0.000000
4A	0.493288	-0.303804	-0.897767
5A	0.493288	-0.303804	0.897767
6A	-0.464423	-0.819003	-0.551002
7A	-0.464424	-0.819003	0.551002
8A	-1.063230	-0.085460	-0.000001
9A	-0.500794	0.927349	0.000000
10A	0.464763	0.774308	-0.583771
11A	0.464763	0.774308	0.583770
12A	1.370762	-0.915332	0.588577
13A	1.370763	-0.915333	-0.588577
14A	-0.473880	0.245745	-0.913020
15A	-0.473880	0.245745	0.913019
16B	1.598766	0.300740	1.197839
17B	1.598766	0.300740	-1.197840
18B	-0.229507	-2.052683	0.000000
19A	0.379043	-1.397646	0.963969
20A	0.379043	-1.397646	-0.963969
21B	1.596577	1.216596	0.000000
22B	-1.563779	-1.317346	-0.000001
23B	2.370782	-0.197167	0.000000
24B	0.269844	1.981624	-0.000001
25B	-1.533722	-0.399278	-1.239976
26B	-1.533723	-0.399278	1.239975
27B	0.294468	0.487014	1.952703
28B	0.294469	0.487014	-1.952703
29B	-0.530432	1.512783	1.210415
30B	-0.530431	1.512783	-1.210416
31B	1.015741	-0.881669	1.968762
32B	1.015742	-0.881670	-1.968763
33A	1.037176	-1.817013	0.000000
34B	2.326127	-1.710446	0.000000
35A	-1.421561	0.762558	-0.578401
36A	-1.421562	0.762558	0.578399
37A	-0.257851	-0.648496	-1.605032
38A	-0.257852	-0.648495	1.605031
39B	1.429799	-2.146742	-1.195701
40B	1.429799	-2.146742	1.195701
41B	-0.847041	-1.793192	-1.363510
42B	-0.847042	-1.793192	1.363509
43B	-2.373603	0.034038	-0.000001
44B	-1.348057	1.959487	-0.000001

45B	1.004869	1.724971	-1.341707
46B	1.004869	1.724972	1.341706
47B	2.449068	-0.974680	-1.357947
48B	2.449068	-0.974680	1.357947

$E49/\varepsilon$ =-264.629464

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.072956	0.000000	0.000000
3A	-0.429039	-0.983443	0.000000
4A	0.503948	-0.769671	0.565302
5A	0.496567	-0.758398	-0.533498
6A	0.492280	0.235566	-0.936457
7A	-0.412760	-0.357015	-0.936457
8A	0.478911	0.950225	-0.073288
9A	-1.062452	-0.058994	-0.073288
10A	0.485422	0.335622	0.889656
11A	-0.501726	-0.310721	0.889656
12A	-0.524571	0.801168	0.463012
13A	1.406571	-1.066793	-0.055966
14A	0.415353	-1.715800	-0.055966
15A	-0.463495	0.707888	-0.652100
16B	-0.325273	-1.675809	1.097704
17B	1.666068	-0.371963	1.097703
18B	0.486024	-0.742296	-1.868283
19A	-0.216421	-1.426284	-0.992869
20A	1.393834	-0.371958	-0.992869
21B	-0.441858	0.674843	1.789257
22B	0.394798	-0.602967	1.867000
23B	-1.608533	-1.097496	0.592537
24B	1.649134	1.035487	0.592536
25B	1.171713	-1.789537	1.074708
26B	0.354070	1.695951	0.992408
27B	-1.696044	0.353623	0.992408
28B	-0.352426	0.538254	-1.931198
29A	-1.280490	-0.965659	-0.680572
30A	1.397123	0.787529	-0.680572
31B	2.375852	-0.039978	-0.221835
32B	-0.913381	-2.193629	-0.221835
33B	-0.378689	1.959825	-0.312243
34B	-1.644898	1.130765	-0.312242
35A	1.012563	-1.546469	-1.003871
36B	1.583574	-2.418564	-0.236230
37A	0.414960	1.285405	-1.131827
38A	-1.344096	0.133650	-1.131826
39B	1.237400	0.591443	-1.954299
40B	-1.036897	-0.897668	-1.954298
41B	0.293045	-2.630137	-1.076008
42B	2.293536	-1.320302	-1.076007
43B	-2.360675	-0.222569	-0.380942
44B	1.147956	2.074734	-0.380942
45B	1.091672	0.765479	2.000590
46B	-1.138141	-0.694508	2.000590
47B	-1.186692	1.812415	1.013141
48B	2.570345	-1.439245	0.454118
49B	0.291380	-2.931416	0.454118

$E50/\varepsilon$ =-271.536410

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.075219	0.000000	0.000000
3A	0.492675	-0.953435	0.000000
4A	0.484257	-0.298973	0.865150
5A	0.490337	0.745395	0.598184
6A	-0.446297	0.250442	0.956655
7A	-0.446098	-0.788267	0.593817
8A	-1.062651	-0.037173	0.105511
9A	-0.520553	0.297484	-0.860718
10A	0.455030	0.807565	-0.529316
11A	0.454967	-0.305076	-0.917284
12A	1.373971	-0.861674	0.683472
13A	1.374401	0.250991	1.073017
14A	-0.481810	0.938475	0.087056
15A	-0.481303	-0.791850	-0.513425
16A	0.402604	-1.341351	1.032978
17A	0.395415	0.392006	1.669454
18A	-0.210581	-0.574671	1.643211
19A	0.954636	-0.611079	1.753367
20B	1.590892	1.227031	0.116661
21B	1.593308	-1.038088	-0.671383
22B	-1.512721	-0.450215	1.294490
23B	1.583009	0.397602	-1.148220
24B	2.367874	-0.069213	0.190285
25B	0.248112	0.643886	-1.857303
26B	-1.524113	1.019870	0.834405
27B	-1.516989	-1.325601	0.031314
28B	1.013698	1.538980	1.501137
29B	0.279380	-1.698721	-1.071175
30B	0.280832	1.995314	0.209427
31B	1.020553	-2.145454	0.215931
32B	-0.549737	1.631867	-1.009453
33B	-0.548530	-0.658128	-1.804350
34B	2.284312	-0.569616	1.622588
35A	-1.436549	-0.316738	-0.874122
36A	-1.438125	0.785381	-0.493892
37A	-0.247872	-1.747240	0.142219
38B	-0.769044	-1.792435	1.374373
39A	-0.254106	1.286771	1.186703
40B	-0.799313	0.585050	2.171477
41B	1.447257	-1.838367	1.653293
42B	1.478054	0.426243	2.425530
43B	0.232958	-0.330348	2.843076
44B	-2.368460	-0.017248	0.032798
45B	-1.378110	0.627843	-1.816577
46B	0.983835	-0.714569	-2.058726
47B	0.983916	1.834417	-1.174499
48B	2.454957	-1.602810	0.480411
49B	2.463615	0.957621	1.356683
50A	0.281477	-1.436219	2.123550

s = 1.5

$E5/\varepsilon$ =-9.184718

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
4B	0.562000	-0.324470	1.239161
5B	0.562000	-0.324470	-1.239161

$E6/\varepsilon$ = -12.968869

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.184180	0.000000	0.000000
3B	0.592090	-1.242964	0.000000
4B	0.592090	0.000000	1.242964
5B	0.592090	0.000000	-1.242964
6B	0.592090	1.242964	0.000000

$E7/\varepsilon$ = -16.609636

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.409860	0.000000	0.000000
3B	0.394643	-1.341452	0.000000
4B	0.396357	1.048084	0.837272
5B	0.396357	1.048084	-0.837272
6A	0.454748	-0.338539	0.966493
7A	0.454748	-0.338539	-0.966493

$E8/\varepsilon$ = -20.714043

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.372614	0.000000	0.000000
3B	0.234630	-1.361777	0.000000
4B	0.234631	0.916203	-1.007477
5A	0.494380	-0.428603	-0.969103
6B	0.359385	1.191352	0.630439
7B	0.359385	-0.335126	1.305551
8B	-0.886536	-0.420728	-0.951297

$E9/\varepsilon$ = -25.991730

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.381971	0.000000	0.000000
3B	0.365941	-1.332641	0.000000
4B	-0.650092	-0.558001	-1.084371
5B	0.365939	0.774640	-1.084373
6B	0.352503	-0.268752	1.308953
7B	-1.084383	0.826753	-0.224581
8B	0.352503	1.221321	0.542183
9B	-1.084381	-0.663321	0.542187

$E10/\varepsilon$ = -30.931901

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.377337	0.000000	0.000000
3B	0.300770	-1.344097	0.000000
4B	0.321982	1.018262	0.855047
5B	-0.923376	-0.536571	0.855046
6B	0.321988	1.018267	-0.855040
7B	-0.923379	-0.536577	-0.855040
8B	-1.099417	0.880588	-0.000002
9A	0.446546	-0.357665	-0.967696
10A	0.446550	-0.357669	0.967696

$E11/\varepsilon$ = -35.487787

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.401505	0.000000	0.000000
3B	0.386899	-1.347044	0.000000
4B	0.386899	0.764212	-1.109282
5B	-0.627707	-0.582832	-1.109283
6B	0.404461	-0.304646	1.294483
7B	0.404462	1.238831	0.483520
8B	-1.079036	-0.730738	0.483518
9B	-1.079036	0.812740	-0.327446
10A	-0.644098	0.485139	0.923348
11A	0.750149	-0.565019	-1.075380

$E12/\varepsilon$ = -40.000211

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.353576	0.000000	0.000000
3B	-1.011156	-0.943526	0.000000
4B	-1.011156	0.599713	-0.728411
5A	0.398240	0.409974	-0.949630
6A	0.398241	-0.993708	-0.287090
7A	-0.233240	-0.485510	-1.028619
8B	0.249759	1.383608	0.007340
9B	0.249760	-0.873768	1.072826
10B	-0.887621	0.443736	0.940118
11A	0.490164	0.457250	0.968745
12B	1.054580	-0.698142	-1.479108

$E13/\varepsilon$ = -45.475297

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.148432	0.000000	0.000000
3A	0.608462	-0.973997	0.000000
4B	-1.399472	-0.189028	-0.000001
5B	-0.581152	1.287056	0.000000
6B	-0.532776	0.295362	1.314231
7B	-0.532774	0.295363	-1.314233
8A	0.596870	-0.330896	-0.894069
9A	0.596869	-0.330896	0.894069
10A	0.568801	0.751724	0.570125
11A	0.568802	0.751725	-0.570124

12A	-0.336183	-0.880685	-0.570125
13A	-0.336183	-0.880685	0.570124

$E14/\varepsilon$ = -50.489724

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.094025	0.000000	0.000000
3B	0.547011	-1.254801	0.000000
4B	0.547013	0.004236	-1.254794
5A	0.547012	-0.187034	0.941602
6A	0.547013	0.942228	-0.183855
7B	-0.283451	0.941508	0.944690
8B	1.377474	0.941507	0.944691
9B	1.849169	-0.676771	0.915917
10B	-0.755145	0.918197	-0.673676
11B	1.849171	0.918195	-0.673674
12B	-0.755146	-0.676770	0.915916
13B	-0.862167	-0.757487	-0.760051
14B	1.956191	-0.757490	-0.760050

$E15/\varepsilon$ = -55.390724

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.122549	0.000000	0.000000
3B	0.598787	-1.252248	0.000000
4B	0.598788	-0.069271	1.250331
5B	-0.257103	0.966310	-0.914256
6A	0.579437	-0.148324	-0.935716
7A	0.579437	0.926079	0.199859
8B	1.412328	0.970903	-0.918600
9B	-0.632827	-0.774610	-0.990758
10B	-0.632828	0.946391	0.828229
11B	-0.830798	-0.784893	0.742611
12B	1.868914	-0.652634	-0.947016
13B	1.868914	0.909463	0.704021
14B	2.028662	-0.758148	0.717306
15A	-1.133718	0.194065	-0.183613

$E16/\varepsilon$ = -60.928253

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.064317	0.000000	0.000000
3B	0.532160	-1.285279	0.000000
4B	0.532158	1.349602	-0.000001
5A	0.492746	0.365301	-0.917049
6A	0.571572	0.365303	0.917049
7B	1.827087	0.694077	-0.908862
8B	-0.762771	0.694076	0.908860
9B	1.306307	-0.702544	1.305576
10B	-0.241987	-0.702546	-1.305577
11A	-0.063660	-0.526681	0.984620
12A	1.127979	-0.526681	-0.984621
13B	-0.853744	0.743508	-0.757964
14B	1.918061	0.743511	0.757962
15B	-1.123959	-0.749962	0.104479
16B	2.188279	-0.749959	-0.104480

$E17/\varepsilon$ = -66.446027

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.358945	0.000000	0.000000
3A	0.440918	-1.001977	0.000000
4A	0.361735	-0.438820	-0.917340
5B	-0.875867	-0.983423	-0.453749
6B	0.332215	-1.835488	-1.122328
7B	-0.687997	0.482927	-1.122327
8A	-0.306922	-0.733061	0.777358
9B	0.296164	0.421626	1.282122
10B	0.951863	-1.068438	1.282121
11B	1.571511	-0.805777	-1.465421
12B	0.908428	0.701067	-1.465420
13B	0.258759	1.338920	-0.075413
14B	1.602932	-1.715689	-0.075415
15B	-1.185784	0.380180	0.499586
16B	-0.079820	-2.133106	0.499585
17B	0.029909	-0.584839	-2.212341

$E18/\varepsilon$ = -71.703520

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.066074	0.000000	0.000000
3B	0.532339	-1.344414	0.000000
4A	0.568306	-0.339225	-0.909851
5B	0.540400	1.284827	0.003268
6B	-0.740246	-0.708806	-0.927625
7B	1.308140	0.715200	-1.310797
8B	1.890910	-0.748084	-0.793595
9A	0.497238	-0.366538	0.917182
10A	-0.071312	0.544733	-0.970674
11B	1.833420	-0.706415	0.884917
12B	-0.852566	-0.754735	0.743173
13B	-0.247130	0.695568	1.293786
14B	-1.139207	0.725392	-0.112702
15A	1.136875	0.521481	0.984590
16B	2.194667	0.739070	0.092547
17B	0.119538	-0.033830	-2.202529
18B	0.624179	-1.503827	-1.636823

$E19/\varepsilon$ = -78.191386

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
4B	0.553068	0.562672	-1.157945
5B	0.553066	0.562672	1.157945
6B	-0.781595	-1.271141	-0.000001
7B	1.887729	-1.271141	0.000002
8A	0.006883	-0.666108	0.923839
9A	1.099249	-0.666108	0.923840
10A	1.099251	-0.666109	-0.923839
11A	0.006885	-0.666108	-0.923840
12B	1.392642	1.374024	0.000000
13B	-0.286508	1.374024	-0.000001
14B	0.553066	-1.957967	0.854950
15B	0.553068	-1.957968	-0.854950
16B	-1.079203	0.169300	-0.840167
17B	2.185336	0.169301	0.840166
18B	2.185338	0.169300	-0.840164
19B	-1.079204	0.169300	0.840164

$E20/\varepsilon$ = -83.514565

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.197703	0.000000	0.000000
3A	0.598852	-0.912246	0.000000
4A	0.598852	-0.295459	-0.892984
5A	0.598852	-0.295459	0.892984
6A	0.598852	0.751774	-0.554425
7A	0.598852	0.751774	0.554425
8B	-0.433863	-1.188890	0.829699
9B	-0.433863	-1.188890	-0.829699
10B	1.631567	-1.188889	0.829698
11B	1.631567	-1.188889	-0.829698
12B	1.679741	0.394639	1.330827
13B	-0.482038	0.394639	-1.330827
14B	1.679741	0.394639	-1.330827
15B	-0.482038	0.394639	1.330827
16B	1.692956	1.362047	0.000000
17B	-0.495252	1.362047	0.000000
18B	-1.370553	-0.077970	0.000000
19B	2.568256	-0.077969	0.000000
20B	0.598852	-2.261996	0.000000

$E21/\varepsilon$ = -89.330178

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.198969	0.000000	0.000000
3A	0.599485	-0.917149	0.000000
4A	0.599485	-0.289503	-0.870259
5B	1.604291	-1.202290	-0.867111
6B	-0.405320	-1.202291	-0.867114
7A	0.599485	0.752681	-0.563269
8A	0.599484	-0.296883	0.891998
9A	0.599484	0.756326	0.545475
10B	1.646633	-1.188716	0.799331
11B	-0.447665	-1.188717	0.799328
12B	1.646634	0.383238	-1.380256
13B	-0.447663	0.383237	-1.380258
14B	1.701885	0.390351	1.293750
15B	-0.502918	0.390350	1.293748
16B	-0.502917	1.350821	-0.037989
17B	1.701886	1.350821	-0.037987
18B	-1.364218	-0.091215	-0.065789
19B	2.563187	-0.091213	-0.065785
20B	0.599486	-2.266918	-0.014293
21B	0.599487	-0.729130	-2.146507

$E22/\varepsilon$ = -95.143253

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.078302	0.000000	0.000000
3A	0.513393	-0.948242	0.000000
4B	1.290068	-0.768547	1.161497
5A	-0.035671	-0.608753	0.905029
6A	0.518346	0.321207	0.905027
7B	0.377391	1.323254	-0.001144
8B	-0.983968	-0.961889	-0.001138
9B	-0.851960	0.507551	0.919351
10B	1.274692	-0.759391	-1.155039
11B	0.096449	-1.952827	0.862660
12B	1.763208	0.844953	0.862655
13A	-0.061938	-0.598133	-0.923409
14A	0.496498	0.339243	-0.923411
15B	0.158467	-0.094399	2.168585
16B	-0.902937	0.537918	-0.821507
17B	1.537972	-1.898995	0.003978
18B	2.402194	-0.448334	0.003976
19B	1.769287	0.852091	-0.824232
20B	0.093061	-1.961577	-0.824228
21B	-1.109911	-1.026460	1.644587
22B	0.374212	1.464757	1.644580

$E23/\varepsilon$ =-101.901346

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.161114	0.000000	0.000000
3A	0.580557	-1.005554	0.000000
4A	0.580557	-0.335185	-0.857079
5A	0.580557	-0.335184	0.857079
6A	0.580557	0.740722	-0.571010
7A	0.580557	0.740723	0.571009
8A	-0.351206	-0.873138	0.571010
9A	-0.351206	-0.873138	-0.571009
10A	1.512319	-0.873138	0.571010
11A	1.512319	-0.873138	-0.571010
12B	-0.504936	0.291524	-1.324520
13B	-0.504935	0.291525	1.324519
14B	1.666049	0.291525	1.324519
15B	1.666050	0.291524	-1.324519
16B	0.580557	-1.588603	1.324520
17B	0.580556	-1.588604	-1.324519
18B	1.424022	-2.122218	0.000000
19B	-1.388792	-0.172131	0.000000
20B	-0.262908	-2.122218	0.000000
21B	2.549905	-0.172131	0.000000
22B	-0.545327	1.288794	-0.000001

23B	1.706441	1.288793	-0.000001

$E24/\varepsilon$ =-107.064064

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.157329	0.000000	0.000000
3A	0.590476	-1.009004	0.000000
4A	0.588234	-0.333039	0.858882
5A	0.576931	-0.339653	-0.858341
6A	-0.318850	-0.863871	0.554668
7A	-0.350938	-0.882649	-0.563555
8A	1.510674	-0.872480	0.584872
9A	0.569734	0.735395	0.584872
10A	1.517175	-0.879530	-0.563330
11A	0.566771	0.744517	-0.563329
12B	0.544797	-1.569333	1.358834
13B	-0.510889	0.234621	1.358834
14B	-1.401601	-0.232672	0.046091
15B	-0.298871	-2.117012	0.046090
16B	-0.534599	0.281005	-1.291047
17B	0.573623	-1.612721	-1.291048
18B	1.663621	0.296285	1.336716
19B	1.662708	0.295752	-1.311590
20B	-0.579679	1.254272	0.044233
21B	1.400075	-2.128725	0.044232
22B	1.691927	1.291587	0.012718
23B	2.545226	-0.166528	0.012717
24B	-1.198357	-1.378563	1.403470

$E25/\varepsilon$ =-112.963841

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.139519	0.000000	0.000000
3A	0.565278	-0.999312	0.000000
4A	0.573240	-0.332085	0.865833
5A	0.550263	-0.330668	-0.865672
6A	-0.334091	-0.856908	0.578485
7A	0.567087	0.721468	0.624596
8B	0.543270	-1.557292	1.378233
9A	1.491287	-0.874797	0.575815
10A	-0.387209	-0.867912	-0.545783
11A	-0.383862	0.194944	1.002629
12A	1.484919	-0.876878	-0.576035
13A	0.552260	0.758868	-0.543819
14B	1.695163	0.270053	1.319818
15B	-1.399267	-0.176630	0.122253
16B	-0.570540	0.317257	-1.245579
17B	0.529441	-1.605480	-1.288921
18B	-0.306149	-2.107689	0.060343
19B	1.633220	0.312139	-1.312476
20B	-0.567090	1.265832	0.119551
21B	1.376889	-2.123590	0.038019
22B	1.680824	1.287200	0.028012
23B	2.531109	-0.185378	-0.018754
24B	0.316156	-0.044672	2.163237
25B	-1.058539	-0.838260	1.695343

$E26/\varepsilon$ =-120.425633

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.118544	0.000000	0.000000
3A	0.559271	-0.968687	0.000000
4A	0.559271	-0.322896	0.913287
5A	0.559272	0.720572	0.597243
6A	0.559272	-0.322895	-0.878443
7A	-0.344399	-0.844629	0.597243
8A	1.462941	-0.844630	0.597243
9A	0.559270	-1.415077	1.000610
10A	0.559273	0.769286	-0.543967
11A	-0.386585	0.223196	1.000610
12A	1.505128	0.223194	1.000611
13A	1.505128	-0.868986	-0.543967
14A	-0.386585	-0.868985	-0.543968
15B	1.390851	-2.097898	0.110000
16B	-0.272310	-2.097897	0.109999
17B	0.559272	0.637331	1.941250
18B	2.512258	-0.155566	0.110001
19B	1.680679	0.324548	-1.247964
20B	-1.393715	-0.155562	0.110000
21B	-0.562134	0.324550	-1.247965
22B	1.680679	1.284774	0.110002
23B	1.390851	-0.803009	1.941250
24B	-0.272310	-0.803008	1.941249
25B	-0.562133	1.284777	0.110001
26B	0.559271	-1.617783	-1.247965

$E27/\varepsilon$ =-125.697620

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	-0.323070	0.913182
5A	0.559572	-0.323069	-0.876086
6A	1.462517	-0.844385	0.596550
7A	-0.343372	-0.844385	0.596550
8A	0.559572	0.719561	0.596550
9A	-0.383820	-0.867737	-0.548724
10A	1.502964	-0.867737	-0.548725
11A	0.559572	0.766266	-0.548724
12A	1.505079	0.222819	1.001119
13A	-0.385935	0.222819	1.001119
14A	0.559572	-1.414847	1.001118
15B	1.692751	0.331172	-1.235277
16B	-0.573609	0.331173	-1.235275
17B	0.559571	-1.631553	-1.235276
18B	-0.274469	-2.097746	0.114972
19B	-0.560323	1.286569	0.114973
20B	2.513507	-0.158031	0.114972
21B	1.393613	-2.097746	0.114971
22B	1.679466	1.286569	0.114971
23B	-1.394364	-0.158032	0.114973
24B	-0.272233	-0.803314	1.940815
25B	1.391378	-0.803313	1.940815
26B	0.559572	0.637416	1.940816
27B	0.559570	-0.323069	-2.250492

$E28/\varepsilon$ =-131.301741

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.124603	0.000000	0.000000
3A	0.562301	-0.963801	0.000000
4A	0.562300	-0.313790	-0.912747
5A	0.562301	-0.313844	0.878177
6A	0.562301	0.751682	0.548015
7A	0.562301	0.726461	-0.588572
8A	1.464206	-0.840672	-0.600696
9A	-0.339605	-0.840671	-0.600696
10B	1.721039	0.306148	1.231920
11B	-0.596438	0.306147	1.231920
12A	-0.383956	-0.869556	0.541977
13A	1.508557	-0.869556	0.541977
14A	0.562300	-1.406078	-1.004399
15A	1.505476	0.239229	-0.996615
16A	-0.380875	0.239229	-0.996615
17B	0.562300	-1.612533	1.245336
18B	-0.546031	1.294628	-0.080451
19B	1.670632	1.294628	-0.080451
20B	2.518564	-0.151917	-0.130910
21B	-1.393963	-0.151917	-0.130909
22B	1.392518	-2.093931	-0.113360
23B	-0.267918	-2.093931	-0.113360
24B	-0.269014	-0.783259	-1.942985
25B	1.393614	-0.783259	-1.942985
26B	0.562300	0.657394	-1.934244
27B	0.562300	-0.270900	2.249663
28B	0.562300	1.368918	1.752056

$E29/\varepsilon$ =-137.929835

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.091230	0.000000	0.000000
3A	0.545615	-0.945033	0.000000
4A	0.545616	-0.315010	-0.910215
5A	0.545613	-0.315011	0.910215
6A	-0.367975	-0.842472	-0.578446
7A	0.545615	0.739912	0.578445
8A	1.459204	-0.842472	0.578446
9A	-0.367976	-0.842473	0.578443
10A	0.545616	0.739912	-0.578444
11A	1.459205	-0.842473	-0.578444
12A	1.501942	0.237126	0.974081
13A	0.545613	-1.419285	0.974080
14A	0.545616	-1.419284	-0.974081
15A	-0.410716	0.237126	0.974079
16A	-0.410713	0.237127	-0.974081
17A	1.501946	0.237126	-0.974079
18B	-1.381226	-0.145774	-0.000003
19B	-0.271243	-2.068322	-0.000002
20B	1.655599	1.269063	0.000002
21B	-0.564368	1.269064	-0.000001
22B	1.362472	-2.068322	0.000001
23B	2.472455	-0.145776	0.000003
24B	-0.285861	-0.795061	1.921471
25B	0.545611	0.645091	1.921473
26B	-0.285855	-0.795060	-1.921474
27B	1.377082	-0.795061	1.921474
28B	0.545617	0.645092	-1.921472
29B	1.377088	-0.795061	-1.921472

$E30/\varepsilon$ =-143.322385

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.107729	0.000000	0.000000
3A	0.537017	-0.940517	0.000000
4A	0.521180	-0.319450	0.913820
5A	0.536804	-0.324356	-0.921839
6A	0.554122	0.716324	-0.584682
7A	0.531109	0.729409	0.581423
8A	-0.389668	-0.841646	-0.553673
9A	-0.387993	-0.835434	0.575650
10B	1.752089	0.408443	-1.167824
11A	1.460184	-0.843584	-0.588759
12A	1.426049	-0.860310	0.599258
13A	-0.438493	0.217793	-0.957394
14B	-0.535123	1.292176	-0.042032
15A	1.470438	0.207932	1.011196
16A	0.509449	-1.422412	0.975404
17A	-0.425209	0.252688	0.965506
18A	0.493599	-1.435436	-0.955075
19B	1.668236	1.296018	0.181787
20B	0.371133	0.605308	-1.975226
21B	-1.392853	-0.111875	0.013244
22B	1.334509	-2.070670	-0.006538
23B	-0.302031	-2.070478	0.018956
24B	2.491908	-0.186853	0.151626
25B	0.519135	0.646165	1.926642
26B	1.327958	-0.816585	1.943489
27B	-0.330331	-0.783002	1.916258
28B	-0.392429	-0.848069	-1.885644
29B	1.251590	-0.910946	-1.966467
30B	0.747904	1.956061	-1.048390

$E31/\varepsilon$ =-149.398191

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.099627	0.000000	0.000000
3A	0.549814	-0.939102	0.000000

4A	0.549813	-0.299276	-0.910130
5A	0.549813	-0.299275	0.910130
6A	0.549813	0.744576	-0.557218
7A	0.549813	0.744577	0.557216
8B	-0.597325	1.251339	-0.000002
9B	1.696951	1.251340	-0.000002
10A	-0.360181	-0.836621	-0.586318
11A	-0.360180	-0.836620	0.586318
12A	1.459807	-0.836621	-0.586319
13A	1.459807	-0.836620	0.586319
14A	1.505509	0.254089	-0.970058
15A	-0.405884	0.254089	-0.970057
16A	1.505509	0.254091	0.970057
17A	-0.405884	0.254091	0.970056
18A	0.549813	-1.403306	-0.982203
19A	0.549813	-1.403305	0.982204
20B	0.549812	0.696064	-1.896743
21B	0.549812	0.696068	1.896741
22B	-1.382464	-0.167468	0.000000
23B	2.482090	-0.167467	0.000000
24B	-0.266345	-2.058232	0.000001
25B	1.365972	-2.058232	0.000001
26B	-0.278359	-0.755761	-1.929185
27B	-0.278359	-0.755757	1.929186
28B	1.377983	-0.755761	-1.929186
29B	1.377983	-0.755757	1.929187
30B	0.549813	2.065096	-0.868167
31B	0.549813	2.065099	0.868161

$E32/\varepsilon$ =-155.872192

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.143923	0.000000	0.000000
3A	-1.143923	-0.000871	0.000000
4A	-0.541869	0.947053	0.000199
5A	0.541148	0.947465	0.000199
6A	0.548495	0.281982	0.888285
7A	-0.548709	0.281937	-0.888167
8A	-0.548709	0.281565	0.888285
9A	0.548495	0.282355	-0.888167
10A	-0.545384	-0.764705	0.550041
11A	0.545966	-0.764290	0.550041
12A	-0.545384	-0.764475	-0.550360
13A	0.545966	-0.764060	-0.550360
14B	-0.000566	1.487471	1.173636
15B	-0.000566	1.487963	-1.173010
16B	1.622236	1.116512	-0.826587
17B	-1.623085	1.115277	-0.826588
18B	-1.623084	1.114931	0.827057
19B	1.622235	1.116165	0.827058
20B	0.000222	-0.583033	1.799973
21B	0.000222	-0.582279	-1.800216
22B	0.000722	-1.899234	-0.000398
23B	1.617039	-0.444798	-1.333963
24B	-1.616699	-0.446028	-1.333963
25B	-1.616698	-0.446586	1.333779
26B	1.617038	-0.445356	1.333779
27B	-1.615457	-1.410686	-0.000294
28B	1.616530	-1.409456	-0.000294
29B	0.826771	2.312008	0.000486
30B	-0.828529	2.311378	0.000485
31B	-2.523068	-0.014280	-0.000001
32B	2.523078	-0.012361	0.000000

$E33/\varepsilon$ =-162.262866

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.321573	0.000000	0.000000
3A	0.049854	-1.130394	0.000000
4A	0.049853	1.130396	0.000000
5B	-1.840696	0.000000	0.000001
6A	-0.720427	0.548135	0.573103
7A	-0.720428	0.548135	-0.573102
8A	-0.720427	-0.548134	0.573103
9A	-0.720428	-0.548134	-0.573102
10B	-0.425575	0.000001	1.832113
11B	-0.425577	0.000001	-1.832113
12B	-1.287936	1.645046	0.000001
13B	-1.287935	-1.645045	0.000001
14A	0.348844	0.538346	0.859409
15A	0.348844	-0.538345	0.859409
16A	0.348843	0.538346	-0.859409
17A	0.348843	-0.538345	-0.859410
18B	-0.301670	-1.620676	-1.332293
19B	-0.301669	1.620677	1.332293
20B	-0.301670	1.620676	-1.332293
21B	-0.301669	-1.620675	1.332294
22B	1.279881	1.491046	-0.814053
23B	1.279881	-1.491045	-0.814053
24B	1.279882	-1.491045	0.814053
25B	1.279882	1.491046	0.814053
26B	1.286963	0.000001	1.685024
27B	1.286961	0.000001	-1.685024
28B	-1.779308	0.847093	1.403087
29B	-1.779307	-0.847091	1.403087
30B	-1.779309	0.847092	-1.403085
31B	-1.779309	-0.847091	-1.403085
32B	0.187752	2.486328	0.000000
33B	0.187753	-2.486327	0.000001

$E34/\varepsilon$ =-169.250795

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.141387	0.000000	0.000000
3A	-1.141385	-0.002418	0.000000
4B	-0.001998	1.885038	-0.000573
5A	-0.543776	0.753781	-0.564192
6A	-0.543777	0.754124	0.563733
7A	0.542177	0.754932	-0.564192
8A	0.542177	0.755274	0.563733
9A	-0.547965	-0.305340	-0.883521
10A	-0.547965	-0.304803	0.883706
11A	0.548610	-0.304178	-0.883521
12A	0.548610	-0.303641	0.883706
13A	-0.543322	-0.949334	0.000289
14A	0.545332	-0.948181	0.000289
15B	1.619341	1.375352	-0.000417
16B	-1.622253	1.371917	-0.000417
17B	-0.000518	0.488208	-1.831811
18B	-0.000519	0.489322	1.831514
19B	1.623368	0.398100	1.332301
20B	-1.624207	0.393849	-1.332541
21B	1.623369	0.397290	-1.332541
22B	-1.624208	0.394659	1.332301
23B	0.001631	-1.539116	-1.118184
24B	0.001630	-1.538436	1.119120
25B	-1.612360	-1.162071	0.821949
26B	-1.612360	-1.162570	-0.821241
27B	1.614820	-1.159151	-0.821242
28B	1.614819	-1.158651	0.821949
29B	-0.839356	1.843433	1.399148
30B	0.835448	1.844357	-1.400268
31B	0.835447	1.845208	1.399147
32B	-0.839355	1.842582	-1.400268
33B	-2.521052	-0.029854	0.000009
34B	2.521110	-0.024512	0.000009

$E35/\varepsilon$ =-175.447948

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.141995	0.000000	0.000000
3A	-1.142920	-0.004446	0.000000
4B	-0.003624	1.888661	0.002970
5A	0.541020	0.756915	0.563935
6A	0.541018	0.758685	-0.561552
7A	-0.545000	0.756105	0.563365
8A	-0.545003	0.757873	-0.560979
9A	0.544367	-0.953878	-0.001499
10A	-0.533885	-0.960675	-0.001507
11A	0.550142	-0.300520	0.878980
12A	0.550138	-0.297755	-0.879921
13A	-0.550897	-0.299545	0.877515
14A	-0.550904	-0.296784	-0.878446
15B	1.618613	1.377352	0.002163
16B	-1.625168	1.372146	0.002163
17B	-0.001528	0.488977	-1.829705
18B	-0.001519	0.483223	1.831237
19B	1.622889	0.399088	1.333178
20B	1.622883	0.403276	-1.331920
21B	-1.626249	0.392461	1.332804
22B	-1.626257	0.396650	-1.331550
23B	-0.007386	-1.495799	-1.182695
24B	-0.007380	-1.499510	1.177991
25B	1.614321	-1.154842	0.823016
26B	1.614317	-1.152249	-0.826646
27B	-1.608850	-1.163708	0.817991
28B	-1.608856	-1.161130	-0.821633
29B	-0.840873	1.839989	1.403150
30B	-0.840879	1.844391	-1.397351
31B	0.832623	1.843210	1.403239
32B	0.832617	1.847612	-1.397438
33B	2.520262	-0.024028	-0.000041
34B	-2.522069	-0.031799	-0.000041
35B	0.764167	-2.329880	-0.003662

$E36/\varepsilon$ =-182.632268

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.142878	0.000000	0.000000
3A	-1.142878	-0.000431	0.000000
4A	0.542529	0.747295	-0.578072
5A	-0.542810	0.747091	-0.578072
6A	-0.542815	0.771521	0.545030
7A	0.542524	0.771725	0.545030
8B	-0.000356	1.891210	-0.041140
9A	0.540603	-0.957529	0.020829
10A	-0.540242	-0.957732	0.020829
11A	-0.550628	-0.315884	-0.871872
12A	0.550747	-0.315677	-0.871872
13A	0.550742	-0.277465	0.884775
14A	-0.550637	-0.277673	0.884775
15B	-1.619148	1.382025	-0.030072
16B	1.618628	1.382633	-0.030071
17B	-0.000100	0.529535	1.818024
18B	-0.000084	0.449979	-1.839335
19B	0.000277	-1.471139	1.208239
20B	0.000287	-1.522288	-1.143129
21B	1.623078	0.379382	-1.342095
22B	-1.623220	0.378772	-1.342096
23B	-1.623233	0.436773	1.324336
24B	1.623068	0.437384	1.324337
25B	1.620304	-1.157727	-0.800183
26B	-1.619868	-1.158336	-0.800183
27B	1.620298	-1.121836	0.849777
28B	-1.619875	-1.122446	0.849777
29B	-0.835404	1.819170	-1.440342
30B	0.834721	1.819485	-1.440340
31B	0.834709	1.880395	1.359863
32B	-0.835417	1.880081	1.359863
33B	-2.523359	-0.012562	0.000260
34B	2.523364	-0.011613	0.000261
35B	0.823299	-2.326991	0.050620
36B	-0.822423	-2.327301	0.050619

$E37/\varepsilon$ =-188.761434

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.138623	0.000000	0.000000
3A	-1.143771	-0.004669	0.000000
4A	0.540354	0.506129	0.794287

5B	-0.002822	-0.132101	1.888866
6A	-0.547466	0.500080	0.796730
7A	-0.544218	-0.616249	0.722958
8A	0.538507	0.052897	-0.952905
9A	0.539966	-0.614537	0.723284
10A	-0.544064	0.046383	-0.954421
11A	0.550619	0.907394	-0.244763
12B	-0.019128	1.772026	0.642849
13B	-0.017303	1.227810	-1.446318
14A	-0.548795	0.894247	-0.242524
15A	0.548297	-0.862544	-0.346447
16A	-0.551715	-0.864075	-0.345954
17B	1.614103	-0.104543	1.386496
18B	-1.623872	-0.103257	1.380875
19B	-0.002248	-1.865420	0.373582
20B	-0.002328	-1.097269	-1.559020
21B	1.631165	1.278557	0.504556
22B	1.628077	0.863083	-1.086159
23B	-1.626664	1.290043	0.494295
24B	-1.622942	0.877559	-1.086007
25B	1.616286	-1.371608	0.327752
26B	-1.623187	-1.370278	0.325998
27B	1.614577	-0.774799	-1.186655
28B	-1.622757	-0.770028	-1.184736
29B	0.833976	1.263248	1.947410
30B	2.521375	-0.024011	-0.006388
31B	0.821030	0.118094	-2.324448
32B	-0.837659	-1.526579	1.759520
33B	0.829207	-1.528190	1.760643
34B	-2.525576	-0.014422	-0.010573
35B	-0.851693	1.255164	1.955432
36B	-0.833829	0.108689	-2.329675
37B	0.911337	2.266727	-0.600699

$E38/\varepsilon$ =-195.963276

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.138584	0.000000	0.000000
3A	-1.138580	-0.003196	0.000000
4B	-0.002641	1.880919	0.001930
5A	0.543922	0.753050	0.561971
6A	-0.546034	0.751520	0.561971
7A	0.543920	0.754201	-0.560425
8A	-0.546036	0.752671	-0.560425
9B	-0.000791	0.562674	-1.809950
10B	-0.000785	0.558962	1.811102
11A	-0.541524	-0.313280	0.900434
12A	0.542400	-0.311759	0.900434
13A	-0.541527	-0.311434	-0.901071
14A	0.542398	-0.309912	-0.901071
15A	-0.548807	-0.932754	-0.000955
16A	0.551422	-0.931210	-0.000955
17B	-1.626341	1.371892	0.001410
18B	1.622482	1.376452	0.001410
19B	1.620271	0.403182	1.329609
20B	-1.621398	0.398632	1.329609
21B	-1.621402	0.401357	-1.328782
22B	1.620267	0.405908	-1.328782
23B	0.002249	-1.602858	-1.035703
24B	0.002252	-1.604978	1.032416
25B	1.621646	-1.159322	0.810381
26B	-1.618386	-1.163870	0.810381
27B	1.621644	-1.157658	-0.812759
28B	-1.618389	-1.162206	-0.812759
29B	-2.520567	-0.026370	-0.000022
30B	2.520630	-0.019294	-0.000022
31B	-0.856299	1.872635	1.384452
32B	0.851038	1.875032	1.384452
33B	-0.856303	1.875469	-1.380605
34B	0.851033	1.877866	-1.380605
35B	-0.832320	-0.786580	2.200393
36B	-0.832326	-0.782068	-2.201997
37B	0.834522	-0.784241	2.200393
38B	0.834516	-0.779728	-2.201997

$E39/\varepsilon$ =-202.040051

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.134713	0.000000	0.000000
3A	-1.140312	-0.001014	0.000000
4A	0.540368	0.303371	-0.898998
5A	0.540368	0.304736	0.898536
6B	-0.006694	-1.889625	0.001435
7A	-0.548157	-0.759862	-0.557521
8A	-0.548157	-0.759015	0.558674
9A	0.540972	-0.760447	-0.557879
10A	0.540972	-0.759599	0.559034
11B	-0.003295	-0.573247	1.806997
12B	-0.003295	-0.575991	-1.806124
13A	-0.546191	0.298658	-0.901132
14A	-0.546191	0.300026	0.900677
15A	0.551929	0.945682	-0.000718
16B	-0.016202	1.571354	1.068460
17B	-0.016202	1.569730	-1.070844
18A	-0.546560	0.932015	-0.000708
19B	1.614998	-1.392375	0.001058
20B	-1.628260	-1.383881	0.001051
21B	1.614903	-0.424208	1.331377
22B	1.614903	-0.426230	-1.330730
23B	-1.626082	-0.416755	-1.326915
24B	-1.626083	-0.414739	1.327546
25B	1.630713	1.126613	-0.819384
26B	1.630713	1.127856	0.817672
27B	-1.621434	1.147125	-0.814125
28B	-1.621434	1.148360	0.812382
29B	2.519615	-0.007425	0.000006
30B	-2.523938	0.013439	-0.000010
31B	0.834722	0.757188	-2.210841
32B	0.834721	0.760546	2.209689
33B	-0.860363	-1.885846	1.383031
34B	-0.860363	-1.887945	-1.380166
35B	0.844817	-1.893878	-1.380380
36B	0.844817	-1.891779	1.383255
37B	-0.848216	0.750555	-2.218123
38B	-0.848217	0.753923	2.216981
39B	0.919001	2.366230	-0.001796

$E40/\varepsilon$ =-209.230681

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.132965	0.000000	0.000000
3A	-1.132936	-0.008220	0.000000
4A	-0.537776	-0.770854	0.533362
5A	0.543353	-0.766932	0.533362
6A	-0.537777	-0.770652	-0.533651
7A	0.543352	-0.766731	-0.533651
8B	-0.005367	1.479223	-1.139144
9B	-0.005365	1.478794	1.139702
10A	-0.542217	0.241335	0.914188
11A	-0.542218	0.241680	-0.914096
12A	0.540450	0.245263	0.914189
13A	0.540449	0.245607	-0.914096
14A	-0.548772	0.923289	0.000175
15A	0.542058	0.927247	0.000175
16B	0.002839	-0.782824	-1.760434
17B	0.002842	-0.783487	1.760139
18B	-1.635764	1.039359	0.827534
19B	1.628179	1.051199	0.827533
20B	-1.635766	1.039671	-0.827137
21B	1.628178	1.051511	-0.827138
22B	-1.613603	-0.560191	1.295686
23B	1.617624	-0.548470	1.295686
24B	-1.613606	-0.559702	-1.295893
25B	1.617622	-0.547981	-1.295894
26A	0.005603	-1.544721	-0.000291
27A	1.456871	-1.072494	-0.000203
28A	-1.449053	-1.083035	-0.000202
29B	-0.875383	-2.022412	0.898063
30B	-0.875384	-2.022073	-0.898823
31B	0.890031	-2.016009	0.898062
32B	0.890030	-2.015670	-0.898822
33B	2.505750	-0.110772	-0.000022
34B	-2.504882	-0.128948	-0.000021
35B	0.833392	0.573638	2.224754
36B	-0.837533	0.567576	2.224754
37B	0.833388	0.574476	-2.224538
38B	-0.837537	0.568415	-2.224537
39B	0.848678	2.281771	0.000430
40B	-0.865212	2.275554	0.000430

$E41/\varepsilon$ =-215.407179

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.133834	0.000000	0.000000
3A	-1.130450	-0.003499	0.000000
4A	0.529580	-0.776333	0.531613
5A	0.529579	-0.775005	-0.533547
6A	-0.548384	-0.766292	-0.547942
7A	-0.548381	-0.767656	0.546033
8A	0.553613	0.259022	0.905428
9A	0.553611	0.261279	-0.904779
10A	-0.531936	0.263348	0.911534
11A	-0.531939	0.265620	-0.910871
12B	0.021791	1.503219	-1.125043
13B	0.021794	1.500409	1.128791
14A	0.554666	0.932083	0.001163
15A	-0.535567	0.933983	0.001166
16B	0.039657	-0.678832	1.783979
17B	0.039652	-0.674381	-1.785664
18A	-0.057901	-1.568938	-0.001955
19B	1.618568	-0.529666	-1.290151
20B	1.618571	-0.532882	1.288824
21B	1.649720	1.062394	-0.816996
22B	1.649722	1.060353	0.819641
23B	-1.609890	1.084989	0.830739
24B	-1.609892	1.087057	-0.828025
25B	-1.612316	-1.425124	-0.001774
26B	-1.599481	-0.495756	1.340203
27B	-1.599485	-0.492413	-1.341430
28B	0.939422	-2.008372	0.856037
29B	0.939420	-2.006231	-0.861043
30A	1.465177	-1.048088	-0.001308
31B	-0.689735	-1.977444	-1.202281
32B	-0.689732	-1.980436	1.197350
33B	2.517953	-0.105474	-0.000134
34B	-2.503965	-0.039366	-0.000046
35B	-0.810267	0.646922	2.235158
36B	-0.810272	0.652495	-2.233534
37B	-0.832455	2.307450	0.002879
38B	0.885195	2.298186	0.002866
39B	0.882916	0.643066	2.222437
40B	0.882912	0.648606	-2.220827
41B	-0.141191	-2.955065	-0.003683

$E42/\varepsilon$ =-221.319539

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.066727	0.000000	0.000000
3A	0.453774	-0.952288	0.000000
4A	0.485722	-0.281128	-0.903408
5A	-0.462493	0.955018	0.020844
6A	-1.064421	-0.021418	-0.017058
7A	0.453557	-0.319748	0.917584
8A	-0.465717	0.246337	0.925913
9A	-0.495764	-0.784454	-0.558251
10A	0.498239	0.804137	-0.553182
11A	-0.492906	-0.799154	0.544595
12A	0.481875	0.754416	0.580407
13A	-0.459944	0.317123	-0.901014

14B	1.700673	0.325712	-1.186277
15B	0.432056	0.649036	1.915590
16B	-1.601134	-0.249679	-1.287902
17B	-0.448066	-0.773468	1.880743
18A	-1.352233	0.793569	0.640756
19A	1.336583	-0.878498	0.609905
20B	-0.337829	-2.080394	0.068343
21B	-0.523123	1.667512	-1.155973
22B	1.707868	1.212401	0.177983
23B	0.333968	2.062137	0.193205
24A	1.359846	-0.869658	-0.607323
25B	0.316842	0.569843	-1.993979
26B	-1.698869	-1.241313	0.019424
27A	0.327855	-1.397699	-0.962983
28A	-1.418383	-0.287095	0.984722
29A	-0.429808	1.323423	1.052437
30A	1.410058	0.182955	1.022837
31A	-1.417764	0.880695	-0.503420
32A	-0.277223	-0.594257	-1.606180
33A	0.418475	-1.411853	0.987326
34B	1.268399	-2.077274	-0.021962
35B	2.430955	-0.286024	0.141298
36B	1.036670	-0.933958	-1.998896
37B	-1.242821	0.682267	1.984775
38B	-1.314464	2.067317	0.240671
39B	1.218016	-0.821494	1.962579
40B	-2.444026	0.206717	0.120258
41B	-0.939461	-1.772028	-1.420527
42B	1.110727	1.849765	-1.250149

$E43/\varepsilon$ =-227.979704

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.071204	0.000000	0.000000
3A	0.496923	-0.948970	0.000000
4A	-0.466250	0.282157	0.953503
5A	0.466685	0.776693	0.579253
6A	-0.471575	-0.773734	0.579252
7A	0.466832	-0.282509	0.886211
8A	-0.466154	0.952654	0.059461
9A	-1.060193	-0.028965	0.059460
10A	-0.485919	0.294061	-0.888978
11A	0.485390	-0.293739	-0.929036
12A	0.471889	0.774989	-0.548972
13A	-0.467651	-0.777553	-0.548972
14B	-1.605771	-0.370481	1.285026
15B	-0.416697	1.594403	1.285027
16B	1.701015	-1.029389	-0.661433
17B	0.440742	2.016687	-0.057951
18B	-1.582110	-1.325973	-0.057952
19A	-1.370968	0.829659	-0.520561
20A	1.374754	-0.831949	0.676109
21A	1.347746	0.295572	1.039790
22A	0.363363	-1.331071	1.039789
23A	-0.252070	-0.583099	1.635353
24A	0.399629	0.493801	1.635353
25B	0.310394	-1.743375	-1.115832
26B	1.688431	0.533763	-1.115831
27B	-0.555912	-0.626050	-1.907564
28B	0.296731	0.782900	-1.907563
29A	-1.396788	0.845284	0.626982
30A	-0.450305	1.386521	-0.933755
31A	-1.437200	-0.244272	-0.933756
32A	-0.252143	-1.733164	0.132270
33A	1.418430	1.027372	0.132271
34B	1.077507	-0.652067	2.027398
35B	1.227571	1.601988	1.381865
36B	-0.849729	-1.830644	1.381863
37B	-2.429972	0.141192	-0.043628
38B	-1.252323	2.087196	-0.043626
39B	-1.356455	0.820877	-1.857665
40B	1.071695	-2.187849	0.300998
41B	2.435349	0.065520	0.300999
42B	1.081654	-0.654574	-2.132678
43B	-0.726405	0.439593	2.394677

$E44/\varepsilon$ =-234.297422

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.073556	0.000000	0.000000
3A	0.472550	-0.971526	0.000000
4A	-0.469799	-0.804174	-0.591771
5A	0.492505	0.773822	-0.576145
6A	-1.057677	-0.042125	-0.063024
7A	-0.462572	0.962506	-0.028301
8A	0.474496	-0.304567	-0.873322
9A	-0.478651	-0.818354	0.514919
10A	-0.480633	0.285857	0.889120
11A	-0.451463	0.271808	-0.930438
12A	0.495848	0.785571	0.572327
13A	0.476073	-0.294306	0.896402
14B	-1.583872	-0.280675	-1.372072
15B	-0.475984	1.524982	-1.364255
16B	-0.316096	-2.093386	-0.028375
17B	1.726321	1.196043	-0.064895
18B	-0.473499	1.617332	1.219948
19B	-1.686424	-1.273364	-0.109107
20B	0.365017	2.062016	-0.092263
21B	0.503895	-1.564411	1.274655
22A	1.383977	0.255582	-1.031170
23A	0.387895	-1.376957	-1.022195
24A	0.388018	0.439940	-1.631435
25A	-0.227322	-0.556533	-1.637906
26A	1.352140	-0.857043	-0.664818
27A	-1.375239	0.803405	0.570764
28A	-1.395180	-0.364205	0.905915
29B	1.709723	0.197202	1.218928
30B	0.330015	0.465010	2.021412
31A	-1.388750	0.827414	-0.605314
32B	1.090126	-0.686808	-2.016977
33A	-0.431207	-0.555747	1.568115
34A	1.435544	-0.907298	0.486074
35B	-2.427244	0.166274	0.040391
36B	-1.343733	0.449314	1.964106
37B	2.450674	-0.250922	-0.213945
38B	-0.856215	-1.755222	-1.530834
39B	1.293391	-2.103778	-0.169162
40B	1.158696	1.547326	-1.540246
41B	-1.165552	-1.673785	1.378137
42B	-1.349026	2.062303	-0.062847
43B	1.148874	1.752484	1.360174
44B	-0.620267	0.378577	-2.536969

$E45/\varepsilon$ =-240.654799

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.079134	0.000000	0.000000
3A	0.473022	-0.969938	0.000000
4A	0.509199	0.772326	0.589571
5A	-0.470976	-0.796212	0.589570
6A	0.484561	-0.302801	0.871092
7A	-0.441340	0.971637	0.046898
8A	-1.066773	-0.029221	0.046897
9A	-0.436180	0.272567	0.936463
10A	-0.474978	0.296812	-0.890266
11A	0.508397	0.798090	-0.524090
12A	-0.494484	-0.806784	-0.524090
13A	0.488154	-0.305046	-0.891372
14B	-0.422619	1.528195	1.386723
15B	-1.558808	-0.290007	1.386722
16B	0.564918	-1.600882	-1.236769
17B	1.686516	0.193968	-1.236768
18B	-0.485911	1.600140	-1.217207
19B	-1.651216	-0.264655	-1.217207
20B	-0.311718	-2.086988	0.045543
21B	1.739172	1.194976	0.045543
22B	-1.687834	-1.253566	0.087039
23B	0.386883	2.066527	0.087040
24A	0.391138	-1.370431	1.024977
25A	1.403209	0.249148	1.024978
26A	0.413567	0.434003	1.638579
27A	-0.208807	-0.561958	1.638579
28A	1.363139	-0.851822	0.662570
29A	-0.332778	-0.566633	-1.566000
30A	0.363428	0.547481	-1.566000
31A	-1.380913	0.862929	-0.497280
32A	-1.347372	0.841969	0.646692
33B	1.110067	-0.693678	2.012676
34A	1.449875	-0.906023	-0.473300
35B	2.462240	-0.246998	0.198987
36B	1.301291	-2.104822	0.198987
37B	1.206597	1.533281	1.537580
38B	-0.849239	-1.756595	1.537579
39B	-2.454909	0.250052	0.113580
40B	-1.300823	2.096894	0.113581
41B	-0.729687	0.455980	-2.365903
42B	1.117881	1.713444	-1.395302
43B	-1.050057	-1.755827	-1.395302
44B	0.727260	-0.454463	-2.404789
45B	-0.593430	0.370832	2.544795

$E46/\varepsilon$ =-247.137015

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.174039	0.000000	0.000000
3A	0.500979	-1.006225	0.000000
4A	-0.509323	1.010035	0.000000
5A	0.551231	-0.318951	-0.849854
6A	0.551231	-0.318952	0.849853
7A	0.574923	0.888081	0.000000
8A	0.016317	0.625478	-0.896836
9A	0.016318	0.625478	0.896837
10B	-0.421254	-0.267387	-1.817091
11B	-0.421253	-0.267388	1.817091
12A	-0.415004	-0.823761	-0.566507
13A	-0.415003	-0.823762	0.566507
14A	-0.912190	0.143950	-0.567007
15A	-0.912190	0.143949	0.567007
16B	-1.661588	-0.858099	0.000000
17B	0.458384	-1.586365	1.309322
18B	0.458383	-1.586364	-1.309323
19B	1.811499	1.385841	-0.000001
20A	1.091630	0.628768	0.929291
21A	1.091629	0.628769	-0.929292
22A	1.430443	-0.903990	0.560942
23A	1.430442	-0.903990	-0.560942
24B	0.441383	1.935463	-0.817401
25B	0.441384	1.935462	0.817401
26B	2.339793	0.061951	-0.819180
27B	2.339794	0.061951	0.819177
28B	-0.415209	-2.070790	-0.000001
29B	-1.926691	0.855626	0.000001
30B	-1.052405	1.294833	-1.329618
31B	-1.052404	1.294832	1.329619
32B	1.273362	-2.158372	-0.000001
33B	1.265512	-0.275161	1.980094
34B	1.265509	-0.275159	-1.980097
35B	0.379123	1.080644	2.174140
36B	0.379120	1.080646	-2.174141
37B	2.669580	-1.308984	-0.000002
38B	-0.982012	2.282486	0.000001
39B	-1.993678	-0.083285	1.398661
40B	-1.993679	-0.083283	-1.398660
41B	-1.222245	-1.616410	1.381112
42B	-1.222246	-1.616408	-1.381112
43B	1.897876	1.429259	-1.664827
44B	1.897877	1.429261	1.664823
45B	2.101907	-1.621868	-1.499297
46B	2.101909	-1.621871	1.499293

$E47/\varepsilon$ =-253.365117

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.108782	0.000000	0.000000
3A	0.513684	-0.962192	0.000000
4A	-0.438103	0.268841	-0.973515
5A	-0.439590	-0.791365	-0.605676
6A	0.487419	-0.307372	-0.848446
7A	0.505358	0.737613	-0.586085
8A	0.509170	0.770619	0.534051
9A	-0.481721	0.946139	-0.097353
10A	0.522000	-0.295014	0.894900
11A	-1.080762	-0.028238	-0.070765
12A	-0.468328	-0.791165	0.513442
13A	-0.498845	0.299086	0.866484
14A	0.459143	-1.338323	-1.088933
15A	-0.152702	-0.574022	-1.663620
16A	1.394948	-0.849366	-0.676638
17A	0.442585	0.398280	-1.636662
18A	1.379062	0.231746	-1.043471
19B	1.642896	1.321126	-0.221637
20A	0.997654	-0.575702	-1.724139
21B	-0.112152	1.635159	-1.345996
22B	1.683550	-1.080338	0.678408
23B	-1.522384	-0.506556	-1.373221
24B	1.688435	0.463844	1.162852
25B	-1.569119	1.045103	-0.924805
26B	0.244523	-1.744664	1.124962
27B	0.227049	0.705414	1.912372
28B	-1.526482	-1.445156	-0.039533
29B	-1.611282	1.062806	0.717909
30A	0.332073	1.683375	-0.047289
31A	-0.298427	1.426361	0.865204
32B	2.482634	-0.080717	-0.316798
33B	-0.704033	0.488204	-2.352456
34B	-0.714151	-1.912062	-1.419116
35B	1.058391	-2.230789	-0.271465
36B	-1.579006	-0.466550	1.255176
37A	-0.207751	-1.750444	-0.163019
38B	1.424460	1.308779	-1.862524
39A	-0.269643	-0.543243	1.590517
40B	0.844593	0.103547	-2.891950
41B	2.263833	-0.157721	-1.985540
42B	1.745121	-1.712057	-1.664302
43B	0.374353	-1.458332	-2.550153
44B	0.944979	1.967296	1.136053
45B	-0.874772	2.306525	-0.043716
46B	1.011040	-0.708532	2.140211
47B	-2.473718	-0.083353	-0.096142

$E48/\varepsilon$ =-260.451080

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.095930	0.000000	0.000000
3A	0.541814	-0.950976	0.000000
4A	0.550579	0.988193	-0.002180
5A	-0.587370	-0.959479	-0.000991
6A	1.667833	-0.970621	0.001045
7A	0.547240	0.311124	-0.866425
8A	0.001703	-0.627354	-0.867906
9A	0.546983	0.312332	0.866065
10A	-0.000544	-0.626686	0.866244
11A	1.085569	-0.630593	-0.867080
12A	1.083844	-0.629928	0.867878
13A	-0.368008	0.840832	-0.579012
14A	-0.909562	-0.091862	-0.583907
15B	-0.338887	0.201628	-1.861733
16A	-0.365096	0.842623	0.573434
17B	-1.613398	0.929838	0.005119
18A	-0.918016	-0.089072	0.585443
19B	-0.350464	0.203814	1.854563
20B	0.552060	1.565106	-1.330520
21A	1.468351	0.841238	-0.584991
22B	-1.084451	-1.251160	-1.335191
23A	1.467753	0.842481	0.582551
24A	-0.007374	-1.688430	-0.583898
25A	-0.010114	-1.688140	0.583696
26B	0.552958	1.568149	1.325923
27A	2.009058	-0.105268	-0.584149
28A	2.008096	-0.104489	0.585418
29A	1.082854	-1.693458	-0.584577
30A	1.081040	-1.693144	0.585569
31B	-0.312754	2.079809	-0.003284
32B	1.453939	0.206112	-1.849106
33B	0.540916	-1.364641	-1.849653
34B	1.453164	0.208695	1.848611
35B	0.535741	-1.365020	1.848475
36B	-1.096573	-1.242515	1.325765
37B	-1.959964	-0.752377	-0.011367
38B	2.170490	-1.263104	-1.329793
39B	2.167740	-1.262276	1.332494
40B	1.400237	2.081105	-0.003081
41B	-1.118959	-2.240088	-0.003078
42B	2.183265	-2.259836	0.001887
43B	3.043995	-0.784554	0.002038
44B	2.704053	0.921654	-0.000090
45B	0.530777	-2.803567	0.000521
46B	-1.110910	1.616131	-1.419025
47B	-1.949442	0.168697	-1.430035
48B	-1.110817	1.616246	1.417370

$E49/\varepsilon$ =-267.906522

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.094017	0.000000	0.000000
3A	0.539861	-0.951537	0.000000
4A	-0.589381	-0.962357	0.000000
5A	0.546184	0.987513	0.000000
6A	1.665823	-0.970141	0.000001
7A	-0.001952	-0.627536	-0.866554
8A	0.544845	0.311366	-0.866555
9A	-0.001953	-0.627536	0.866554
10A	0.544845	0.311366	0.866554
11A	1.082297	-0.630308	0.867467
12A	1.082298	-0.630308	-0.867466
13B	-1.611266	0.938368	-0.000001
14A	-0.913184	-0.092337	0.578600
15A	-0.370314	0.839820	-0.578601
16A	-0.370315	0.839820	0.578600
17A	-0.913183	-0.092337	-0.578601
18B	-0.344737	0.200767	1.859063
19B	-0.344736	0.200767	-1.859064
20B	0.548957	1.565920	1.328623
21B	-1.091089	-1.250194	-1.328623
22B	-1.091090	-1.250193	1.328623
23B	0.548958	1.565920	-1.328623
24A	-0.009898	-1.689535	0.583590
25A	-0.009898	-1.689536	-0.583590
26A	1.464613	0.842339	0.583590
27A	1.464614	0.842339	-0.583590
28B	-1.963316	-0.748895	-0.000001
29B	-0.317469	2.077177	-0.000001
30A	1.080522	-1.693375	0.585173
31A	1.080523	-1.693375	-0.585171
32A	2.006039	-0.104176	0.585173
33A	2.006040	-0.104176	-0.585171
34B	0.535519	-1.364208	-1.849153
35B	1.450800	0.207415	-1.849153
36B	0.535517	-1.364207	1.849154
37B	1.450798	0.207416	1.849155
38B	2.166993	-1.262013	1.331345
39B	2.166995	-1.262014	-1.331341
40B	1.394985	2.081389	0.000000
41B	-1.121940	-2.240405	0.000000
42B	3.041643	-0.783203	0.000002
43B	2.182153	-2.259029	0.000002
44B	2.700517	0.922842	0.000001
45B	0.529961	-2.804206	0.000001
46B	-1.111540	1.616970	-1.421920
47B	-1.954891	0.168858	-1.421921
48B	-1.954892	0.168858	1.421919
49B	-1.111542	1.616970	1.421919

$E50/\varepsilon$ =-274.312888

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.093271	0.000000	0.000000
3A	0.542471	-0.950805	0.000000
4A	0.542216	0.989942	-0.001169
5A	-0.586131	-0.964094	0.001154
6A	1.669753	-0.963572	-0.003390
7A	0.543167	0.312010	-0.866595
8A	-0.000602	-0.628054	-0.866292
9A	0.545060	0.313583	0.865457
10A	0.000900	-0.626908	0.867077
11A	1.083360	-0.627805	-0.867591
12A	1.084664	-0.628280	0.867495
13B	-1.612862	0.935001	-0.000162
14A	-0.373044	0.838208	-0.579735
15A	-0.371944	0.839959	0.577665
16A	-0.913055	-0.095372	-0.577981
17A	-0.911949	-0.094028	0.579126
18B	-0.346164	0.198405	-1.859334
19B	-0.342602	0.202986	1.858549
20B	0.542581	1.563374	-1.332876
21A	1.456998	0.839439	-0.576586
22B	1.430809	0.196828	-1.862073
23A	2.006374	-0.093132	-0.593285
24A	1.462001	0.846577	0.579492
25B	0.549229	1.571034	1.321512
26B	-1.088388	-1.253979	-1.326984
27B	-1.086092	-1.251571	1.330310
28B	-0.319372	2.077339	-0.004950
29A	-0.005082	-1.689982	-0.583219
30A	-0.003554	-1.689520	0.584787
31A	2.004868	-0.099631	0.583872
32A	1.085778	-1.690021	-0.586719
33B	-1.960794	-0.753748	0.002203
34A	1.087818	-1.690092	0.583095
35B	0.537764	-1.363123	-1.849453
36B	1.453374	0.213957	1.845863
37B	0.541581	-1.363427	1.848893
38B	2.169820	-1.252072	-1.335829
39B	1.396582	2.082806	-0.012564
40B	2.173720	-1.255361	1.327804
41B	2.702271	0.924593	0.016286
42B	-1.114807	-2.243317	0.002524
43B	3.043337	-0.769571	-0.006537
44B	2.191272	-2.250067	-0.004881
45B	0.539481	-2.802337	-0.000235
46B	-1.116239	1.613113	-1.423598
47B	-1.955696	0.162870	-1.420803
48B	-1.111895	1.617929	1.419681
49B	-1.952599	0.166878	1.423172
50B	2.212557	1.595409	-1.419669

s = 1.6

$E5/\varepsilon$ =-9.201428

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
4B	0.561986	-0.324462	1.301696
5B	0.561986	-0.324462	-1.301696

$E6/\varepsilon$ = -13.138655

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.161602	0.000000	0.000000
3B	0.580800	-1.312441	0.000000
4B	0.580800	0.000000	1.312441
5B	0.580800	0.000000	-1.312441
6B	0.580800	1.312441	0.000000

$E7/\varepsilon$ = -16.634759

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.462464	0.000000	0.000000
3B	0.351120	-1.413250	0.000000
4B	0.354329	1.096111	-0.891534
5B	0.354329	1.096111	0.891534
6A	0.435898	-0.346080	0.973719
7A	0.435898	-0.346080	-0.973719

$E8/\varepsilon$ = -20.902561

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.422607	0.000000	0.000000
3B	0.210330	-1.439661	0.000000
4B	0.210329	0.964521	1.068795
5A	0.454391	-0.431815	0.971339
6B	-0.989290	-0.415740	0.935180
7B	0.313550	-0.351685	-1.382000
8B	0.313550	1.261604	-0.664802

$E9/\varepsilon$ = -26.148194

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.411875	0.000000	0.000000
3B	0.113788	-1.407282	0.000000
4B	-1.043285	-0.295742	0.906118
5B	0.210696	1.063726	-0.906118
6B	0.210696	1.063726	0.906118
7B	-1.043285	-0.295741	-0.906118
8A	0.405251	-0.373806	0.974336
9A	0.405251	-0.373806	-0.974336

$E10/\varepsilon$ = -31.451692

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.418215	0.000000	0.000000
3B	0.152584	-1.409983	0.000000
4B	0.240116	1.057487	0.914001
5B	-1.025516	-0.352496	0.914001
6B	0.240117	1.057487	-0.914002
7B	-1.025515	-0.352497	-0.914001
8A	-0.835835	0.750264	-0.000001
9A	0.417918	-0.375132	-0.972696
10A	0.417917	-0.375132	0.972696

$E11/\varepsilon$ = -35.603591

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.457006	0.000000	0.000000
3B	-0.989940	-1.064991	0.000000
4B	-0.989941	0.380077	-0.994858
5A	0.423851	0.005391	-1.007602
6A	0.423851	-0.943174	-0.354561
7B	0.328819	-0.817361	1.125619
8B	0.328820	1.343198	-0.361822
9B	-0.999143	0.557312	0.809518
10A	0.444109	0.587216	0.852952
11B	-0.243561	-1.113469	-1.617352

$E12/\varepsilon$ = -40.269325

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.428326	0.000000	0.000000
3B	-1.053626	-1.006925	0.000000
4B	-1.053626	0.619471	-0.793825
5A	0.407656	-0.992294	-0.290954
6A	0.407656	0.381091	-0.961287
7B	0.288479	-0.913985	1.130890
8B	0.288480	1.453846	-0.024820
9A	-0.230310	-0.506631	-1.037992
10B	-0.933819	0.477277	0.977846
11A	0.491027	0.470707	0.964387
12B	1.077587	-0.760542	-1.558207

$E13/\varepsilon$ = -45.438215

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.482393	0.000000	0.000000
3B	0.396676	-1.428334	0.000000
4A	-0.470450	1.057273	0.000000
5A	-1.144606	0.170375	0.000000
6B	0.494120	-0.375595	1.398251
7B	0.494120	-0.375595	-1.398251
8A	-0.551530	0.419233	0.891251
9A	-0.551530	0.419233	-0.891251
10A	-0.679210	-0.655097	-0.570594
11A	-0.679210	-0.655097	0.570593
12A	0.449455	0.829740	-0.570593
13A	0.449455	0.829740	0.570593

$E14/\varepsilon$ = -51.095901

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.069407	0.000000	0.000000
3A	0.534703	-0.972693	0.000000
4A	0.534703	-0.333352	-0.913788
5A	0.534703	0.333353	0.913787
6A	0.534703	0.972693	-0.000002
7B	-0.368819	-0.778883	1.113231
8B	-0.368820	0.778882	-1.113232
9B	1.438224	-0.778883	1.113232
10B	1.438225	0.778883	-1.113232
11B	-0.754620	-0.966557	-0.676261
12B	-0.754621	0.966557	0.676260
13B	1.824025	0.966558	0.676261
14B	1.824026	-0.966557	-0.676262

$E15/\varepsilon$ = -56.181783

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.150794	0.000000	0.000000
3B	0.575396	-1.315325	0.000000
4B	0.575396	-0.042743	1.302121
5A	0.575397	-0.155419	-0.897578
6B	-0.300233	0.989926	-1.010308
7B	1.451029	0.989925	-1.010307
8A	0.575397	0.925001	0.148999
9B	-0.711676	-0.718679	-1.070075
10B	1.862470	-0.718680	-1.070074
11B	-0.750447	0.997973	0.710125
12B	1.901240	0.997972	0.710127
13B	2.115973	-0.774525	0.710306
14B	-0.965181	-0.774524	0.710305
15B	0.575399	-0.000195	-2.278691

$E16/\varepsilon$ = -61.799365

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.092841	0.000000	0.000000
3A	0.540055	-0.950073	0.000000
4B	0.476565	-0.277281	1.288451
5B	0.480136	1.303232	0.183264
6B	-0.895711	-1.061437	0.183253
7B	1.380720	-0.803345	-1.168291
8A	0.538168	0.333024	-0.903158
9A	-0.023564	-0.632432	-0.903161
10B	1.875394	-1.091172	0.504611
11B	-0.898209	0.522610	-0.937409
12B	0.189434	-2.066890	-0.820913
13B	1.890488	0.856728	-0.820910
14B	0.410162	-2.017891	0.948801
15B	1.956978	0.640605	0.948800
16B	-1.009681	0.587464	0.845461

$E17/\varepsilon$ = -67.449039

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.085938	0.000000	0.000000
3A	0.542969	-0.940450	0.000000
4B	0.542969	-0.313483	1.276333
5A	-0.014554	-0.635370	-0.897392
6A	1.100493	-0.635370	-0.897392
7A	0.542969	0.330290	-0.897392
8B	0.542969	1.295469	0.166473
9B	1.936363	-1.117959	0.166473
10B	-0.850424	-1.117959	0.166473
11B	1.960157	0.504730	-0.977814
12B	-0.874218	0.504730	-0.977815
13B	0.542970	-1.949910	-0.977814
14B	0.542970	-0.313481	-2.164474
15B	-0.975732	0.563339	0.840733
16B	0.542970	-2.067128	0.840733
17B	2.061671	0.563339	0.840733

$E18/\varepsilon$ = -73.165711

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	0.301581	0.886291
5B	0.546598	-0.294839	-1.274867
6B	0.546598	1.301887	-0.131557
7A	1.108507	-0.644818	0.900541
8A	-0.015308	-0.644819	0.900541
9B	-0.848071	-1.113101	-0.173369
10B	-0.848072	0.522693	0.997919
11B	1.941270	-1.113099	-0.173369
12B	1.941270	0.522696	0.997916
13B	0.546601	-1.958603	0.963004
14B	0.546600	-0.280735	2.164415
15B	-0.972928	0.587369	-0.820308
16B	2.066123	0.587370	-0.820310
17B	0.546600	-2.051610	-0.856304
18B	0.546598	1.471553	1.666399

$E19/\varepsilon$ = -79.045725

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.094865	0.000000	0.000000
3A	-0.007244	-1.094842	0.000000
4A	0.543810	-0.547421	0.776744
5A	0.543810	-0.547421	-0.776744
6B	1.401250	-1.410551	0.000000
7B	0.475301	0.892473	0.966182
8B	0.475301	0.892473	-0.966182
9B	-0.895599	-0.469388	0.966181
10B	-0.895599	-0.469388	-0.966181
11B	1.874829	-0.200230	-1.188968
12B	0.187822	-1.876114	1.188968
13B	1.874829	-0.200230	1.188968
14B	0.187822	-1.876114	-1.188968
15B	-1.013067	1.019790	0.000000
16B	-1.149659	-1.948798	0.000000
17B	1.956359	1.136741	0.000000
18B	0.403349	-0.406027	2.189058
19B	0.403349	-0.406027	-2.189058

$E20/\varepsilon$ = -84.683290

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.089526	0.000000	0.000000
3A	0.000000	-1.089526	0.000000
4A	1.089526	-1.089526	0.000000
5A	0.544763	-0.544763	-0.770411
6A	0.544763	-0.544763	0.770411
7B	0.544763	0.856273	-0.990681
8B	0.544763	0.856273	0.990681
9B	-0.856273	-0.544762	0.990682
10B	-0.856273	-0.544762	-0.990682
11B	1.945799	-0.544763	-0.990682
12B	0.544763	-1.945799	0.990681
13B	1.945799	-0.544763	0.990682
14B	0.544763	-1.945799	-0.990681
15B	-0.986360	0.986360	0.000000
16B	0.544762	-0.544762	2.165335
17B	0.544762	-0.544762	-2.165335
18B	2.075886	0.986360	0.000000
19B	2.075886	-2.075886	0.000000
20B	-0.986362	-2.075884	0.000000

*E*21/ε = -90.570373

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.115920	0.000000	0.000000
3A	0.557960	-0.910668	0.000000
4A	0.557960	0.368390	-0.832829
5B	0.557960	0.730814	1.122384
6A	1.093899	-0.607693	-0.933294
7A	0.022022	-0.607693	-0.933294
8B	1.974579	-1.191211	-0.016313
9B	1.974580	0.466958	-1.095990
10B	-0.858659	0.466958	-1.095991
11B	-0.858659	-1.191211	-0.016313
12A	1.110667	-0.578570	0.932155
13A	0.005253	1.086527	-0.152034
14A	0.005253	-0.578570	0.932154
15A	1.110667	1.086527	-0.152034
16B	0.557960	-1.946179	-0.938923
17B	0.557960	-0.071389	-2.159650
18B	0.557961	1.630802	-1.399651
19B	0.557960	-1.939722	0.925213
20B	-1.123347	0.445231	0.683788
21B	2.239267	0.445231	0.683789

*E*22/ε = -96.512158

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.210237	0.000000	0.000000
3A	0.605118	-0.926448	0.000000
4A	0.605118	-0.289333	0.876166
5A	0.605118	-0.289333	-0.876166
6B	-0.464180	-1.219483	0.879925
7B	-0.464181	-1.219483	-0.879924
8B	1.674413	-1.219487	0.879925
9B	1.674414	-1.219487	-0.879925
10A	0.605120	0.751026	-0.548082
11A	0.605120	0.751026	0.548082
12B	1.671507	0.456721	1.428819
13B	1.671507	0.456721	-1.428818
14B	-0.461268	0.456725	-1.428818
15B	-0.461268	0.456725	1.428819
16B	1.675653	1.493587	0.000000
17B	-0.465410	1.493592	0.000000
18B	2.634041	-0.008756	0.000000
19B	-1.423803	-0.008747	0.000001
20B	0.605114	-2.349172	0.000000
21B	0.605117	-0.746398	-2.225541
22B	0.605117	-0.746398	2.225541

*E*23/ε =-103.276147

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.210250	0.000000	0.000000
3A	0.605124	-1.048108	0.000000
4A	0.605124	-0.349369	0.826000
5A	0.605125	-0.349369	-0.825999
6A	-0.326605	-0.887303	0.567184
7A	-0.326605	-0.887303	-0.567186
8A	1.536853	-0.887304	0.567185
9A	0.605124	0.726499	0.567185
10A	1.536853	-0.887304	-0.567185
11A	0.605125	0.726499	-0.567186
12B	0.605124	-1.603096	-1.413658
13B	1.690884	0.277494	-1.413657
14B	-0.480634	0.277494	-1.413658
15B	-0.480636	0.277495	1.413655
16B	0.605123	-1.603097	1.413656
17B	1.690884	0.277495	1.413656
18B	1.501393	-2.195604	-0.000001
19B	2.652145	-0.202446	0.000000
20B	-0.545625	1.349942	-0.000001
21B	-0.291148	-2.195603	-0.000001
22B	1.755875	1.349941	-0.000001
23B	-1.441897	-0.202445	-0.000002

*E*24/ε =-108.932853

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	-0.352781	0.826095
5A	0.608699	-0.344442	-0.826467
6A	0.608699	0.703938	0.555585
7A	0.608699	0.732035	-0.561267
8B	-0.447072	0.294688	1.438839
9B	1.664469	0.294687	1.438840
10A	-0.322879	-0.881022	0.577263
11A	1.540276	-0.881022	0.577263
12A	1.546846	-0.883012	-0.560582
13A	-0.329450	-0.883012	-0.560582
14B	-0.517358	1.375848	0.035496
15B	1.734756	1.375848	0.035496
16B	-0.487701	0.297950	-1.387466
17B	1.705098	0.297950	-1.387466
18B	0.608698	-1.597188	1.426569
19B	0.608698	-1.604417	-1.400653
20B	2.649390	-0.174483	0.033153
21B	-1.431993	-0.174482	0.033153
22B	1.505344	-2.190092	0.013679
23B	-0.287948	-2.190092	0.013678
24B	0.608698	1.787590	1.431848

*E*25/ε =-114.879107

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.104644	0.000000	0.000000
3A	0.552322	-0.956649	0.000000
4A	1.105582	-0.638308	-0.869473
5A	-0.000940	-0.638308	-0.869472
6A	0.552321	0.319969	-0.869471
7B	-0.816274	0.471276	-1.235863
8B	1.920914	0.471277	-1.235867
9B	0.552321	-1.899198	-1.235869
10B	0.552323	0.728600	1.076815
11B	-0.354825	-0.842628	1.076813
12B	1.459474	-0.842628	1.076811
13B	0.552319	-0.318881	-2.137622
14A	1.487552	-1.486876	-0.238343
15A	-0.382907	-1.486877	-0.238340
16A	1.096219	1.075046	-0.238338
17A	-0.926805	-0.544820	-0.238338
18A	2.031449	-0.544819	-0.238343
19A	0.008424	1.075047	-0.238337
20B	0.552324	-2.286537	0.513649
21B	-1.151715	0.664941	0.513656
22B	2.256360	0.664942	0.513651
23B	2.184060	-1.260966	-1.510704
24B	0.552319	1.565291	-1.510696
25B	-1.079420	-1.260968	-1.510699

*E*26/ε =-122.006208

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.129285	0.000000	0.000000
3A	0.564642	-0.977990	0.000000
4A	0.564642	-0.325997	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	1.510811	-0.872268	-0.542029
12A	0.564642	0.766545	-0.542029
13A	1.510811	0.220274	1.003059
14A	-0.381528	-0.872267	-0.542029
15B	-0.321550	-2.155437	0.126388
16B	1.450830	-2.155438	0.126388
17B	1.705890	1.356186	0.126387
18B	0.564640	-1.643796	-1.320753
19B	2.592079	-0.178739	0.126388
20B	0.564641	0.697286	1.990037
21B	1.450830	-0.837639	1.990037
22B	-0.576605	0.332903	-1.320754
23B	-1.462795	-0.178738	0.126387
24B	-0.321550	-0.837639	1.990037
25B	1.705890	0.332903	-1.320754
26B	-0.576605	1.356187	0.126387

*E*27/ε =-127.430425

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	-0.330718	0.922477
5A	0.568125	0.709409	0.599911
6A	-0.332678	-0.845786	0.599911
7A	0.552726	-0.320151	-0.870640
8A	1.462524	-0.847126	0.599264
9A	-0.355743	0.206053	0.991281
10A	-0.398351	-0.867712	-0.529368
11A	0.554468	0.777286	-0.529367
12A	1.506105	0.226076	1.008134
13A	0.553286	-1.418922	1.008133
14A	1.503250	-0.870715	-0.545375
15B	-1.473715	-0.167386	0.187106
16B	-0.588081	1.361622	0.187108
17B	-0.358133	-0.813556	1.989484
18B	0.527501	0.715451	1.989484
19B	-0.607710	0.351999	-1.276118
20B	1.419667	-0.822304	1.999391
21B	-0.334361	-2.155504	0.131405
22B	1.703370	1.362544	0.131406
23B	1.436801	-2.155988	0.124136
24B	0.544862	-1.639357	-1.316913
25B	2.585064	-0.173565	0.124137
26B	1.693125	0.343066	-1.316913
27B	-1.328676	0.769596	1.795513

*E*28/ε =-133.017782

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.097111	0.000000	0.000000
3A	0.494536	-0.970528	0.000000

4A	0.475929	-0.277290	0.937182
5A	0.524061	-0.314605	-0.880621
6B	-0.811580	0.532315	-0.976871
7B	-0.871442	0.562919	0.905943
8A	0.553419	0.737526	-0.569985
9A	0.527017	0.749718	0.566301
10A	1.368764	-0.833311	0.625946
11A	-0.422775	-0.792525	0.580397
12B	1.711312	0.271737	-1.324940
13A	-0.413233	-0.820124	-0.598581
14B	1.674478	1.357359	0.059031
15A	1.454610	-0.890567	-0.516771
16A	0.449339	-1.375770	1.013734
17A	1.445191	0.245610	1.001557
18B	0.531184	-1.645709	-1.316940
19B	-0.438915	-2.094726	0.096391
20B	2.532359	-0.205335	0.169042
21B	1.337244	-2.155643	0.178828
22B	1.346153	-0.800694	2.012286
23B	0.522046	0.764451	1.971656
24B	-0.421645	-0.765486	1.984952
25B	-0.091578	1.873446	-0.021010
26B	-1.696608	-0.714491	-0.012858
27B	0.220720	-0.131133	-2.234236
28B	0.522582	1.562278	-1.693405

$E29/\varepsilon$ =-139.739463

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.094292	0.000000	0.000000
3A	0.547146	-0.947685	0.000000
4A	0.547147	-0.315895	0.919466
5A	0.547146	-0.315895	-0.919466
6A	-0.361611	-0.840567	0.579040
7A	-0.361612	-0.840567	-0.579039
8A	0.547146	0.733448	-0.579040
9A	0.547146	0.733448	0.579040
10A	1.455904	-0.840566	-0.579040
11A	1.455904	-0.840567	0.579039
12A	1.504658	0.236925	-0.974509
13A	0.547146	-1.421535	0.974509
14A	0.547146	-1.421535	-0.974509
15A	-0.410366	0.236925	0.974509
16A	-0.410367	0.236924	-0.974508
17A	1.504660	0.236925	0.974509
18B	-1.450358	-0.166051	0.000000
19B	-0.581376	1.339071	0.000000
20B	1.416129	-2.120707	-0.000001
21B	1.675669	1.339071	0.000000
22B	-0.321836	-2.120707	0.000000
23B	2.544651	-0.166051	-0.000001
24B	-0.337466	-0.826626	1.970744
25B	-0.337468	-0.826627	-1.970744
26B	0.547147	0.705567	1.970744
27B	0.547143	0.705568	-1.970744
28B	1.431759	-0.826627	1.970744
29B	1.431757	-0.826625	-1.970745

$E30/\varepsilon$ =-145.480894

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.110012	0.000000	0.000000
3A	0.575570	-0.951018	0.000000
4A	0.553540	0.967676	-0.000001
5A	-0.557873	0.959112	0.000000
6B	1.343723	-0.762382	1.250581
7B	1.343722	-0.762384	-1.250581
8A	-0.538559	-0.972859	0.000001
9A	-1.111378	-0.011720	0.000001
10A	0.532116	0.322046	-0.884782
11A	0.532116	0.322047	0.884781
12A	0.000429	-0.625584	0.884606
13A	0.000427	-0.625586	-0.884605
14A	-0.552085	0.303626	0.883196
15A	-0.552086	0.303624	-0.883196
16B	-0.031372	1.578491	-1.186247
17B	-0.031371	1.578493	1.186245
18B	1.741811	0.987932	0.884137
19B	1.741811	0.987931	-0.884139
20B	-1.377059	-0.819581	-1.151288
21B	-1.377057	-0.819580	1.151291
22B	0.032029	-2.006462	0.878355
23B	0.032027	-2.006464	-0.878351
24B	-0.031393	0.005594	2.159577
25B	-0.031395	0.005591	-2.159576
26B	-1.750912	0.986234	0.876720
27B	-1.750912	0.986233	-0.876720
28B	2.498238	-0.371923	-0.000001
29B	1.596463	-1.957796	0.000001
30B	1.014092	2.341037	-0.000002

$E31/\varepsilon$ =-152.530780

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.111655	0.000000	0.000000
3A	0.549155	-0.966542	0.000000
4A	-0.543364	-0.968461	0.000000
5A	0.573624	0.950853	0.000000
6B	1.345605	0.766203	1.249307
7B	-0.001465	-1.548455	-1.249307
8B	1.345605	0.766203	-1.249307
9B	-0.001465	-1.548455	1.249307
10A	-1.110490	-0.004729	0.000000
11A	-0.544464	0.967869	0.000000
12A	0.537141	-0.312600	-0.883861
13A	0.537141	-0.312600	0.883861
14A	-0.002246	0.627668	-0.882948
15A	-0.002246	0.627668	0.882948
16A	-0.546844	-0.308111	0.882948
17A	-0.546844	-0.308111	-0.882948
18B	1.731064	-1.007432	-0.878621
19B	1.731064	-1.007432	0.878621
20B	-1.384138	0.805532	-1.146673
21B	-1.384138	0.805532	1.146673
22B	0.026032	2.006569	-0.877599
23B	0.026032	2.006569	0.877599
24B	-1.731781	-1.013867	0.877599
25B	-1.731781	-1.013867	-0.877599
26B	-0.034039	0.019812	-2.161164
27B	-0.034039	0.019812	2.161164
28B	2.496930	0.358889	0.000000
29B	0.921427	-2.348281	0.000000
30B	1.593947	1.958895	0.000000
31B	-0.915789	-2.353563	0.000000

$E32/\varepsilon$ =-158.700621

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.109419	0.000000	0.000000
3A	-0.546424	-0.969308	0.000000
4A	0.573324	-0.953146	0.000000
5A	-1.111540	-0.033924	0.000000
6A	0.546824	0.970669	0.000000
7A	-0.571168	0.951843	0.000000
8B	1.348077	-0.760762	-1.248369
9B	1.348077	-0.760762	1.248369
10B	-1.328880	-0.801599	-1.249084
11B	-1.328880	-0.801599	1.249084
12A	0.008753	-0.623296	0.882506
13A	0.008753	-0.623296	-0.882506
14A	0.534477	0.326489	0.881747
15A	0.534477	0.326489	-0.881747
16A	-0.549212	0.303555	0.881234
17A	-0.549212	0.303555	-0.881234
18B	-0.042727	1.582394	1.178321
19B	-0.042727	1.582394	-1.178321
20B	0.027593	-2.004220	-0.878582
21B	0.027593	-2.004220	0.878582
22B	1.741787	0.991782	-0.883207
23B	1.741787	0.991782	0.883207
24B	-1.762319	0.959537	-0.876624
25B	-1.762319	0.959537	0.876624
26B	-0.001363	0.028465	2.160625
27B	-0.001363	0.028465	-2.160625
28B	1.591467	-1.959546	0.000000
29B	-1.537647	-2.003470	0.000000
30B	2.500099	-0.368701	0.000000
31B	-2.489404	-0.431081	0.000000
32B	1.012489	2.343453	0.000000

$E33/\varepsilon$ =-165.783355

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.110416	0.000000	0.000000
3A	-0.555210	-0.961648	0.000000
4A	-0.555208	0.961650	-0.000002
5A	0.540981	-0.969723	0.000000
6A	-1.110296	0.016358	-0.000002
7A	0.569313	0.953366	-0.000001
8B	-0.011430	-1.551391	1.245128
9B	-0.011429	-1.551392	-1.245128
10B	-1.337832	0.785596	1.245124
11B	1.349259	0.765798	-1.245128
12B	-1.337830	0.785591	-1.245132
13B	1.349257	0.765800	1.245127
14A	0.004606	0.625384	0.881184
15A	-0.543901	-0.308702	-0.881186
16A	0.004607	0.625382	-0.881187
17A	-0.543902	-0.308700	0.881185
18A	0.539294	-0.316682	-0.881186
19A	0.539293	-0.316680	0.881186
20B	0.014763	2.004044	-0.877172
21B	-1.742937	-0.989236	0.877166
22B	-1.742936	-0.989238	-0.877169
23B	0.014760	2.004047	0.877163
24B	1.728172	-1.014807	0.877168
25B	1.728172	-1.014808	-0.877167
26B	0.000001	-0.000002	-2.163218
27B	-0.000003	0.000002	2.163216
28B	2.498055	0.353020	0.000000
29B	1.583853	1.963750	-0.000002
30B	-2.492584	0.389783	-0.000004
31B	0.908728	-2.353532	0.000001
32B	-0.943306	-2.339889	0.000000
33B	-1.554753	1.986870	-0.000007

$E34/\varepsilon$ =-171.326596

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.618302	0.000000	0.000000
3B	-1.618285	-0.008059	0.000000
4A	-0.544558	-0.761444	-0.554486
5A	-0.544557	-0.761736	0.554087
6A	0.548341	-0.759015	0.554087
7A	0.548341	-0.758724	-0.554486
8A	-0.547642	0.292006	0.894201
9A	-0.547644	0.292477	-0.894046
10A	0.546178	0.295201	-0.894046
11A	0.546179	0.294730	0.894202
12A	-0.548320	0.940366	0.000249
13A	0.543627	0.943087	0.000249
14A	0.003797	-1.525526	-0.000401
15B	0.004593	-1.845978	1.365047
16B	0.004591	-1.845259	-1.366018
17B	-1.380424	-1.771869	-0.000463
18B	1.389227	-1.764974	-0.000463
19A	-0.003098	1.243455	-0.900533
20A	-0.003097	1.242981	0.901190
21A	0.001157	-0.465120	1.458638

22A	0.001155	-0.464352	-1.458881
23B	-0.005738	2.302391	0.000607
24B	-0.001789	0.717492	2.188162
25B	-0.001791	0.718644	-2.187783
26B	-1.393761	-0.547120	1.671351
27B	-1.393764	-0.546239	-1.671636
28B	1.396465	-0.539290	-1.671636
29B	1.396466	-0.540172	1.671352
30B	-1.401657	1.418966	1.028970
31B	-1.401659	1.419507	-1.028219
32B	1.394570	1.425929	1.028971
33B	1.394569	1.426470	-1.028220
34B	0.007355	-2.954436	-0.000778

$E35/\varepsilon$ =-177.660242

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.109480	0.000000	0.000000
3A	-0.554485	-0.960986	0.000000
4A	0.565808	-0.954264	0.013740
5A	0.543769	0.966690	-0.027756
6A	-0.554485	0.960100	-0.041226
7A	-1.109067	-0.013312	-0.027210
8B	-1.379087	-0.773058	1.183843
9B	-0.023736	1.605884	1.149589
10B	1.358816	-0.756628	1.217422
11A	-0.554745	0.328621	0.872832
12A	0.529189	0.335126	0.886126
13A	-0.007394	-0.606695	0.899687
14B	1.357617	-0.791298	-1.237771
15B	-1.317261	-0.807347	-1.270578
16B	0.006892	1.516830	-1.304044
17A	-0.529736	0.288811	-0.902534
18A	0.014590	-0.641338	-0.875827
19A	0.548208	0.295278	-0.889314
20B	-1.763793	1.016012	0.772887
21B	0.001462	-2.000467	0.859496
22B	1.731990	1.036988	0.815761
23B	1.734919	0.988625	-0.928359
24B	-1.723367	0.967874	-0.970773
25B	0.022953	-2.016249	-0.885093
26B	0.026958	-0.046680	-2.175177
27B	0.849314	0.562066	2.265423
28B	-0.022247	-0.967717	2.287450
29B	-0.911300	0.551501	2.243830
30B	-0.951384	2.343862	-0.115327
31B	0.925734	2.355125	-0.092304
32B	-2.502566	-0.378803	-0.076122
33B	-1.554683	-1.998552	-0.029617
34B	1.578809	-1.979750	0.008815
35B	2.508045	-0.348738	-0.014670

$E36/\varepsilon$ =-184.177344

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.154512	0.000000	0.000000
3A	-1.154496	-0.006374	0.000000
4A	-0.552026	0.596382	0.709352
5A	0.548723	0.599421	0.709352
6A	-0.546362	-0.478976	0.806677
7A	0.548998	-0.475952	0.806677
8B	-0.005195	1.881359	0.632465
9A	-0.550136	0.886881	-0.346966
10A	0.545230	0.889905	-0.346966
11A	0.551522	-0.931716	-0.176642
12A	-0.546370	-0.934747	-0.176642
13A	0.558494	-0.093719	-0.914764
14A	-0.557969	-0.096802	-0.914764
15B	-0.002587	0.936753	-1.695580
16B	-1.679966	1.379866	0.443093
17B	1.672320	1.389122	0.443092
18B	0.004901	-1.775037	0.886541
19A	-0.000355	0.128598	1.518807
20B	-1.697416	0.721207	-1.188682
21B	1.693406	0.730569	-1.188683
22B	1.666056	-1.321570	0.677619
23B	-1.658733	-1.330750	0.677619
24A	-1.463557	0.075049	1.065316
25A	1.463120	0.083130	1.065316
26B	0.908563	1.077137	1.998487
27B	-0.914499	1.072102	1.998488
28B	-0.899643	-0.742490	2.151832
29B	0.903730	-0.737509	2.151832
30B	0.003561	-1.290045	-1.453559
31B	1.686007	-0.988827	-1.029253
32B	-1.680523	-0.998122	-1.029253
33B	0.864834	2.232744	-0.859561
34B	-0.877151	2.227934	-0.859560
35B	-2.619140	-0.020379	0.129931
36B	2.619211	-0.005916	0.129930

$E37/\varepsilon$ =-190.811208

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.150537	0.000000	0.000000
3A	-1.149780	-0.041732	0.000000
4A	-0.552248	0.226903	0.905705
5A	0.543656	0.246785	0.905704
6A	0.538184	0.923707	0.066199
7A	-0.571334	0.903578	0.066200
8B	-0.031558	1.739423	-0.913514
9A	-0.554498	0.342633	-0.881853
10A	0.541704	0.362520	-0.881853
11B	0.010416	-0.574227	-1.865591
12A	0.552614	-0.767811	0.541150
13A	-0.524400	-0.787350	0.541150
14A	0.559113	-0.719087	-0.565667
15A	-0.532664	-0.738894	-0.565666
16B	0.010268	-0.565858	1.924832
17B	-1.713489	1.199826	-0.682384
18B	1.668839	1.261189	-0.682388
19A	-0.021219	1.169626	0.966478
20B	-1.669776	-0.441465	-1.348102
21B	1.684687	-0.380608	-1.348105
22B	1.650716	-0.466021	1.410198
23B	-1.632723	-0.525591	1.410201
24B	-1.542472	-1.567734	-0.009070
25B	1.598322	-1.510753	-0.009072
26A	-1.489316	0.760168	0.685376
27A	1.460765	0.813689	0.685373
28B	-0.932614	0.995798	2.023689
29B	0.895884	1.028972	2.023687
30B	0.882847	2.178457	0.612067
31B	-0.961282	2.145000	0.612069
32B	0.036384	-2.005551	-0.809700
33B	0.036708	-2.023345	0.930529
34B	0.861027	0.926029	-2.196418
35B	-0.894055	0.894189	-2.196416
36B	-2.600681	-0.067816	0.083844
37B	2.601429	0.026562	0.083839

$E38/\varepsilon$ =-197.608976

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.155549	0.000000	0.000000
3A	-1.155547	-0.003219	0.000000
4A	-0.548423	-0.759408	-0.539851
5A	-0.548423	-0.759340	0.539946
6A	0.550534	-0.757878	-0.539851
7A	0.550534	-0.757811	0.539946
8B	0.001114	-0.801061	1.826460
9B	0.001114	-0.801289	-1.826360
10A	-0.547396	0.262185	0.923629
11A	-0.547396	0.262070	-0.923662
12A	0.546662	0.263594	-0.923662
13A	0.546662	0.263709	0.923630
14A	-0.562478	0.912410	-0.000057
15A	0.559933	0.913974	-0.000057
16B	-0.002230	1.600563	1.094585
17B	-0.002231	1.600427	-1.094784
18B	-1.671833	-0.572444	1.354807
19B	-1.671833	-0.572613	-1.354736
20B	1.673419	-0.567954	-1.354736
21B	1.673418	-0.567786	1.354808
22A	0.002117	-1.521390	0.000095
23B	1.693393	1.116275	-0.856765
24B	1.693394	1.116381	0.856627
25B	-1.696499	1.111660	0.856626
26B	-1.696499	1.111552	-0.856765
27A	1.463687	-1.068858	0.000067
28A	-1.460707	-1.072931	0.000067
29B	-0.903758	-2.088446	-0.905070
30B	-0.903758	-2.088333	0.905331
31B	0.909568	-2.085921	-0.905070
32B	0.909568	-2.085808	0.905330
33B	2.623797	-0.128552	0.000008
34B	-2.623433	-0.135860	0.000008
35B	0.867431	0.651884	2.315249
36B	0.867431	0.651596	-2.315329
37B	-0.869247	0.649176	-2.315330
38B	-0.869247	0.649466	2.315248

$E39/\varepsilon$ =-204.172478

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.136410	0.000000	0.000000
3A	-1.143537	-0.002641	0.000000
4A	0.538178	0.773548	-0.537200
5A	0.538178	0.773564	0.537177
6A	0.548433	-0.257702	-0.883426
7A	0.548433	-0.257677	0.883433
8A	0.540885	-0.946045	0.000013
9A	-0.547538	0.764642	-0.536506
10A	-0.547538	0.764657	0.536483
11A	-0.543943	-0.266603	-0.881634
12A	-0.543943	-0.266578	0.881642
13A	-0.551512	-0.946508	0.000013
14B	-0.009551	-1.487040	1.271062
15B	-0.009551	-1.487076	-1.271021
16B	-0.054985	1.972658	-0.000029
17B	1.679712	-1.075571	0.888129
18B	1.679712	-1.075596	-0.888098
19B	1.623520	1.494286	-0.000022
20B	-1.741000	1.317435	-0.000020
21A	-0.007169	0.503796	-1.437652
22A	-0.007170	0.503838	1.437637
23B	-1.720512	-1.028916	0.875359
24B	-1.720512	-1.028940	-0.875330
25A	1.468090	0.376603	0.978114
26A	1.468090	0.376574	-0.978125
27B	0.931836	-0.178252	2.230395
28B	0.931836	-0.178317	-2.230391
29B	0.901036	1.568928	1.626183
30B	0.901037	1.568880	-1.626230
31B	-0.891673	-0.216592	2.250495
32B	-0.891673	-0.216658	-2.250489
33B	-0.904933	1.586391	1.606767
34B	-0.904931	1.586345	-1.606814
35A	-1.433638	0.363338	1.034265
36A	-1.433637	0.363309	-1.034276
37B	0.853293	-2.355343	0.000033
38B	2.584732	0.100668	-0.000001
39B	-0.907274	-2.335082	0.000032

$E40/\varepsilon$ =-210.847376

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.144330	0.000000	0.000000
3A	-1.144293	-0.009329	0.000000
4A	0.542524	0.770811	-0.536078

5A	0.542525	0.770753	0.536161
6A	-0.548790	0.766305	0.536162
7A	-0.548791	0.766363	-0.536078
8A	0.550508	-0.258313	-0.880661
9A	-0.548384	-0.262887	0.880632
10A	-0.548385	-0.262791	-0.880660
11A	0.550509	-0.258409	0.880632
12A	-0.541928	-0.950186	-0.000051
13A	0.549654	-0.945737	-0.000052
14B	0.006046	-1.483861	-1.273857
15B	0.006048	-1.484000	1.273695
16B	-0.008054	1.975970	0.000107
17B	1.687869	-1.070780	0.892077
18B	-1.679086	-1.084404	-0.892194
19B	-1.679084	-1.084502	0.892079
20B	1.687867	-1.070683	-0.892197
21B	1.644248	1.476813	0.000079
22B	-1.656231	1.463362	0.000080
23A	-0.002048	0.502298	-1.433953
24A	-0.002046	0.502142	1.434008
25A	1.470605	0.374303	-0.981848
26A	-1.473607	0.362197	0.981888
27A	-1.473609	0.362304	-0.981847
28A	1.470606	0.374196	0.981888
29B	-0.921378	-0.189469	2.232891
30B	0.922890	-0.181709	-2.232911
31B	-0.921381	-0.189227	-2.232910
32B	0.922893	-0.181953	2.232890
33B	0.900681	1.570707	-1.622090
34B	-0.913455	1.563136	1.622260
35B	-0.913458	1.563311	-1.622090
36B	0.900684	1.570530	1.622260
37B	0.883144	-2.351986	-0.000129
38B	-0.863945	-2.359107	-0.000128
39B	2.601826	0.088001	0.000003
40B	-2.602458	0.066791	0.000007

$E41/\varepsilon$ =-216.848113

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.140841	0.000000	0.000000
3A	-1.140761	-0.005391	0.000000
4A	0.526343	0.557824	0.780325
5A	0.538910	-0.531443	0.752808
6A	0.553749	0.895774	-0.253561
7A	-0.541168	0.900826	-0.274735
8A	-0.534478	0.043311	-0.929723
9A	-0.551755	-0.560085	0.740905
10A	0.563634	0.050496	-0.923694
11A	-0.553513	0.570727	0.749324
12A	0.563377	-0.882515	-0.341952
13B	0.038142	-0.952281	-1.733237
14A	-0.531198	-0.890830	-0.346136
15B	0.050698	-1.849455	0.577274
16B	0.016708	1.946126	0.489965
17A	-0.070667	-0.000376	1.546151
18B	-1.657813	0.034370	1.437117
19B	1.693281	-1.298702	0.455340
20B	-1.663878	-1.358424	0.394740
21B	1.716956	-0.690529	-1.213193
22B	-1.652380	-0.726934	-1.257305
23B	1.641799	1.390221	0.494780
24B	-1.646911	1.440383	0.406154
25A	0.020733	0.945432	-1.198266
26B	0.954904	-0.907062	2.025769
27B	0.995472	0.872680	2.064413
28A	-1.453838	0.659805	-0.836583
29A	1.486317	0.675444	-0.798160
30A	1.480763	0.019525	1.028027
31B	0.942776	1.999237	-1.047848
32B	-0.882687	0.558850	-2.197260
33B	-0.892786	2.001535	-1.091503
34B	0.951203	0.574782	-2.177146
35B	-0.673550	1.351445	1.937894
36B	-0.754799	-1.312153	1.970887
37B	-2.591971	0.084691	-0.069387
38B	-0.824696	-2.225283	-0.887339
39B	2.613113	0.093509	0.031197
40B	0.938148	-2.205765	-0.875082
41B	-0.271373	0.013807	2.975001

$E42/\varepsilon$ =-223.652390

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.079447	0.000000	0.000000
3A	0.539723	-0.995012	0.000000
4A	0.539723	-0.321118	0.896033
5A	0.539724	-0.321118	-0.896032
6A	0.539724	0.923037	0.000000
7A	1.614951	1.017331	0.000000
8A	-0.535504	1.017332	-0.000001
9A	0.001601	0.621520	0.898884
10A	1.077846	0.621519	0.898884
11A	0.001602	0.621520	-0.898884
12A	1.077847	0.621519	-0.898884
13B	0.539724	1.989826	0.867888
14B	0.539725	1.989826	-0.867887
15A	-0.921060	0.141479	-0.559048
16A	2.000508	0.141478	-0.559047
17A	-0.921061	0.141479	0.559047
18A	2.000508	0.141478	0.559048
19A	-0.387013	-0.841443	-0.557660
20A	1.466460	-0.841444	-0.557659
21A	1.466459	-0.841443	0.557659
22A	-0.387013	-0.841443	0.557659
23B	1.641452	-0.333741	-1.847459
24B	-0.562003	-0.333740	-1.847460
25B	1.641452	-0.333741	1.847460
26B	-0.562006	-0.333741	1.847459
27B	0.539723	-1.628457	-1.377154
28B	0.539722	-1.628456	1.377154
29B	2.140820	1.334209	-1.413776
30B	-1.061372	1.334210	1.413776
31B	-1.061370	1.334210	-1.413777
32B	2.140818	1.334209	1.413777
33B	2.776614	-0.911491	0.000001
34B	-1.697167	-0.911489	0.000000
35B	0.539723	0.942280	2.211803
36B	0.539725	0.942282	-2.211803
37B	1.459799	-2.152966	0.000001
38B	-0.380354	-2.152965	0.000000
39B	3.078280	0.883781	0.000001
40B	-1.998832	0.883783	-0.000001
41B	-0.957071	2.375869	-0.000001
42B	2.036521	2.375868	0.000000

$E43/\varepsilon$ =-230.062836

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.091241	0.000000	0.000000
3A	0.545620	-0.995625	0.000000
4A	0.545620	0.925731	-0.037968
5A	-0.558158	1.002593	-0.000912
6A	1.649398	1.002593	-0.000913
7B	0.545621	2.049912	0.695760
8A	0.545621	-0.305620	0.884513
9A	0.545620	-0.323758	-0.875085
10A	1.097743	0.612831	-0.893883
11A	-0.006503	0.612831	-0.893883
12A	0.011088	0.648636	0.873861
13A	1.080153	0.648636	0.873861
14A	-0.381824	-0.841263	-0.576753
15A	1.473065	-0.841263	-0.576754
16A	-0.924324	0.118295	-0.566526
17A	2.015564	0.118295	-0.566527
18A	-0.377612	-0.841271	0.563390
19A	1.468853	-0.841271	0.563389
20A	-0.913306	0.131081	0.569621
21A	2.004547	0.131082	0.569620
22B	-0.417439	-0.260031	-1.904414
23B	1.508678	-0.260031	-1.904415
24B	-0.489767	-0.282226	1.862788
25B	1.581009	-0.282226	1.862788
26B	0.545619	1.317641	-1.972492
27B	0.545621	-1.618934	1.378379
28B	0.545620	-1.633319	-1.377647
29B	2.233286	1.274808	-1.403638
30B	-1.142048	1.274809	-1.403636
31A	1.082446	1.683706	-0.650473
32A	0.008793	1.683706	-0.650473
33B	-1.055428	1.352969	1.393076
34B	2.146669	1.352970	1.393074
35B	0.545621	1.091799	2.139981
36B	-1.684868	-0.934837	0.014654
37B	2.776109	-0.934837	0.014652
38B	1.460259	-2.152250	0.001298
39B	-0.369018	-2.152250	0.001299
40B	3.113684	0.829824	0.030024
41B	-2.022444	0.829823	0.030026
42B	2.153210	2.365138	-0.022472
43B	-1.061971	2.365138	-0.022470

$E44/\varepsilon$ =-237.368902

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.071802	0.000000	0.000000
3A	0.512712	-0.941215	0.000000
4B	-0.948092	0.563175	0.767588
5A	1.646268	-0.977897	-0.036770
6A	-0.634431	-0.909000	0.039983
7A	0.494759	0.991966	0.039982
8A	1.082206	-0.642839	0.871997
9A	1.043342	-0.619754	-0.885706
10A	0.519736	0.330863	-0.872022
11A	-0.041928	-0.614685	-0.872022
12A	-0.009906	-0.616021	0.898621
13A	0.536227	0.303383	0.898621
14B	-0.441293	0.262131	-1.900688
15A	1.968139	-0.088771	-0.610358
16A	1.019443	-1.685879	-0.610358
17A	1.418402	0.867278	-0.565026
18A	-0.083096	-1.660462	-0.565026
19A	1.058690	-1.704810	0.532165
20A	2.003538	-0.114179	0.532164
21A	1.441396	0.843838	0.573804
22A	-0.051512	-1.669441	0.573805
23A	-0.384903	0.853248	-0.578725
24A	-0.933414	-0.070158	-0.578724
25B	1.434260	0.259867	-1.918322
26B	0.457893	-1.383823	-1.918322
27B	1.617153	0.246004	1.850568
28B	0.557559	-1.537799	1.850569
29B	-1.216964	-1.230075	-1.357306
30B	0.498052	1.657114	-1.357308
31B	2.223746	-1.320923	1.318452
32B	2.149156	-1.276618	-1.439686
33B	0.468235	1.574212	1.428062
34B	-1.158424	-1.164232	1.428064
35B	-0.083531	0.049620	2.177798
36B	0.448893	-2.863222	-0.023576
37B	2.729105	0.975465	-0.023578
38B	2.170468	-2.353694	-0.079401
39B	3.105198	-0.780097	-0.079402
40B	-1.243656	-2.241041	0.055178
41B	1.373074	2.164166	0.055176
42B	-0.460381	2.107991	0.046154
43B	-2.071385	-0.604100	0.046156
44B	-1.763339	1.047438	-0.775909

$E45/\varepsilon$ =-243.724171

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.095586	0.000000	0.000000
3B	0.549776	-2.164716	0.000000
4A	0.548740	-0.861015	0.327050
5A	0.545758	0.942487	-0.315102
6A	-0.558142	-0.950999	0.320286
7A	1.655247	-0.950275	0.318352
8A	0.551327	0.003201	-0.935250
9A	-0.005424	-0.292629	1.041882
10A	0.546775	0.587057	0.722029
11A	1.096559	-0.291323	1.044222
12A	0.015898	-0.896253	-0.620985
13A	1.085136	-0.895558	-0.621106
14A	-0.927175	0.067783	0.574351
15B	-0.353606	0.837929	1.765762
16A	-0.394579	0.977052	0.286340
17B	0.553247	-0.674599	2.285477
18B	-1.121487	-0.779173	1.749182
19A	1.475761	0.980458	0.280539
20A	2.017782	0.066036	0.578943
21A	-0.909162	-0.316094	-0.497842
22A	1.471689	0.616175	-0.801804
23A	2.010037	-0.307642	-0.496616
24A	-0.365832	0.609817	-0.807424
25A	0.014299	-1.374568	1.137682
26A	1.087915	-1.373377	1.138383
27B	1.510460	0.849800	1.725283
28B	-0.488921	-0.337021	-1.853141
29B	1.588421	-0.335615	-1.851776
30B	2.229435	-0.769734	1.741810
31B	0.550667	1.087637	-1.825093
32B	0.541568	1.985022	0.785720
33B	-2.013660	-0.805216	0.251748
34B	-1.045708	-1.741719	-0.864921
35B	-1.680959	0.858031	-0.397510
36B	2.143494	-1.742917	-0.866932
37B	0.549411	-1.724692	-1.674801
38B	-0.368729	2.030758	-0.687869
39B	2.779151	0.877620	-0.306876
40B	1.459799	2.036697	-0.686212
41B	3.111497	-0.807869	0.246509
42B	-1.028918	-2.253941	0.804847
43B	2.128299	-2.253876	0.804512
44B	0.550261	-2.504616	1.778491
45B	-2.028350	0.662199	1.294033

$E46/\varepsilon$ =-251.048217

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.096126	0.000000	0.000000
3B	0.560782	-2.165423	0.000000
4A	0.551329	-0.861354	-0.326656
5A	0.547697	0.940826	0.318518
6A	-0.556120	-0.950132	-0.321746
7A	1.657999	-0.949627	-0.319642
8A	0.552700	0.000703	0.935918
9A	0.544605	0.588134	-0.720938
10A	-0.004297	-0.294873	-1.041021
11A	1.096971	-0.289889	-1.043916
12B	-0.361831	0.829750	-1.763356
13A	0.018624	-0.897812	0.619892
14A	-0.391341	0.980634	-0.278730
15A	1.088606	-0.896107	0.620601
16A	-0.927026	0.073607	-0.578416
17B	0.555092	-0.674522	-2.285184
18B	-1.114567	-0.794906	-1.748636
19A	1.476734	0.979615	-0.278166
20B	0.553797	1.984809	-0.776075
21A	2.018528	0.067443	-0.579877
22A	-0.907086	-0.317925	0.497086
23A	-0.365688	0.608301	0.809222
24A	1.473841	0.612708	0.803248
25A	2.012831	-0.307861	0.494050
26B	-1.682406	0.851108	0.389838
27B	1.505208	0.851599	-1.725967
28A	0.020103	-1.377978	-1.134731
29A	1.092693	-1.371959	-1.139749
30B	-0.489247	-0.341192	1.852334
31B	1.597796	-0.340573	1.849885
32B	2.231170	-0.764228	-1.744098
33B	0.558942	1.074835	1.835850
34B	-2.005944	-0.819374	-0.247794
35B	-0.352104	2.026726	0.714904
36B	-1.037184	-1.748276	0.867881
37B	2.148651	-1.743620	0.862299
38B	0.555463	-1.724991	1.674744
39B	1.464648	2.031667	0.697578
40B	2.781054	0.877484	0.306996
41B	3.114682	-0.805169	-0.249983
42B	-1.017638	-2.263237	-0.799553
43B	2.135921	-2.250868	-0.810430
44B	0.557256	-2.504386	-1.779977
45B	-2.062064	0.603269	-1.308708
46B	-1.205891	2.054251	-0.819538

$E47/\varepsilon$ =-258.224693

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.099025	0.000000	0.000000
3A	0.554605	-0.948825	0.000000
4A	0.547016	0.997605	0.000349
5A	-0.585223	-0.975683	0.000350
6A	1.693966	-0.971969	0.001835
7A	0.003269	-0.633246	0.867557
8A	0.548353	0.316736	0.867557
9A	1.097637	-0.629805	0.871332
10A	0.010500	-0.635303	-0.871347
11A	0.553777	0.311529	-0.871347
12A	1.103220	-0.633010	-0.869787
13B	-0.348661	0.200057	1.928054
14A	-0.923633	-0.098103	0.579510
15A	-0.381401	0.846909	0.579509
16A	-0.910415	-0.111076	-0.585472
17A	-0.363532	0.842043	-0.585473
18B	0.564933	1.623510	1.378616
19B	-1.116545	-1.307002	1.378619
20A	0.010272	-1.698387	0.572628
21A	1.471458	0.848196	0.572626
22A	0.010514	-1.696405	-0.578354
23A	1.469868	0.846985	-0.578356
24A	1.105413	-1.694880	-0.576179
25A	2.021075	-0.099047	-0.576180
26A	1.104355	-1.694202	0.577243
27A	2.019956	-0.098474	0.577242
28B	-1.673060	0.959973	-0.075698
29B	1.497766	0.230951	1.901988
30B	0.556437	-1.409615	1.901990
31B	-0.385398	0.221133	-1.909762
32B	0.562554	-1.405890	-1.906301
33B	1.497634	0.223786	-1.906303
34B	-1.116005	-1.295639	-1.397085
35B	0.555393	1.617305	-1.397088
36B	2.234221	-1.281958	1.386830
37B	2.239379	-1.284919	-1.382984
38B	-0.345620	2.154836	-0.018616
39B	-2.034754	-0.789019	-0.018613
40B	1.453667	2.159660	-0.010578
41B	-1.130936	-2.344838	-0.010573
42B	3.150172	-0.765841	0.002887
43B	2.250860	-2.333180	0.002888
44B	0.561480	-2.882844	-0.001539
45B	2.772197	0.970036	-0.001541
46B	-1.182581	1.686944	1.458000
47B	-2.053165	0.169673	1.458001

$E48/\varepsilon$ =-264.768267

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.097566	0.000000	0.000000
3B	0.548780	-2.166060	0.000000
4A	0.548784	0.939782	0.318824
5A	0.548782	-0.861152	-0.326706
6A	-0.559829	-0.948190	-0.323345
7A	1.657391	-0.948192	-0.323347
8A	0.548783	-0.005237	0.936911
9A	0.548782	0.588938	-0.717850
10A	1.100695	-0.292088	-1.040859
11A	-0.003133	-0.292087	-1.040858
12B	-0.367091	0.834444	-1.756109
13B	1.464652	0.834443	-1.756112
14A	-0.391347	0.980746	-0.274905
15A	1.488913	0.980745	-0.274908
16A	0.013554	-0.900281	0.618338
17A	1.084010	-0.900281	0.618337
18A	-0.927957	0.076023	-0.577559
19A	2.025521	0.076021	-0.577563
20B	0.548783	1.982605	-0.765255
21B	0.548779	-0.677538	-2.283625
22B	-1.118903	-0.787580	-1.747437
23B	2.216463	-0.787583	-1.747442
24A	-0.365282	0.605896	0.810354
25A	1.462850	0.605895	0.810353
26A	-0.909077	-0.317202	0.495072
27A	2.006643	-0.317204	0.495070
28B	2.780492	0.851668	0.395069
29B	-1.682925	0.851671	0.395074
30A	1.084370	-1.376463	-1.135203
31A	0.013190	-1.376462	-1.135201
32B	-0.501054	-0.346520	1.850327
33B	1.598622	-0.346523	1.850325
34B	0.548786	1.060267	1.848360
35B	1.451041	2.022765	0.725519
36B	-0.353471	2.022766	0.725522
37B	-2.010135	-0.815192	-0.247477
38B	3.107697	-0.815197	-0.247482
39B	2.141311	-1.749664	0.864400
40B	-1.043748	-1.749660	0.864404
41B	0.548782	-1.725165	1.674687
42B	-1.027248	-2.259718	-0.804295
43B	2.124807	-2.259721	-0.804299
44B	0.548778	-2.504171	-1.781013
45B	2.305132	2.058349	-0.809090
46B	-1.207566	2.058351	-0.809085
47B	3.163505	0.609913	-1.303016
48B	-2.065943	0.609918	-1.303010

$E49/\varepsilon$ =-271.973689

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.104542	0.000000	0.000000
3A	0.567341	-0.947701	0.000000
4A	0.544068	0.994643	-0.000001
5A	-0.573951	-0.977703	0.000000
6A	1.707621	-0.967960	0.000001
7A	0.018343	-0.638755	0.868337
8A	0.557476	0.312354	0.868337
9A	0.018343	-0.638756	-0.868337
10A	0.557476	0.312353	-0.868337
11A	1.112199	-0.630447	0.871128
12A	1.112200	-0.630447	-0.871128
13B	-1.666965	0.944914	-0.000001
14B	-0.324287	0.183822	1.939863
15B	-0.324286	0.183820	-1.939864
16A	-0.910521	-0.111898	0.595469
17A	-0.371674	0.838706	-0.595470
18A	-0.371674	0.838706	0.595469
19A	-0.910521	-0.111898	-0.595469

20B	-1.090991	-1.325027	-1.389456
21B	0.576498	1.616664	-1.389457
22B	-1.090991	-1.325026	1.389456
23B	0.576497	1.616666	1.389455
24A	0.028367	-1.701005	-0.571645
25A	0.028367	-1.701005	0.571646
26A	1.474040	0.849371	0.571646
27A	1.474040	0.849370	-0.571646
28B	-0.343050	2.143455	-0.000001
29B	-2.015299	-0.806633	0.000000
30A	1.122240	-1.693126	0.574702
31A	2.029140	-0.093224	0.574702
32A	2.029140	-0.093224	-0.574701
33A	1.122240	-1.693127	-0.574700
34B	0.580605	-1.416885	1.900730
35B	1.513917	0.229612	1.900730
36B	0.580606	-1.416887	-1.900729
37B	1.513918	0.229610	-1.900729
38B	2.253906	-1.277620	-1.382513
39B	2.253905	-1.277619	1.382516
40B	1.453524	2.163181	-0.000001
41B	-1.109426	-2.358232	0.000001
42B	3.164016	-0.753476	0.000002
43B	2.271659	-2.327721	0.000002
44B	2.776407	0.979780	0.000000
45B	0.585426	-2.885426	0.000002
46B	-2.032980	0.138483	-1.501668
47B	-1.163046	1.673172	-1.501669
48B	-1.163046	1.673174	1.501666
49B	-2.032980	0.138485	1.501667

$E50/\varepsilon$ =-278.361820

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.105597	0.000000	0.000000
3A	0.565175	-0.947598	0.000000
4A	0.546246	0.994536	0.000854
5A	-0.575824	-0.976992	-0.000036
6A	1.707219	-0.966528	0.003223
7A	0.559434	0.313576	0.867074
8A	0.017872	-0.637445	0.868648
9A	0.555437	0.310115	-0.868839
10A	0.015269	-0.639686	-0.868629
11A	1.107639	-0.633850	-0.871642
12A	1.112395	-0.631202	0.868274
13B	-0.335137	0.186077	1.934601
14B	-1.666683	0.947482	-0.003064
15B	-0.325110	0.182788	-1.940963
16A	-0.371835	0.839233	0.593147
17A	-0.370431	0.839494	-0.595340
18A	-0.912318	-0.110546	0.593055
19A	-0.911058	-0.110465	-0.595992
20B	0.572175	1.613067	1.388464
21A	1.481851	0.851576	0.569334
22B	1.469182	0.192822	1.929550
23A	2.033826	-0.081595	0.577979
24A	1.468308	0.845652	-0.576474
25B	-0.338612	2.144378	-0.001936
26B	0.577208	1.614762	-1.392521
27B	-1.094805	-1.322559	1.386839
28A	0.026593	-1.701272	-0.571483
29A	0.025820	-1.700547	0.570672
30B	-1.093576	-1.324858	-1.390117
31B	-2.017482	-0.804630	-0.002888
32A	1.121146	-1.693809	-0.572044
33A	1.120430	-1.693581	0.574475
34A	2.021312	-0.102625	-0.582030
35B	0.576358	-1.423852	1.896507
36B	1.511410	0.225163	-1.902800
37B	0.577218	-1.420700	-1.900233
38B	2.253530	-1.273462	1.382268
39B	2.250261	-1.283589	-1.383540
40B	1.457471	2.159574	-0.005281
41B	2.787235	0.968748	-0.093910
42B	-1.112012	-2.357635	-0.000746
43B	3.160452	-0.754751	-0.001467
44B	2.270036	-2.328395	0.003111
45B	0.582852	-2.885863	0.001149
46B	-1.166273	1.677134	1.497017
47B	-1.161084	1.674153	-1.503403
48B	-2.033215	0.140330	-1.503880
49B	-2.039897	0.141540	1.496064
50B	2.338086	1.622684	1.452093

s = 1.7

$E5/\varepsilon$ =-9.218112

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.123943	0.000000	0.000000
3A	0.561972	-0.973363	0.000000
4B	0.561972	-0.324454	1.363623
5B	0.561972	-0.324454	-1.363623

$E6/\varepsilon$ = -13.273980

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.147934	0.000000	0.000000
3B	0.573968	-1.380046	0.000000
4B	0.573968	0.000000	-1.380046
5B	0.573968	0.000000	1.380046
6B	0.573968	1.380046	0.000000

$E7/\varepsilon$ = -16.781371

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.494896	0.000000	0.000000
3B	0.226754	-1.477598	0.000000
4A	0.431686	-0.370492	-0.985394
5B	0.212747	1.111237	-0.957496
6B	-1.066107	-0.378840	-0.957498
7B	0.268773	-0.230673	1.444600

$E8/\varepsilon$ = -21.283208

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.476483	0.000000	0.000000
3B	0.189751	-1.464238	0.000000
4B	0.181498	1.137998	-0.923048
5B	-1.105234	-0.326240	-0.923053
6A	0.398347	-0.350055	-0.990428
7B	0.233847	1.071423	0.992854
8B	-1.032489	-0.369599	0.992850

$E9/\varepsilon$ = -26.529040

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.478641	0.000000	0.000000
3B	0.131687	-1.472765	0.000000
4B	0.207750	1.118229	-0.950898
5B	0.207750	1.118229	0.950898
6B	-1.095284	-0.306511	-0.950898
7B	-1.095284	-0.306511	0.950898
8A	0.405574	-0.370928	0.980663
9A	0.405574	-0.370928	-0.980663

$E10/\varepsilon$ = -31.799676

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.488577	0.000000	0.000000
3B	0.173092	-1.478479	0.000000
4B	0.242325	1.108858	-0.963106
5B	-1.073159	-0.369619	-0.963106
6B	0.242325	1.108861	0.963103
7B	-1.073160	-0.369619	0.963104
8A	-0.842779	0.749868	-0.000001
9A	0.421389	-0.374933	0.976951
10A	0.421390	-0.374935	-0.976951

$E11/\varepsilon$ = -35.917049

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.109981	0.000000	0.000000
3A	0.550457	-0.963875	0.000000
4A	0.550457	0.324801	-0.907502
5A	-0.009067	-0.639074	-0.907502
6B	-0.934490	-1.117627	0.176158
7B	-0.934490	0.542467	-0.992899
8B	0.507086	-0.294360	1.345217
9B	0.507085	1.365732	0.176160
10B	-1.073661	0.623252	0.885036
11B	1.446211	-0.839517	-1.192136

$E12/\varepsilon$ = -40.619462

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.111221	0.000000	0.000000
3A	0.558816	-0.960488	0.000000
4B	0.477618	-0.274691	1.353294
5A	0.548765	0.330028	-0.902350
6A	-0.009296	-0.640293	-0.902349
7B	-0.917482	-1.127058	0.193252
8B	0.512788	1.359809	0.193251
9B	-0.932567	0.536348	-1.002646
10B	1.431292	-0.823180	-1.224818
11B	-1.092795	0.628498	0.865257
12B	1.949159	-1.121019	0.558597

$E13/\varepsilon$ = -45.844938

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.098475	0.000000	0.000000
3A	0.565285	-0.962062	0.000000
4A	0.565284	0.325900	0.905181
5B	0.659059	1.367074	-0.200141
6B	0.659059	-0.274791	-1.354045
7B	-0.278410	-0.865782	1.231902
8A	1.147460	-0.632389	0.899814
9B	-0.826410	0.889660	0.878687
10B	-0.826408	-1.128111	-0.539403
11B	2.054716	-1.076162	-0.221597
12B	2.054715	0.573049	0.937470
13B	-0.915931	0.695361	-0.989416

$E14/\varepsilon$ = -51.987964

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.084094	0.000000	0.000000
3A	0.542048	-0.965664	0.000000
4A	0.542048	0.315693	-0.912604
5A	0.542047	0.965664	0.000000
6A	0.542046	-0.315693	0.912604
7B	-0.408088	-0.821624	-1.153616
8B	1.492184	0.821623	1.153615
9B	1.492187	-0.821623	-1.153614
10B	-0.408091	0.821623	1.153614
11B	-0.776883	1.013946	-0.722151
12B	-0.776884	-1.013947	0.722148
13B	1.860978	1.013947	-0.722148
14B	1.860978	-1.013946	0.722151

$E15/\varepsilon$ = -57.624738

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.100216	0.000000	0.000000
3A	0.541721	-0.957608	0.000000
4A	0.541722	0.325724	0.900509

5A	-0.016772	-0.631884	0.900509
6A	1.088811	-0.635014	0.904970
7B	-0.914081	0.533110	1.033898
8B	0.553983	-0.323093	-1.333194
9B	-0.914082	-1.153582	-0.149647
10B	0.553985	1.363598	-0.149648
11B	1.997365	-1.164901	-0.133156
12B	0.529600	-1.995220	1.050150
13B	0.529602	-0.308872	2.233454
14B	1.997367	0.521447	1.050149
15B	-1.040411	0.606787	-0.864740

$E16/\varepsilon$ = -63.402124

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.092802	0.000000	0.000000
3A	0.546400	-0.957918	0.000000
4A	0.546401	0.329363	0.899515
5A	1.099424	-0.630159	0.901810
6A	-0.006623	-0.630159	0.901810
7B	0.546401	1.367243	-0.147652
8B	0.546401	-0.331453	-1.334651
9B	-0.909303	0.531810	1.035867
10B	2.002104	0.531810	1.035868
11B	-0.909303	-1.155565	-0.143221
12B	2.002103	-1.155566	-0.143222
13B	0.546400	-0.303710	2.231805
14B	0.546400	-1.991309	1.052559
15B	-1.039787	0.604163	-0.864607
16B	2.132589	0.604161	-0.864607

$E17/\varepsilon$ = -69.267007

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.095706	0.000000	0.000000
3A	0.547853	-0.948909	0.000000
4B	0.547853	-0.316303	1.336609
5A	1.101603	-0.636012	-0.900052
6A	-0.005899	-0.636012	-0.900052
7A	0.547852	0.323113	-0.900052
8B	2.003727	-1.156853	0.145759
9B	0.547853	1.364797	0.145759
10B	-0.908022	-1.156852	0.145761
11B	-0.908447	0.524492	-1.038369
12B	0.547852	-1.997893	-1.038369
13B	2.004151	0.524492	-1.038370
14B	0.547851	-0.316303	-2.230094
15B	-1.041823	0.601498	0.862083
16B	2.137530	0.601497	0.862082
17B	0.547852	-2.151903	0.862083

$E18/\varepsilon$ = -75.146699

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.098807	0.000000	0.000000
3A	0.549403	-0.947064	0.000000
4A	0.549404	0.313261	0.893755
5B	0.549403	-0.308909	-1.335734
6B	0.549403	1.362725	-0.150302
7A	-0.005203	-0.638880	0.900916
8A	1.104010	-0.638881	0.900916
9B	2.005997	-1.155522	-0.145957
10B	2.005999	0.519951	1.042200
11B	-0.907190	0.519954	1.042200
12B	-0.907192	-1.155521	-0.145954
13B	0.549405	-0.315503	2.229550
14B	0.549402	-1.999692	1.035214
15B	2.141990	0.606241	-0.854890
16B	-1.043184	0.606241	-0.854889
17B	0.549401	-2.146192	-0.866354
18B	0.549406	1.527487	1.738820

$E19/\varepsilon$ = -81.113225

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.097440	0.000000	0.000000
3A	0.551390	-0.948865	0.000000
4A	0.551391	0.314240	-0.895320
5A	0.005339	-0.634624	-0.895320
6B	-0.904958	-1.156397	0.146057
7B	-0.904958	0.520786	-1.042770
8B	0.545158	1.363454	0.146056
9B	0.545158	-0.313727	1.334884
10A	1.109139	-0.638285	-0.900484
11B	0.555409	-1.997717	-1.039902
12B	0.555409	-0.319625	-2.229374
13B	2.006317	0.523499	-1.039901
14B	2.006316	-1.154589	0.149570
15B	-1.047331	0.602715	0.850303
16B	2.135405	0.608309	0.858193
17B	0.546947	1.522433	-1.746294
18B	0.546946	-2.151940	0.858192
19B	-1.041519	-1.237814	-1.746293

$E20/\varepsilon$ = -87.167631

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.551213	0.000000	0.000000
3A	0.775607	-0.775607	0.000000
4A	0.775607	0.775607	0.000000
5A	0.775607	0.000000	-0.775607
6A	0.775606	0.000000	0.775607
7B	1.804352	-1.028745	1.028748
8B	-0.253139	1.028747	-1.028747
9B	1.804353	1.028746	1.028747
10B	-0.253139	-1.028747	-1.028747
11B	-0.253141	1.028748	1.028745
12B	-0.253140	-1.028747	1.028745
13B	1.804354	-1.028746	-1.028746
14B	1.804354	1.028746	-1.028747
15B	-1.476414	0.000000	-0.000001
16B	3.027627	0.000000	0.000001
17B	0.775609	2.252021	-0.000001
18B	0.775608	-2.252021	0.000000
19B	0.775603	0.000001	2.252021
20B	0.775607	0.000000	-2.252021

$E21/\varepsilon$ = -92.763166

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.080670	0.000000	0.000000
3A	0.540335	-0.936392	0.000000
4B	0.540333	1.433377	-0.014161
5A	0.540334	0.311136	0.916306
6A	1.089668	-0.629797	0.912376
7A	-0.008998	-0.629798	0.912375
8B	-0.980427	-1.184897	0.000810
9B	2.061098	-1.184894	0.000810
10A	1.088686	-0.631807	-0.914470
11A	-0.008017	-0.631808	-0.914469
12A	0.540334	0.312974	-0.920232
13B	-0.918472	0.546370	0.991743
14B	1.999139	0.546374	0.991742
15B	0.540336	-2.008997	0.984834
16B	-0.929879	0.535873	-0.980464
17B	2.010545	0.535877	-0.980465
18B	0.540336	-2.012332	-0.980200
19B	0.540333	-0.379992	2.248061
20B	0.540332	-0.326520	-2.248192
21B	0.540332	1.457974	1.859014

$E22/\varepsilon$ = -98.657162

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.080166	0.000000	0.000000
3A	0.537051	-0.937195	0.000000
4A	0.539366	0.313202	0.916544
5A	-0.003578	-0.623697	0.916544
6B	0.537718	1.433746	-0.014299
7B	-0.976626	-1.179392	-0.014299
8B	-0.925255	0.536197	0.991542
9A	1.090877	-0.632176	0.903187
10B	2.060393	-1.194022	0.000692
11A	1.091881	-0.632758	-0.912098
12A	0.544279	0.314472	-0.920278
13A	-0.002238	-0.628591	-0.920278
14B	1.994172	0.546795	0.997923
15B	0.517064	-2.002086	0.997923
16B	0.624682	-0.362010	2.249728
17B	-0.927411	0.537446	-0.980389
18B	0.538760	-2.014147	-0.974849
19B	2.015424	0.533967	-0.974849
20B	0.556237	-0.322346	-2.249475
21B	0.519161	1.463225	1.855599
22B	-1.011431	-1.177947	1.855600

$E23/\varepsilon$ =-105.416880

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.195733	0.000000	0.000000
3A	0.597867	-0.883559	0.000000
4A	0.597866	0.441778	-0.765185
5A	0.597866	0.441781	0.765184
6B	-0.894416	0.580791	-1.005966
7B	-0.894415	-1.161588	0.000000
8B	-0.894417	0.580794	1.005962
9B	2.090147	0.580796	1.005964
10B	2.090149	0.580793	-1.005964
11B	2.090149	-1.161586	0.000003
12A	0.059043	-0.544232	-0.942636
13A	1.136690	-0.544230	0.942637
14A	1.136690	1.088462	-0.000002
15A	1.136692	-0.544232	-0.942635
16A	0.059041	1.088462	-0.000002
17A	0.059041	-0.544230	0.942636
18B	0.597867	-1.939277	0.994039
19B	0.597868	0.108774	-2.176484
20B	0.597868	-1.939280	-0.994035
21B	0.597865	0.108781	2.176483
22B	0.597866	1.830498	-1.182450
23B	0.597864	1.830502	1.182443

$E24/\varepsilon$ =-111.349064

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.194980	0.000000	0.000000
3A	0.599952	-0.884471	0.000000
4A	0.599952	0.440134	0.767184
5A	0.594547	0.442608	-0.764199
6B	-0.892109	0.569130	1.014782
7B	-0.892108	-1.163428	0.011321
8A	0.078809	-0.540325	0.932915
9B	-0.902176	0.577205	-0.996592
10B	2.091484	0.586002	1.002862
11B	2.091484	-1.161484	-0.009246
12B	2.083263	0.584250	-1.008756
13A	1.151207	-0.546477	0.943537
14A	0.054110	-0.546348	-0.940055
15A	0.054110	1.087273	0.006104
16A	1.131655	1.089105	0.001578
17A	1.131656	-0.543334	-0.943897
18B	0.604632	-1.937691	0.998087
19B	0.604631	0.098508	2.177412
20B	0.592311	-1.941520	-0.989661
21B	0.592310	1.824572	1.191581
22B	0.586196	0.110160	-2.174964
23B	0.586196	1.831729	-1.177867

24B	-0.850991	-1.111039	1.918299

*E*25/ε =-117.418348

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.196787	0.000000	0.000000
3A	0.598393	-0.884357	0.000000
4A	0.598393	0.436607	-0.769065
5A	0.598393	0.443549	0.761851
6B	-0.893475	-1.163850	-0.005175
7B	-0.893476	0.570092	-1.014675
8B	2.090260	0.570092	-1.014678
9B	2.090260	-1.163850	-0.005177
10A	1.131087	-0.543107	-0.932854
11A	0.065697	-0.543108	-0.932854
12B	0.598392	-1.939568	-0.996389
13B	0.598391	0.091073	-2.178629
14B	-0.894783	0.581493	0.998788
15B	2.091569	0.581494	0.998788
16A	0.059310	-0.545589	0.940706
17A	1.137477	1.087425	-0.010035
18A	1.137477	-0.545589	0.940706
19A	0.059309	1.087425	-0.010034
20B	0.598391	1.816378	-1.203319
21B	0.598393	-1.943192	0.985501
22B	0.598392	1.833598	1.170165
23B	0.598393	0.112363	2.172267
24B	2.048133	-1.118184	-1.920621
25B	-0.851352	-1.118184	-1.920618

*E*26/ε =-123.754916

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.139234	0.000000	0.000000
3A	0.569616	-0.986607	0.000000
4A	0.569617	-0.328869	-0.930182
5A	0.569617	-0.328869	0.860239
6A	-0.322638	-0.844012	-0.596807
7A	1.461871	-0.844013	-0.596806
8A	0.569617	0.701419	-0.596807
9A	1.515944	-0.875232	0.540130
10A	-0.376711	0.217495	-1.005219
11A	0.569616	-1.421595	-1.005220
12A	1.515946	0.217494	-1.005219
13A	-0.376712	-0.875232	0.540128
14A	0.569617	0.763857	0.540129
15B	2.669819	-0.204100	-0.144317
16B	-0.372431	-2.210082	-0.144320
17B	1.511663	-0.872761	-2.035579
18B	-0.588540	0.339792	1.394036
19B	-0.588539	1.427573	-0.144318
20B	1.727774	1.427573	-0.144318
21B	1.511661	-2.210083	-0.144318
22B	-0.372430	-0.872759	-2.035580
23B	1.727772	0.339792	1.394037
24B	-1.530586	-0.204098	-0.144320
25B	0.569618	0.758912	-2.035580
26B	0.569614	-1.666192	1.394037

*E*27/ε =-130.980905

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.096518	0.000000	0.000000
3A	0.548259	-0.949613	0.000000
4A	0.548259	0.316538	-0.895303
5A	-0.548259	-0.316537	0.895304
6A	-0.548260	0.316539	-0.895303
7A	-0.000001	-0.633074	-0.895303
8A	-0.548258	0.949613	0.000001
9A	-0.548260	-0.949612	0.000000
10A	0.000001	0.633075	0.895304
11A	-1.096518	0.000001	0.000001
12A	0.548259	-0.316538	0.895303
13A	0.548260	0.949613	0.000000
14B	-1.439447	0.831067	1.175307
15B	1.439449	0.831066	1.175305
16B	0.000000	1.662133	-1.175304
17B	-1.439450	-0.831064	-1.175304
18B	1.439447	-0.831065	-1.175305
19B	0.000000	-1.662132	1.175305
20B	0.000001	2.099190	0.742176
21B	0.000002	0.000000	2.226527
22B	1.817952	1.049595	-0.742176
23B	-1.817952	1.049597	-0.742173
24B	-1.817952	-1.049593	0.742177
25B	1.817951	-1.049595	0.742176
26B	-0.000001	0.000001	-2.226527
27B	-0.000002	-2.099189	-0.742176

*E*28/ε =-136.064944

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094810	0.000000	0.000000
3A	0.546122	-0.950607	0.000000
4A	0.546123	0.950607	-0.000001
5A	0.546123	0.323893	0.893727
6A	0.546122	-0.323892	-0.893727
7A	0.012423	-0.630473	0.899088
8A	0.012424	0.630474	-0.899088
9A	-0.549226	-0.315030	-0.893240
10A	-0.549225	0.315032	0.893240
11A	-0.549225	0.947131	-0.008165
12A	-0.549226	-0.947129	0.008166
13B	1.476086	0.803249	-1.145474
14B	1.476086	-0.803249	1.145474
15A	-1.098110	0.000001	0.000000
16B	-0.037500	-1.668964	-1.170340
17B	-0.037497	1.668965	1.170340
18B	-1.430408	0.830838	-1.184815
19B	-1.430409	-0.830835	1.184815
20B	1.754018	1.144839	0.802804
21B	1.754016	-1.144840	-0.802804
22B	0.015404	2.095208	-0.749787
23B	0.015401	-0.008958	-2.225308
24B	0.015401	-2.095206	0.749788
25B	0.015403	0.008960	2.225308
26B	-1.825893	1.043567	0.731787
27B	-1.825895	-1.043562	-0.731786
28A	2.199118	0.000000	0.000000

*E*29/ε =-142.945508

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.098350	0.000000	0.000000
3A	0.556309	-0.947044	0.000000
4A	0.556309	-0.318403	-0.891915
5B	-0.042519	-1.665055	-1.173567
6B	1.414147	0.880005	-1.173566
7B	1.414146	-0.809387	1.223339
8A	-0.547297	-0.315840	-0.893217
9A	0.539693	0.951761	0.002852
10A	0.539693	0.322675	0.895399
11A	-0.004873	-0.628780	0.895398
12A	-0.004872	0.631875	-0.893216
13A	-0.547297	-0.947408	0.002852
14A	-1.098561	-0.001197	-0.000843
15A	-0.555383	0.947833	-0.000843
16A	-0.555383	0.317874	0.892941
17B	-0.018584	1.666677	1.174710
18B	-1.446494	-0.828138	1.174710
19B	-1.446493	0.827902	-1.174876
20B	1.791667	1.079373	0.760767
21B	-0.023212	-2.091549	0.760766
22B	-0.023212	0.013287	-2.225571
23B	-0.022486	0.012870	2.227549
24B	-0.022486	2.102206	-0.736797
25B	-1.824001	-1.045367	-0.736798
26B	-1.827786	1.046135	0.737339
27B	1.571883	-0.899667	-1.781663
28B	1.571883	-1.980423	-0.248289
29B	2.503756	-0.352271	-0.248288

*E*30/ε =-148.313123

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.098428	0.000000	0.000000
3A	0.530294	-0.961942	0.000000
4A	0.530285	-0.313190	-0.909532
5B	-0.018592	-1.648552	-1.175879
6B	1.434733	0.812168	-1.175876
7B	1.434738	-0.847374	1.150765
8A	0.549737	0.948046	0.003070
9A	0.549739	0.311571	0.895391
10A	-0.564846	-0.939123	0.003067
11A	-0.007458	-0.631852	0.895390
12A	-0.564853	-0.302864	-0.888948
13A	-0.007466	0.640884	-0.888947
14A	-1.100588	0.014573	0.010401
15A	-0.544100	0.956798	0.010402
16A	-0.544097	0.321348	0.901283
17B	0.002221	1.662637	1.185931
18B	-1.454975	-0.804629	1.185926
19B	-1.454986	0.859332	-1.146892
20B	1.788286	1.085460	0.774235
21B	-0.087246	-2.090116	0.774231
22B	-0.087263	0.051541	-2.228308
23A	1.418598	-0.837842	-0.597632
24B	0.013469	-0.007957	2.227772
25B	0.013460	2.103797	-0.732845
26B	-1.835887	-1.027449	-0.732850
27B	-1.809064	1.068452	0.762118
28B	2.657351	-0.255069	-0.181933
29B	1.506282	-2.204020	-0.181932
30B	1.506264	-0.889610	-2.024717

E31/ =-154.937882

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2B	2.031831	0.000000	0.000000
3A	0.769048	-0.780275	0.000000
4A	0.769048	0.013329	0.780161
5A	0.769047	-0.013329	-0.780161
6A	0.769047	0.780275	0.000000
7A	0.001294	0.787410	0.774072
8A	0.001294	-0.787410	-0.774072
9B	-0.052073	-2.041023	0.048516
10B	-0.052073	-0.013643	2.041554
11B	-0.052073	2.041023	-0.048515
12B	-0.052073	0.013642	-2.041554
13A	-0.006098	-0.765755	0.778950
14A	-0.006098	0.765755	-0.778950
15A	-0.778887	0.008792	0.770854
16A	-0.778887	-0.770892	0.004378
17A	-0.778887	-0.008792	-0.770854
18A	-0.778887	0.770892	-0.004377
19B	-2.044411	0.000000	0.000000
20B	1.252810	-1.287643	1.309831
21B	1.252810	1.287643	-1.309831
22B	-1.325792	1.280999	1.259301
23B	-1.325792	-1.281000	-1.259300
24B	-1.309131	-1.265506	1.287312
25B	-1.309131	1.265507	-1.287311
26B	1.742902	1.794356	0.445880
27B	1.742902	-0.476468	-1.786476
28B	1.742902	0.476467	1.786477
29B	1.742902	-1.794356	-0.445879
30B	0.413007	-1.795939	-1.765516
31B	0.413007	1.795938	1.765517

$E32/\varepsilon$ =-161.073978

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.703492	0.000000	0.000000
3B	-1.703486	-0.004558	0.000000
4A	-0.551229	-0.269446	0.901102
5A	-0.551229	-0.269443	-0.901103
6A	0.551947	-0.267968	-0.901103
7A	0.551947	-0.267970	0.901103
8A	-0.553814	-0.931997	-0.000002
9A	0.556306	-0.930512	-0.000001
10A	0.548583	0.773400	0.539414
11A	0.548583	0.773401	-0.539412
12A	-0.550650	0.771931	-0.539412
13A	-0.550651	0.771929	0.539414
14B	0.003142	-2.347590	-0.000004
15B	0.000920	-0.688488	2.250927
16B	0.000920	-0.688482	-2.250930
17A	0.001621	-1.211894	-0.898907
18A	0.001621	-1.211896	0.898903
19A	-0.000694	0.518579	1.446864
20A	-0.000694	0.518583	-1.446863
21B	-0.002638	1.971567	-1.197668
22B	-0.002638	1.971564	1.197671
23B	-1.417572	-1.469155	1.091663
24B	-1.417572	-1.469150	-1.091669
25B	1.421498	-1.465351	-1.091670
26B	1.421498	-1.465353	1.091667
27B	-1.428423	0.609198	-1.727051
28B	-1.428423	0.609191	1.727053
29B	1.426787	0.613011	1.727053
30B	1.426787	0.613013	-1.727053
31B	-1.449533	1.820421	0.000001
32B	1.444657	1.824293	0.000001

$E33/\varepsilon$ =-169.571951

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.698927	0.000000	0.000000
3B	-1.698927	0.000000	0.000000
4A	-0.551860	-0.904135	-0.263812
5A	-0.551859	0.886526	-0.318009
6A	0.551859	-0.028494	-0.941406
7A	0.551859	0.576397	0.744865
8A	-0.551859	-0.530293	0.778362
9A	0.551859	-0.530293	0.778362
10A	0.551859	0.886525	-0.318010
11A	-0.551859	0.576396	0.744866
12A	0.551859	-0.904135	-0.263812
13A	-0.551859	-0.028493	-0.941406
14B	-0.000002	-2.272880	-0.663189
15B	0.000001	1.448987	1.872496
16B	0.000001	-0.071629	-2.366575
17B	-0.000001	2.228612	-0.799435
18B	0.000001	-1.333089	1.956701
19A	0.000001	0.046162	1.525175
20A	0.000000	-0.933821	-1.206759
21A	0.000000	0.859129	-1.261026
22A	0.000000	1.464792	0.427402
23A	0.000000	-1.436262	0.515208
24B	-1.425402	0.055439	1.831645
25B	1.425402	-1.724867	0.618732
26B	1.425402	1.759130	0.513283
27B	-1.425403	-1.121462	-1.449248
28B	-1.425402	1.759129	0.513287
29B	1.425402	1.031763	-1.514418
30B	1.425402	-1.121465	-1.449246
31B	-1.425402	1.031762	-1.514419
32B	-1.425403	-1.724866	0.618736
33B	1.425403	0.055439	1.831645

$E34/\varepsilon$ =-175.526184

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.645347	0.000000	0.000000
3A	-1.147867	0.000000	0.000000
4A	-0.567728	0.928892	-0.003088
5A	-0.567728	0.289980	0.882475
6A	-0.567728	0.284106	-0.884383
7A	-0.567728	-0.753305	-0.543491
8A	-0.567728	-0.749674	0.548487
9A	0.514265	0.298863	0.909508
10A	0.514266	0.292810	-0.911475
11A	0.514265	0.957347	-0.003182
12A	0.514265	-0.772639	0.565290
13A	0.514266	-0.776381	-0.560140
14B	-1.578631	-1.633954	0.005432
15B	-1.578631	-0.510086	-1.552304
16B	-1.578631	-0.499754	1.555661
17B	-1.578631	1.318704	-0.964809
18B	-1.578631	1.325090	0.956020
19A	-0.062820	1.248944	0.901083
20A	-0.062819	1.242925	-0.909366
21A	-0.062819	-0.480774	-1.463102
22A	-0.062820	-0.471036	1.466266
23A	-0.062819	-1.540060	0.005120
24B	-0.100990	2.368142	-0.007872
25B	-0.100989	0.739283	2.249805
26B	-0.100989	0.724309	-2.254669
27B	-0.100989	-1.911240	1.398328
28B	-0.100989	-1.920495	-1.385590
29B	1.366894	1.489877	-1.090042
30B	1.366894	1.497091	1.080114
31B	1.366894	-1.846047	0.006138
32B	1.366894	-0.564623	1.757591
33B	1.366894	-0.576297	-1.753798
34B	-2.588879	0.000001	0.000000

$E35/\varepsilon$ =-181.357766

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.644227	0.000000	0.000000
3A	-0.562714	-0.931722	0.000000
4A	-0.562715	-0.290606	0.885242
5A	-1.146309	-0.004781	0.003461
6A	-0.572486	0.752609	-0.545062
7A	-0.570550	0.750841	0.543964
8A	-0.570549	-0.282642	-0.883049
9A	0.517313	-0.957232	-0.001610
10A	0.517312	-0.297032	0.909982
11A	0.509416	0.778419	-0.563753
12A	0.513518	-0.286749	-0.912606
13A	0.513517	0.777644	0.557087
14B	-1.557542	-1.343233	0.972803
15A	-0.060541	-1.251697	0.906513
16B	-1.573052	-1.328469	-0.955235
17B	-1.573056	0.493231	1.560132
18B	-1.589328	0.501055	-1.546693
19B	-1.589330	1.625813	0.006351
20B	-0.080548	-2.363618	-0.049007
21B	-0.080551	-0.690653	2.260993
22B	1.356989	-1.506154	1.090801
23A	-0.068699	1.542577	-0.000781
24A	-0.068698	0.481872	-1.465383
25A	-0.058959	0.487095	1.454188
26A	-0.058957	-1.229720	-0.916359
27B	-0.112952	1.920800	-1.391098
28B	-0.106880	-0.718502	-2.261161
29B	-0.106882	1.924260	1.387916
30B	1.368853	-1.480704	-1.098223
31B	1.368851	0.581602	1.749376
32B	1.362797	0.582208	-1.755056
33B	1.362796	1.849095	-0.005761
34B	-2.585727	-0.022514	0.016299
35B	-0.201658	-2.465318	1.785450

$E36/\varepsilon$ =-188.040054

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.718279	0.000000	0.000000
3B	-1.717912	-0.035490	0.000000
4A	-0.602771	0.892156	-0.000068
5A	0.584216	0.904416	-0.000068
6A	-0.547492	-0.745423	-0.565785
7A	-0.547493	-0.745338	0.565895
8A	0.562772	-0.733956	-0.565785
9A	0.562771	-0.733871	0.565895
10A	-0.548581	0.311177	-0.899989
11A	0.542037	0.322441	-0.899989
12A	-0.548582	0.311312	0.899941
13A	0.542036	0.322576	0.899941
14A	-0.013513	1.308363	0.785023
15A	-0.013512	1.308245	-0.785220
16B	-0.008907	0.862418	-2.177872
17B	-0.008911	0.862744	2.177742
18B	-1.466326	1.451759	1.077402
19B	1.436028	1.481736	1.077402
20B	-1.466324	1.451598	-1.077624
21B	1.436029	1.481575	-1.077623
22B	0.019410	-1.879188	-1.397942
23B	0.019405	-1.878978	1.398223
24A	0.004462	-0.431985	1.471086
25A	0.004464	-0.432205	-1.471022
26A	0.015389	-1.489967	0.000112
27A	0.520560	1.977726	-0.000148
28A	-0.561298	1.966552	-0.000148
29B	-1.419026	-0.521408	1.761399
30B	1.429493	-0.491989	1.761399
31B	-1.419023	-0.521671	-1.761326
32B	1.429496	-0.492250	-1.761325
33B	-1.390492	-1.847627	0.000138
34B	1.428358	-1.818513	0.000140
35B	-0.027907	2.701876	1.193773
36B	-0.027903	2.701697	-1.194178

$E37/\varepsilon$ =-194.081783

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.719197	0.000000	0.000000
3B	-1.718786	-0.037621	0.000000
4A	0.538989	0.510524	-0.811484
5A	-0.550031	0.498607	-0.811485
6A	0.560722	-0.591742	-0.714735
7A	-0.547640	-0.603870	-0.714734
8A	-0.605322	0.868297	0.195148
9A	0.586175	0.881335	0.195149
10A	-0.546619	-0.849912	0.393061
11A	0.565085	-0.837747	0.393061
12A	0.543927	0.119738	0.948533
13A	-0.546417	0.107807	0.948533
14A	-0.012102	1.105864	1.048944
15A	-0.015835	1.447043	-0.476616
16B	-0.014581	1.332635	-1.927011
17B	-0.004053	0.370401	2.313632
18B	-1.470939	1.647320	-0.731837
19B	1.434538	1.679115	-0.731834
20B	0.016861	-1.541039	-1.761880
21B	-1.464205	1.181720	1.371654
22B	1.437994	1.213480	1.371653
23A	0.001111	-0.101518	-1.534850
24B	-1.432622	-0.128630	-1.819031
25B	1.435094	-0.097252	-1.819030
26B	0.023390	-2.137636	0.958047
27A	0.008110	-0.741176	1.343254
28A	0.015885	-1.451768	-0.319252
29A	0.520127	1.929474	0.428887
30A	-0.562228	1.917630	0.428887

31B	1.432924	-0.861323	1.612811
32B	-1.413733	-0.892472	1.612812
33B	1.428155	-1.771979	-0.402479
34B	-1.389039	-1.802806	-0.402479
35B	-0.031676	2.894691	-0.579148
36B	-0.026008	2.376670	1.752561
37B	0.001867	-0.170570	-3.041564

$E38/\varepsilon$=-200.368418

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.137213	0.000000	0.000000
3A	-1.137199	-0.005664	0.000000
4B	0.005080	-2.039816	0.000072
5A	-0.541954	-0.778384	0.538207
6A	-0.541954	-0.778422	-0.538152
7A	0.545825	-0.775675	0.538207
8A	0.545824	-0.775713	-0.538152
9A	-0.547915	0.261424	0.889862
10A	-0.547915	0.261361	-0.889881
11A	0.546606	0.264087	-0.889881
12A	0.546605	0.264150	0.889862
13B	-0.003806	1.527952	-1.332985
14B	-0.003806	1.528047	1.332875
15A	-0.555119	0.950102	-0.000034
16A	0.550379	0.952855	-0.000034
17B	1.805752	-1.356259	0.000048
18B	-1.798974	-1.365237	0.000048
19A	0.001273	-0.511348	1.439376
20A	0.001273	-0.511450	-1.439340
21B	1.787982	1.047550	-0.913217
22B	1.787982	1.047615	0.913141
23B	-1.793178	1.038631	-0.913216
24B	-1.793179	1.038695	0.913142
25B	0.939400	-1.635747	-1.659277
26B	0.939400	-1.635629	1.659393
27B	-0.931242	-1.640405	-1.659277
28B	-0.931242	-1.640287	1.659393
29B	0.937356	0.174803	-2.330139
30B	0.937356	0.174969	2.330126
31B	-0.938216	0.170132	-2.330139
32B	-0.938216	0.170297	2.330126
33A	-1.429576	-0.379020	1.032124
34A	-1.429576	-0.379092	-1.032098
35A	1.431446	-0.371894	1.032124
36A	1.431446	-0.371967	-1.032098
37B	0.928734	2.429357	-0.000087
38B	-0.940824	2.424701	-0.000087

$E39/\varepsilon$=-206.281050

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.076031	0.000000	0.000000
3A	0.523664	-0.934425	0.000000
4A	0.407631	0.835267	-0.533327
5A	-0.471304	-0.749066	-0.610432
6A	-0.487715	-0.747547	0.587823
7A	0.488882	-0.270255	-0.902861
8A	0.494818	-0.272325	0.918095
9A	0.454457	0.772509	0.564055
10A	-0.477011	0.292482	-0.927862
11A	-0.526261	0.950263	0.036712
12B	1.713951	-1.041307	-0.944029
13A	-1.057920	-0.012639	-0.025597
14A	-0.462927	0.282888	0.936936
15B	1.726132	-1.025683	0.923753
16B	0.314301	2.168338	0.255551
17B	-0.177951	-0.653923	-2.118981
18A	1.338932	0.414894	-0.951840
19A	1.319231	1.075917	-0.021225
20B	-1.837470	-0.273412	1.145893
21A	-0.305351	-1.626994	-0.007558
22B	-0.597785	1.679593	-1.298319
23B	-1.782772	-0.361691	-1.251484
24B	-0.286694	-0.692707	2.086084
25B	0.560461	0.925814	1.984753
26B	2.565076	0.356123	-0.084733
27B	1.283907	1.807316	-1.316723
28A	-1.325696	-1.102730	-0.026534
29A	0.392310	0.600032	-1.580810
30A	0.301068	-1.429120	-0.948730
31A	1.433699	0.424381	0.919692
32A	0.285718	-1.429984	0.940621
33B	0.883492	-2.436439	-0.000104
34B	-1.032720	-2.067799	-1.164410
35B	-1.107094	-2.046142	1.108110
36B	-1.068844	1.525574	1.346069
37B	-1.988779	1.118509	-0.185978
38B	1.538690	0.153479	-2.376259
39B	1.973991	1.796002	1.065461

$E40/\varepsilon$=-213.220313

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.085044	0.000000	0.000000
3A	-0.451604	-0.986597	0.000000
4A	0.449191	0.346518	-0.929894
5A	-0.502035	-0.264212	-0.929893
6A	0.456239	-0.710603	-0.592579
7A	0.510057	0.306482	0.902828
8A	-0.490964	-0.336218	0.902828
9A	0.498420	-0.776300	0.522980
10A	0.491982	0.938376	0.013885
11A	-1.058004	-0.056784	0.013886
12B	1.729689	-0.647282	1.249130
13B	-0.131357	-1.842157	1.249130
14A	-0.492205	0.766621	-0.570437
15A	-0.488698	0.761160	0.523591
16B	1.776149	1.132608	0.704312
17B	-1.769092	-1.143596	0.704314
18B	1.114134	-1.735291	-1.427192
19B	-0.489558	0.762496	-2.039311
20A	1.367501	-1.043463	-0.140662
21A	0.379623	-1.677725	-0.140662
22A	0.310701	-0.483926	-1.648845
23A	1.321735	-0.314929	-1.043210
24A	-0.263763	-1.332889	-1.043211
25B	-1.949669	0.351547	-1.001760
26B	0.491818	1.919090	-1.001762
27B	-1.779733	0.644372	1.124848
28B	0.154833	1.886450	1.124846
29A	-0.331837	0.516846	1.574635
30A	1.419740	0.774509	-0.684099
31A	-1.295146	-0.968568	-0.684097
32A	0.311514	-0.485189	1.615095
33B	-0.906338	-2.413674	-0.355630
34B	2.571905	-0.180487	-0.355630
35B	-1.229676	1.915250	-0.144279
36B	1.329900	0.589032	-2.156637
37B	-1.089109	-0.964076	-2.156635
38B	-0.975573	-0.563182	2.330319
39B	0.918127	0.652659	2.330318
40B	1.517299	-2.363228	0.460949

$E41/\varepsilon$=-219.743606

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.081992	0.000000	0.000000
3A	0.473128	-0.979220	0.000000
4A	0.463004	-0.290261	-0.881200
5A	0.515293	0.751052	0.559339
6A	-0.498483	0.287537	-0.931038
7A	-0.519820	0.943526	-0.027687
8A	0.471263	0.764049	-0.565254
9A	0.475434	-0.314870	0.905210
10A	-0.455842	-0.774861	-0.557066
11A	-0.481762	0.258774	0.880529
12A	-1.075834	-0.026220	-0.025846
13B	1.693657	1.411446	-0.154998
14A	-0.457947	-0.804793	0.562706
15B	-0.194098	1.804861	-1.296470
16B	1.113657	-0.701115	-2.142124
17B	1.727318	0.257662	1.337594
18B	-0.572941	-2.135140	-0.149420
19B	-1.787317	0.808294	1.017424
20B	-1.712935	-0.773558	-1.212920
21A	0.369940	-1.348402	-1.025921
22B	-1.793891	1.024066	-0.811389
23A	1.341832	-0.843601	-0.674397
24A	-0.329045	1.307975	0.984838
25A	-0.265597	-0.558813	-1.612049
26A	1.368600	0.252279	-1.025952
27A	0.339379	0.454606	-1.628488
28B	-0.685783	-0.527208	2.044599
29B	0.525367	-1.709566	1.308909
30A	0.284911	0.545308	1.603806
31A	0.268213	1.694642	0.096282
32B	0.886720	1.935694	1.446129
33A	1.455574	-0.916949	0.457915
34B	-1.891782	-1.036581	0.651107
35B	1.306784	-2.235159	-0.300494
36B	2.576977	-0.221209	-0.275545
37B	-0.916259	0.473062	-2.399076
38B	-1.033473	2.369064	0.291573
39B	1.463500	1.289078	-2.041858
40B	-0.473358	-1.935055	-2.055859
41B	-0.661730	1.345582	2.409737

$E42/\varepsilon$=-226.250732

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.050909	0.000000	0.000000
3A	-0.477127	-0.985715	0.000000
4A	-0.477129	0.785095	-0.596035
5A	-0.450110	-0.297058	-0.882552
6A	0.463332	-0.791460	0.583016
7A	0.463331	0.982911	-0.014218
8A	0.494308	0.289889	-0.903992
9A	0.494308	-0.777509	-0.544718
10B	1.702632	-0.438857	-1.303839
11A	-1.050319	-0.009988	-0.029671
12A	0.426126	0.301174	0.894783
13A	-0.506991	-0.313871	0.891411
14A	-0.506992	0.789001	0.520197
15B	-1.083222	-0.724309	-2.151905
16B	0.584004	-2.159101	-0.180108
17B	0.584001	1.610761	-1.449001
18B	-1.952954	-0.832149	0.692378
19B	-1.952956	1.081443	0.048283
20B	0.326213	-0.327006	2.164419
21B	0.326212	1.569217	1.526172
22A	-0.329399	-1.347349	-1.035138
23A	-0.329400	0.447207	-1.639166
24B	-0.461654	-1.746785	1.284684
25B	-0.461657	2.168080	-0.033016
26A	-1.339771	-0.843669	-0.686243
27A	-1.339772	0.257004	-1.056718
28A	1.334126	-0.270999	1.007946
29A	1.334125	0.825322	0.638936
30A	0.276253	-0.537816	-1.597839
31B	2.533818	0.084229	0.250242
32A	1.446805	0.841671	-0.525009
33A	1.446807	-0.987827	0.090780
34B	-1.277778	0.586521	1.742548
35B	-1.274262	1.580491	-1.646451
36B	-1.274259	-2.254388	-0.355673
37B	1.426220	2.177949	0.125928
38B	1.426224	-1.658533	1.417245
39B	0.620612	0.242099	-2.751931

40B	0.620612	-1.856845	-2.045452
41B	1.919457	0.664572	1.974431
42B	-2.669721	-0.339221	-1.007809

$E43/\varepsilon$ =-233.255889

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.078586	0.000000	0.000000
3A	0.534401	-0.993548	0.000000
4B	-0.881798	1.427298	-0.000002
5A	0.565285	-0.309707	0.896296
6A	0.565290	-0.309705	-0.896297
7A	0.528554	0.940833	0.000001
8A	1.630218	0.998897	0.000004
9A	-0.025714	0.614715	-0.895947
10A	-0.025719	0.614712	0.895947
11A	-0.360798	-0.848862	-0.563807
12A	-0.360802	-0.848864	0.563800
13A	-0.932880	0.059096	0.560602
14A	-0.932876	0.059098	-0.560610
15A	1.089745	0.623343	-0.883941
16A	1.089739	0.623341	0.883944
17B	0.438248	-1.590283	1.519865
18B	0.438256	-1.590281	-1.519869
19B	0.556709	1.992868	-1.009237
20B	0.556702	1.992863	1.009246
21A	2.001665	0.112516	0.553365
22A	2.001669	0.112517	-0.553356
23A	1.448697	-0.861168	0.554648
24A	1.448700	-0.861168	-0.554645
25B	0.578450	0.538988	2.249024
26B	0.578460	0.539003	-2.249023
27B	-0.567927	-2.167764	-0.000006
28B	2.803126	-1.013407	0.000007
29B	2.215930	1.270659	-1.512057
30B	2.215919	1.270652	1.512074
31B	1.342162	-2.233219	0.000000
32A	-0.351055	-0.269429	1.477050
33A	-0.351045	-0.269424	-1.477057
34A	-1.286745	-0.835882	-0.000007
35B	-1.576354	-1.043943	-1.404201
36B	-1.576364	-1.043947	1.404184
37B	1.998193	-0.567233	-1.845684
38B	1.998190	-0.567243	1.845690
39B	3.176144	0.825028	0.000011
40B	-1.240218	0.879221	-1.736723
41B	-1.240227	0.879216	1.736717
42B	-2.296232	0.218891	-0.000010
43B	2.092040	2.391950	0.000011

$E44/\varepsilon$ =-240.201249

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.104889	0.000000	0.000000
3A	0.552444	-0.940171	0.000000
4A	0.552445	-0.289602	0.894457
5A	0.552444	0.304356	-0.869573
6A	0.552444	0.921042	-0.021701
7B	0.552445	2.197061	0.508959
8B	0.552440	0.192544	-2.247007
9A	0.013361	-0.638030	-0.903101
10A	1.091527	0.662656	0.885189
11A	1.091526	-0.638030	-0.903101
12A	0.013362	0.662655	0.885190
13A	-0.527912	0.317093	-0.912382
14A	1.632800	0.965694	-0.020634
15A	-0.527912	0.965693	-0.020632
16A	1.632799	0.317093	-0.912383
17B	-0.464913	-0.257572	1.951901
18B	-0.464915	-1.936333	-0.356196
19B	1.569804	-0.257571	1.951900
20B	1.569803	-1.936332	-0.356198
21B	-1.892333	0.575401	-0.418509
22B	2.997221	0.575403	-0.418514
23A	0.010285	1.258773	-0.915548
24A	1.094602	1.258773	-0.915549
25A	-0.905016	-0.519524	-0.309868
26A	2.009906	0.134773	0.589710
27A	-0.905016	0.134772	0.589712
28A	2.009905	-0.519523	-0.309870
29A	-0.362517	-0.823366	0.598863
30A	1.467407	-0.823366	0.598863
31B	0.552445	-1.745948	1.269889
32B	-1.159359	-0.707798	-1.761343
33B	-1.159357	1.457677	1.215931
34B	2.264243	-0.707797	-1.761346
35B	2.264246	1.457679	1.215929
36B	0.552445	1.297448	2.114413
37B	0.552443	-1.611953	-1.885663
38B	2.100764	1.181634	-2.006823
39B	-0.995884	2.273220	-0.506014
40B	2.100772	2.273221	-0.506018
41B	-0.995882	1.181635	-2.006819
42B	0.552443	2.347847	-1.707659
43B	-1.812493	-1.016549	0.739371
44B	2.917382	-1.016547	0.739369

$E45/\varepsilon$ =-247.677700

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.106159	0.000000	0.000000
3A	0.545095	-0.962529	0.000000
4A	0.548248	-0.319578	-0.844954
5B	0.525911	-0.306559	-2.223057
6A	-0.544020	-0.944249	-0.016519
7A	0.553558	0.938689	-0.016520
8A	0.002383	-0.635128	0.882606
9A	0.553833	0.310906	0.882605
10A	1.633718	-0.952306	-0.017745
11A	1.097423	-0.639696	0.879452
12A	-0.537400	-0.317285	-0.915111
13A	0.011265	0.623971	-0.915112
14A	-0.004102	-1.252277	-0.917210
15A	1.087650	0.620667	-0.917210
16A	1.086026	-1.258071	-0.917559
17A	1.629887	-0.325056	-0.917560
18B	-0.441958	0.257621	1.954310
19B	-1.906933	-0.558866	-0.402222
20B	-0.453404	1.934721	-0.402223
21A	-0.904514	0.527246	-0.319484
22A	-0.908604	-0.101218	0.585814
23A	-0.359669	0.840503	0.585813
24B	0.541089	-1.436084	1.967977
25B	1.516252	0.236846	1.967977
26B	-0.930374	-2.290266	-0.419239
27B	1.534408	1.938168	-0.419242
28B	1.997740	-2.305802	-0.430077
29B	2.990850	-0.602083	-0.430078
30B	-1.269132	-1.345124	1.245558
31B	0.545057	1.767192	1.245557
32A	2.015431	0.525751	-0.324542
33A	0.535684	-2.012815	-0.324541
34A	1.479442	0.844256	0.588892
35A	-0.005589	-1.703375	0.588893
36A	1.084751	-1.709772	0.585984
37A	2.022309	-0.101354	0.585984
38B	-1.172966	0.683728	-1.773009
39B	2.351208	-1.370535	1.238696
40B	0.527550	-2.277123	-1.805624
41B	2.241411	0.663074	-1.805626
42B	0.536910	1.532012	-1.952624
43B	-1.068507	-1.222144	-1.952622
44B	2.121297	-1.236520	-1.974527
45B	-1.803502	1.051272	0.731993

$E46/\varepsilon$ =-255.625219

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.100033	0.000000	0.000000
3A	0.550015	-0.961916	0.000000
4A	0.550016	-0.318211	0.846270
5A	0.550018	0.941283	0.016768
6B	0.550016	-0.290983	2.223876
7A	0.550017	0.309197	-0.885687
8A	1.638951	-0.946925	0.017469
9A	-0.538922	-0.946922	0.017469
10A	1.096775	-0.637438	-0.882061
11A	0.003255	-0.637436	-0.882062
12A	0.012373	0.625285	0.915060
13A	1.087663	0.625283	0.915060
14A	1.633717	-0.317915	0.914883
15A	-0.533685	-0.317911	0.914883
16A	1.095349	-1.252687	0.917156
17A	0.004679	-1.252684	0.917156
18B	-0.439070	0.255099	-1.956311
19B	1.539104	0.255096	-1.956311
20B	-0.453561	1.936697	0.396888
21B	1.553601	1.936694	0.396889
22B	3.000855	-0.564382	0.407946
23B	-1.900824	-0.564372	0.407946
24A	-0.903378	0.527277	0.319738
25A	2.003413	0.527272	0.319738
26A	-0.360258	0.840487	-0.588281
27A	1.460294	0.840484	-0.588282
28A	-0.907374	-0.103597	-0.585283
29A	2.007407	-0.103602	-0.585283
30B	0.550020	1.767536	-1.249195
31B	0.550015	-1.428855	-1.971359
32B	2.016650	-2.293164	0.425421
33B	-0.916626	-2.293158	0.425421
34B	2.362930	-1.351215	-1.242420
35B	-1.262902	-1.351209	-1.242421
36A	0.550012	-2.011320	0.324799
37A	0.004350	-1.705332	-0.588593
38A	1.095677	-1.705334	-0.588593
39B	2.263818	0.685622	1.776593
40B	-1.163783	0.685629	1.776592
41B	0.550012	-2.268624	1.809881
42B	0.550019	1.547035	1.937471
43B	-1.047052	-1.218155	1.961112
44B	2.147080	-1.218162	1.961112
45B	-1.805084	1.045950	-0.731954
46B	2.905122	1.045941	-0.731952

$E47/\varepsilon$ =-263.555682

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.102045	0.000000	0.000000
3A	0.551023	-0.954400	0.000000
4A	0.551023	-0.318133	0.847406
5A	-0.538988	-0.947453	0.017680
6A	1.641035	-0.947451	0.017679
7A	0.551021	0.940504	0.017679
8B	0.551024	-0.318132	2.224727
9A	1.096796	-0.633236	-0.884966
10A	0.005248	-0.633237	-0.884966
11A	0.551021	0.312072	-0.884966
12A	1.089804	0.622407	0.914846
13A	0.012240	0.622406	0.914847
14A	1.634946	-0.321803	0.914846
15A	-0.532899	-0.321805	0.914847
16A	1.096164	-1.255002	0.914846
17A	0.005884	-1.255003	0.914847
18B	0.551022	-1.457329	-1.958478
19B	1.537591	0.251465	-1.958479
20B	-0.435552	0.251463	-1.958477
21B	-1.900125	-0.573297	0.402997
22B	-0.895525	-2.313311	0.402996
23B	-0.453579	1.932203	0.402995

24B	3.002171	-0.573291	0.402993
25B	1.997575	-2.313308	0.402995
26B	1.555619	1.932205	0.402993
27A	2.007079	0.522523	0.320149
28A	-0.905035	0.522520	0.320152
29A	0.551024	-1.999443	0.320151
30A	1.463210	0.839163	-0.587668
31A	-0.907320	-0.106804	-0.587665
32A	-0.361169	0.839162	-0.587667
33A	1.097176	-1.686760	-0.587667
34A	2.009364	-0.106801	-0.587668
35A	0.004870	-1.686761	-0.587666
36B	-1.255279	-1.361004	-1.245781
37B	2.357323	-1.361000	-1.245784
38B	0.551019	1.767603	-1.245784
39B	-1.163214	0.671580	1.780590
40B	2.265259	0.671585	1.780586
41B	0.551026	-2.297563	1.780589
42B	2.150247	-1.241442	1.946399
43B	-1.048198	-1.241447	1.946401
44B	0.551022	1.528491	1.946399
45B	-1.805626	1.042472	-0.731834
46B	2.907664	1.042479	-0.731841
47B	0.551025	-3.039353	-0.731837

*E*48/ε =-270.247871

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.084436	0.000000	0.000000
3A	0.542218	-0.947195	0.000000
4A	0.542218	-0.310199	-0.894961
5A	0.542218	0.311706	0.894518
6A	0.542218	0.947270	0.001569
7A	1.632022	-0.942960	-0.001016
8A	-0.547587	-0.309772	-0.890627
9A	-0.547587	-0.942960	-0.001016
10A	1.632022	-0.309772	-0.890627
11A	1.086951	-0.631246	0.891165
12A	-0.002516	-0.631246	0.891165
13A	-0.002516	0.635293	-0.888284
14A	1.086951	0.635293	-0.888284
15A	-0.001363	-1.255487	-0.893603
16A	1.085799	-1.255486	-0.893603
17B	-0.444585	0.259253	1.968303
18B	1.529021	1.944662	-0.399648
19B	1.529021	0.259252	1.968303
20B	-0.444586	1.944662	-0.399647
21B	-1.904203	-0.572263	-0.407313
22B	2.988638	-0.572263	-0.407313
23A	1.449101	0.843924	0.600671
24A	-0.364666	0.843924	0.600671
25A	1.995720	-0.100808	0.597876
26A	-0.911285	0.531892	-0.291048
27A	-0.911285	-0.100808	0.597876
28A	1.995720	0.531892	-0.291048
29B	0.542218	1.773267	1.262138
30B	0.542217	-1.421412	1.983410
31B	0.542217	1.408532	-1.992577
32B	-0.937162	-2.274548	-0.430663
33B	-0.937162	-1.151810	-2.008077
34B	2.021598	-1.151810	-2.008077
35B	2.021598	-2.274548	-0.430663
36B	-1.272019	0.745310	-1.682755
37B	-1.272019	-1.345875	1.255299
38B	2.356453	-1.345876	1.255299
39B	2.356454	0.745310	-1.682756
40A	1.089072	-1.694781	0.601854
41A	-0.004637	0.013637	-1.798423
42A	-0.004637	-1.694781	0.601854
43A	1.089072	0.013637	-1.798423
44A	0.542218	-2.008301	-0.291788
45A	0.542218	-0.933400	-1.801993
46B	0.542219	-2.393973	-1.703931
47B	-1.810970	1.050468	0.747679
48B	2.895405	1.050467	0.747679

*E*49/ε =-278.200778

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.086440	0.000000	0.000000
3A	0.543219	-0.940884	0.000000
4A	0.543218	-0.313626	0.895587
5A	0.543220	0.945848	0.000630
6A	1.633958	-0.943367	0.000635
7A	-0.547519	-0.943366	0.000631
8A	0.543221	0.314218	-0.893804
9A	-0.000511	-0.627553	-0.893803
10A	1.086953	-0.627554	-0.893802
11A	-0.001863	-1.258073	0.890447
12A	1.088298	-1.258073	0.890449
13A	1.088593	0.630651	0.890445
14A	1.633674	-0.313456	0.890448
15A	-0.002157	0.630651	0.890444
16A	-0.547238	-0.313456	0.890445
17B	0.543222	-1.450105	-1.970543
18B	1.527437	0.254605	-1.970545
19B	-0.440991	0.254605	-1.970548
20B	-1.902405	-0.583929	0.403944
21B	-0.445503	1.939497	0.403941
22B	-0.913683	-2.296447	0.403949
23B	1.531942	1.939496	0.403945
24B	2.988842	-0.583930	0.403952
25B	2.000119	-2.296448	0.403954
26A	-0.365408	0.841851	-0.600333
27A	1.451851	0.841851	-0.600330
28A	-0.911769	-0.104472	-0.600332
29A	1.089580	-1.678266	-0.600326
30A	-0.003140	-1.678266	-0.600328
31A	1.998211	-0.104473	-0.600328
32A	-0.912456	0.526808	0.291123
33A	0.543218	-1.994496	0.291130
34A	1.998894	0.526807	0.291127
35B	0.543222	1.772439	-1.259059
36B	-1.263368	-1.356664	-1.259056
37B	2.349811	-1.356666	-1.259050
38B	-0.938639	-1.169173	1.997861
39B	2.025070	-1.169173	1.997866
40B	0.543216	1.397475	1.997859
41B	0.543216	-2.409819	1.684611
42B	2.358574	0.734473	1.684608
43B	-1.272141	0.734473	1.684602
44A	0.543216	-0.945653	1.799539
45A	1.090569	0.002390	1.799538
46A	-0.004137	0.002390	1.799536
47B	-1.811842	1.046069	-0.747539
48B	2.898285	1.046067	-0.747529
49B	0.543220	-3.033024	-0.747524

*E*50/ε =-286.133713

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.088368	0.000000	0.000000
3A	0.544184	-0.942555	0.000000
4A	0.544184	-0.314184	-0.888649
5A	0.544184	0.314372	0.892225
6A	-0.002812	-1.258548	-0.889930
7A	1.091179	-1.258549	-0.889930
8A	0.544184	0.945988	-0.001014
9A	1.088530	-0.628464	0.892224
10A	1.088530	0.631710	-0.889928
11A	-0.000163	0.631711	-0.889928
12A	-0.000163	-0.628464	0.892224
13A	1.635525	-0.944271	-0.001016
14A	-0.547158	-0.944271	-0.001016
15A	1.635525	-0.315713	-0.889929
16A	-0.547158	-0.315713	-0.889929
17B	1.530300	0.255149	1.966333
18B	-0.441933	0.255149	1.966333
19B	1.530300	1.938927	-0.414885
20B	0.544183	-1.452855	1.966332
21B	-0.441933	1.938927	-0.414885
22B	0.544183	1.369594	-2.025207
23B	-1.900127	-0.586737	-0.414887
24B	-0.914010	-2.294742	-0.414889
25B	-0.914010	-1.156071	-2.025209
26B	2.988494	-0.586737	-0.414887
27B	2.002376	-2.294742	-0.414889
28B	2.002376	-1.156071	-2.025210
29A	0.544183	-1.996687	-0.296991
30A	-0.912906	0.527067	-0.296989
31A	2.001274	0.527067	-0.296989
32A	1.090977	-1.680997	0.595919
33A	0.544183	-0.945565	-1.783499
34A	1.090977	0.001509	-1.783499
35A	-0.002610	-1.680996	0.595919
36A	-0.366113	0.842758	0.595920
37A	2.001274	-0.104316	0.595920
38A	1.454480	0.842758	0.595921
39A	-0.912906	-0.104316	0.595920
40A	-0.002610	0.001509	-1.783498
41B	0.544184	1.773226	1.253862
42B	-1.263568	-1.357891	1.253860
43B	-1.263568	0.729523	-1.698184
44B	2.351935	-1.357891	1.253860
45B	2.351935	0.729523	-1.698185
46B	0.544183	-2.401594	-1.698187
47B	-1.812835	1.046641	0.740089
48B	2.901203	1.046641	0.740089
49B	0.544182	-3.035836	0.740086
50B	0.544182	-0.314181	-3.108910

s = 1.8

*E*5/ε =-9.234711

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.123913	0.000000	0.000000
3A	0.561956	-0.973337	0.000000
4B	0.561956	-0.324446	1.425019
5B	0.561956	-0.324446	-1.425019

*E*6/ε = -13.373777

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.138310	0.000000	0.000000
3B	0.569155	-1.447142	0.000000
4B	0.569155	0.000000	-1.447142
5B	0.569155	0.000000	1.447142
6B	0.569155	1.447142	0.000000

*E*7/ε = -17.140302

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2B	1.500436	0.000000	0.000000
3B	0.000000	-1.500436	0.000000
4B	0.000000	-0.000003	1.500436
5B	0.000000	0.000000	-1.500436
6B	0.000000	1.500436	0.000003
7B	-1.500436	-0.000001	0.000000

*E*8/ε = -21.521513

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2B	1.545837	0.000000	0.000000
3B	-1.158888	-1.023030	0.000000
4B	0.205433	-0.507000	1.445810
5B	0.181520	-0.516040	-1.445811
6A	0.398252	-1.052915	-0.000001

7B	0.241249	1.356174	-0.711700
8B	-1.078370	0.857041	0.711706

*E*9/ε = -26.756037

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.548819	0.000000	0.000000
3B	0.151097	-1.541431	0.000000
4B	0.210451	1.172601	-0.998247
5B	-1.146478	-0.323841	0.998247
6B	0.210451	1.172601	0.998247
7B	-1.146478	-0.323842	-0.998247
8A	0.406857	-0.368926	0.983734
9A	0.406857	-0.368926	-0.983734

*E*10/ε = -32.012806

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.561100	0.000000	0.000000
3B	0.191721	-1.549282	0.000000
4B	0.246484	1.161961	-1.012977
5B	-1.122894	-0.387321	1.012977
6B	0.246484	1.161961	1.012977
7B	-1.122894	-0.387321	-1.012977
8A	-0.846201	0.747938	0.000000
9A	0.423100	-0.373970	0.978059
10A	0.423100	-0.373970	-0.978059

*E*11/ε = -36.270022

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.115837	0.000000	0.000000
3A	0.563637	-0.963018	0.000000
4A	0.011437	-0.646385	0.909476
5A	0.563637	0.316633	0.909477
6B	0.530937	-0.304441	-1.405353
7B	-0.963650	-1.179196	-0.174557
8B	0.530937	1.427316	-0.174555
9B	-0.963650	0.552562	1.056243
10B	-1.140458	0.653945	-0.920113
11B	1.514179	-0.868237	1.221628

*E*12/ε = -41.305141

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.073230	0.000000	0.000000
3B	0.536613	-1.459962	0.000000
4A	0.536616	0.604067	-0.765074
5B	0.536616	-0.097163	1.448691
6B	1.543136	-0.427382	-1.387976
7B	-0.469908	-0.427379	-1.387976
8A	0.536616	0.929763	0.302368
9B	-0.852703	1.223350	-0.302978
10B	1.925937	1.223346	-0.302978
11B	2.332630	-0.634646	0.526392
12B	-1.259402	-0.634638	0.526396

*E*13/ε = -46.632565

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.096848	0.000000	0.000000
3A	0.548423	-0.949898	0.000000
4A	1.100931	-0.635623	-0.916547
5A	-0.004085	-0.635622	-0.916547
6A	0.548424	0.321351	-0.916546
7B	0.548424	-0.316633	1.397943
8B	0.548424	1.418903	0.177106
9B	-0.954595	-1.184399	0.177103
10B	2.051442	-1.184401	0.177102
11B	2.086067	0.571127	-0.990498
12B	0.548422	-2.092149	-0.990500
13B	-0.989219	0.571129	-0.990495

*E*14/ε = -53.222502

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.563886	0.000000	0.000000
3A	0.781943	-0.781943	0.000000
4A	0.781943	0.781943	0.000000
5A	0.781943	0.000000	0.781943
6A	0.781943	0.000000	-0.781943
7B	1.847476	-1.065533	-1.065533
8B	1.847476	1.065533	-1.065533
9B	-0.283590	1.065533	1.065533
10B	-0.283590	1.065533	-1.065533
11B	-0.283590	-1.065533	-1.065533
12B	-0.283590	-1.065533	1.065533
13B	1.847476	-1.065533	1.065533
14B	1.847476	1.065533	1.065533

*E*15/ε = -58.931166

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.105864	0.000000	0.000000
3A	0.554549	-0.956771	0.000000
4A	0.003234	-0.639089	-0.902491
5A	0.554549	0.317683	-0.902490
6A	1.108564	-0.638781	-0.902056
7B	-0.945224	0.544662	-1.093846
8B	0.575153	1.425879	0.150568
9B	-0.945223	-1.212637	0.150564
10B	0.575154	-0.331419	1.394978
11B	2.062066	-1.188213	0.163975
12B	0.558891	-2.059460	-1.066358
13B	0.558891	-0.322044	-2.296690
14B	2.062066	0.549203	-1.066356
15B	-1.102983	0.635563	0.897515

*E*16/ε = -64.728570

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.104490	0.000000	0.000000
3A	0.552245	-0.957109	0.000000
4A	0.552244	0.309453	-0.905702
5A	1.105409	-0.643996	-0.900585
6A	-0.000920	-0.643996	-0.900584
7B	0.552244	1.435735	0.116636
8B	0.552245	-0.353831	1.396331
9B	-0.947824	0.538834	-1.095720
10B	-0.947822	-1.211085	0.155625
11B	2.052312	0.538835	-1.095722
12B	2.052313	-1.211085	0.155623
13B	0.552243	-0.336557	-2.296919
14B	0.552245	-2.064734	-1.061122
15B	2.206920	0.640517	0.895718
16B	-1.102430	0.640517	0.895719

*E*17/ε = -70.600218

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.105626	0.000000	0.000000
3A	0.552812	-0.957500	0.000000
4B	0.552812	-0.319167	1.396975
5A	1.103751	-0.637252	-0.902296
6A	0.001871	-0.637252	-0.902295
7A	0.552812	0.317004	-0.902295
8B	-0.965809	-1.195943	0.128708
9B	2.071433	-1.195944	0.128705
10B	0.552814	1.434386	0.128707
11B	0.552810	-2.048854	-1.097590
12B	2.050765	0.545677	-1.097590
13B	-0.945141	0.545677	-1.097588
14B	0.552810	-0.319165	-2.297809
15B	2.216974	0.641635	0.890250
16B	-1.111347	0.641638	0.890250
17B	0.552812	-2.240774	0.890249

*E*18/ε = -76.485964

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.106359	0.000000	0.000000
3A	0.553180	-0.957072	0.000000
4A	0.553179	0.325196	-0.900131
5B	0.553180	1.423012	0.172226
6B	0.553180	-0.321532	1.396868
7A	1.101865	-0.633289	-0.902144
8A	0.004493	-0.633289	-0.902143
9B	2.070080	0.524238	-1.087681
10B	-0.963721	-1.201093	0.123477
11B	-0.963722	0.524239	-1.087680
12B	2.070082	-1.201094	0.123473
13B	0.553178	-0.337353	-2.297932
14B	0.553179	-2.046588	-1.098077
15B	-1.119049	0.628629	0.895501
16B	2.225409	0.628628	0.895500
17B	0.553181	-2.242392	0.889292
18B	0.553179	1.598307	-1.806815

*E*19/ε = -82.446070

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.104730	0.000000	0.000000
3A	0.550209	-0.957967	0.000000
4A	-0.004312	-0.636981	0.902590
5A	0.550209	0.320986	0.902589
6B	-0.957755	-1.191999	-0.164504
7B	0.556629	1.424189	-0.164506
8B	-0.957755	0.554398	1.067972
9B	0.556630	-0.322209	-1.396982
10A	1.096198	-0.634537	0.899127
11B	2.069913	0.518533	1.087281
12B	0.581272	-0.336470	2.298806
13B	0.581272	-2.053177	1.087283
14B	2.069913	-1.198173	-0.124242
15B	-1.108959	0.641920	-0.909592
16B	2.225258	0.631297	-0.894536
17B	0.560861	-2.244050	-0.894534
18B	-1.103541	-1.280607	1.814598
19B	0.560859	1.594739	1.814595

*E*20/ε = -89.054680

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.088685	0.000000	0.000000
3A	0.544342	-0.942829	0.000000
4B	-1.035919	-1.226638	0.000000
5B	2.124601	-1.226641	0.000000
6B	0.544344	1.510452	0.000001
7A	1.091792	-0.630347	0.911055
8A	1.091792	-0.630347	-0.911055
9A	-0.003109	-0.630346	-0.911055
10A	-0.003109	-0.630346	0.911055
11A	0.544343	0.317866	0.911054
12A	0.544342	0.317866	-0.911054
13B	-0.969733	0.559878	-1.031320
14B	-0.969733	0.559878	1.031320
15B	2.058419	0.559874	1.031321
16B	2.058418	0.559876	-1.031320
17B	0.544340	-2.062580	-1.031321
18B	0.544340	-2.062581	1.031320
19B	0.544341	-0.314272	-2.303205
20B	0.544341	-0.314273	2.303205

*E*21/ε = -94.850253

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000

2A	1.084632	0.000000	0.000000
3A	0.542316	-0.945400	0.000000
4B	0.542316	1.499873	-0.029780
5A	0.542314	0.317776	0.922584
6B	2.124237	-1.231648	0.003753
7B	-1.039606	-1.231647	0.003746
8A	1.089953	-0.629799	0.906819
9A	-0.005325	-0.629799	0.906818
10A	-0.006452	-0.640595	-0.908629
11A	1.091087	-0.640596	-0.908627
12B	-0.975361	0.555857	1.025969
13B	2.059988	0.555856	1.025975
14A	0.542318	0.302664	-0.920601
15B	0.542314	-2.067200	1.025756
16B	2.057776	0.547656	-1.034804
17B	-0.973139	0.547657	-1.034809
18B	0.542318	-2.071535	-1.027016
19B	0.542311	-0.421060	2.307605
20B	0.542320	-0.342910	-2.304920
21B	0.542312	1.514912	1.937818

$E22/\varepsilon$ =-100.718586

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.083967	0.000000	0.000000
3A	0.530704	-0.945164	0.000000
4B	0.552938	1.500214	0.027551
5B	-1.037397	-1.216630	0.027550
6A	-0.011848	-0.624701	-0.925082
7A	0.538909	0.316182	-0.925082
8B	-0.981216	0.574368	-1.002103
9B	2.124209	-1.243430	-0.009049
10B	0.526630	-2.063382	-1.030503
11B	2.057004	0.551023	-1.030502
12A	1.084282	-0.634696	-0.891631
13A	1.097639	-0.642515	0.902076
14A	0.553462	0.306145	0.920548
15A	0.004029	-0.632478	0.920548
16B	0.688731	-0.403155	-2.314261
17B	-0.956848	0.560102	1.048167
18B	0.543106	-2.070536	1.025481
19B	2.071307	0.540160	1.025482
20B	0.575232	-0.336719	2.306780
21B	0.524132	1.515661	-1.937176
22B	-1.064970	-1.199071	-1.937177

$E23/\varepsilon$ =-107.744490

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.172287	0.000000	0.000000
3A	0.586143	-0.898535	0.000000
4A	0.586143	0.449266	0.778155
5A	0.586143	0.449268	-0.778154
6B	-0.968149	-1.190651	0.000000
7B	-0.968149	0.595323	1.031136
8B	-0.968150	0.595325	-1.031133
9B	2.140434	0.595327	-1.031134
10B	2.140435	-1.190652	-0.000002
11B	2.140435	0.595325	1.031134
12A	0.047706	-0.542019	0.938801
13A	1.124582	-0.542019	0.938801
14A	1.124580	1.084035	0.000001
15A	1.124580	-0.542017	-0.938802
16A	0.047705	-0.542017	-0.938802
17A	0.047704	1.084035	0.000002
18B	0.586142	-1.983780	-1.056589
19B	0.586143	-1.983782	1.056588
20B	0.586144	0.076853	2.246299
21B	0.586141	0.076859	-2.246299
22B	0.586142	1.906921	1.189713
23B	0.586140	1.906924	-1.189708

$E24/\varepsilon$ =-113.721598

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.175892	0.000000	0.000000
3A	0.588254	-0.896377	0.000000
4A	0.588254	0.450739	0.774807
5A	0.588988	0.447671	-0.778343
6B	-0.962894	-1.192211	-0.008864
7B	-0.962893	0.607159	1.026061
8A	0.052179	-0.540338	0.939457
9B	-0.966126	0.593740	-1.032304
10B	2.146794	-1.186055	-0.000576
11B	2.146793	0.596901	1.024909
12B	2.143681	0.594999	-1.034493
13A	1.127058	-0.541130	0.940835
14A	0.052466	-0.541022	-0.939845
15A	0.052466	1.084430	-0.004951
16A	1.128966	-0.541807	-0.938910
17A	1.128966	1.084017	-0.003802
18B	0.607095	-1.992752	1.037950
19B	0.607093	0.104868	2.244417
20B	0.592342	-1.982343	-1.057523
21B	0.592342	1.910909	1.181719
22B	0.589480	1.904391	-1.195336
23B	0.589480	0.075603	-2.247180
24B	-0.926933	-1.142309	1.986073

$E25/\varepsilon$ =-119.874315

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.180185	0.000000	0.000000
3A	0.590092	-0.893890	0.000000
4A	0.590092	0.454618	0.769650
5A	0.590092	0.444630	-0.779041
6B	-0.965041	-1.187961	-0.004100
7B	2.145225	0.607708	1.020765
8B	-0.965042	0.607708	1.020763
9B	2.145225	-1.187962	-0.004098
10A	0.055021	-0.537680	0.942072
11A	1.125161	-0.537680	0.942072
12B	0.590091	-2.006373	1.011808
13B	0.590091	0.149230	2.242101
14B	-0.965973	0.591347	-1.036106
15B	2.146159	0.591348	-1.036105
16A	0.051644	-0.542299	-0.938846
17A	1.128541	1.084162	-0.010558
18A	1.128542	-0.542299	-0.938846
19A	0.051643	1.084162	-0.010558
20B	0.590092	-1.980678	-1.060282
21B	0.590091	1.920257	1.166144
22B	0.590093	0.070261	-2.247843
23B	0.590093	1.899683	-1.203717
24B	-0.902841	-1.140087	1.997551
25B	2.083022	-1.140087	1.997553

$E26/\varepsilon$ =-125.890569

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.183360	0.000000	0.000000
3A	0.591769	-0.891974	0.000000
4B	-0.959959	-1.188960	-0.004592
5A	0.592849	0.453360	-0.769845
6A	0.591793	0.446292	0.775816
7B	-0.962697	0.606709	-1.022543
8B	2.150928	-1.183434	0.003436
9B	-0.961029	0.604304	1.030338
10B	2.148770	0.607930	-1.022999
11A	0.059396	-0.536248	-0.943714
12A	1.129372	-0.537288	-0.942384
13A	0.055151	-0.540611	0.940155
14B	0.595181	-2.004166	-1.014130
15B	0.595034	0.149800	-2.243009
16B	2.152216	0.592798	1.030320
17A	1.130241	-0.540981	0.940859
18A	0.056378	1.084690	0.005424
19A	1.132827	1.084142	0.007218
20B	0.612055	-1.988971	1.042957
21B	0.610820	0.098972	2.246111
22B	0.594049	1.918889	-1.170578
23B	0.596091	1.904389	1.195230
24B	-0.896597	-1.139340	-2.002345
25B	2.088137	-1.139290	-1.998319
26B	-0.924935	-1.144759	1.987535

$E27/\varepsilon$ =-133.907416

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.097842	0.000000	0.000000
3A	0.000000	-1.097842	0.000000
4A	-0.548921	0.548921	-0.776292
5A	0.000000	1.097842	0.000000
6A	0.548921	-0.548921	0.776292
7A	-0.548921	-0.548921	-0.776292
8A	0.548921	0.548921	0.776292
9A	-0.548921	0.548921	0.776292
10A	0.548921	-0.548921	-0.776292
11A	-0.548921	-0.548921	0.776292
12A	0.548921	0.548921	-0.776292
13A	-1.097842	0.000000	0.000000
14B	0.000000	0.000000	2.105807
15B	1.489031	-1.489031	0.000000
16B	-1.489031	1.489031	0.000000
17B	1.489031	1.489031	0.000000
18B	-1.489031	-1.489031	0.000000
19B	0.000000	0.000000	-2.105807
20B	1.872748	0.000000	1.324233
21B	1.872748	0.000000	-1.324233
22B	0.000000	-1.872748	1.324233
23B	0.000000	1.872748	1.324233
24B	0.000000	-1.872748	-1.324233
25B	-1.872748	0.000000	1.324233
26B	0.000000	1.872748	-1.324233
27B	-1.872748	0.000000	-1.324233

$E28/\varepsilon$ =-138.966341

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.097418	0.000000	0.000000
3B	1.523756	-1.445742	0.000000
4B	1.523756	1.445742	-0.000001
5A	0.545234	0.544878	0.781901
6A	0.545234	0.544877	-0.781901
7A	0.545235	-0.544877	-0.781901
8A	0.545234	-0.544877	0.781901
9A	-0.552280	0.551385	-0.771643
10A	-0.552281	-0.551385	0.771642
11A	-0.552281	0.551386	0.771641
12A	-0.552280	-0.551385	-0.771643
13A	0.012151	-1.097330	0.000000
14A	0.012151	1.097330	-0.000001
15A	-1.098924	0.000000	-0.000001
16B	-1.476579	-1.501475	-0.000001
17B	-1.476580	1.501474	-0.000003
18B	-0.061421	-0.000001	-2.111577
19B	-0.061424	0.000002	2.111575
20B	1.798220	-0.000001	-1.457157
21B	1.798219	0.000000	1.457157
22B	0.022439	-1.871621	-1.321647
23B	0.022438	-1.871619	1.321648
24B	0.022439	1.871620	-1.321649
25B	0.022438	1.871622	1.321644
26B	-1.896143	-0.000001	-1.296418
27B	-1.896146	0.000001	1.296413
28A	2.210264	0.000000	0.000000

$E29/\varepsilon$ =-145.342393

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.103368	0.000000	0.000000
3A	0.555143	-0.953540	0.000000
4A	0.555141	-0.319172	0.898536
5B	-0.076024	-1.717836	1.212792
6B	1.446314	0.930003	1.212795
7B	1.446321	-0.831541	-1.282305
8A	-0.012390	-0.626320	-0.898115
9A	-0.556447	-0.309619	0.890809
10A	0.535037	0.325834	-0.898113
11A	0.535034	0.955372	-0.006418
12A	-0.556444	-0.943063	-0.006421
13A	-0.012396	0.636663	0.890811
14A	-0.559802	0.951491	-0.003571
15A	-1.103943	0.005054	-0.003573
16A	-0.559799	0.321849	-0.895414
17B	-1.510631	0.868512	1.202048
18B	-0.032385	1.729136	-1.220772
19B	-1.510622	-0.842003	-1.220778
20B	-0.058962	-2.149079	-0.799361
21B	1.827583	1.132237	-0.799357
22B	-0.058971	0.033901	2.292676
23B	-0.042652	0.024526	-2.299334
24B	-1.901037	-1.057410	0.746522
25B	-0.042663	2.174907	0.746530
26B	-1.887349	1.085104	-0.766092
27B	1.612160	-0.926891	1.861979
28B	1.612164	-2.064824	0.250181
29B	2.595573	-0.354357	0.250182

$E30/\varepsilon$ =-151.524277

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	2.094427	0.000000	0.000000
3B	0.027929	-2.094241	0.000000
4B	0.027928	-0.027558	2.094059
5A	-0.001465	-0.781642	0.771423
6A	0.781552	0.011889	0.771423
7A	0.781553	-0.771199	-0.022038
8A	-0.774554	-0.778587	-0.002954
9A	-0.003038	0.774583	0.778557
10A	-0.774555	-0.007292	0.778558
11A	0.768189	0.013282	-0.784761
12A	-0.003037	-0.768298	-0.784761
13A	0.768188	0.784868	-0.002954
14A	-0.783140	0.002053	-0.772806
15A	-0.012497	0.783043	-0.772806
16A	-0.783141	0.772765	0.008115
17B	-0.022739	0.022438	-2.108977
18B	-0.022742	2.109089	0.005314
19B	-2.109205	-0.005388	0.005315
20B	1.309517	-1.292169	-1.373808
21B	-1.339103	-1.327491	1.310134
22B	1.309515	1.356687	1.310134
23A	1.023152	-1.009597	0.996399
24B	-1.320938	1.303437	1.347578
25B	1.312577	1.338559	-1.321058
26B	-1.320935	-1.330311	-1.321059
27B	-1.344727	1.326911	-1.309566
28B	0.437000	-1.978874	1.953003
29B	1.984526	-0.410571	1.953003
30B	1.984527	-1.958237	0.384838

$E31/\varepsilon$ =-156.759040

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.483113	0.000000	0.000000
3A	-0.745299	-0.775715	0.000000
4A	-0.745299	-0.013269	0.775602
5A	-0.745300	0.775715	0.000001
6A	-0.745300	0.013269	-0.775601
7A	0.019510	-0.796374	-0.810116
8A	0.019511	0.796373	0.810115
9A	0.315270	-1.006262	0.215514
10A	0.315270	0.232697	-1.002428
11A	0.315270	1.006262	-0.215515
12A	0.315270	-0.232697	1.002428
13B	-1.786635	-1.052941	-1.071110
14B	-1.786636	1.052940	1.071110
15B	-0.569351	-2.257340	0.065430
16B	-0.569351	0.104039	-2.255890
17B	-0.569350	-0.104039	2.255891
18B	-0.569351	2.257340	-0.065431
19B	-1.925242	-1.029988	1.012516
20B	-1.925242	1.029987	-1.012516
21A	-0.414059	1.046430	-1.028680
22A	-0.414059	-1.046431	1.028680
23A	-1.518940	0.000000	0.000000
24B	0.997459	-1.499364	1.473929
25B	0.997458	1.499363	-1.473930
26B	1.278800	-0.493121	-1.906255
27B	1.278800	1.897540	0.525659
28B	1.278801	0.493121	1.906254
29B	1.278800	-1.897540	-0.525660
30B	-0.185063	1.852530	1.884499
31B	-0.185063	-1.852531	-1.884499

$E32/\varepsilon$ =-163.768277

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.775560	0.000000	0.000000
3B	-1.772348	-0.060145	0.000000
4A	0.561860	0.299996	-0.894499
5A	0.561860	0.300044	0.894482
6A	0.548791	0.948054	-0.000026
7A	-0.566451	0.938983	-0.000026
8A	0.551368	-0.764814	-0.554809
9A	0.551367	-0.764785	0.554850
10A	-0.551307	0.296861	-0.896907
11A	-0.551307	0.296909	0.896890
12A	-0.556146	-0.760238	-0.568150
13A	-0.556146	-0.760207	0.568190
14B	-0.033819	2.446862	-0.000066
15B	0.037402	0.785055	2.318609
16B	0.037401	0.784930	-2.318652
17A	-0.005561	1.238880	0.890559
18A	-0.005561	1.238832	-0.890627
19B	-1.477699	1.515727	1.115029
20B	-1.477698	1.515668	-1.115112
21A	0.008939	-0.452112	1.454691
22A	0.008940	-0.452190	-1.454667
23B	1.457384	1.568493	-1.092306
24B	1.457384	1.568553	1.092220
25B	1.466818	-0.583443	-1.814311
26B	1.466817	-0.583347	1.814342
27B	1.437379	-1.910512	0.000051
28B	-0.002313	-1.953199	1.451987
29B	-0.002312	-1.953277	-1.451883
30A	-0.036920	-1.527302	0.000041
31B	-1.441149	-0.504701	1.871198
32B	-1.441147	-0.504803	-1.871173

$E33/\varepsilon$ =-172.578008

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.778289	0.000000	0.000000
3B	-1.778287	0.000000	0.000000
4A	0.557436	-0.626313	-0.705635
5A	-0.557434	-0.626313	-0.705635
6A	0.557436	-0.864640	0.377606
7A	0.557436	0.091937	0.939008
8A	-0.557434	0.091937	0.939008
9A	-0.557434	0.921460	0.202732
10A	0.557435	0.477557	-0.813713
11A	-0.557434	-0.864640	0.377606
12A	0.557436	0.921460	0.202732
13A	-0.557434	0.477557	-0.813713
14B	0.000001	-2.235288	0.976196
15B	0.000000	1.234592	-2.103630
16B	0.000003	-1.619160	-1.824225
17B	0.000001	2.382181	0.524108
18B	0.000001	0.237677	2.427547
19A	0.000001	1.009433	1.137274
20A	0.000001	-0.148174	-1.513404
21A	0.000001	1.393544	-0.608590
22A	0.000001	-1.485121	-0.326746
23A	0.000001	-0.769680	1.311464
24B	-1.458213	1.749620	-0.764097
25B	1.458214	1.749620	-0.764098
26B	-1.458212	1.267361	1.427870
27B	-1.458212	-0.966348	1.646569
28B	-1.458212	-0.186037	-1.900107
29B	-1.458211	-1.864597	-0.410237
30B	1.458214	1.267361	1.427869
31B	1.458214	-0.966348	1.646568
32B	1.458215	-0.186033	-1.900107
33B	1.458215	-1.864597	-0.410236

$E34/\varepsilon$ =-179.450528

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.727309	0.000000	0.000000
3A	-0.570518	-0.929829	0.000000
4A	-0.570518	0.752248	0.546540
5A	-0.570518	0.752248	-0.546540
6A	-0.570518	-0.287332	0.884320
7A	-0.570518	-0.287332	-0.884320
8A	-1.153850	0.000001	0.000000
9A	0.521250	-0.957555	0.000000
10A	0.521250	0.774678	-0.562836
11A	0.521250	-0.295900	-0.910689
12A	0.521250	0.774678	0.562836
13A	0.521250	-0.295900	0.910689
14B	-1.601390	1.711513	0.000000
15B	-1.601391	-1.384641	-1.006002
16B	-1.601391	0.528888	-1.627745
17B	-1.601391	-1.384642	1.006002
18B	-1.601391	0.528887	1.627745
19B	-0.105091	-2.436410	0.000000
20B	-0.105090	1.971098	1.432086
21B	-0.105089	-0.752891	2.317164
22B	-0.105090	1.971098	-1.432086
23B	-0.105089	-0.752891	-2.317164
24A	-0.055847	1.533886	0.000000
25A	-0.055848	0.473997	1.458811
26A	-0.055848	-1.240939	0.901595
27A	-0.055848	-1.240938	-0.901595
28A	-0.055848	0.473997	-1.458811
29B	1.401632	0.593389	-1.826258
30B	1.401631	1.920242	0.000000
31B	1.401631	-1.553508	-1.128690
32B	1.401632	0.593389	1.826258
33B	1.401631	-1.553509	1.128690
34B	-2.658391	0.000002	0.000000

$E35/\varepsilon$ =-185.635002

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.083613	0.000000	0.000000
3A	0.520798	-0.950256	0.000000
4A	0.520799	0.729996	0.608352
5A	-0.389855	-0.807551	0.608352
6A	-0.389855	0.230902	0.984334
7A	-0.017400	1.048759	-0.272062
8A	-0.928054	-0.488787	-0.272063
9A	-0.928054	0.549666	0.103920

10A	0.545415	0.318763	-0.880415
11A	-0.017400	-0.631493	-0.880415
12A	0.555725	-0.329143	0.909085
13A	-0.555724	0.329143	-0.909084
14B	0.311503	0.994403	2.074490
15B	-0.722314	-0.751091	2.074489
16B	1.984252	-1.175227	0.266397
17B	1.984252	0.732272	0.957028
18B	0.311502	-2.091997	0.957026
19B	-1.236174	-1.175341	-1.574745
20B	0.436577	1.648928	-1.574743
21B	0.436576	-0.258573	-2.265374
22B	-2.269991	0.165564	-0.457282
23B	-1.236174	1.911059	-0.457281
24B	2.109199	0.412722	-1.139926
25B	0.651779	-2.047985	-1.139927
26B	0.651779	2.303061	0.435415
27B	-1.706377	-1.678446	0.435413
28B	-1.706376	1.010648	1.409028
29A	-0.412103	-1.456169	-0.275301
30A	1.078901	1.061240	-0.275300
31A	-1.333594	-0.260954	0.720748
32A	-0.412102	1.294890	0.720749
33A	1.078901	-0.639008	-0.890893
34B	1.300890	-0.770490	2.128064
35B	-1.300889	0.770489	-2.128064

*E*36/ε=-191.280568

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.084726	0.000000	0.000000
3A	0.551281	-0.934195	0.000000
4A	0.524831	0.319712	0.893850
5A	-0.008615	-0.614483	0.893850
6A	-0.931626	-0.089907	-0.551401
7A	-0.396040	0.848035	-0.551400
8A	0.512180	0.331316	-0.894432
9A	-0.025038	-0.609484	-0.894432
10A	-0.391578	0.847381	0.548378
11A	-0.928795	-0.093419	0.548378
12A	0.553454	0.966039	0.001143
13A	-0.550702	-0.967610	0.001142
14B	1.994519	0.625164	1.025731
15B	0.475246	-2.035456	1.025729
16A	1.096039	-0.625862	0.910402
17B	0.313832	1.607222	1.640080
18B	0.438517	-2.036829	-1.015158
19B	-1.224688	-1.087105	1.640077
20B	1.977036	0.657496	-1.015156
21B	0.599644	-0.342411	2.330145
22B	2.109324	-1.204470	-0.079995
23B	-0.724615	2.207434	0.004246
24B	0.303523	1.620344	-1.637134
25B	-1.241227	-1.084891	-1.637137
26B	-2.269366	-0.497802	0.004243
27B	-1.716302	0.980049	-1.425614
28B	-1.716400	0.980102	1.428557
29B	0.635598	-0.362938	-2.326306
30A	-1.338405	0.764259	0.001951
31A	-0.420703	0.240232	-1.463121
32A	-0.423427	0.241786	1.448375
33A	1.059904	-0.605228	-0.919699
34B	1.306761	2.255671	0.011728
35B	-1.278524	-2.271794	0.011723
36B	2.218434	-1.266774	1.842697

*E*37/ε=-198.154921

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.746929	0.000000	0.000000
3A	0.544057	-0.923272	0.000000
4A	-0.607940	-0.893779	0.000000
5A	-0.567675	-0.311854	-0.886891
6A	-0.567675	-0.311855	0.886891
7A	-0.553281	0.739024	0.558396
8A	-0.553281	0.739024	-0.558395
9A	0.515403	-0.327994	0.910551
10A	0.515403	-0.327994	-0.910551
11A	-1.163373	0.029303	0.000000
12A	0.538454	0.749012	0.574670
13A	0.538454	0.749013	-0.574669
14B	-1.636222	-1.375026	-1.005754
15B	-1.636221	-1.375027	1.005754
16A	-0.060362	-1.323858	-0.797418
17A	-0.060362	-1.323858	0.797418
18B	-0.109645	-0.880477	2.242826
19B	-0.109646	-0.880476	-2.242826
20B	-1.574619	1.700580	0.000001
21B	1.423159	-1.553854	-1.116263
22B	1.423159	-1.553855	1.116262
23B	-1.591660	0.517878	-1.629801
24B	-1.591660	0.517877	1.629802
25B	-0.070962	1.935598	1.440736
26B	-0.070962	1.935599	-1.440734
27A	-0.050034	0.432977	-1.475952
28A	-0.050034	0.432976	1.475953
29A	-0.033605	1.506322	0.000001
30A	0.443253	-1.997331	0.000000
31B	1.406518	0.513658	-1.847409
32B	1.406518	0.513658	1.847409
33A	-0.633986	-1.963823	0.000000
34B	1.413783	1.907569	0.000001
35B	-0.172411	-2.769706	-1.218540
36B	-0.172411	-2.769707	1.218539
37B	-2.668959	0.017330	0.000000

*E*38/ε=-204.430886

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.071855	0.000000	0.000000
3A	0.467541	-0.964510	0.000000
4A	-0.016280	-0.624047	0.893326
5A	0.554448	0.286857	-0.893326
6A	-0.016279	-0.624047	-0.893326
7A	0.554448	0.286857	0.893326
8A	-0.345189	0.850352	0.564991
9A	-0.345189	0.850352	-0.564991
10A	-0.915760	-0.060303	-0.564991
11A	-0.915760	-0.060303	0.564991
12A	0.581684	0.963454	0.000000
13A	-0.613235	-0.943685	0.000000
14B	2.033215	0.564558	-1.018635
15B	0.378867	-2.075849	1.018636
16B	2.033214	0.564559	1.018637
17B	0.378868	-2.075849	-1.018636
18A	1.120299	-0.701924	-0.798832
19A	1.120298	-0.701923	0.798832
20B	0.747926	-0.468612	-2.237235
21B	0.747925	-0.468612	2.237235
22B	-2.258043	-0.427412	0.000000
23B	-0.600349	2.218338	0.000000
24B	-1.245774	-1.056051	1.641769
25B	0.406884	1.581658	-1.641769
26B	-1.245773	-1.056052	-1.641769
27B	0.406883	1.581658	1.641769
28B	-1.637504	1.025980	-1.439470
29B	-1.637504	1.025980	1.439469
30A	-0.366632	0.229713	1.481240
31A	-0.366631	0.229713	-1.481241
32A	-1.284659	0.804903	0.000000
33A	1.393853	-1.509317	0.000001
34A	1.966157	-0.595897	0.000001
35B	2.335362	-1.463221	1.230918
36B	2.335365	-1.463222	-1.230914
37B	-1.353439	-2.242214	0.000000
38B	1.427288	2.195944	0.000000

*E*39/ε=-210.627234

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.750821	0.000000	0.000000
3B	-1.636644	-1.699792	0.000000
4B	-1.636642	-0.499806	1.624652
5A	-0.611200	-0.718792	0.530909
6A	0.547820	-0.739308	0.546061
7A	-0.566254	-0.776173	-0.528786
8A	-0.566253	0.277185	0.897346
9A	-0.550916	0.263697	-0.889129
10A	-0.550915	0.927361	0.009400
11A	0.516868	0.278096	0.926699
12A	0.516867	-0.803962	-0.538290
13A	-1.162345	0.025503	-0.018836
14A	0.540766	0.260930	-0.906462
15A	0.540767	0.943114	0.017139
16B	1.424100	-1.910420	0.025821
17B	1.424100	-0.586421	1.818373
18A	-0.059817	-0.589647	1.423652
19A	-0.059818	-1.534097	0.144970
20B	-0.107530	0.622908	2.326381
21B	-0.107533	-2.040380	-1.279420
22B	-1.572730	1.368112	-1.010502
23B	-1.589256	-0.549164	-1.620942
24B	-1.589252	1.387812	1.001512
25A	0.429990	-1.597508	1.179937
26A	-0.638301	-1.579719	1.166799
27B	-0.172406	-1.471159	2.636658
28B	-0.172408	-2.952680	0.630839
29B	-0.066837	0.701404	-2.309129
30B	-0.066833	2.413290	0.008577
31A	-0.048036	1.225866	0.929805
32A	-0.048039	-0.528248	-1.445075
33A	-0.030778	1.212180	-0.895331
34B	1.408895	-0.686099	-1.789873
35B	1.408897	1.509008	1.182061
36B	1.416927	1.533836	-1.132915
37B	-2.667659	0.012585	-0.009291
38B	1.322890	-2.593547	1.915622
39B	-1.691512	-2.486499	1.836558

*E*40/ε=-216.945765

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	2.343246	0.000000	0.000000
3B	1.452637	-1.838654	0.000000
4B	-0.614446	-0.837399	2.100482
5B	0.276164	1.001259	2.100480
6A	0.170361	-0.082519	1.054752
7A	0.930296	-0.450617	0.282540
8A	-0.553544	-0.724510	0.596882
9A	0.939109	0.537750	-0.128423
10A	0.160227	-1.070247	-0.128422
11A	0.225338	0.883487	0.596880
12A	-0.341686	-0.463024	-0.911312
13A	0.151496	0.555146	-0.911313
14A	-1.055015	-0.117501	-0.186458
15A	-0.561833	0.900669	-0.186459
16A	0.735322	-0.356176	-0.775222
17A	-0.760438	0.368342	0.744704
18A	0.455740	-1.104462	0.974968
19A	1.149153	0.327083	0.974967
20B	-0.436173	-2.272211	0.653877
21B	1.512519	1.750851	0.653873
22B	0.017579	-0.008517	-2.296378
23B	-2.060036	0.997839	-0.185197
24B	0.019390	-1.833130	-1.414628
25B	1.450404	1.121189	-1.414630
26B	-0.618059	2.123111	0.687250
27B	-2.049071	-0.831207	0.687252
28A	0.845640	-0.409610	1.818478

29A	1.554719	-0.753076	1.097942
30B	2.211081	0.315351	2.025601
31B	1.123264	-1.930440	2.025604
32B	-1.800747	-0.727487	-1.425338
33B	-0.545501	1.863960	-1.425340
34A	-0.908416	-1.207063	-0.318590
35A	0.383983	1.461087	-0.318592
36A	-0.920501	0.445871	-1.118404
37B	-1.705471	0.826096	1.807926
38B	1.772612	-0.858619	-1.726351
39B	0.907560	-0.439601	3.347184
40B	2.919532	-1.414164	1.302704

$E41/\varepsilon$ =-223.258093

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.094698	0.000000	0.000000
3A	0.550723	-0.948256	0.000000
4A	0.550722	-0.293426	-0.901715
5A	0.545886	0.313295	0.879071
6A	0.545886	0.932871	0.025903
7A	1.090124	-0.648204	0.910058
8A	1.090123	0.664815	-0.897995
9A	0.012126	0.663778	-0.893212
10A	0.012127	-0.643977	0.907593
11A	-0.538857	0.963299	0.014652
12A	-0.538857	0.312011	0.911488
13B	-0.495981	-2.009435	0.355615
14B	-0.495982	-0.283633	-2.020850
15B	1.602652	-0.288549	-2.018917
16B	1.602653	-2.009116	0.350340
17B	-1.964974	0.581746	0.422470
18B	0.662669	0.191892	2.315067
19B	0.662667	2.260823	-0.533890
20A	-0.904369	-0.525966	0.303786
21A	-0.904370	0.126121	-0.594152
22A	-0.360797	-0.829287	-0.602232
23A	1.462754	-0.829212	-0.602178
24A	2.001984	-0.520755	0.303415
25A	2.001984	0.127383	-0.589084
26B	1.356552	1.746319	1.268187
27B	0.549457	-1.816407	-1.319084
28A	1.625118	0.308006	0.917633
29A	1.625117	0.967903	0.008941
30B	3.040487	0.618663	0.449276
31B	-1.213657	-0.753452	1.792687
32B	-1.213660	1.471554	-1.271193
33A	-0.009298	1.263179	0.917329
34B	2.352885	1.449188	-1.265641
35B	2.352887	-0.755093	1.769697
36B	0.557717	1.337412	-2.209958
37B	0.557720	-1.687651	1.955615
38B	-1.870562	-1.053427	-0.765001
39B	2.984438	-1.032670	-0.749931
40B	-1.002219	1.198903	2.083826
41B	-1.002221	2.352535	0.495252

$E42/\varepsilon$ =-230.236470

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.123900	0.000000	0.000000
3A	0.582476	-0.914367	0.000000
4A	0.582474	0.777239	-0.481629
5A	0.744658	0.813152	0.617477
6A	0.744660	-0.365955	0.953190
7A	0.687468	-0.273582	-0.960891
8A	-0.225629	-0.783477	-0.736218
9A	-0.225630	0.278185	-1.038491
10B	0.674822	-1.952381	1.078036
11B	0.674816	2.227422	-0.112026
12B	0.659293	1.113254	-1.949763
13B	0.659297	-1.973307	-1.070967
14B	2.759148	-0.030299	-0.106427
15B	-1.526973	0.327720	1.151047
16A	-0.999333	0.481942	-0.315683
17A	-0.999332	-0.575950	-0.014482
18A	-0.253423	-0.735382	0.758216
19A	-0.253426	1.024475	0.257155
20B	-0.197937	-0.642089	-2.255181
21A	-0.074741	0.299614	1.052323
22B	-0.117939	-0.570741	2.275207
23B	-0.117943	1.683577	1.633364
24A	1.603833	0.981942	0.004034
25A	1.603836	-0.832552	0.520652
26A	1.653745	0.251928	0.884828
27A	1.538605	-0.819670	-0.570431
28A	1.538603	0.396280	-0.916633
29B	-1.395373	-1.785313	-1.006109
30B	-1.395376	0.987609	-1.795610
31B	1.795795	-0.579355	-2.034851
32A	0.865707	0.471077	1.654538
33B	1.868375	1.646870	1.363568
34B	1.868379	-0.681643	2.026537
35A	-0.333004	1.318317	-0.783317
36A	-0.332999	-1.533211	0.028563
37B	-1.455296	1.933197	0.024790
38B	-1.455289	-1.630222	1.039359
39A	-1.130970	-0.308866	-1.084808
40B	-2.466915	-0.129332	-0.454236
41B	2.360727	1.681463	-1.099492
42B	2.360732	-2.008431	-0.048917

$E43/\varepsilon$ =-237.073585

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.096375	0.000000	0.000000
3A	0.560099	-0.922144	0.000000
4B	-0.870880	0.529779	1.386183
5A	0.541201	-0.357098	-0.968401
6B	1.977234	0.490110	1.411713
7B	0.573804	-2.039840	-0.946402
8A	0.542545	0.707399	-0.606445
9A	0.553655	0.324284	0.887372
10B	0.464088	0.906079	-2.082968
11A	-0.001730	-0.646496	0.880957
12A	1.130873	-0.652597	0.877390
13A	-0.361886	0.210781	-1.008381
14A	-0.345986	-0.837391	-0.617806
15A	1.460696	-0.794846	-0.648150
16A	-0.933973	0.544418	-0.150476
17A	-0.005796	1.063046	0.241759
18A	-0.921244	-0.515952	0.242226
19A	2.044085	-0.486020	0.204987
20B	0.749899	2.233797	-0.614844
21A	1.122747	1.049026	0.253325
22A	2.015031	0.568174	-0.151114
23A	1.414011	0.261359	-1.012137
24B	0.595872	-2.098357	1.210040
25B	-0.518388	-0.816013	-2.104064
26B	1.560258	-0.741311	-2.138087
27B	0.567655	1.877908	1.386015
28B	0.538184	-0.464262	2.291793
29B	2.717524	-1.665907	-0.644810
30B	-1.617979	0.935981	-1.551269
31B	-1.582202	-1.763817	-0.553302
32B	2.416112	1.228442	-1.500766
33A	1.487111	-1.454212	0.201013
34B	-1.264367	-1.378399	1.453857
35A	-0.343874	-1.478282	0.241361
36A	2.369478	-0.208260	-0.860339
37A	-1.277969	-0.312831	-0.790536
38A	-0.369642	1.263684	-0.789519
39B	-1.202868	2.038710	0.190199
40B	2.456306	-1.385763	1.371257
41B	3.452093	0.125436	0.151447
42B	-2.354925	0.046930	0.203611
43B	2.434316	1.984165	0.318821

$E44/\varepsilon$ =-244.756631

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.100400	0.000000	0.000000
3A	0.553444	-0.969252	0.000000
4B	0.653308	-0.367093	-2.274355
5A	0.548761	0.944750	-0.023252
6A	0.548637	-0.312745	-0.847779
7A	0.551327	0.311736	0.889624
8A	-0.547181	-0.943105	-0.015191
9A	-0.003111	-0.621731	0.892704
10A	1.094218	0.630612	-0.923892
11A	1.094748	-0.654998	0.877881
12A	0.011218	0.628590	-0.924479
13A	-0.535419	-0.324028	-0.920562
14A	1.649028	-0.309492	-0.920590
15B	1.174981	-2.377874	0.053152
16A	1.665786	-0.936321	-0.033524
17B	-0.472157	0.280889	2.024300
18B	1.548746	0.261562	2.029951
19B	-0.481478	2.001060	-0.416243
20B	1.576490	2.007555	-0.413529
21B	-1.974445	-0.573710	-0.414000
22A	0.010063	-1.266215	-0.910006
23A	-0.901498	0.525092	-0.319941
24A	1.999078	0.539121	-0.305460
25A	-0.358361	0.843871	0.587007
26A	-0.912272	-0.097972	0.587010
27A	1.448384	0.850609	0.592117
28A	1.997867	-0.091642	0.603428
29B	0.544365	1.837058	1.291902
30A	1.094132	-1.239724	-0.936805
31B	3.119225	-0.491468	-0.344577
32B	-1.337141	-1.364900	1.295521
33B	-0.884608	-2.384977	-0.397761
34B	0.547652	-1.490860	2.021588
35B	2.354032	0.693511	-1.802219
36B	-1.224263	0.710857	-1.812610
37B	2.392673	-1.399174	1.270041
38B	0.560193	1.564644	-2.033068
39B	-1.078850	-1.258692	-2.020322
40B	0.551223	-2.360219	-1.838959
41A	-0.012849	-1.671833	0.617488
42B	-1.856658	1.084533	0.755187
43B	2.291219	-1.389015	-1.840921
44B	2.919721	1.126199	0.807909

$E45/\varepsilon$ =-251.897352

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.103619	0.000000	0.000000
3A	0.547040	-0.958501	0.000000
4B	0.536492	-0.311528	-2.277691
5A	0.548165	-0.318307	-0.848450
6A	-0.546218	-0.947970	-0.017571
7A	0.552568	0.944281	-0.017569
8A	0.553357	0.312505	0.889358
9A	0.002874	-0.635498	0.889357
10A	1.640379	-0.952530	-0.017978
11A	1.098919	-0.638117	0.887469
12A	0.007954	0.629675	-0.920609
13A	-0.542934	-0.319026	-0.920610
14A	1.088863	0.627220	-0.923080
15A	-0.005017	-1.256584	-0.923081
16A	1.092822	-1.260594	-0.922659
17A	1.636522	-0.324272	-0.922659
18B	-0.465327	0.270202	2.026641
19B	-1.981040	-0.566043	-0.397218
20B	-0.490350	2.001120	-0.397217
21A	-0.904198	0.525046	-0.312204
22A	-0.906583	-0.104775	0.591655

23A	-0.358377	0.839306	0.591655
24B	0.543669	-1.483559	2.029638
25B	1.557963	0.263186	2.029639
26B	-0.951388	-2.367693	-0.403963
27B	1.584771	1.999902	-0.403960
28B	2.027896	-2.378698	-0.410649
29B	3.071098	-0.582168	-0.410648
30B	-1.321849	-1.376208	1.296831
31B	0.540030	1.830189	1.296833
32B	-1.238452	0.719140	-1.799655
33B	2.406958	-1.397665	1.291628
34A	0.539752	-2.004699	-0.317037
35A	2.008636	0.524909	-0.317036
36A	1.472531	0.844093	0.594451
37A	-0.003197	-1.697302	0.594449
38A	2.016855	-0.101506	0.592219
39A	1.087871	-1.701337	0.592218
40B	2.312276	0.703891	-1.826929
41B	0.534814	-2.357128	-1.826931
42B	0.540179	1.605143	-2.011384
43B	-1.126320	-1.264785	-2.011386
44B	2.198617	-1.276684	-2.021370
45B	-1.854172	1.076672	0.775017

$E46/\varepsilon$ =-260.391381

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.099820	0.000000	0.000000
3A	0.549910	-0.958060	0.000000
4B	0.549909	-0.303028	2.278093
5A	0.549910	-0.316959	0.849198
6A	0.549910	0.945359	0.017924
7A	0.549911	0.310582	-0.891240
8A	-0.543076	-0.949407	0.017949
9A	1.642897	-0.949407	0.017951
10A	0.002670	-0.637289	-0.889242
11A	1.097152	-0.637289	-0.889241
12A	0.009660	0.630614	0.921041
13A	1.090159	0.630614	0.921042
14A	-0.540085	-0.318944	0.920292
15A	1.639904	-0.318944	0.920293
16A	0.000849	-1.256334	0.922815
17A	1.098970	-1.256334	0.922815
18B	1.563387	0.269978	-2.027533
19B	-0.463564	0.269978	-2.027534
20B	1.587737	2.003140	0.393835
21B	-0.487917	2.003140	0.393834
22B	-1.976569	-0.568074	0.400749
23B	3.076389	-0.568074	0.400753
24A	-0.902297	0.526369	0.312316
25A	2.002118	0.526369	0.312318
26A	-0.357971	0.840727	-0.593600
27A	1.457792	0.840727	-0.593599
28A	-0.905410	-0.104983	-0.591304
29A	2.005232	-0.104983	-0.591303
30B	0.549911	1.829720	-1.299578
31B	0.549912	-1.480610	-2.030971
32B	-0.941458	-2.369271	0.407887
33B	2.041278	-2.369271	0.407889
34B	2.416917	-1.379354	-1.294602
35B	-1.317095	-1.379353	-1.294605
36B	2.331637	0.721361	1.801483
37B	-1.231819	0.721361	1.801481
38A	0.549910	-2.003433	0.317241
39A	1.095919	-1.698720	-0.594082
40A	0.003902	-1.698720	-0.594083
41B	0.549909	-2.351316	1.829217
42B	0.549909	1.611394	2.004639
43B	2.213044	-1.262051	2.015113
44B	-1.113226	-1.262051	2.015111
45B	-1.854466	1.074753	-0.774170
46B	2.954288	1.074753	-0.774167

$E47/\varepsilon$ =-268.881577

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.100898	0.000000	0.000000
3A	0.550449	-0.953405	0.000000
4B	0.550452	-0.317801	-2.278481
5A	0.550449	-0.317802	-0.849884
6A	0.550449	0.944742	-0.018265
7A	-0.542946	-0.949074	-0.018265
8A	1.643844	-0.949074	-0.018263
9A	1.096874	-0.633280	0.891088
10A	0.550448	0.313156	0.891087
11A	0.004023	-0.633280	0.891087
12A	1.640087	-0.322301	-0.920691
13A	1.099165	-1.259206	-0.920691
14A	1.091371	0.628102	-0.920692
15A	0.009527	0.628102	-0.920692
16A	0.001734	-1.259206	-0.920692
17A	-0.539188	-0.322302	-0.920692
18B	-0.462954	0.267286	2.028388
19B	0.550447	-1.487975	2.028389
20B	1.563849	0.267287	2.028389
21B	-0.936395	-2.376220	-0.397579
22B	-1.975615	-0.576238	-0.397580
23B	-0.488772	1.999052	-0.397579
24B	1.589669	1.999053	-0.397578
25B	3.076514	-0.576237	-0.397576
26B	2.037294	-2.376220	-0.397576
27A	-0.903832	0.521828	-0.312594
28A	0.550449	-1.997061	-0.312593
29A	2.004730	0.521828	-0.312593
30A	1.097338	-1.684112	0.593096
31A	-0.359367	0.838975	0.593094
32A	1.460263	0.838975	0.593095
33A	2.007153	-0.108267	0.593095
34A	0.003558	-1.684112	0.593095
35A	-0.906256	-0.108267	0.593094
36B	-1.308341	-1.390974	1.297244
37B	0.550448	1.828544	1.297244
38B	2.409237	-1.390973	1.297247
39B	2.332738	0.711202	-1.803622
40B	-1.231837	0.711202	-1.803624
41B	0.550451	-2.375810	-1.803622
42B	2.211247	-1.276663	-2.008361
43B	-1.110344	-1.276662	-2.008365
44B	0.550450	1.599920	-2.008364
45B	-1.855642	1.071354	0.773208
46B	0.550448	-3.096115	0.773210
47B	2.956538	1.071356	0.773210

$E48/\varepsilon$ =-275.324355

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.085833	0.000000	0.000000
3A	0.542917	-0.946590	0.000000
4A	0.542917	-0.311201	-0.893972
5A	0.542917	0.313530	0.898385
6A	0.542917	0.951523	0.000748
7A	1.088867	-0.631998	0.896287
8A	-0.003033	0.638690	-0.891531
9A	-0.003034	-0.631998	0.896287
10A	1.088867	0.638690	-0.891531
11A	-0.551242	-0.946114	-0.001054
12A	-0.551241	-0.312039	-0.893177
13A	1.637076	-0.946114	-0.001053
14A	1.637076	-0.312039	-0.893176
15A	-0.004238	-1.259899	-0.895471
16A	1.090073	-1.259899	-0.895471
17B	-0.472406	0.275810	2.032999
18B	1.558239	2.010667	-0.407890
19B	-0.472404	2.010667	-0.407891
20B	1.558238	0.275810	2.032999
21B	-1.975328	-0.584153	-0.415187
22B	3.061163	-0.584153	-0.415185
23A	-0.364290	0.844720	0.600383
24A	1.450123	0.844720	0.600383
25A	-0.911576	-0.101867	0.597862
26A	1.997409	0.531140	-0.292757
27A	-0.911575	0.531140	-0.292758
28A	1.997409	-0.101867	0.597863
29B	0.542917	1.836142	1.305034
30B	0.542916	-1.474942	2.037895
31B	0.542918	1.439714	-2.062934
32B	2.053528	-2.343541	-0.425782
33B	-0.967693	-1.172578	-2.073293
34B	2.053529	-1.172578	-2.073292
35B	-0.967693	-2.343542	-0.425783
36B	-1.326520	0.775746	-1.726477
37B	2.412355	-1.375472	1.300222
38B	-1.326521	-1.375473	1.300220
39B	2.412356	0.775746	-1.726475
40B	0.542918	-2.458591	-1.747438
41A	1.090535	-1.692777	0.601268
42A	1.090536	0.011328	-1.796355
43A	-0.004700	0.011328	-1.796355
44A	-0.004701	-1.692778	0.601267
45A	0.542918	-0.936357	-1.799041
46A	0.542917	-2.006875	-0.292855
47B	-1.864210	1.080244	0.767780
48B	2.950043	1.080244	0.767782

$E49/\varepsilon$ =-283.859545

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.087342	0.000000	0.000000
3A	0.543671	-0.941666	0.000000
4A	0.543671	-0.313888	-0.894504
5A	1.088825	-0.628633	0.898124
6A	-0.001483	-0.628633	0.898124
7A	0.543671	0.315601	0.898124
8A	0.543671	0.950169	-0.000832
9A	-0.551035	-0.945917	-0.000832
10A	1.638377	-0.945917	-0.000832
11A	1.092015	-1.261502	-0.893173
12A	-0.551158	-0.314961	-0.893173
13A	-0.004672	-1.261502	-0.893173
14A	1.638501	-0.314961	-0.893172
15A	1.090157	0.634798	-0.893172
16A	-0.002815	0.634798	-0.893172
17B	-0.471061	0.271967	2.034171
18B	0.543671	-1.485599	2.034172
19B	1.558402	0.271967	2.034172
20B	-0.957295	-2.354295	-0.411290
21B	-0.472890	2.006190	-0.411290
22B	2.044637	-2.354295	-0.411290
23B	1.560232	2.006190	-0.411290
24B	-1.973856	-0.593560	-0.411290
25B	3.061198	-0.593559	-0.411290
26A	1.452380	0.842722	0.600101
27A	-0.365038	0.842722	0.600101
28A	1.090971	-1.679159	0.600101
29A	-0.003629	-1.679159	0.600101
30A	1.999680	-0.105229	0.600101
31A	-0.912338	-0.105229	0.600101
32A	-0.912507	0.526837	-0.292581
33A	1.999849	0.526837	-0.292581
34A	0.543671	-1.995338	-0.292582
35B	0.543671	1.834412	1.303080
36B	-1.316812	-1.388039	1.303080
37B	2.404154	-1.388038	1.303080
38B	0.543671	1.430877	-2.066478
39B	-0.967339	-1.186270	-2.066478
40B	2.054682	-1.186270	-2.066479
41B	0.543671	-2.473726	-1.727603
42B	2.414146	0.766031	-1.727602
43B	-1.326804	0.766031	-1.727602

44A	0.543671	-0.946457	-1.797280
45A	-0.004150	0.002397	-1.797280
46A	1.091492	0.002397	-1.797280
47B	0.543671	-3.095039	0.767489
48B	-1.864877	1.076687	0.767489
49B	2.952218	1.076688	0.767490

$E50/\varepsilon$ =-292.387819

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.088858	0.000000	0.000000
3A	0.544429	-0.942979	0.000000
4A	0.544429	-0.314326	0.889049
5A	1.090108	-0.629374	-0.896595
6A	1.090107	0.635527	0.892244
7A	-0.001250	-0.629374	-0.896595
8A	-0.005329	-1.261824	0.892245
9A	0.544429	0.315769	-0.896595
10A	1.639865	-0.946777	0.001156
11A	1.094186	-1.261824	0.892245
12A	-0.551007	-0.316681	0.892244
13A	0.544429	0.950574	0.001154
14A	1.639865	-0.316681	0.892245
15A	-0.001250	0.635527	0.892244
16A	-0.551007	-0.946777	0.001155
17B	0.544429	-1.487370	-2.030477
18B	1.560314	0.272194	-2.030477
19B	0.544429	1.418565	2.079129
20B	-0.471456	0.272194	-2.030478
21B	-0.956298	-1.180769	2.079131
22B	-0.471456	2.005085	0.420196
23B	1.560313	2.005085	0.420197
24B	2.045154	-1.180770	2.079132
25B	-0.956297	-2.353813	0.420199
26B	3.061040	-0.594249	0.420199
27B	-1.972182	-0.594249	0.420197
28B	2.045154	-2.353814	0.420200
29A	-0.913188	-0.104956	-0.596319
30A	1.091917	-1.681346	-0.596318
31A	-0.365700	0.843321	-0.596319
32A	2.002047	-0.104956	-0.596318
33A	-0.913188	0.527230	0.297725
34A	2.002046	0.527230	0.297726
35A	0.544429	-1.997438	0.297727
36A	0.544429	-0.946510	1.783961
37A	1.454558	0.843322	-0.596319
38A	1.091917	0.001767	1.783960
39A	-0.003059	-1.681346	-0.596318
40A	-0.003060	0.001768	1.783960
41B	0.544429	1.835215	-1.297695
42B	-1.317129	0.760446	1.742217
43B	-1.317129	-1.389098	-1.297693
44B	2.405987	0.760446	1.742218
45B	2.405987	-1.389098	-1.297692
46B	0.544428	-2.463867	1.742219
47B	0.544429	-0.314323	3.173848
48B	2.954388	1.077066	-0.761600
49B	-1.865530	1.077066	-0.761601
50B	0.544429	-3.097109	-0.761598

s = 1.9

$E5/\varepsilon$ =-9.251172

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.123881	0.000000	0.000000
3A	0.561940	-0.973310	0.000000
4B	0.561940	-0.324440	-1.485951
5B	0.561940	-0.324440	1.485951

$E6/\varepsilon$ = -13.439465

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.131135	0.000000	0.000000
3B	0.565569	-1.514218	0.000000
4B	0.565569	0.000000	1.514218
5B	0.565569	1.514218	0.000000
6B	0.565569	0.000000	-1.514218

$E7/\varepsilon$ = -17.672694

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.562405	0.000000	0.000000
3B	0.000000	-1.562405	0.000000
4B	0.000000	0.000000	1.562405
5B	0.000000	1.562405	0.000000
6B	0.000000	0.000000	-1.562405
7B	-1.562405	0.000000	0.000000

$E8/\varepsilon$ = -21.634684

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.617923	0.000000	0.000000
3B	-1.210707	-1.073251	0.000000
4B	0.186920	-0.542957	-1.512593
5B	0.220297	-0.530298	1.512592
6A	0.399619	-1.053226	-0.000001
7B	0.248859	1.420621	-0.745382
8B	-1.128594	0.897978	0.745388

$E9/\varepsilon$ = -26.868864

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.621957	0.000000	0.000000
3B	0.172073	-1.612804	0.000000
4B	0.216387	1.226774	1.047547
5B	-1.196896	-0.345312	-1.047545
6B	0.216389	1.226775	-1.047547
7B	-1.196894	-0.345316	1.047549
8A	0.408694	-0.367410	-0.983815
9A	0.408695	-0.367411	0.983815

$E10/\varepsilon$ = -32.132430

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.635017	0.000000	0.000000
3B	0.209709	-1.621513	0.000000
4B	-1.173836	-0.405379	-1.063514
5B	0.251472	1.216135	-1.063513
6B	0.251472	1.216135	1.063513
7B	-1.173836	-0.405379	1.063514
8A	0.423561	-0.372309	-0.976758
9A	0.423561	-0.372309	0.976758
10A	-0.847122	0.744619	0.000000

$E11/\varepsilon$ = -36.549295

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.120471	0.000000	0.000000
3A	0.027058	-1.120144	0.000000
4A	0.573765	-0.560072	-0.782668
5A	0.573764	-0.560072	0.782668
6B	-0.994581	-0.580585	1.110193
7B	-0.994581	-0.580584	-1.110194
8B	0.556396	1.008312	-1.110192
9B	0.556397	1.008311	1.110194
10B	-1.207030	1.178224	0.000001
11B	1.576504	-1.538883	0.000000

$E12/\varepsilon$ = -41.889065

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.082056	0.000000	0.000000
3B	0.541029	-1.523346	0.000000
4A	0.541027	0.607566	-0.759451
5B	0.541029	-0.087182	1.521290
6B	1.597495	-0.418365	-1.446637
7B	-0.515441	-0.418367	-1.446636
8A	0.541027	0.923992	0.310233
9B	1.954644	1.304390	-0.287458
10B	-0.872591	1.304388	-0.287459
11B	-1.326162	-0.627849	0.559569
12B	2.408220	-0.627847	0.559566

$E13/\varepsilon$ = -47.448527

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.099049	0.000000	0.000000
3A	0.549524	-0.951804	0.000000
4A	1.102304	-0.636417	-0.914313
5A	-0.003258	-0.636417	-0.914312
6A	0.549523	0.321028	-0.914313
7B	0.549525	-0.317267	1.461358
8B	-1.005170	-1.214872	0.202459
9B	0.549524	1.477939	0.202454
10B	2.104219	-1.214872	0.202453
11B	0.549522	-2.146348	-1.024026
12B	-1.034507	0.597270	-1.024026
13B	2.133552	0.597271	-1.024030

$E14/\varepsilon$ = -54.331902

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.564018	0.000000	0.000000
3A	0.782009	-0.782008	0.000000
4A	0.782009	0.000000	0.782008
5A	0.782009	0.782008	0.000000
6A	0.782009	0.000000	-0.782008
7B	-0.319972	1.101982	1.101982
8B	-0.319972	-1.101982	-1.101982
9B	1.883991	-1.101982	-1.101982
10B	-0.319972	-1.101982	1.101982
11B	1.883991	1.101982	1.101982
12B	-0.319972	1.101982	-1.101982
13B	1.883991	1.101982	-1.101982
14B	1.883991	-1.101982	1.101982

$E15/\varepsilon$ = -59.981696

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.111168	0.000000	0.000000
3A	0.018393	-1.111016	0.000000
4A	0.564781	-0.555508	-0.779184
5A	0.564780	-0.555508	0.779184
6A	1.123499	-1.105054	0.000000
7B	-0.980898	-0.608006	1.121302
8B	-0.980897	-0.608006	-1.121303
9B	0.591683	0.990827	1.121303
10B	0.591683	0.990826	-1.121303
11B	0.586711	-2.117647	1.098326
12B	2.127067	-0.551577	1.098327
13B	0.586712	-2.117647	-1.098325
14B	2.127069	-0.551578	-1.098324
15B	-1.171161	1.151929	0.000000

$E16/\varepsilon$ = -65.711712

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.114201	0.000000	0.000000
3A	0.557100	-0.957730	0.000000
4A	0.557101	0.293209	0.911743
5A	1.110589	-0.655981	0.900025
6A	0.003614	-0.655980	0.900026
7B	0.557100	1.503697	-0.090051
8B	0.557100	-0.374631	-1.459063
9B	-0.992154	0.546102	1.148509
10B	-0.992154	-1.260551	-0.168262

11B	2.106357	0.546101	1.148508
12B	2.106355	-1.260551	-0.168265
13B	0.557102	-0.369864	2.364437
14B	0.557102	-2.137670	1.075980
15B	2.282020	0.681973	-0.935689
16B	-1.167820	0.681972	-0.935688

$E17/\varepsilon$ = -71.481302

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.114445	0.000000	0.000000
3A	0.557222	-0.965138	0.000000
4B	0.557223	-0.321713	-1.457634
5A	1.106448	-0.638808	0.904592
6A	0.007994	-0.638808	0.904591
7A	0.557221	0.312481	0.904591
8B	0.557222	1.502800	-0.118718
9B	2.137297	-1.233969	-0.118713
10B	-1.022852	-1.233968	-0.118718
11B	-0.986589	0.569607	1.148560
12B	0.557220	-2.104349	1.148564
13B	2.101030	0.569608	1.148564
14B	0.557219	-0.321711	2.368524
15B	2.300517	0.684778	-0.930082
16B	0.557223	-2.334696	-0.930082
17B	-1.186071	0.684779	-0.930087

$E18/\varepsilon$ = -77.246409

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.113254	0.000000	0.000000
3A	0.556628	-0.965603	0.000000
4A	0.556626	0.334386	-0.905855
5B	0.556628	-0.332165	1.458397
6B	0.556628	1.483186	0.193427
7A	1.101903	-0.629779	-0.903794
8A	0.011349	-0.629779	-0.903793
9B	2.131310	-1.245347	0.113402
10B	2.131307	0.537649	-1.129020
11B	-1.018053	-1.245347	0.113408
12B	-1.018055	0.537649	-1.129017
13B	0.556626	-2.101455	-1.146192
14B	0.556625	-0.347541	-2.368350
15B	-1.200775	0.658978	0.945696
16B	2.314031	0.658977	0.945693
17B	0.556630	-2.343790	0.930669
18B	0.556625	1.684733	-1.876479

$E19/\varepsilon$ = -83.597114

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.093952	0.000000	0.000000
3A	0.546976	-0.947390	0.000000
4B	-1.095636	-1.264158	-0.008058
5B	2.189588	-1.264160	-0.008057
6B	0.546977	1.580929	-0.008056
7A	0.000156	-0.631502	-0.910475
8A	1.093797	-0.631503	-0.910475
9A	0.546977	0.315618	-0.910474
10B	-1.008130	0.582047	-1.100913
11B	2.102085	0.582045	-1.100912
12B	0.546976	-2.111479	-1.100915
13A	0.546976	0.316233	0.920837
14A	1.094330	-0.631813	0.920837
15A	-0.000379	-0.631813	0.920837
16B	2.127316	0.596612	1.036929
17B	-1.033364	0.596613	1.036927
18B	0.546976	-2.140618	1.036926
19B	0.546978	-0.315794	-2.368135

$E20/\varepsilon$ = -90.753192

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.096330	0.000000	0.000000
3A	0.548165	-0.949450	0.000000
4B	0.548164	1.582194	-0.000002
5B	2.192468	-1.265822	-0.000002
6B	-1.096138	-1.265823	0.000003
7A	1.096016	-0.632787	-0.907570
8A	0.000314	-0.632786	0.907570
9A	1.096019	-0.632786	0.907569
10A	0.548163	0.316122	-0.907570
11A	0.548166	0.316123	0.907570
12A	0.000311	-0.632787	-0.907569
13B	-1.012034	0.584298	1.079087
14B	-1.012037	0.584297	-1.079085
15B	0.548167	-2.118046	1.079087
16B	0.548164	-2.118047	-1.079085
17B	2.108362	0.584298	-1.079089
18B	2.108366	0.584299	1.079084
19B	0.548168	-0.316483	2.362757
20B	0.548161	-0.316486	-2.362757

$E21/\varepsilon$ = -96.404037

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.089331	0.000000	0.000000
3A	0.544665	-0.953798	0.000000
4B	0.544668	1.568893	-0.046102
5A	0.544666	0.324401	0.925481
6B	2.188512	-1.276941	0.004810
7B	-1.099185	-1.276937	0.004810
8B	-1.027177	0.571777	1.065438
9B	2.116510	0.571772	1.065437
10A	1.091105	-0.630809	0.903413
11A	-0.001776	-0.630808	0.903413
12A	-0.004605	-0.647401	-0.904668
13A	1.093934	-0.647402	-0.904668
14A	0.544665	0.295040	-0.920269
15B	0.544663	-2.130183	1.062884
16B	-1.018340	0.562511	-1.088516
17B	2.107672	0.562507	-1.088517
18B	0.544663	-2.130367	-1.078414
19B	0.544662	-0.434743	2.368615
20B	0.544663	-0.349900	-2.365756
21B	0.544669	1.600468	2.016277

$E22/\varepsilon$ =-102.128446

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.088471	0.000000	0.000000
3A	0.526247	-0.952803	0.000000
4B	-1.100219	-1.254103	0.042132
5B	0.565861	1.569413	0.042130
6A	0.539929	0.319280	-0.930696
7A	-0.018443	-0.626996	-0.930696
8B	-1.033752	0.609988	-1.021570
9B	2.187366	-1.290705	-0.014576
10B	2.119359	0.566848	-1.059383
11B	0.528461	-2.129256	-1.059382
12A	1.079868	-0.637201	-0.886131
13A	1.101743	-0.650109	0.895463
14A	0.008328	-0.635507	0.920514
15A	0.560323	0.299962	0.920513
16B	0.730889	-0.431279	-2.379671
17B	-0.990548	0.584496	1.115693
18B	0.546629	-2.127107	1.081381
19B	2.126262	0.549907	1.081381
20B	0.584578	-0.344942	2.368634
21B	-1.131475	-1.230850	-2.020261
22B	0.530394	1.585528	-2.020262

$E23/\varepsilon$ =-109.579428

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.162754	0.000000	0.000000
3A	0.581377	-0.909517	0.000000
4A	0.581377	0.454759	-0.787665
5A	0.581377	0.454759	0.787665
6B	-1.031964	0.615238	-1.065624
7B	2.194720	0.615238	-1.065624
8B	-1.031964	0.615238	1.065624
9B	2.194720	0.615238	1.065624
10B	2.194721	-1.230476	0.000000
11B	-1.031965	-1.230477	0.000000
12A	1.120326	-0.539676	-0.934746
13A	0.042429	-0.539676	-0.934746
14A	1.120326	-0.539676	0.934746
15A	0.042429	-0.539676	0.934746
16A	0.042429	1.079352	0.000000
17A	1.120326	1.079352	0.000000
18B	0.581378	-2.025358	-1.125032
19B	0.581378	0.038371	-2.316527
20B	0.581378	-2.025358	1.125032
21B	0.581378	1.986987	-1.191492
22B	0.581378	0.038371	2.316527
23B	0.581378	1.986987	1.191492

$E24/\varepsilon$ =-115.433419

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.168864	0.000000	0.000000
3A	0.589442	-0.909949	0.000000
4A	0.582339	0.447612	0.786594
5A	0.582338	0.447611	-0.786595
6B	-1.027893	0.583501	1.079633
7B	-1.027896	0.583499	-1.079631
8A	0.030551	1.087853	0.000000
9B	-1.020430	-1.245038	0.000003
10B	2.203639	0.610355	-1.058998
11B	2.203641	0.610356	1.058993
12B	2.206193	-1.233796	-0.000002
13A	1.109748	1.080371	-0.000002
14A	0.054272	-0.550172	0.930570
15A	0.054269	-0.550173	-0.930569
16A	1.131502	-0.544199	-0.931913
17A	1.131504	-0.544198	0.931913
18B	0.605191	1.954005	-1.238290
19B	0.605195	1.954008	1.238287
20B	0.595392	0.018791	-2.316060
21B	0.595396	0.018795	2.316060
22B	0.597067	-2.031980	-1.122231
23B	0.597070	-2.031979	1.122232
24B	-1.018548	2.370061	0.000000

$E25/\varepsilon$ =-121.508101

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.175604	0.000000	0.000000
3A	0.587803	-0.910182	0.000000
4A	0.587802	0.438496	-0.786185
5A	0.587802	0.438496	0.786185
6B	2.205660	0.582696	-1.071142
7B	2.205662	0.582696	1.071140
8B	-1.030057	0.582691	1.071143
9B	-1.030059	0.582692	-1.071141
10A	1.125697	1.088745	0.000000
11A	0.049904	1.088744	0.000000
12B	0.587799	1.908842	-1.307812
13B	0.587800	1.908842	1.307812
14B	-1.026504	-1.247450	0.000001
15B	2.202112	-1.247446	-0.000003
16A	0.048955	-0.554850	0.927199
17A	0.048953	-0.554850	-0.927199
18A	1.126651	-0.554848	-0.927200
19A	1.126653	-0.554849	0.927199
20B	0.587801	-0.014058	-2.317151

21B	0.587805	-0.014058	2.317150
22B	0.587803	-2.038553	-1.118988
23B	0.587806	-2.038555	1.118985
24B	-0.954232	2.383332	0.000001
25B	2.129827	2.383337	-0.000001

$E26/\varepsilon$ =-127.784324

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.157525	0.000000	0.000000
3A	0.578761	-1.002446	0.000000
4A	0.578761	-0.334149	-0.945115
5A	1.461061	-0.843547	-0.596477
6A	0.578762	0.684644	-0.596477
7A	0.578762	-0.334148	0.844315
8A	-0.303541	-0.843545	-0.596476
9A	1.525257	0.212309	-1.009090
10A	-0.367734	0.212311	-1.009089
11A	0.578759	-1.427068	-1.009089
12A	1.525257	-0.880609	0.536531
13A	-0.367735	-0.880607	0.536532
14A	0.578763	0.758770	0.536531
15B	0.578762	0.884099	-2.119940
16B	1.633793	-0.943276	-2.119940
17B	-1.662598	-0.258346	-0.182680
18B	1.633793	-2.313125	-0.182681
19B	1.765088	0.350775	1.540182
20B	-0.476277	-2.313122	-0.182680
21B	-0.607561	1.569026	-0.182681
22B	1.765089	1.569024	-0.182683
23B	-0.476277	-0.943273	-2.119939
24B	2.820121	-0.258351	-0.182682
25B	-0.607562	0.350778	1.540184
26B	0.578760	-1.703998	1.540184

$E27/\varepsilon$ =-135.837752

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.100073	0.000000	0.000000
3A	0.550037	-0.952692	0.000000
4A	-0.550037	0.317563	-0.898206
5A	-0.550036	-0.317564	0.898206
6A	0.550037	0.317564	-0.898206
7A	0.000000	0.635128	0.898206
8A	-0.550037	0.952691	0.000000
9A	-0.550037	-0.952692	0.000000
10A	0.550037	-0.317564	0.898206
11A	0.550037	0.952691	0.000000
12A	0.000000	-0.635128	-0.898206
13A	-1.100073	0.000000	0.000000
14B	-1.540941	0.889663	1.258173
15B	0.000000	1.779325	-1.258173
16B	-1.540941	-0.889663	-1.258172
17B	0.000001	-1.779326	1.258173
18B	1.540941	0.889663	1.258173
19B	1.540942	-0.889663	-1.258173
20B	1.931098	1.114919	-0.788368
21B	0.000000	-2.229839	-0.788368
22B	1.931098	-1.114920	0.788368
23B	0.000000	2.229839	0.788368
24B	-1.931097	-1.114920	0.788368
25B	0.000000	-0.000001	-2.365102
26B	0.000001	0.000000	2.365102
27B	-1.931098	1.114919	-0.788368

$E28/\varepsilon$ =-140.858567

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.100343	0.000000	0.000000
3B	1.577099	-1.492933	0.000000
4B	1.577099	1.492933	0.000000
5A	-0.555523	0.553027	0.772386
6A	-0.555523	0.553027	-0.772386
7A	-0.555523	-0.553028	0.772386
8A	-0.555523	-0.553028	-0.772386
9A	0.544966	-0.544689	0.785701
10A	0.544965	-0.544689	-0.785701
11A	0.544966	0.544689	0.785701
12A	0.544965	0.544689	-0.785701
13A	0.013684	-1.098421	0.000000
14A	0.013683	1.098421	0.000000
15A	-1.100941	-0.000001	0.000000
16B	-1.519732	1.563355	0.000000
17B	-1.519731	-1.563357	0.000000
18B	-0.090050	0.000000	-2.187161
19B	-0.090048	0.000000	2.187161
20B	1.844755	0.000000	-1.516981
21B	1.844756	0.000000	1.516980
22B	0.033112	-1.928359	1.363730
23B	0.033112	-1.928359	-1.363730
24B	0.033111	1.928359	-1.363730
25B	0.033111	1.928359	1.363730
26B	-1.974771	-0.000001	1.314023
27B	-1.974772	-0.000001	-1.314021
28A	2.222730	0.000000	-0.000001

$E29/\varepsilon$ =-146.434540

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.120537	0.000000	0.000000
3A	0.591990	-0.951394	0.000000
4B	1.528408	-0.849107	-1.296302
5B	0.092298	-1.746727	1.273001
6B	1.531824	0.844447	1.273000
7A	0.515005	-0.286111	0.897577
8A	0.540695	0.947367	0.015992
9A	-0.518710	-0.959580	0.015993
10A	0.543741	0.328984	-0.891316
11A	0.007938	-0.635470	-0.891315
12A	-0.566562	0.945979	-0.001779
13A	-1.102505	-0.018728	-0.001778
14A	-0.556447	0.309134	-0.895672
15A	-0.034176	0.648075	0.904110
16A	-0.568305	-0.313365	0.904111
17B	-1.535515	-0.913341	-1.244601
18B	-0.035752	1.786258	-1.244604
19B	-1.581817	0.878780	1.236916
20B	-0.002697	-2.227593	-0.791315
21B	1.889918	1.179147	-0.791316
22B	-1.889997	-1.169903	0.803894
23B	-0.005193	2.222777	0.803890
24B	-0.029831	0.016571	-2.362223
25B	-0.046317	0.025732	2.372851
26B	-1.949620	1.083112	-0.805433
27A	1.433542	-0.796405	0.721804
28B	2.858044	-0.367774	0.216498
29B	1.822189	-2.232331	0.216497

$E30/\varepsilon$ =-153.819680

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	2.164714	0.000000	0.000000
3B	0.039654	-2.164351	0.000000
4B	0.039654	-0.038933	2.164001
5A	0.005029	-0.784704	0.770713
6A	0.784664	-0.770420	-0.023210
7A	0.784664	0.009348	0.770713
8A	-0.773189	-0.782853	-0.001679
9A	-0.773189	-0.012403	0.782757
10A	0.768558	0.787400	-0.001680
11A	-0.001762	0.773287	0.782756
12A	-0.001763	-0.768719	-0.787242
13A	0.768558	0.015844	-0.787242
14A	-0.015548	0.785954	-0.771941
15A	-0.786107	0.771836	0.012739
16A	-0.786107	0.001148	-0.771940
17B	-0.026233	2.180918	0.013477
18B	-0.026234	0.025757	-2.180807
19B	-2.181033	-0.013722	0.013479
20B	1.356529	-1.331903	-1.410495
21B	1.356529	1.386308	1.357060
22B	-1.361225	-1.381696	1.357062
23A	1.034531	-1.015750	0.997639
24B	-1.358183	1.333529	1.400360
25B	-1.358185	-1.376145	-1.358502
26B	1.351035	1.383164	-1.358503
27B	-1.392766	1.367481	-1.343098
28B	0.532738	-2.063788	2.026992
29B	2.073201	-0.494842	2.026992
30B	2.073202	-2.035565	0.458299

$E31/\varepsilon$ =-158.954495

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.543352	0.000000	0.000000
3A	-0.747400	-0.780149	0.000000
4A	-0.747400	-0.002455	0.780146
5A	-0.747404	0.002451	-0.780140
6A	-0.747404	0.780145	0.000007
7A	0.020882	-0.807899	-0.810446
8A	0.020884	0.807898	0.810447
9A	0.315865	-1.012115	0.221644
10A	0.315865	-0.224831	1.011412
11A	0.315861	1.012115	-0.221645
12A	0.315860	0.224832	-1.011412
13B	-1.861373	1.084131	1.087562
14B	-1.861372	-1.084141	-1.087550
15B	-0.594432	-0.120525	2.327816
16B	-0.594442	2.328179	-0.113187
17B	-0.594442	0.120520	-2.327811
18B	-0.594431	-2.328183	0.113191
19B	-1.999873	1.048128	-1.044831
20B	-1.999862	-1.048139	1.044844
21A	-0.429040	1.030115	-1.026875
22A	-0.429030	-1.030119	1.026880
23A	-1.514301	-0.000004	0.000005
24B	0.972441	-1.555388	1.550496
25B	0.972424	1.555392	-1.550500
26B	1.338852	-0.502769	-1.980719
27B	1.338851	1.979124	0.509008
28B	1.338857	0.502774	1.980718
29B	1.338857	-1.979122	-0.509013
30B	-0.186526	-1.924618	-1.930689
31B	-0.186527	1.924615	1.930690

$E32/\varepsilon$ =-165.730628

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.813105	0.000000	0.000000
3A	-0.562109	-0.935866	0.000000
4A	-0.562112	0.778000	-0.520151
5A	-0.561621	-0.269047	-0.886493
6A	0.537965	0.798645	-0.523522
7A	0.537968	-0.954898	0.008671
8A	0.536777	-0.274936	-0.905902
9A	-1.186081	-0.008649	-0.028490
10A	0.512890	-0.289379	0.919410
11A	0.512889	0.751573	0.603486
12A	-0.597832	-0.294047	0.867977
13A	-0.597833	0.726864	0.558135
14B	-0.124993	-0.723918	-2.385271
15B	-1.641712	-1.404045	-1.027013
16B	-1.641716	0.596393	-1.634137
17B	-0.032390	-2.493702	-0.011346
18B	-0.032402	2.066755	-1.395424
19B	-0.205093	-0.487973	2.348765
20B	-0.205096	1.711097	1.681357
21A	-0.038986	0.509334	-1.429866

22A	-0.038983	-1.218133	-0.905588
23B	-1.586316	-1.555098	1.051189
24B	-1.586323	1.877024	0.009557
25A	-0.048574	1.535190	0.084390
26A	-0.048570	-1.229328	0.923409
27B	1.447512	0.628857	-1.890842
28B	1.447515	-1.573698	-1.222382
29B	1.429785	1.997896	0.178875
30B	1.429789	-1.561463	1.259134
31B	-1.893633	0.431475	1.421696
32B	1.498091	0.575988	1.897836

$E33/\varepsilon$ =-174.297678

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.806439	0.000000	0.000000
3A	-0.573899	-0.929597	0.000000
4A	-0.573899	-0.287262	-0.884098
5A	-0.573899	-0.287262	0.884098
6A	-0.573900	0.752058	-0.546403
7A	-0.573900	0.752058	0.546403
8A	0.526471	-0.959169	0.000000
9A	0.526471	-0.296400	-0.912223
10A	0.526471	-0.296400	0.912223
11A	0.526470	0.775983	-0.563786
12A	0.526470	0.775983	0.563785
13A	-1.180166	-0.000001	0.000000
14B	-0.109663	2.029753	1.474703
15B	-0.109663	2.029752	-1.474704
16B	-0.109662	-0.775299	2.386119
17B	-0.109662	-0.775300	-2.386119
18B	-0.109662	-2.508916	0.000000
19B	-1.645968	1.767782	0.000000
20B	-1.645966	-1.430169	1.039077
21B	-1.645966	-1.430170	-1.039077
22B	-1.645968	0.546272	-1.681262
23B	-1.645967	0.546273	1.681262
24A	-0.052949	0.473064	1.455947
25A	-0.052949	0.473064	-1.455947
26A	-0.052949	1.530872	0.000000
27A	-0.052948	-1.238504	0.899824
28A	-0.052948	-1.238504	-0.899824
29B	1.437110	-1.615414	1.173664
30B	1.437110	-1.615413	-1.173664
31B	1.437109	0.617030	-1.899031
32B	1.437109	0.617031	1.899031
33B	1.437109	1.996759	0.000000

$E34/\varepsilon$ =-182.112852

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.810719	0.000000	0.000000
3A	-0.572256	-0.932108	0.000000
4A	-0.572256	-0.288037	0.886487
5A	-0.572256	-0.288037	-0.886487
6A	-0.572256	0.754091	-0.547879
7A	-0.572256	0.754091	0.547879
8A	0.529639	0.774862	-0.562971
9A	0.529639	-0.295971	-0.910906
10A	0.529639	-0.295971	0.910906
11A	0.529639	0.774863	0.562970
12A	0.529639	-0.957783	0.000000
13A	-1.159435	0.000000	0.000000
14B	-1.630023	0.551639	-1.697771
15B	-1.630023	-1.444210	-1.049280
16B	-1.630023	1.785142	0.000000
17B	-1.630023	-1.444210	1.049280
18B	-1.630023	0.551639	1.697771
19B	-0.100720	-0.775411	2.386470
20B	-0.100718	-2.509282	0.000000
21B	-0.100719	2.030052	1.474919
22B	-0.100719	2.030052	-1.474920
23B	-0.100720	-0.775411	-2.386470
24B	-0.047348	0.472737	1.454935
25A	-0.047348	1.529809	0.000000
26A	-0.047348	0.472737	-1.454935
27A	-0.047348	-1.237641	-0.899199
28A	-0.047348	-1.237641	0.899199
29B	1.442393	-1.614632	1.173100
30B	1.442393	-1.614632	-1.173100
31B	1.442393	0.616734	-1.898115
32B	1.442393	0.616734	1.898115
33B	1.442393	1.995795	0.000000
34B	-2.735158	0.000000	0.000000

$E35/\varepsilon$ =-189.341608

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.086526	0.000000	0.000000
3A	0.540692	-0.942439	0.000000
4A	0.524337	0.325605	0.894199
5A	-0.021497	-0.616834	0.894199
6A	-0.385306	0.852444	0.552645
7A	0.524336	0.325605	-0.894199
8A	-0.021498	-0.616834	-0.894199
9A	-0.931140	-0.089995	0.552646
10A	-0.385306	0.852444	-0.552645
11A	-0.931140	-0.089995	-0.552645
12A	0.562868	0.971848	0.000000
13A	-0.562867	-0.971848	0.000000
14B	2.052297	0.639398	-1.057471
15B	2.052297	0.639398	1.057471
16B	-1.273887	-1.090230	-1.711024
17B	-2.349621	-0.467196	0.000000
18B	0.311723	1.647489	1.711024
19B	0.466687	-2.098322	-1.057471
20B	-0.764012	2.270524	0.000000
21B	-1.273886	-1.090230	1.711025
22B	0.466688	-2.098322	1.057471
23B	0.311722	1.647490	-1.711024
24B	-1.752264	1.014862	1.471205
25B	-1.752264	1.014862	-1.471204
26B	0.669306	-0.387642	-2.380458
27B	2.165919	-1.254438	0.000000
28B	0.669307	-0.387642	2.380458
29A	-1.327606	0.768912	0.000000
30A	-0.410252	0.237607	1.459110
31A	-0.410252	0.237607	-1.459109
32A	1.074057	-0.622063	-0.901779
33A	1.074057	-0.622063	0.901779
34B	-1.346032	-2.324064	0.000000
35B	1.346033	2.324065	0.000000

$E36/\varepsilon$ =-194.828824

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.087917	0.000000	0.000000
3A	0.549502	-0.938941	0.000000
4A	0.528338	0.320878	0.895243
5A	-0.010077	-0.618063	0.895243
6A	-0.393249	0.853576	-0.551748
7A	-0.935318	-0.091738	-0.551748
8A	0.513355	0.335865	-0.895085
9A	-0.030580	-0.612702	-0.895085
10A	-0.388193	0.852838	0.547256
11A	-0.932128	-0.095729	0.547256
12A	0.560555	0.971335	0.002228
13A	-0.555190	-0.974411	0.002228
14B	2.056862	0.631166	1.059433
15B	0.494178	-2.094002	1.059434
16B	2.037483	0.657187	-1.063852
17B	0.307881	1.648989	1.703249
18B	-1.267671	-1.098619	1.703249
19B	0.461930	-2.090418	-1.063853
20B	0.608431	-0.348890	2.400713
21B	2.168114	-1.243256	-0.094544
22B	-2.352258	-0.475906	0.001620
23B	-1.281386	-1.089972	-1.711613
24B	0.293492	1.656459	-1.711612
25B	-0.777380	2.270525	0.001620
26A	1.098715	-0.630033	0.912581
27B	-1.765561	1.012421	-1.466458
28B	-1.763504	1.011241	1.470548
29B	0.651942	-0.373840	-2.393801
30A	-1.334244	0.765092	0.002012
31A	-0.420646	0.241210	-1.459607
32A	-0.422651	0.242360	1.442757
33A	1.053466	-0.604087	-0.918809
34B	-1.332442	-2.329237	0.002002
35B	1.337266	2.326471	0.002002
36B	2.316720	-1.328469	1.924244

$E37/\varepsilon$ =-200.863152

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.826224	0.000000	0.000000
3A	-0.612460	-0.892002	0.000000
4A	0.543091	-0.928664	-0.000003
5A	-0.571739	-0.310856	-0.889898
6A	-0.571736	-0.310862	0.889900
7A	-0.553685	0.743844	0.557725
8A	-0.553687	0.743849	-0.557716
9A	0.517880	-0.337383	0.913238
10A	0.517878	-0.337376	-0.913240
11B	-1.698540	-1.401488	-1.038181
12B	-1.698536	-1.401496	1.038178
13A	0.549068	0.744969	0.575654
14A	0.549067	0.744974	-0.575647
15A	-1.172111	0.033019	0.000003
16A	-0.066255	-1.336133	-0.799076
17A	-0.066252	-1.336140	0.799070
18B	-0.118386	-0.897743	2.312147
19B	-0.118392	-0.897725	-2.312150
20B	-1.580504	1.801104	0.000011
21B	-1.612279	0.561162	-1.704080
22B	-1.612275	0.561149	1.704091
23B	1.467250	-1.616332	-1.150305
24B	1.467252	-1.616341	1.150293
25B	-0.049942	1.995859	-1.483907
26B	-0.049939	1.995847	1.483926
27A	-0.013455	1.500642	0.000007
28A	-0.039711	0.434380	-1.467984
29A	-0.039707	0.434369	1.467990
30A	0.433172	-2.001507	-0.000007
31B	1.445217	0.522460	-1.924642
32B	1.445221	0.522445	1.924646
33A	-0.642221	-1.958981	-0.000005
34B	1.465195	1.984001	0.000008
35B	-0.196814	-2.871227	1.203537
36B	-0.196817	-2.871215	-1.203558
37B	-2.752467	0.075879	0.000006

$E38/\varepsilon$ =-208.347221

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.074152	0.000000	0.000000
3A	0.469631	-0.966048	0.000000
4A	-0.017516	-0.626767	-0.894968
5A	0.556031	0.289783	-0.894968
6A	0.556030	0.289783	0.894968
7A	-0.017517	-0.626767	0.894967
8A	-0.919763	-0.064810	-0.562252
9A	-0.343842	0.855534	-0.562252
10A	-0.919765	-0.064810	0.562249
11A	-0.343843	0.855534	0.562250
12B	2.088919	0.591897	1.051301
13B	0.380971	-2.137473	-1.051300
14B	0.380968	-2.137473	1.051300
15B	2.088921	0.591896	-1.051299

16A	0.589637	0.969472	0.000000
17A	-0.614108	-0.954158	-0.000001
18A	1.127026	-0.705256	0.802614
19A	1.127027	-0.705257	-0.802613
20B	0.753510	-0.471522	-2.306584
21B	0.753506	-0.471520	2.306584
22B	-0.669441	2.282091	-0.000002
23B	-2.345107	-0.395684	-0.000003
24B	0.387988	1.619933	1.715125
25B	-1.287271	-1.057192	1.715124
26B	0.387991	1.619932	-1.715128
27B	-1.287267	-1.057193	-1.715128
28B	-1.692399	1.059048	1.476880
29B	-1.692396	1.059048	-1.476885
30A	-0.372649	0.233191	1.471665
31A	-0.372646	0.233190	-1.471667
32A	-1.282693	0.802668	-0.000002
33A	1.966306	-0.595979	0.000001
34A	1.395689	-1.507848	0.000001
35B	2.407984	-1.506839	1.232414
36B	2.407987	-1.506840	-1.232409
37B	-1.432923	-2.288397	-0.000003
38B	1.431604	2.289223	-0.000001

*E*39/ε =-214.480766

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2B	2.407432	0.000000	0.000000
3B	1.473740	-1.903633	0.000000
4A	0.929934	-0.456113	-0.296730
5A	0.166272	-0.081553	-1.057052
6A	0.942644	0.533719	0.125997
7A	0.155023	-1.072102	0.125996
8A	-0.566651	-0.718580	-0.596591
9A	0.221321	0.887957	-0.596591
10A	-1.058185	-0.105701	0.192148
11A	-0.564200	0.901446	0.192148
12A	-0.333453	-0.461744	0.918027
13A	0.160988	0.546334	0.918027
14B	-0.670112	-0.837311	-2.156671
15B	0.251871	1.042450	-2.156671
16A	0.748216	-0.366984	0.768446
17A	-0.767070	0.376232	-0.748507
18A	1.150209	0.330027	-0.985665
19A	0.443153	-1.111537	-0.985665
20B	1.542512	1.813600	-0.659897
21B	-0.489803	-2.329931	-0.659897
22B	-0.012864	0.006310	2.379426
23B	1.486485	1.182259	1.453100
24B	-0.024879	-1.899146	1.453100
25B	-2.124102	1.041827	0.272709
26B	-0.621312	2.214514	-0.657081
27B	-2.131431	-0.864351	-0.657082
28A	1.556665	-0.763512	-1.117439
29B	-1.850296	-0.736596	1.487183
30B	-0.550232	1.914004	1.487183
31A	0.380920	1.451060	0.328705
32A	-0.914215	-1.189491	0.328705
33A	-0.909376	0.446030	1.127208
34A	0.834628	-0.409367	-1.830944
35B	2.231261	0.313381	-2.115212
36B	1.118094	-1.956170	-2.115212
37B	1.802247	-0.883964	1.803079
38B	-1.812271	0.888881	-1.797123
39B	3.006139	-1.474448	-1.353025

*E*40/ε =-220.807300

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2B	2.404690	0.000000	0.000000
3B	-0.682101	-2.305921	0.000000
4B	0.242964	-1.614871	1.765132
5B	1.479624	-0.691051	-1.765133
6A	0.928930	-0.444735	-0.312717
7A	0.162973	-1.016927	0.312717
8A	0.157080	-0.272663	-1.043983
9A	-0.567345	-0.813829	-0.452462
10A	0.941331	0.313196	0.452461
11A	0.216907	-0.227970	1.043982
12A	-1.057663	0.144432	-0.171304
13A	-0.329601	0.688315	-0.765795
14A	-0.566552	0.511306	0.765794
15A	0.161510	1.055190	0.171303
16A	-0.769515	-0.556585	0.621188
17A	0.752000	0.580030	-0.621188
18A	0.438338	-1.321793	-0.672447
19A	1.143165	-0.795267	0.672446
20B	-0.490833	-1.455916	-1.933092
21B	1.535343	0.057696	1.933091
22B	1.485911	1.785561	0.571593
23B	-2.133707	-0.918399	-0.571596
24B	-0.629390	0.205370	2.298820
25B	-0.018407	0.661791	-2.298822
26B	-0.010200	2.220525	-0.863993
27B	-2.126429	0.639642	0.863990
28A	0.831645	-1.862524	0.293332
29A	1.550123	-1.325800	-0.293334
30B	2.245157	-1.807966	1.095545
31B	1.096856	-2.665779	-1.095547
32B	-0.551942	2.088315	1.234588
33B	-1.845981	1.121630	-1.234591
34A	0.376552	0.839430	1.229128
35A	-0.911763	-0.122979	-1.229129
36A	-0.908451	1.216084	-0.000001
37B	1.804948	1.360313	-1.478497
38B	-1.816424	-1.344954	1.478494
39B	2.988624	-1.823609	-0.852325
40B	0.900970	-3.383146	0.852324

*E*41/ε =-226.951993

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.067006	0.000000	0.000000
3A	-0.902651	-0.568966	0.000000
4A	0.462818	-0.174529	-0.945432
5A	-0.298462	-0.394437	0.945432
6A	0.551667	-0.836210	0.447892
7A	-0.020794	-1.001574	-0.447892
8A	-0.372793	0.672881	0.761949
9A	0.530669	0.933860	0.136403
10A	-0.946895	0.507043	-0.136403
11A	-0.043433	0.768022	-0.761948
12B	-0.646669	0.370252	2.275996
13B	0.349630	0.658049	-2.275996
14B	-2.357727	-0.124013	-0.401457
15B	2.060688	1.152314	0.401457
16B	0.382561	-1.416753	-1.909905
17B	0.431831	-1.402521	1.909904
18B	-1.275574	-1.895732	-0.761833
19B	2.089966	-0.923543	0.761833
20B	0.679877	-2.353609	0.000000
21A	-0.617025	-0.161502	-0.958537
22A	0.608102	0.192395	0.958537
23A	1.115318	-0.924305	-0.542127
24A	-0.450648	-1.376659	0.542127
25A	1.101109	0.675445	-0.828365
26A	-1.291672	-0.015747	0.828365
27B	-1.755309	1.484749	0.847662
28B	0.693212	2.192043	-0.847661
29B	0.344814	1.952757	1.312702
30B	-1.332980	1.468101	-1.312701
31A	-0.423339	1.465525	0.000000
32A	1.957480	-0.094150	-0.588504
33A	-1.605757	-1.123447	0.588504
34A	-1.034190	-0.958340	1.482890
35A	1.385913	-0.259256	-1.482890
36B	2.372281	0.978068	-1.696587
37B	-2.528410	-0.437571	1.696587
38B	2.395531	-1.478548	-1.257948
39B	-1.238123	-2.528185	1.257948
40B	1.448897	0.409340	2.263387
41B	-1.443991	-0.426316	-2.263387

*E*42/ε =-233.679219

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.121913	0.000000	0.000000
3A	0.586700	-0.916266	0.000000
4A	0.586699	0.781839	-0.477778
5A	0.751320	0.822430	0.621834
6A	0.751320	-0.377520	0.959451
7A	0.709937	-0.272895	-0.969919
8B	0.682761	2.297003	-0.115002
9B	0.682761	-2.019971	1.099620
10B	2.848720	-0.018287	-0.064993
11B	0.696312	-2.041388	-1.081226
12B	0.696312	1.178099	-1.987058
13A	-0.209649	0.276431	-1.048260
14A	-0.209648	-0.782479	-0.750325
15B	-1.569161	0.335707	1.193157
16A	-0.991193	-0.580175	-0.022222
17A	-0.991193	0.483469	-0.321488
18A	-0.254768	1.027827	0.271361
19A	-0.254768	-0.735533	0.767500
20B	-0.180280	-0.656004	-2.331557
21B	-0.096842	1.713376	1.716521
22B	-0.096843	-0.566939	2.358109
23A	-0.061812	0.297950	1.058966
24A	1.608698	-0.838612	0.518435
25A	1.608698	0.985910	0.005088
26A	1.560407	0.402879	-0.905331
27A	1.560406	-0.815847	-0.562431
28A	1.651174	0.246917	0.877585
29B	-1.417819	1.018590	-1.862283
30B	-1.417815	-1.840222	-1.057932
31B	1.991415	-0.685303	2.046559
32B	1.991416	1.651919	1.388959
33B	1.919514	-0.578809	-2.057190
34B	-1.481693	-1.704188	1.064941
35B	-1.481691	2.009470	0.020070
36A	0.895715	0.465010	1.652725
37A	-0.336288	-1.520090	0.020463
38A	-0.336288	1.307745	-0.775175
39A	-1.119405	-0.306656	-1.089905
40B	-2.537271	-0.139946	-0.497374
41B	2.467779	1.737095	-1.077912
42B	2.467779	-2.044309	-0.013980

*E*43/ε =-240.538283

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.131377	0.000000	0.000000
3A	0.580176	-0.912895	0.000000
4A	0.580174	0.789469	0.458384
5A	0.737823	0.789551	-0.648207
6A	0.737825	-0.357323	-0.957018
7A	0.728109	-0.260951	0.969127
8B	2.829952	-0.019708	0.073206
9B	0.645431	-2.005917	-1.113735
10B	0.645424	2.293942	0.044059
11B	0.683031	-2.047374	1.083227
12B	0.683025	1.226651	1.964803
13A	-0.188254	0.283330	1.069915
14A	-0.188253	-0.782253	0.782993
15A	-0.259429	-0.709083	-0.763414
16A	-0.259432	0.996538	-0.304153
17A	-0.956699	0.480751	0.369969
18A	-0.956698	-0.601526	0.078552
19B	-0.115247	-0.565753	-2.384995
20B	-0.115251	1.686816	-1.778462

21B	-0.174875	-0.632960	2.350706
22A	-0.081353	0.302926	-1.125023
23A	-1.008771	0.174400	-0.647702
24B	-2.421988	-0.047651	0.176950
25B	-1.556626	-1.464835	-1.104944
26B	-1.556632	1.821595	-0.220030
27A	1.593105	0.993973	-0.038649
28A	1.593109	-0.840176	-0.532518
29A	1.651037	0.240356	-0.892637
30A	1.552147	-0.837330	0.550764
31A	1.552144	0.447572	0.896742
32B	-1.453384	1.050632	1.806604
33B	-1.453379	-1.815724	1.034800
34B	1.914991	-0.549079	2.039198
35B	1.975247	-0.701801	-2.060417
36B	1.975243	1.641500	-1.429452
37A	-0.348959	1.318403	0.738000
38A	-0.348955	-1.510720	-0.023778
39A	0.897631	0.452980	-1.682293
40A	-1.123631	-0.300386	1.115574
41B	-1.856944	0.506562	-1.881306
42B	2.445228	1.788033	1.013708
43B	2.445235	-2.055284	-0.021159

$E44/\varepsilon$ =-248.636081

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.106139	0.000000	0.000000
3A	0.553070	-0.924395	0.000000
4A	0.553070	0.704833	0.598094
5B	0.553072	-2.124273	0.946608
6B	0.553072	1.007253	2.096199
7B	-0.918289	0.530072	-1.443938
8B	2.024425	0.530075	-1.443942
9A	0.553071	-0.355266	0.967757
10A	0.553069	0.325121	-0.885642
11A	-0.343503	0.222225	1.019991
12A	-0.343503	-0.829387	0.633942
13A	1.449645	0.222226	1.019990
14A	1.449646	-0.829387	0.633940
15A	1.118958	1.070558	-0.250896
16A	-0.012820	1.070558	-0.250895
17A	1.118958	-0.653948	-0.883967
18A	-0.012820	-0.653949	-0.883965
19A	-0.932796	0.538796	0.159891
20A	2.038936	0.538798	0.159887
21A	2.038936	-0.514271	-0.226697
22A	-0.932797	-0.514273	-0.226693
23B	-0.507616	-0.802824	2.186925
24B	1.613763	-0.802824	2.186921
25B	0.553069	-2.226511	-1.204099
26B	0.553069	2.476737	0.522472
27B	2.717377	0.968122	1.656856
28B	2.717379	-1.810176	0.636935
29B	-1.611234	0.968120	1.656862
30B	-1.611235	-1.810179	0.636943
31B	0.553068	-0.534256	-2.363413
32B	0.553067	1.936512	-1.456389
33B	-2.437792	0.054514	-0.148495
34B	3.543931	0.054518	-0.148503
35B	-1.365164	2.039319	-0.166887
36B	2.471300	-1.446963	-1.446715
37B	2.471302	2.039322	-0.166891
38B	-1.365165	-1.446966	-1.446708
39A	1.470357	1.267108	0.772843
40A	-0.364216	1.267107	0.772846
41A	1.470357	-1.466184	-0.230554
42A	-0.364217	-1.466185	-0.230551
43A	2.373466	-0.299269	0.815221
44A	-1.267324	-0.299271	0.815227

$E45/\varepsilon$ =-255.883412

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.095783	0.000000	0.000000
3A	0.537665	-0.924597	0.000000
4A	0.537663	0.732908	0.563671
5B	2.037670	0.492396	-1.447911
6A	0.513706	-0.325872	0.958246
7B	0.494926	-2.108463	0.956830
8B	0.494922	1.088014	2.043861
9A	0.554227	0.301635	-0.886976
10A	-0.013945	-0.645489	-0.879416
11A	-0.013947	1.047791	-0.303580
12A	-0.926961	-0.495389	-0.257229
13A	-0.926963	0.549498	0.098108
14A	-0.376907	-0.814346	0.618444
15A	-0.376909	0.268485	0.986684
16A	1.412113	0.252461	1.017337
17A	1.412114	-0.820327	0.652512
18A	1.117594	1.065107	-0.298653
19A	1.117596	-0.662217	-0.886067
20A	-0.555816	0.313256	-0.921152
21A	2.023640	0.538048	0.160257
22A	2.023642	-0.524196	-0.200982
23B	1.519989	-0.750872	2.207986
24B	0.379328	1.679863	-1.658940
25B	0.379332	-0.320240	-2.339117
26B	0.549587	2.469619	0.278973
27B	0.549593	-2.127689	-1.284440
28B	-0.595750	-0.733341	2.156424
29B	-1.331768	1.943520	-0.452702
30B	-1.331764	-1.264608	-1.543695
31B	-2.374096	0.119720	-0.352058
32B	2.665223	-1.805841	0.721192
33B	2.665219	0.991790	1.672588
34B	-1.681425	1.055086	1.501340
35B	-1.681420	-1.751627	0.546857
36B	3.529631	0.033463	-0.098389
37A	1.451678	-1.473720	-0.207732
38A	1.451675	1.294831	0.733774
39A	-0.384526	1.311531	0.690854
40A	-0.384522	-1.460798	-0.251936
41A	-1.301564	-0.256985	0.755671
42A	2.331643	-0.287080	0.844182
43B	2.524357	2.005326	-0.182489
44B	2.524360	-1.478323	-1.367181
45B	-1.437441	0.731508	-2.151052

$E46/\varepsilon$ =-263.282585

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.098640	0.000000	0.000000
3A	0.550909	-0.950532	0.000000
4A	0.544366	-0.313684	0.865023
5A	0.552416	0.949031	0.018733
6A	-0.544083	-0.953834	0.018732
7A	0.000776	-0.634276	-0.896435
8A	0.549156	0.317384	-0.896435
9A	1.097047	-0.632159	-0.900113
10A	1.647606	-0.949411	0.005470
11B	0.867541	-0.499910	2.319711
12A	1.100737	0.627811	0.923655
13A	0.008786	-1.267161	0.923655
14A	0.005358	0.633009	0.919511
15A	-0.544986	-0.322058	0.919511
16B	-0.499847	0.288030	-2.092073
17B	0.550112	-1.527286	-2.095797
18B	1.597241	0.289904	-2.095797
19B	-0.980214	-2.430577	0.426240
20B	1.611379	2.066875	0.426241
21B	-2.043811	-0.602539	0.428254
22B	-0.503555	2.070421	0.428255
23A	1.106221	-1.265318	0.909890
24A	1.649449	-0.322600	0.909891
25A	-0.911609	-0.110495	-0.590284
26A	-0.361526	0.844120	-0.590284
27A	1.461968	0.843669	-0.594554
28A	0.003168	-1.687934	-0.594554
29A	1.102500	-1.686342	-0.595362
30A	2.011848	-0.108259	-0.595362
31A	-0.907060	0.522680	0.310333
32A	2.008035	0.523197	0.305123
33A	0.554260	-1.999685	0.305123
34B	-1.368964	-1.428208	-1.337707
35B	0.549204	1.900582	-1.337706
36B	2.472060	-1.424490	-1.342418
37B	3.139957	-0.611104	0.439290
38B	2.103244	-2.410217	0.439290
39B	-1.322779	0.762231	1.822840
40B	0.579904	-2.504586	1.809829
41B	2.457728	0.754191	1.809829
42B	-1.045989	-1.253533	2.131968
43B	0.560032	1.533556	2.131969
44B	-1.919231	1.105929	-0.781073
45B	3.025171	1.097889	-0.783232
46B	0.567085	-3.167877	-0.783233

$E47/\varepsilon$ =-271.372063

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.102506	0.000000	0.000000
3A	0.551253	-0.954799	0.000000
4B	0.551250	-0.318269	-2.330576
5A	0.551253	-0.318267	-0.850810
6A	-0.545444	-0.951445	-0.020429
7A	1.647950	-0.951445	-0.020430
8A	0.551253	0.948090	-0.020430
9A	0.002969	-0.634819	0.896663
10A	1.099538	-0.634819	0.896663
11A	0.551253	0.314839	0.896663
12A	1.103762	-1.264169	-0.929493
13A	0.008332	0.633172	-0.929494
14A	-0.544178	-0.323804	-0.929493
15A	-0.001258	-1.264169	-0.929493
16A	1.646682	-0.323804	-0.929494
17A	1.094172	0.633172	-0.929494
18B	1.596471	0.285191	2.098981
19B	0.551254	-1.525179	2.098983
20B	-0.493963	0.285190	2.098983
21B	1.622533	2.068271	-0.403315
22B	-0.520029	2.068271	-0.403314
23B	-0.979910	-2.439291	-0.403312
24B	3.153695	-0.583779	-0.403315
25B	2.082414	-2.439293	-0.403313
26B	-2.051190	-0.583779	-0.403312
27A	-0.903213	0.521469	-0.311119
28A	2.005718	0.521470	-0.311121
29A	0.551252	-1.997739	-0.311119
30A	-0.907963	-0.109538	0.595706
31A	-0.359120	0.841088	0.595705
32A	1.461626	0.841088	0.595704
33A	0.002409	-1.686350	0.595706
34A	1.100097	-1.686350	0.595705
35A	2.010470	-0.109537	0.595704
36B	2.469011	-1.425484	1.347064
37B	-1.366504	-1.425484	1.347066
38B	0.551253	1.896170	1.347064
39B	2.395973	0.746783	-1.842095
40B	0.551251	-2.448369	-1.842092
41B	-1.293471	0.746783	-1.842092
42B	0.551252	-3.165093	0.805123
43B	-1.914171	1.105147	0.805124
44B	3.016677	1.105148	0.805120
45B	0.551251	1.682090	-2.094389
46B	2.283612	-1.318447	-2.094388
47B	-1.181111	-1.318447	-2.094387

$E48/\varepsilon$ =-278.085201

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.089206	0.000000	0.000000
3A	0.544602	-0.946432	0.000000
4A	0.544603	-0.313460	-0.893015
5A	0.544603	0.316231	0.902200
6A	0.544603	0.956016	-0.000426
7A	1.092402	-0.632769	0.901784
8A	-0.003197	0.641313	-0.895727
9A	1.092403	0.641313	-0.895726
10A	-0.003198	-0.632769	0.901783
11A	1.644088	-0.950336	-0.001148
12A	-0.554883	-0.950335	-0.001149
13A	-0.554882	-0.315836	-0.896318
14A	1.644089	-0.315837	-0.896317
15A	-0.006898	-1.266270	-0.897536
16A	1.096104	-1.266270	-0.897536
17B	1.590508	2.078473	-0.421744
18B	-0.501301	2.078473	-0.421744
19B	-0.501302	0.290451	2.100847
20B	1.590506	0.290450	2.100848
21B	3.137627	-0.603753	-0.427940
22B	-2.048422	-0.603751	-0.427942
23A	-0.365254	0.846131	0.599741
24A	1.454459	0.846131	0.599742
25A	-0.913835	0.529484	-0.296227
26A	-0.913836	-0.104142	0.597711
27A	2.003041	-0.104143	0.597712
28A	2.003041	0.529484	-0.296226
29B	0.544601	-1.538850	2.091803
30B	0.544604	1.464073	-2.144804
31B	0.544603	1.903315	1.349078
32B	2.083508	-2.421809	-0.418512
33B	-0.994304	-2.421807	-0.418513
34B	2.083509	-1.196999	-2.146508
35B	-0.994303	-1.196998	-2.146510
36B	-1.386631	-1.408961	1.347734
37B	2.475834	-1.408962	1.347736
38B	2.475836	0.805018	-1.775810
39B	-1.386628	0.805020	-1.775811
40A	-0.004645	0.006492	-1.794406
41A	1.093851	0.006491	-1.794405
42A	-0.004646	-1.690980	0.600435
43A	1.093850	-1.690980	0.600435
44A	0.544602	-2.006677	-0.295099
45A	0.544603	-0.943058	-1.795682
46B	0.544603	-2.533080	-1.795455
47B	3.013534	1.109481	0.786407
48B	-1.924329	1.109482	0.786405

*E*49/ε =-286.985560

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.090020	0.000000	0.000000
3A	0.545010	-0.943985	0.000000
4A	0.545010	-0.314662	-0.893188
5A	-0.002377	-0.630695	0.902382
6A	0.545010	0.317406	0.902381
7A	1.092397	-0.630695	0.902382
8A	0.545010	0.955235	-0.001274
9A	-0.554753	-0.949610	-0.001274
10A	1.644773	-0.949610	-0.001274
11A	1.093028	0.639394	-0.896579
12A	1.645255	-0.317092	-0.896579
13A	-0.555236	-0.317092	-0.896579
14A	-0.007217	-1.266288	-0.896579
15A	1.097237	-1.266288	-0.896579
16A	-0.003009	0.639394	-0.896579
17B	-0.503624	0.290768	2.099909
18B	0.545010	-1.525519	2.099910
19B	1.593644	0.290768	2.099909
20B	3.138769	-0.604507	-0.424082
21B	-1.002882	-2.416001	-0.424080
22B	-0.500857	2.076522	-0.424081
23B	2.092903	-2.416001	-0.424080
24B	1.590876	2.076522	-0.424081
25B	-2.048749	-0.604508	-0.424081
26A	-0.365528	0.845162	0.599240
27A	1.455548	0.845163	0.599240
28A	-0.004158	-1.683123	0.599241
29A	2.004716	-0.106025	0.599240
30A	-0.914696	-0.106025	0.599240
31A	1.094178	-1.683123	0.599241
32A	0.545010	-1.999281	-0.295990
33A	2.003933	0.527648	-0.295991
34A	-0.913913	0.527647	-0.295991
35B	2.465114	-1.423233	1.347617
36B	-1.375094	-1.423234	1.347617
37B	0.545010	1.902483	1.347617
38B	-0.991553	-1.201798	-2.146762
39B	0.545009	1.459609	-2.146762
40B	2.081573	-1.201797	-2.146763
41B	-1.386380	0.800426	-1.776329
42B	0.545010	-2.544839	-1.776328
43B	2.476399	0.800427	-1.776329
44A	1.094005	0.002301	-1.794708
45A	0.545010	-0.948588	-1.794708
46A	-0.003986	0.002301	-1.794708
47B	-1.923987	1.110812	0.785082
48B	0.545010	-3.165613	0.785083
49B	3.014007	1.110813	0.785081

*E*50/ε =-295.883575

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.090767	0.000000	0.000000
3A	0.545383	-0.944632	0.000000
4A	0.545382	-0.314876	0.890607
5A	-0.002210	-0.631031	-0.901601
6A	0.545384	0.317430	-0.901600
7A	1.092976	0.639694	0.895475
8A	-0.007503	-1.266392	0.895475
9A	0.545383	0.955847	0.001256
10A	-0.555096	-0.950239	0.001256
11A	1.645863	-0.950239	0.001259
12A	1.098267	-1.266392	0.895476
13A	1.645861	-0.317931	0.895476
14A	-0.555097	-0.317931	0.895474
15A	-0.002213	0.639694	0.895474
16A	1.092979	-0.631031	-0.901600
17B	1.594043	2.075363	0.425558
18B	3.139721	-0.601829	0.425561
19B	2.091060	-2.418163	0.425561
20B	-1.000295	-2.418163	0.425557
21B	0.545380	1.469919	2.138013
22B	-1.000297	-1.207273	2.138013
23B	-0.503279	2.075362	0.425555
24B	-2.048956	-0.601829	0.425555
25B	2.091057	-1.207272	2.138017
26B	1.594047	0.290568	-2.098522
27B	0.545386	-1.525767	-2.098522
28B	-0.503275	0.290567	-2.098524
29A	-0.365843	0.845076	-0.597561
30A	-0.914779	-0.105708	-0.597561
31A	2.005545	0.528149	0.298850
32A	0.545383	-2.000928	0.298850
33A	-0.914780	0.528148	0.298847
34A	-0.003555	0.002053	1.786876
35A	1.456611	0.845077	-0.597559
36A	1.094317	0.002053	1.786877
37A	0.545381	-0.948732	1.786877
38A	1.094320	-1.684000	-0.597558
39A	-0.003552	-1.684000	-0.597559
40A	2.005547	-0.105708	-0.597558
41B	0.545384	1.902454	-1.345240
42B	2.465650	-1.423543	-1.345236
43B	2.465646	0.793791	1.790544
44B	-1.374881	-1.423544	-1.345240
45B	0.545381	-2.532208	1.790543
46B	-1.374885	0.793790	1.790539
47B	0.545383	-3.166090	-0.785402
48B	-1.923838	1.110729	-0.785408
49B	3.014607	1.110729	-0.785401
50B	0.545378	-0.314874	3.246820

s = 2.0

*E*5/ε =-9.267451

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.123849	0.000000	0.000000
3A	0.561925	-0.973282	0.000000
4B	0.561923	-0.324428	1.546474
5B	0.561923	-0.324428	-1.546474

*E*6/ε = -13.473670

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.125643	0.000000	0.000000
3B	0.562820	-1.581510	0.000000
4B	0.562820	0.000000	1.581510
5B	0.562820	1.581510	0.000000
6B	0.562820	0.000000	-1.581510

*E*7/ε = -18.073138

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.626551	0.000000	0.000000
3B	0.000000	-1.626551	0.000000
4B	0.000000	0.000000	-1.626551
5B	0.000000	0.000000	1.626551
6B	0.000000	1.626551	0.000000
7B	-1.626551	0.000000	0.000000

*E*8/ε = -21.814932

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.621114	0.000000	0.000000
3B	-1.271283	-1.002600	0.000000
4A	0.328350	-0.935257	-0.549449
5A	0.328349	-0.935253	0.549456
6B	-0.139311	0.199148	-1.640945
7B	-0.139321	0.199157	1.640942
8B	0.102540	1.665018	-0.000004

*E*9/ε = -26.901093

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.697957	0.000000	0.000000
3B	0.195785	-1.686632	0.000000
4B	0.224619	1.280199	1.098358
5B	-1.245760	-0.370736	1.098359
6B	-1.245760	-0.370736	-1.098359
7B	0.224619	1.280199	-1.098358
8A	0.411519	-0.366513	0.981291
9A	0.411519	-0.366513	-0.981291

*E*10/ε = -32.187970

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.709625	0.000000	0.000000
3B	0.227591	-1.694408	0.000000
4B	0.256712	1.270807	1.114436
5B	0.256712	1.270807	-1.114436
6B	-1.225321	-0.423600	-1.114437
7B	-1.225321	-0.423600	1.114437
8A	0.423317	-0.370258	-0.974098
9A	0.423317	-0.370258	0.974098

10A	-0.846633	0.740518	0.000000

$E11/\varepsilon$ = -37.111833

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.644798	0.000000	0.000000
3B	0.027246	-1.644572	0.000000
4A	0.356382	-0.350526	0.960456
5A	-0.434601	0.427461	0.927577
6B	0.059200	1.622244	-0.102161
7B	-1.621040	-0.086062	-0.102163
8B	-0.872109	-0.822690	1.916220
9B	0.808132	0.885617	1.916221
10B	1.345872	-1.323760	1.817044
11B	0.067497	-0.066383	-1.628205

$E12/\varepsilon$ = -42.523248

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	1.636574	0.000000	0.000000
3B	-1.635631	-0.055533	0.000000
4B	0.049138	-0.027010	-1.635614
5B	-0.875410	1.931755	0.817724
6B	-0.048194	-0.028524	1.635615
7B	0.809359	1.960278	-0.817889
8A	0.364069	0.951709	0.391607
9A	-0.396152	0.938774	-0.391687
10B	0.027518	-1.621451	0.000068
11B	1.328363	1.779075	1.399308
12B	-1.387962	1.732860	-1.399457

$E13/\varepsilon$ = -48.110134

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.102098	0.000000	0.000000
3A	0.551049	-0.954445	0.000000
4A	1.103931	-0.637354	-0.912164
5A	-0.001831	-0.637354	-0.912165
6A	0.551050	0.320264	-0.912164
7B	0.551049	-0.318148	1.525982
8B	-1.057350	-1.246759	0.223601
9B	0.551048	1.539071	0.223602
10B	2.159448	-1.246758	0.223603
11B	0.551050	-2.197250	-1.068597
12B	-1.076300	0.621403	-1.068597
13B	2.178400	0.621403	-1.068594

$E14/\varepsilon$ = -55.233067

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.564641	0.000000	0.000000
3A	0.782320	-0.782321	0.000000
4A	0.782320	0.782321	0.000000
5A	0.782320	0.000000	0.782321
6A	0.782320	0.000000	-0.782321
7B	-0.357018	1.139338	1.139338
8B	-0.357018	-1.139338	1.139338
9B	1.921658	1.139338	-1.139338
10B	-0.357018	1.139338	-1.139338
11B	-0.357018	-1.139338	-1.139338
12B	1.921658	-1.139338	-1.139338
13B	1.921658	1.139338	1.139338
14B	1.921658	-1.139338	1.139338

$E15/\varepsilon$ = -60.758081

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.115668	0.000000	0.000000
3A	0.029132	-1.115288	0.000000
4A	0.572400	-0.557644	-0.778529
5A	0.572400	-0.557644	0.778529
6A	1.134497	-1.105251	0.000000
7B	0.601631	1.038033	1.163348
8B	-1.021969	-0.628531	1.163348
9B	-1.021969	-0.628531	-1.163348
10B	0.601631	1.038033	-1.163348
11B	2.191190	-0.552243	-1.133482
12B	2.191190	-0.552243	1.133482
13B	0.609271	-2.176023	-1.133483
14B	0.609271	-2.176023	1.133483
15B	-1.249379	1.217171	0.000000

$E16/\varepsilon$ = -66.356133

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.122127	0.000000	0.000000
3A	0.561064	-0.958735	0.000000
4A	0.561063	0.283106	0.915982
5A	1.114826	-0.664241	0.900544
6A	0.007300	-0.664242	0.900543
7B	0.561062	1.568986	-0.078552
8B	0.561065	-0.388259	-1.522216
9B	-1.041720	0.558293	1.191037
10B	-1.041717	-1.302788	-0.181697
11B	2.163847	-1.302784	-0.181694
12B	2.163844	0.558296	1.191039
13B	0.561062	-0.394383	2.434069
14B	0.561064	-2.209069	1.095556
15B	2.364129	0.728800	-0.988064
16B	-1.242002	0.728795	-0.988067

$E17/\varepsilon$ = -71.965936

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.120768	0.000000	0.000000
3A	0.560384	-0.970615	0.000000
4B	0.560384	-0.323540	1.518697
5A	1.109113	-0.640348	-0.906554
6A	0.011651	-0.640348	-0.906553
7A	0.560383	0.310082	-0.906554
8B	-1.077732	-1.269304	0.121887
9B	0.560384	1.567996	0.121881
10B	2.198500	-1.269305	0.121879
11B	2.154935	0.597077	-1.186666
12B	-1.034171	0.597077	-1.186662
13B	0.560380	-2.164770	-1.186664
14B	0.560380	-0.323538	-2.440696
15B	2.390640	0.733160	0.986977
16B	0.560386	-2.436939	0.986978
17B	-1.269872	0.733163	0.986981

$E18/\varepsilon$ = -77.549442

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.117155	0.000000	0.000000
3A	0.558578	-0.971404	0.000000
4A	0.558578	0.337383	0.910933
5B	0.558578	1.544171	-0.208366
6B	0.558578	-0.340919	-1.520413
7A	0.013929	-0.629846	0.904934
8A	1.103227	-0.629846	0.904934
9B	2.187557	0.561667	1.160932
10B	-1.070400	-1.283740	-0.123494
11B	2.187557	-1.283738	-0.123495
12B	-1.070401	0.561667	1.160933
13B	0.558579	-2.164395	1.178051
14B	0.558579	-0.352988	2.438813
15B	2.405585	0.703485	-1.010735
16B	-1.288429	0.703484	-1.010733
17B	0.558579	-2.455498	-0.993817
18B	0.558579	1.784781	1.957471

$E19/\varepsilon$ = -84.509377

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.101571	0.000000	0.000000
3A	0.550786	-0.953989	0.000000
4B	0.550784	1.654522	0.008902
5B	2.259038	-1.304254	0.008899
6B	-1.157464	-1.304258	0.008904
7A	0.003109	-0.634199	0.908158
8A	1.098466	-0.634199	0.908157
9A	0.550787	0.314408	0.908158
10B	-1.055684	0.609498	1.139117
11B	0.550789	-2.172990	1.139114
12B	2.157257	0.609501	1.139113
13A	1.098758	-0.634368	-0.915245
14A	0.550784	0.314749	-0.915245
15A	0.002811	-0.634369	-0.915244
16B	0.550790	-0.317998	2.431932
17B	0.550786	-2.186641	-1.104902
18B	-1.067511	0.616325	-1.104899
19B	2.169077	0.616328	-1.104903

$E20/\varepsilon$ = -91.988950

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.103196	0.000000	0.000000
3A	0.551599	-0.955394	0.000000
4B	-1.157130	-1.304999	0.000000
5B	2.260328	-1.304998	0.000000
6B	0.551599	1.654606	0.000000
7A	1.100080	-0.635130	0.905562
8A	0.551599	0.314868	-0.905562
9A	0.551599	0.314868	0.905562
10A	1.100080	-0.635130	-0.905562
11A	0.003118	-0.635130	0.905563
12A	0.003118	-0.635130	-0.905563
13B	2.160468	0.610417	1.125918
14B	-1.057270	0.610418	1.125918
15B	-1.057270	0.610418	-1.125918
16B	2.160468	0.610417	-1.125918
17B	0.551600	-2.176225	-1.125919
18B	0.551600	-2.176225	1.125919
19B	0.551600	-0.318462	-2.427152
20B	0.551600	-0.318462	2.427152

$E21/\varepsilon$ = -97.424715

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.095033	0.000000	0.000000
3A	0.547516	-0.960634	0.000000
4B	0.547518	1.641156	-0.055345
5A	0.547517	0.327565	0.923595
6B	2.255127	-1.318036	0.004490
7B	-1.160096	-1.318034	0.004492
8B	-1.071832	0.596361	1.112496
9B	2.166867	0.596359	1.112495
10A	1.093797	-0.632884	0.901789
11A	0.001236	-0.632884	0.901789
12A	-0.002342	-0.650473	-0.902842
13A	1.097373	-0.650473	-0.902843
14A	0.547516	0.292643	-0.918712
15B	-1.066298	0.584633	-1.136644
16B	2.161330	0.584630	-1.136646
17B	0.547516	-2.193552	1.103304
18B	0.547514	-2.188511	-1.129710
19B	0.547516	-0.425037	2.431398
20B	0.547514	-0.346643	-2.431049
21B	0.547519	1.719147	2.108114

$E22/\varepsilon$ = -102.921119

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.094493	0.000000	0.000000
3A	0.527952	-0.958740	0.000000

4B	-1.163485	-1.293670	-0.055284
5B	0.571979	1.643203	-0.055286
6B	-1.073777	0.634518	1.072306
7A	0.543579	0.322783	0.927929
8A	-0.020540	-0.631859	0.927929
9B	2.252123	-1.330831	0.016947
10B	2.175936	0.595850	1.094695
11B	0.527664	-2.193469	1.094697
12A	1.080130	-0.638274	0.887977
13A	1.105085	-0.653021	-0.894175
14A	0.563499	0.297819	-0.919488
15A	0.010935	-0.637268	-0.919488
16B	0.713185	-0.421437	2.441152
17B	-1.036065	0.612233	-1.165363
18B	0.552408	-2.184504	-1.135777
19B	2.180018	0.569850	-1.135778
20B	0.581379	-0.343552	-2.435477
21B	-1.231999	-1.299281	2.107125
22B	0.543845	1.705927	2.107123

$E23/\varepsilon$ =-110.903815

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.157324	0.000000	0.000000
3A	0.578662	-0.918600	0.000000
4A	0.578662	0.459300	-0.795532
5A	0.578661	0.459300	0.795531
6B	2.250354	0.637357	1.103931
7B	2.250356	-1.274708	0.000002
8B	2.250354	0.637356	-1.103931
9B	-1.093032	0.637354	1.103930
10B	-1.093031	0.637352	-1.103932
11B	-1.093030	-1.274710	0.000000
12A	0.038964	-0.538019	-0.931874
13A	1.118361	-0.538017	0.931875
14A	1.118359	1.076036	0.000000
15A	1.118362	-0.538019	-0.931874
16A	0.038964	-0.538018	0.931874
17A	0.038962	1.076036	-0.000001
18B	0.578664	-2.068637	-1.194791
19B	0.578663	-0.000408	-2.388888
20B	0.578661	-0.000403	2.388887
21B	0.578659	2.069040	1.194092
22B	0.578663	-2.068635	1.194793
23B	0.578660	2.069039	-1.194094

$E24/\varepsilon$ =-116.521863

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.163942	0.000000	0.000000
3A	0.589907	-0.920286	0.000000
4A	0.577886	0.449793	0.794824
5A	0.577886	0.449793	-0.794824
6B	-1.092317	0.587993	-1.120743
7B	-1.092317	0.587993	1.120743
8A	0.013642	1.088917	0.000000
9B	-1.074354	-1.302616	0.000000
10B	2.259601	0.632406	-1.095900
11B	2.259601	0.632406	1.095900
12B	2.266727	-1.278255	0.000000
13A	1.097625	1.076077	0.000000
14B	0.596919	2.027049	-1.250331
15B	0.596919	2.027049	1.250331
16A	0.054354	-0.553118	0.925885
17A	0.054354	-0.553118	-0.925885
18A	1.132788	-0.543849	0.928387
19A	1.132788	-0.543849	-0.928387
20B	0.596351	-0.023869	2.388153
21B	0.596351	-0.023869	-2.388153
22B	0.602664	-2.078344	1.192753
23B	0.602664	-2.078344	-1.192753
24B	-1.138492	2.464187	0.000000

$E25/\varepsilon$ =-122.388638

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.174028	0.000000	0.000000
3A	0.587013	-0.921645	0.000000
4A	0.587013	0.435987	-0.793776
5A	0.587013	0.435988	0.793776
6B	2.268407	0.582869	-1.111018
7B	-1.094381	0.582872	1.111016
8B	2.268408	0.582870	1.111016
9B	-1.094381	0.582871	-1.111016
10A	1.128345	1.091486	-0.000001
11A	0.045683	1.091486	0.000000
12B	0.587015	1.956827	1.357084
13B	0.587014	1.956826	-1.357086
14B	2.258296	-1.308027	0.000000
15B	-1.084272	-1.308025	0.000000
16A	1.126423	-0.561612	-0.920778
17A	1.126423	-0.561612	0.920778
18A	0.047602	-0.561611	0.920778
19A	0.047602	-0.561612	-0.920778
20B	0.587012	-0.072790	-2.389257
21B	0.587013	-0.072789	2.389256
22B	0.587012	-2.092176	-1.186109
23B	0.587012	-2.092176	1.186109
24B	2.202560	2.473230	-0.000002
25B	-1.028530	2.473233	0.000000

$E26/\varepsilon$ =-129.869161

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.163855	0.000000	0.000000
3A	0.581928	-1.007928	0.000000
4A	0.581928	-0.335976	0.950283
5A	-0.297632	-0.843791	0.596650
6A	0.581928	0.679653	0.596650
7A	1.461489	-0.843790	0.596649
8A	0.581928	-0.335976	-0.839666
9B	1.690844	-0.976210	2.162506
10B	-1.729053	-0.282198	0.199542
11B	-0.620138	1.638502	0.199543
12B	0.581928	0.944490	2.162507
13B	-0.526988	-2.364234	0.199541
14B	-0.620137	0.358036	-1.611310
15B	-0.526989	-0.976210	2.162506
16B	0.581928	-1.723999	-1.611311
17B	1.783993	1.638502	0.199543
18B	1.783992	0.358037	-1.611311
19B	1.690844	-2.364234	0.199541
20B	2.892909	-0.282196	0.199541
21A	-0.364612	0.210508	1.010417
22A	1.528467	-0.882461	-0.535276
23A	-0.364611	-0.882461	-0.535276
24A	0.581928	0.756994	-0.535276
25A	0.581928	-1.428946	1.010417
26A	1.528468	0.210509	1.010417

$E27/\varepsilon$ =-136.658297

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.103094	0.000000	0.000000
3A	0.000000	-1.103094	0.000000
4A	-0.551547	0.551547	-0.780006
5A	-0.551547	0.551547	0.780006
6A	-0.551547	-0.551547	0.780006
7A	-1.103094	0.000000	0.000000
8A	0.000000	1.103094	0.000000
9A	-0.551547	-0.551547	-0.780006
10A	0.551547	0.551547	-0.780006
11A	0.551547	0.551547	0.780006
12A	0.551547	-0.551547	0.780006
13A	0.551547	-0.551547	-0.780006
14B	-1.595543	1.595543	0.000000
15B	0.000000	0.000000	2.256440
16B	-1.595543	-1.595543	0.000000
17B	0.000000	0.000000	-2.256440
18B	1.595543	1.595543	0.000000
19B	1.595543	-1.595543	0.000000
20B	1.993568	0.000000	-1.409666
21B	0.000000	-1.993568	-1.409666
22B	-1.993568	0.000000	-1.409666
23B	-1.993568	0.000000	1.409666
24B	1.993568	0.000000	1.409666
25B	0.000000	1.993568	1.409666
26B	0.000000	1.993568	-1.409666
27B	0.000000	-1.993568	1.409666

$E28/\varepsilon$ =-142.460916

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.084508	0.000000	0.000000
3A	-0.004959	-1.084497	0.000000
4A	0.539774	-0.542248	0.768614
5A	0.539774	-0.542248	-0.768614
6A	-0.523308	0.525706	-0.792733
7A	-0.523308	0.525706	0.792733
8A	-1.085135	-0.033559	0.000000
9A	0.038520	1.084970	0.000000
10A	-0.545524	-0.581447	0.796828
11A	-0.545524	-0.581447	-0.796828
12A	0.583935	0.542859	0.796828
13A	0.583935	0.542859	-0.796828
14B	0.083975	-0.084359	-2.247124
15B	0.083975	-0.084359	2.247124
16B	-1.508609	-1.669681	0.000000
17B	1.676562	1.500959	0.000000
18B	2.073422	-0.372162	1.206923
19B	0.362678	-2.075102	1.206923
20B	2.073422	-0.372162	-1.206923
21B	0.362678	-2.075102	-1.206923
22B	-1.556588	1.563721	0.000000
23A	1.094900	-1.099918	0.000000
24B	-1.961833	-0.036468	-1.416119
25B	-1.961833	-0.036468	1.416119
26B	0.045438	1.961646	1.416118
27B	0.045438	1.961646	-1.416118
28B	2.241923	-2.252199	0.000000

$E29/\varepsilon$ =-148.254717

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.101142	0.000000	0.000000
3A	0.550570	-0.953618	0.000000
4A	0.550570	-0.317873	-0.942694
5A	0.550570	-0.317873	0.942694
6B	1.632073	-2.315921	0.000000
7B	-0.639037	1.617761	0.000000
8B	-1.720542	-0.255461	0.000000
9B	-0.530938	-2.315919	0.000000
10B	1.740178	1.617762	0.000000
11B	2.821682	-0.255461	0.000000
12A	-0.343695	-0.834177	-0.579217
13A	-0.343695	-0.834177	0.579217
14A	1.444836	-0.834178	-0.579217
15A	1.444836	-0.834178	0.579217
16A	0.550571	0.714736	-0.579217
17A	0.550571	0.714736	0.579217
18A	-0.409942	0.236679	0.974382
19A	0.550569	-1.426976	-0.974382
20A	1.511082	0.236679	0.974382
21A	-0.409942	0.236679	-0.974382
22A	0.550569	-1.426976	0.974382
23A	1.511082	0.236679	-0.974382
24B	1.656062	-0.956129	2.140517
25B	0.550570	0.958639	2.140517

26B	-0.554922	-0.956129	2.140517
27B	-0.554922	-0.956129	-2.140517
28B	1.656062	-0.956129	-2.140517
29B	0.550570	0.958639	-2.140517

$E30/\varepsilon$ =-154.825577

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	2.235653	0.000000	0.000000
3B	0.046579	-2.235168	0.000000
4B	0.046578	-0.045617	-2.234703
5A	0.010091	-0.787996	-0.772075
6A	0.788035	0.006329	-0.772075
7A	0.788035	-0.771784	0.022085
8A	-0.774054	-0.785121	0.001300
9A	-0.774054	-0.014724	-0.784983
10A	0.768822	0.790243	0.001301
11A	0.768822	0.017429	0.790052
12A	-0.001407	0.774192	-0.784983
13A	-0.001407	-0.769019	0.790052
14A	-0.789402	0.773122	-0.014162
15A	-0.789402	0.001620	0.773250
16A	-0.018068	0.789196	0.773251
17B	-0.031946	0.031285	2.258136
18B	-0.031945	2.258304	-0.014808
19B	-2.258480	-0.015115	-0.014809
20B	1.399217	-1.370363	1.461085
21B	1.399217	1.432813	-1.399897
22B	-1.403349	-1.428767	-1.399898
23A	1.048506	-1.026883	-1.006135
24B	1.392402	1.429055	1.400182
25B	-1.399737	1.370870	-1.450155
26B	-1.399736	-1.421876	1.400180
27B	-1.442857	1.413100	1.384549
28B	0.586653	-2.148610	-2.105198
29B	2.160367	-0.541758	-2.105198
30B	2.160368	-2.115816	-0.498681

$E31/\varepsilon$ =-160.752462

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2B	2.169144	0.000000	0.000000
3A	0.021713	-1.157094	0.000000
4B	-0.052768	-1.538898	1.647001
5B	-0.052768	-1.538898	-1.647001
6A	0.734349	-0.532364	0.587302
7A	0.734349	-0.532364	-0.587302
8B	-1.593906	-1.811639	0.000000
9A	-0.724577	-0.579148	0.546326
10A	-0.724577	-0.579148	-0.546326
11A	0.715223	0.587671	0.561388
12A	-0.793437	0.509931	0.539784
13A	-0.793437	0.509931	-0.539784
14A	0.715223	0.587671	-0.561388
15A	-0.037916	0.024589	-1.139740
16A	-0.037916	0.024589	1.139740
17A	-0.073411	1.121743	0.000000
18B	-1.728584	-0.069769	1.700972
19B	-1.728584	-0.069769	-1.700972
20B	-0.205394	1.613302	-1.563817
21B	-0.205394	1.613302	1.563817
22B	-1.844272	1.595544	0.000000
23A	-1.543011	-0.089916	0.000000
24B	1.351632	0.119410	2.011012
25B	1.351632	0.119410	-2.011012
26A	1.089454	-1.369130	0.000000
27B	1.315940	2.016966	0.000000
28B	0.411793	-2.849822	0.000000
29B	2.070957	-1.840084	-1.184203
30B	2.070957	-1.840084	1.184203
31B	-3.166058	-0.218070	0.000000

$E32/\varepsilon$ =-167.803356

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.041698	0.000000	0.000000
3B	1.957366	-1.324903	0.000000
4B	1.957359	0.857359	1.010109
5A	-0.120412	-0.488530	1.055425
6A	0.379764	-0.975465	0.234905
7A	0.379759	0.452137	0.895705
8A	-0.957915	-0.209382	0.452341
9A	0.454851	0.410719	-0.887326
10A	0.530848	1.031796	0.007314
11A	0.530853	-0.673257	-0.781910
12B	-0.549176	1.725449	-1.040353
13B	-0.549170	-0.323388	-1.988704
14B	0.019419	-2.273725	-0.688683
15B	0.019406	1.996390	1.287838
16A	-0.518323	-0.789520	-0.446225
17A	-0.518329	0.851101	0.313175
18B	0.445029	-1.953130	1.540919
19B	0.445022	0.089082	2.486204
20B	-1.525858	-0.852329	1.841373
21B	1.218826	1.017004	-2.197154
22A	0.976763	-0.464923	1.004433
23A	-0.946244	0.241837	-0.522479
24B	-2.083630	-1.055831	-0.379527
25B	-2.083638	0.972569	0.559366
26A	-0.658064	-1.285810	0.506563
27A	-0.658070	0.445844	1.308099
28A	1.428810	0.856160	-0.567312
29A	1.428814	-0.121504	-1.019847
30B	1.409670	-1.270270	-2.135000
31B	1.409659	2.449727	-0.413115
32B	2.960195	0.431293	-0.931757

$E33/\varepsilon$ =-175.843136

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.088402	0.000000	0.000000
3A	0.526519	-0.952573	0.000000
4A	-0.382626	-0.813086	0.614090
5A	0.526519	0.728210	0.614090
6A	-0.382626	0.225695	0.993619
7A	0.537927	0.324702	-0.888718
8A	-0.023956	-0.627872	-0.888718
9A	-0.023956	1.052912	-0.274628
10A	-0.933101	-0.488385	-0.274627
11A	-0.933101	0.550396	0.104901
12A	0.575186	-0.339278	0.928614
13A	-0.575186	0.339277	-0.928612
14B	0.688191	-2.164203	-1.216977
15B	-1.801708	1.062750	1.504271
16B	-1.801707	-1.782186	0.464847
17B	0.688192	2.439001	0.464846
18B	2.227034	0.444634	-1.216977
19B	-1.315199	2.037201	-0.453144
20B	-2.419200	0.165559	-0.453143
21B	-1.315198	-1.265247	-1.659723
22B	0.327750	-2.234350	0.992745
23B	0.471114	-0.277890	-2.405432
24B	2.114062	-1.246996	0.247037
25B	0.471116	1.763135	-1.659724
26B	2.114061	0.794029	0.992746
27B	-0.776252	-0.803544	2.199326
28B	0.327748	1.068098	2.199326
29A	-1.326042	-0.264749	0.724627
30A	1.072791	1.061166	-0.276781
31A	-0.409769	-1.452255	-0.276781
32A	-0.409770	1.288630	0.724627
33A	1.072791	-0.632794	-0.895686

$E34/\varepsilon$ =-183.740999

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.090209	0.000000	0.000000
3A	0.527307	-0.954203	0.000000
4A	0.527306	0.729546	0.615033
5A	-0.383489	-0.814387	0.615033
6A	-0.383490	0.226228	0.995144
7A	0.536840	0.324829	-0.889270
8A	-0.024650	-0.626980	-0.889270
9A	-0.024650	1.052544	-0.275780
10A	-0.933159	-0.487514	-0.275780
11A	-0.933160	0.550488	0.103377
12A	0.568195	-0.335189	0.917634
13A	-0.575890	0.339728	-0.930060
14B	-0.806177	-0.801582	2.194456
15B	0.311657	-2.250341	0.973101
16B	0.311654	1.093311	2.194456
17B	2.120347	0.815660	0.973099
18B	2.120348	-1.250832	0.218260
19B	0.683191	2.442703	0.456429
20B	-1.807527	-1.779437	0.456429
21B	2.222542	0.447639	-1.225481
22B	0.683194	-2.161787	-1.225480
23B	-1.807529	1.066295	1.495905
24B	0.467808	-0.275969	-2.407522
25B	0.467809	1.762768	-1.662820
26B	-1.316591	-1.262057	-1.662820
27B	-1.316592	2.036691	-0.457868
28B	-2.419411	0.167247	-0.457870
29A	-1.327178	-0.263289	0.720794
30A	-0.411480	1.288955	0.720794
31A	1.070152	1.061510	-0.279707
32A	-0.411478	-1.450074	-0.279707
33A	1.070152	-0.631303	-0.898051
34B	1.391318	-0.820762	2.246971

$E35/\varepsilon$ =-191.637722

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.090132	0.000000	0.000000
3A	-0.934806	-0.560827	0.000000
4A	-0.934806	0.531541	0.178857
5A	0.528155	0.936722	-0.178862
6A	-0.381142	0.684881	-0.757665
7A	0.528155	-0.830767	-0.468259
8A	-0.381142	-0.407487	-0.936522
9A	-0.025509	-0.984107	0.468264
10A	-0.025509	0.783382	0.757661
11A	0.536468	-0.153340	0.936523
12A	0.570686	0.158055	-0.965317
13A	-0.570687	-0.158055	0.965317
14B	-0.799448	0.378085	-2.309152
15B	0.316429	-1.481896	-1.953997
16B	0.491026	0.735507	2.309148
17B	0.491026	-1.433529	1.954004
18B	0.316428	2.027678	-1.379362
19B	-1.314500	1.575984	1.379351
20B	-1.314499	-1.933591	0.804716
21B	-2.430375	-0.073609	0.449560
22B	2.121954	-0.981835	-0.804709
23B	2.121953	1.187202	-0.449564
24B	2.226649	-0.209907	1.282007
25B	-1.801398	1.665158	-0.792330
26B	-1.801397	-1.325523	-1.282004
27B	0.688071	2.354647	0.792317
28B	0.688073	-2.484377	0.000007
29A	1.070420	0.787647	0.761788
30A	1.070421	-0.989466	0.470815
31A	-0.408866	1.476259	-0.000005
32A	-0.408864	-1.399172	-0.470809
33A	-1.323114	0.124730	-0.761791
34B	-1.396719	-0.386829	2.362546
35B	1.396717	0.386828	-2.362546

$E36/\varepsilon$ =-196.965963

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.090368	0.000000	0.000000
3A	0.527269	-0.954405	0.000000
4A	-0.027016	-0.627377	0.891386
5A	0.536082	0.327030	0.891386
6A	-0.381902	-0.813698	-0.616930
7A	-0.936158	-0.486686	0.274408
8A	-0.026700	1.054771	0.274406
9A	0.527556	0.727760	-0.616932
10A	-0.935005	0.551651	-0.107188
11A	-0.381870	0.225301	-0.996724
12A	-0.570982	0.336880	0.916189
13A	0.569308	-0.335892	-0.917594
14B	0.527444	-0.311189	2.400131
15B	2.128118	-1.255588	-0.174021
16B	0.658566	-2.184831	1.211078
17B	2.230858	0.480076	1.211074
18B	-1.312165	-1.287821	1.652794
19B	2.124675	0.808440	-0.971682
20B	0.492712	1.771300	1.652790
21B	0.319797	-2.250681	-0.971677
22B	0.323064	1.082695	-2.197804
23B	-0.791467	-0.806345	-2.197801
24B	-2.427695	0.159030	0.433529
25B	-1.313164	2.048071	0.433526
26A	1.066127	-0.629013	0.893714
27B	0.688481	2.440985	-0.467429
28B	-1.803679	-1.783023	-0.467423
29B	-1.799742	1.061843	-1.508692
30A	-1.324249	-0.265144	-0.726176
31A	-0.408288	1.287335	-0.726178
32A	1.066086	1.061612	0.273437
33A	-0.413706	-1.446515	0.273440
34B	1.413054	-0.833705	-2.226940
35B	-1.375866	0.811762	2.258113
36A	1.837953	-1.084389	1.540725

$E37/\varepsilon$ =-202.799137

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.076401	0.000000	0.000000
3A	0.468938	-0.965959	0.000000
4A	0.558371	0.292678	0.897899
5A	0.558372	0.292678	-0.897899
6A	-0.346353	0.858289	-0.561943
7A	-0.346353	0.858289	0.561942
8A	-0.015631	-0.629364	-0.899278
9A	-0.015631	-0.629364	0.899278
10A	-0.918484	-0.076048	-0.564296
11A	-0.918485	-0.076048	0.564295
12B	2.152211	0.607587	1.086305
13B	2.152212	0.607587	-1.086304
14A	0.592895	0.975107	0.000000
15A	1.132596	-0.712866	0.805171
16A	1.132596	-0.712866	-0.805171
17B	0.765841	-0.485040	2.378062
18B	0.765842	-0.485039	-2.378061
19B	0.357935	-2.208748	1.073165
20B	0.357936	-2.208747	-1.073165
21A	-0.620627	-0.977892	0.000000
22B	0.374880	1.661253	-1.785320
23B	0.374879	1.661253	1.785321
24B	-0.731730	2.343329	0.000000
25B	-1.760814	1.077550	1.512295
26B	-1.760813	1.077550	-1.512296
27B	-2.394793	-0.463440	-0.000001
28B	-1.325265	-1.077687	1.792778
29B	-1.325264	-1.077687	-1.792779
30A	-0.377224	0.234293	1.468807
31A	-0.377224	0.234294	-1.468808
32A	-1.287012	0.784831	0.000000
33A	1.960932	-0.606148	0.000000
34A	1.387704	-1.515294	0.000000
35B	2.475387	-1.574100	1.225719
36B	2.475388	-1.574099	-1.225717
37B	1.452700	2.375498	0.000001

$E38/\varepsilon$ =-210.677219

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.076990	0.000000	0.000000
3A	0.470478	-0.968792	0.000000
4A	0.559680	0.291320	-0.897419
5A	0.559680	0.291320	0.897419
6A	-0.017561	-0.630714	0.897419
7A	-0.017561	-0.630714	-0.897419
8A	-0.341016	0.861064	0.561267
9A	-0.341016	0.861064	-0.561267
10A	-0.923530	-0.069393	0.561267
11A	-0.923530	-0.069393	-0.561267
12B	0.389283	-2.204420	1.086116
13B	0.389283	-2.204420	-1.086116
14B	2.153015	0.612812	-1.086116
15B	2.153015	0.612812	1.086116
16A	-0.616955	-0.964898	0.000000
17A	0.598449	0.976485	0.000000
18A	1.135619	-0.710955	-0.805030
19A	1.135619	-0.710955	0.805030
20B	0.765091	-0.478986	-2.378095
21B	0.765091	-0.478986	2.378095
22B	0.380965	1.662781	-1.784535
23B	0.380965	1.662781	1.784535
24B	-1.329312	-1.069066	-1.784536
25B	-1.329312	-1.069066	1.784536
26B	-0.720311	2.351144	0.000000
27B	-2.429606	-0.379134	0.000000
28B	-1.748357	1.094562	-1.518473
29B	-1.748357	1.094562	1.518473
30A	-1.279854	0.801254	0.000000
31A	-0.376420	0.235659	-1.464958
32A	-0.376420	0.235659	1.464958
33A	1.966308	-0.597748	0.000000
34A	1.396666	-1.507646	0.000000
35B	2.492749	-1.560589	-1.221309
36B	2.492749	-1.560589	1.221309
37B	-1.503313	-2.352599	0.000000
38B	1.459541	2.380005	0.000000

$E39/\varepsilon$ =-216.589951

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.082588	0.000000	0.000000
3A	0.552598	-0.930931	0.000000
4B	2.152339	0.696257	0.936820
5B	0.499925	-2.206223	0.936816
6A	0.534796	-0.304467	0.963348
7A	0.013091	-0.638980	-0.893954
8A	0.556150	0.314907	-0.893953
9A	-0.362595	-0.823825	0.611865
10A	0.523332	0.732313	0.611867
11A	-0.035041	1.046567	-0.281528
12A	-0.917842	-0.504079	-0.281530
13A	-0.943696	0.537257	0.091601
14A	-0.404492	0.230280	0.988725
15A	1.142547	-0.650464	-0.883705
16A	-0.553373	0.315043	-0.929067
17B	0.537995	-0.306283	-2.392773
18B	0.343344	1.066109	2.182851
19B	-0.741505	-0.839437	2.182848
20B	0.572219	-2.226569	-1.298101
21B	2.206740	0.644480	-1.298097
22B	-1.319580	-1.275408	-1.648316
23B	0.423173	1.785750	-1.648311
24B	-2.439738	0.118842	-0.406838
25B	-1.347537	2.037300	-0.406834
26A	1.426425	-0.812080	0.667219
27B	-1.728966	-1.839662	0.473361
28B	0.699411	2.425799	0.473368
29B	-1.794245	1.021482	1.525657
30A	-0.418621	1.284154	0.717144
31A	-1.317943	-0.295510	0.717142
32A	1.059945	1.059480	-0.275311
33A	-0.370019	-1.452262	-0.275315
34A	1.482506	-1.473893	-0.201427
35A	2.024152	-0.522486	-0.201427
36B	1.438897	-0.819183	2.311081
37B	2.826633	-1.609233	0.754043
38B	2.555041	-1.454612	-1.466799
39B	-1.412234	0.804007	-2.239082

$E40/\varepsilon$ =-223.700145

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.078780	0.000000	0.000000
3B	-1.656201	-0.000017	0.000000
4B	2.734981	0.000016	0.000001
5A	0.539383	0.999057	-0.034117
6A	0.539393	-0.469982	0.882268
7A	0.539394	-0.529075	-0.848150
8B	0.539405	-2.026431	1.375992
9B	0.539374	2.126936	-1.214873
10B	0.539407	-2.115580	-1.234542
11B	0.539392	-0.178430	-2.442936
12B	0.539372	2.204860	1.066944
13B	0.539389	-0.011358	2.449418
14A	0.539386	0.523304	-0.982366
15A	0.539385	0.589102	0.944379
16A	0.539398	-1.112406	0.037989
17A	1.480070	-0.953429	-0.507985
18A	-0.401290	0.916639	-0.571706
19A	1.480070	-0.916552	0.571846
20A	-0.401290	0.953505	0.507841
21A	1.480063	-0.036947	-1.079685
22A	-0.401282	-0.036960	-1.079685
23A	-0.401284	0.036782	1.079691
24A	1.480062	0.036796	1.079692
25A	1.480056	0.916651	-0.571705
26A	1.480055	0.953518	0.507841
27A	-0.401276	-0.916565	0.571845
28A	-0.401275	-0.953441	-0.507985
29B	2.313243	1.184182	1.898318
30B	-1.234482	1.051893	-1.974679
31B	2.313247	1.051920	-1.974677
32B	-1.234484	1.184154	1.898317
33B	-1.234458	-2.236088	0.076361
34B	2.313274	-2.236061	0.076363
35B	-1.342754	-1.156234	-1.853511
36B	2.421554	-1.156205	-1.853510
37B	2.421527	2.183311	-0.074558
38B	-1.342758	-1.027094	1.928070
39B	2.421552	-1.027064	1.928072
40B	-1.342783	2.183282	-0.074559

$E41/\varepsilon$ =-229.365627

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.069745	0.000000	0.000000
3A	0.456888	-0.967267	0.000000
4A	-0.291798	0.862668	-0.561259
5A	-0.904655	-0.104599	-0.561259
6A	-0.021966	-0.625577	-0.908239
7A	0.556269	0.287047	-0.908239
8A	0.535947	0.303946	0.894890
9A	-0.370600	0.878331	0.521191
10A	-0.952474	-0.040035	0.521191
11A	-0.045927	-0.614420	0.894890

12B	0.699804	-0.443392	-2.379141
13B	-0.664869	2.382257	-0.049069
14B	0.355072	-2.185969	1.102301
15B	2.128216	0.612568	1.102302
16B	-2.438014	-0.416280	-0.049070
17B	-1.322112	-1.121538	-1.782907
18B	0.391630	-2.207360	-1.076464
19B	2.163171	0.588648	-1.076463
20B	0.449429	1.674470	-1.782906
21A	0.618736	0.986454	0.015229
22A	-0.627694	-0.980776	0.015229
23A	-1.295363	0.820738	-0.175580
24A	1.107326	-0.701597	0.814861
25A	1.126396	-0.713679	-0.805740
26A	-0.460035	0.291478	-1.459702
27B	-1.802093	1.141801	1.347204
28B	0.705509	-0.447008	2.380893
29B	-1.375328	-1.028324	1.755814
30B	0.342415	1.682774	1.755814
31A	-0.421618	0.267136	1.433390
32A	1.380550	-1.508917	0.019256
33A	-1.030056	1.286847	-1.210838
34A	-1.603508	0.381772	-1.210838
35A	1.954001	-0.603842	0.019256
36B	-2.585314	1.638047	-0.818243
37B	2.455471	-1.555778	1.259679
38B	2.484803	-1.574361	-1.197167
39B	-1.319281	0.835893	-2.765293
40B	-1.510482	-2.380022	0.006083
41B	1.506905	2.382291	0.006084

$E42/\varepsilon$ =-236.995833

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.102676	0.000000	0.000000
3A	0.551337	-0.901954	0.000000
4A	0.551338	-0.227921	-0.872682
5B	2.796708	-0.069194	-0.053439
6B	-1.694033	-0.069192	-0.053444
7B	0.551340	0.876783	-2.159934
8B	0.551334	-1.868275	1.394136
9A	0.551336	-0.309888	0.916055
10A	-0.363073	-0.814002	-0.628712
11A	1.465748	-0.814004	-0.628711
12A	0.551338	0.808018	-0.531313
13A	0.551337	-1.312688	-1.013881
14A	0.551337	0.747750	0.577541
15B	-0.717849	-2.106221	-1.626785
16B	0.551338	2.317101	0.185988
17B	0.551334	0.765472	2.194903
18B	1.820522	-2.106224	-1.626783
19A	-0.391601	-0.858858	0.528089
20A	-0.391599	0.293922	-0.964431
21A	1.494273	-0.858859	0.528092
22A	1.494276	0.293920	-0.964430
23A	-0.018825	-0.618931	-1.668935
24A	-0.018828	-1.771171	-0.177111
25A	1.493832	0.281589	0.937922
26A	-0.391160	0.281589	0.937920
27A	-0.391159	0.978638	0.035442
28A	1.121499	-1.771173	-0.177110
29A	1.121502	-0.618932	-1.668934
30A	1.493834	0.978638	0.035444
31B	2.534803	-0.109965	-2.225230
32B	2.245213	-0.631988	2.018078
33B	-1.142540	1.792880	-1.121437
34B	2.534798	-2.180803	0.455916
35B	2.245218	1.792878	-1.121434
36B	-1.142545	-0.631987	2.018074
37B	-1.432128	-2.180802	0.455913
38B	-1.432124	-0.109961	-2.225235
39B	-1.256166	1.629185	1.258333
40B	0.551334	-3.298994	-0.264181
41B	0.551338	-1.089252	-3.125170
42B	2.358838	1.629183	1.258338

$E43/\varepsilon$ =-243.686941

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.127820	0.000000	0.000000
3A	0.582761	-0.917202	0.000000
4A	0.582758	0.795463	0.456615
5A	0.728721	0.791130	-0.649121
6A	0.728724	-0.362970	-0.956817
7B	2.914107	-0.005342	0.020053
8A	0.746328	-0.260504	0.977095
9B	0.632868	-2.065543	-1.151945
10B	0.632858	2.364865	0.029248
11B	0.717648	-2.111140	1.100024
12B	0.717641	1.283302	2.005018
13A	-0.177054	-0.780636	0.790633
14A	-0.177056	0.283415	1.074320
15A	-0.958988	0.477475	0.374600
16A	-0.958985	-0.600596	0.087175
17A	-0.272106	-0.711311	-0.762236
18A	-0.272111	0.996364	-0.306953
19B	-0.134316	-0.544523	-2.467529
20B	-0.134321	1.700666	-1.868939
21B	-0.162109	-0.646837	2.426142
22A	-0.089847	0.299525	-1.123461
23B	-2.493036	-0.058827	0.220619
24A	-1.024768	0.173293	-0.649999
25B	-1.592114	-1.538006	-1.120984
26B	-1.592122	1.891924	-0.206528
27A	1.590397	1.001395	-0.047346
28A	1.590401	-0.844910	-0.539591
29B	2.062884	-0.696568	-2.098585
30B	2.062879	1.648867	-1.473266
31A	1.637993	0.237943	-0.892468
32B	-1.487166	1.077488	1.871107
33B	-1.487159	-1.865987	1.086346
34A	1.571668	0.453519	0.882706
35A	1.571671	-0.832764	0.539770
36B	2.025957	-0.549210	2.059978
37A	-0.351594	1.311862	0.741556
38A	-0.351589	-1.506918	-0.009961
39A	-1.110279	-0.300615	1.127527
40A	0.901463	0.447719	-1.679297
41B	-1.980036	0.505422	-1.895758
42B	2.532845	1.864618	0.978621
43B	2.532854	-2.104317	-0.079538

$E44/\varepsilon$ =-250.867906

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.083493	0.000000	0.000000
3A	0.550094	-0.928531	0.000000
4B	0.564128	-2.173185	0.956467
5A	0.533304	-0.324376	0.954530
6A	0.538165	0.745380	0.572734
7A	0.539360	0.307564	-0.893286
8A	-0.008778	-0.642322	-0.890478
9B	0.453710	1.094603	2.134389
10A	-0.017143	1.051029	-0.302067
11A	-0.927618	0.552456	0.100917
12A	-0.921334	-0.504809	-0.264410
13A	-0.373290	0.255662	0.988895
14A	-0.361132	-0.825272	0.613159
15A	1.098957	-0.637816	-0.884750
16A	1.451744	-0.793522	0.643548
17A	2.037486	-0.469528	-0.212393
18B	0.532762	-0.294184	-2.389974
19A	-0.567314	0.314306	-0.920320
20B	0.766309	2.411357	0.419869
21B	0.468411	1.737362	-1.683930
22A	1.102737	1.035933	-0.318746
23B	-0.607362	-0.799764	2.204258
24B	0.614846	-2.203254	-1.308142
25A	2.001811	0.568649	0.097725
26A	1.416310	0.298115	0.992745
27B	1.639791	-0.718214	2.241602
28A	1.656671	0.301581	-0.933620
29B	-1.325338	-1.290450	-1.623780
30B	-1.308047	2.049348	-0.428210
31B	-2.424563	0.136506	-0.377247
32B	2.474213	-1.052029	-1.636235
33B	-1.705088	-1.820330	0.534170
34B	-1.731220	1.055473	1.551969
35B	2.531158	1.391478	1.379462
36B	2.793310	-1.772489	0.620920
37A	-0.363238	-1.465194	-0.268230
38A	-1.292880	-0.272329	0.745836
39A	-0.385327	1.309074	0.701999
40B	2.459991	1.786447	-0.882843
41A	2.360740	-0.197889	0.824796
42A	1.500249	-1.421124	-0.246156
43B	3.600902	0.115761	-0.166513
44B	-1.413862	0.792943	-2.235091

$E45/\varepsilon$ =-258.409108

atom	x/σ	y/σ	z/σ
1A	0.000000	0.000000	0.000000
2A	1.102108	0.000000	0.000000
3A	0.541497	-0.927578	0.000000
4A	0.541498	0.729562	0.572835
5B	0.498047	-2.184455	0.959759
6B	0.498049	1.125416	2.103906
7B	2.087498	0.518419	-1.499720
8A	0.520580	-0.331194	0.958102
9A	0.554271	0.307230	-0.888777
10A	-0.017202	1.051562	-0.295300
11A	-0.017203	-0.644712	-0.881663
12A	-0.934861	0.547314	0.099947
13A	-0.934862	-0.492197	-0.259388
14A	-0.376319	0.257998	0.991867
15A	-0.376319	-0.815458	0.620797
16A	1.423066	-0.823551	0.651312
17A	1.423067	0.245516	1.020864
18A	1.117857	1.069217	-0.292176
19A	1.117856	-0.660528	-0.890110
20A	2.037499	-0.521510	-0.207925
21A	2.037500	0.538584	0.158526
22A	-0.559191	0.319410	-0.924011
23B	1.557898	-0.784890	2.270583
24B	0.369029	1.755607	-1.681055
25B	0.369030	-0.342674	-2.406382
26B	-0.630151	-0.767463	2.220175
27B	0.549778	2.541951	0.355890
28B	0.549774	-2.219089	-1.289892
29B	-1.399826	-1.323706	-1.565733
30B	-1.399824	2.008062	-0.414017
31B	-2.471305	0.106692	-0.308642
32B	-1.718021	-1.816808	0.582325
33B	-1.718019	1.069344	1.580001
34B	2.718494	1.007735	1.735919
35B	2.718492	-1.864646	0.742999
36B	3.626353	0.027361	-0.079159
37A	1.468656	1.286056	0.733981
38A	1.468654	-1.464792	-0.216926
39A	-0.391691	1.298956	0.698937
40A	-0.391692	-1.453295	-0.252453
41A	-1.301836	-0.262780	0.760191
42A	2.343803	-0.289873	0.838560
43B	2.592175	-1.532370	-1.412072
44B	2.592180	2.077282	-0.164293
45B	-1.518171	0.757392	-2.191037

$E46/\varepsilon$ =-266.121423

atom	x/σ	y/σ	z/σ

1A	0.000000	0.000000	0.000000
2A	1.087002	0.000000	0.000000
3A	0.543501	-0.928280	0.000000
4A	0.543501	0.735244	0.566675
5B	0.543502	1.132937	2.091636
6B	0.543503	-2.174196	0.965070
7A	0.543502	-0.324798	0.953474
8A	0.543500	0.303459	-0.890832
9B	0.543500	-0.340175	-2.382418
10B	0.543499	1.723798	-1.679331
11A	1.101110	-0.646711	-0.887378
12A	-0.014109	1.053933	-0.308057
13A	1.101110	1.053933	-0.308058
14A	-0.014109	-0.646712	-0.887377
15A	-0.925855	0.550857	0.105765
16A	2.012856	0.550858	0.105763
17A	-0.925854	-0.500871	-0.252504
18A	2.012857	-0.500870	-0.252506
19A	-0.360753	0.263355	0.993949
20A	-0.360752	-0.815353	0.626490
21A	1.447756	0.263356	0.993948
22A	1.447756	-0.815353	0.626489
23A	-0.566828	0.311857	-0.915486
24A	1.653829	0.311858	-0.915487
25B	-0.573403	-0.757914	2.224921
26B	1.660409	-0.757913	2.224920
27B	0.543501	-2.254567	-1.279307
28B	0.543500	2.566690	0.363041
29B	-1.347268	-1.291447	-1.605249
30B	2.434270	-1.291445	-1.605251
31B	2.434268	2.002827	-0.483066
32B	-1.347269	2.002824	-0.483064
33B	3.518331	0.124140	-0.364418
34B	-2.431330	0.124136	-0.364414
35B	2.793254	1.081812	1.558589
36B	-1.706251	1.081809	1.558593
37B	2.793256	-1.808298	0.574080
38B	-1.706250	-1.808300	0.574084
39A	1.466151	-1.456600	-0.250950
40A	1.466150	1.306894	0.690426
41A	-0.379149	1.306893	0.690428
42A	-0.379148	-1.456601	-0.250949
43A	2.375935	-0.259821	0.762730
44A	-1.288932	-0.259823	0.762732
45B	2.448511	0.771582	-2.265043
46B	-1.361513	0.771579	-2.265040

*E*47/ε =-272.215887

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.089437	0.000000	0.000000
3A	0.544719	-0.940223	0.000000
4A	0.544719	0.948652	0.036231
5A	0.544718	-0.306132	0.878324
6B	0.544718	0.152533	2.378892
7A	-0.571593	-0.923113	0.011584
8A	1.661030	-0.923113	0.011585
9A	-0.010164	-0.617578	-0.905754
10A	1.099602	-0.617579	-0.905754
11A	0.544719	0.321367	-0.903647
12B	0.544719	2.129703	-1.014916
13A	-0.005999	0.647990	0.906498
14A	1.095435	0.647989	0.906498
15A	1.648294	-0.295147	0.929952
16A	-0.558858	-0.295146	0.929952
17B	-0.540979	0.433543	-2.137938
18B	1.630419	0.433542	-2.137937
19B	2.140863	-2.432915	0.467479
20B	-1.051428	-2.432914	0.467478
21A	-0.013855	-1.238620	0.915949
22A	1.103291	-1.238620	0.915949
23B	0.544720	-1.484299	-2.182517
24B	3.247010	-0.505109	0.390483
25B	-2.157574	-0.505108	0.390480
26B	0.544718	2.148240	1.378607
27A	1.099419	-1.667936	-0.590560
28A	-0.009982	-1.667936	-0.590560
29A	0.544718	-1.985423	0.318966
30A	1.433772	0.840845	-0.593879
31A	-0.344335	0.840845	-0.593880
32A	-0.901866	0.505913	0.286420
33A	1.991303	0.505913	0.286422
34A	2.015190	-0.083261	-0.622753
35A	-0.925753	-0.083261	-0.622755
36B	2.449561	1.082991	1.700644
37B	-1.360126	1.082991	1.700642
38B	-1.429821	-1.431597	-1.402701
39B	2.519260	-1.431597	-1.402699
40B	0.544717	-2.395756	1.946504
41B	-1.828425	1.458728	-0.621929
42B	2.917863	1.458728	-0.621926
43A	-0.413336	1.481986	0.278757
44A	1.502773	1.481985	0.278758
45B	2.264711	-1.108062	2.204562
46B	-1.175276	-1.108061	2.204560
47B	0.544718	-3.199168	-0.822695

*E*48/ε =-279.832502

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.081390	0.000000	0.000000
3A	0.539429	-0.935779	0.000000
4A	0.525852	-0.320240	0.908849
5A	-0.557075	-0.944491	0.016139
6A	0.509365	0.962323	0.002111
7A	1.627452	-0.977292	0.002110
8A	1.084991	-0.639609	-0.907882
9A	0.529711	0.323669	-0.907882
10B	-0.130899	-0.698822	2.426961
11A	-0.002063	-0.624555	-0.913592
12B	-1.553981	-1.519155	-1.068914
13A	1.637570	-0.327264	0.885854
14A	1.076936	0.645303	0.885855
15A	-0.033371	-1.277774	0.892866
16A	-0.583015	-0.324274	0.892866
17A	-0.021233	0.620513	0.918469
18A	1.065746	-1.265138	0.918469
19B	-0.626505	0.266901	-2.154271
20B	0.456403	-1.611687	-2.154271
21B	1.575893	0.285056	-2.171564
22B	1.565034	2.146281	0.465468
23B	3.181059	-0.657140	0.465467
24B	2.058729	-2.532591	0.439620
25B	-0.620365	2.115000	0.439623
26B	-1.682794	-1.593410	1.237894
27A	1.994794	-0.116054	-0.589205
28A	1.438737	0.848574	-0.589205
29A	1.999714	0.529365	0.306334
30A	-0.002244	-1.653190	-0.612732
31A	-0.892280	-0.109189	-0.612732
32A	-0.887410	0.533123	0.275881
33A	0.556020	-1.970884	0.275881
34A	1.084552	-1.702096	-0.627500
35A	-0.389929	0.855778	-0.627499
36B	-1.681247	0.617873	1.652720
37B	0.231511	-2.700303	1.652721
38B	2.500670	-1.473898	-1.397382
39B	0.517260	1.966847	-1.397380
40B	0.414746	1.423040	2.239123
41B	1.978711	-1.290071	2.239123
42B	2.510977	0.824079	1.853819
43B	-2.150310	0.896420	-0.652619
44B	0.237468	-3.245807	-0.652619
45A	-0.528676	-2.049299	0.241392
46A	-1.498885	-0.366217	0.241392
47B	3.052472	1.136224	-0.798181
48A	1.114969	0.019354	1.770586

*E*49/ε =-287.340181

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094496	0.000000	0.000000
3A	0.547248	-0.947861	0.000000
4A	0.547246	-0.315952	-0.891618
5A	0.547249	0.319489	0.905933
6A	-0.003062	-0.633678	0.905933
7A	1.097561	-0.633678	0.905931
8A	-0.558477	-0.954344	-0.001648
9A	1.652973	-0.954344	-0.001652
10A	0.547248	0.960827	-0.001647
11A	-0.009247	-1.272308	-0.899866
12A	1.097227	0.644163	-0.899865
13A	1.653721	-0.319711	-0.899868
14A	1.103739	-1.272308	-0.899868
15A	-0.002736	0.644163	-0.899864
16A	-0.559229	-0.319712	-0.899864
17B	1.632493	0.310606	2.167687
18B	0.547253	-1.569086	2.167686
19B	-0.537988	0.310606	2.167691
20B	3.221812	-0.617121	-0.443436
21B	-0.529216	2.150873	-0.443424
22B	1.623710	2.150872	-0.443428
23B	-2.127318	-0.617121	-0.443424
24B	2.145350	-2.481609	-0.443438
25B	-1.050855	-2.481610	-0.443430
26A	-0.367049	0.848997	0.597440
27A	-0.918778	-0.106626	0.597440
28A	2.013276	-0.106626	0.597434
29A	1.461547	0.848997	0.597437
30A	-0.004480	-1.690236	0.597436
31A	1.098979	-1.690236	0.597433
32A	0.547247	-2.006885	-0.301535
33A	2.011637	0.529513	-0.301534
34A	-0.917143	0.529513	-0.301528
35B	-1.010252	-1.215170	-2.238710
36B	0.547242	1.482489	-2.238709
37B	2.104737	-1.215169	-2.238717
38B	2.533448	-1.462688	1.392550
39B	0.547251	1.977506	1.392560
40B	-1.438946	-1.462687	1.392559
41B	-1.453838	0.839374	-1.833115
42B	2.548325	0.839374	-1.833124
43B	0.547244	-2.626601	-1.833125
44A	1.098169	0.002126	-1.791686
45A	-0.003682	0.002126	-1.791684
46A	0.547244	-0.952105	-1.791687
47B	-1.990173	1.149027	0.800479
48B	0.547251	-3.245919	0.800464
49B	3.084672	1.149027	0.800468

*E*50/ε =-296.237038

atom	x/σ	*y*/σ	*z*/σ
1A	0.000000	0.000000	0.000000
2A	1.094125	0.000000	0.000000
3A	0.547063	-0.947540	0.000000
4A	0.547062	-0.315847	0.893349
5A	1.097090	0.643744	0.899425
6A	-0.558981	-0.319304	0.899425
7A	1.097090	-0.633405	-0.906736
8A	-0.002965	0.643744	0.899425
9A	-0.002964	-0.633404	-0.906736
10A	1.653106	-0.319304	0.899425
11A	0.547063	0.961302	0.001234
12A	1.653106	-0.954421	0.001234
13A	-0.558981	-0.954421	0.001233
14A	0.547063	0.319271	-0.906736
15A	1.103078	-1.271980	0.899425
16A	-0.008954	-1.271979	0.899425
17B	1.630882	0.309898	-2.171235

18B	-2.130643	-0.610335	0.431571
19B	-1.046826	-1.236078	2.201438
20B	-1.046825	-2.487563	0.431571
21B	2.140949	-1.236078	2.201439
22B	2.140950	-2.487563	0.431571
23B	3.224768	-0.610335	0.431573
24B	-0.536754	0.309897	-2.171236
25B	0.547063	-1.567330	-2.171236
26B	1.630880	2.150359	0.431573
27B	0.547062	1.524616	2.201440
28B	-0.536755	2.150359	0.431572
29A	-0.917791	-0.106416	-0.599655
30A	2.011917	-0.106416	-0.599655
31A	1.460861	0.848040	-0.599654
32A	-0.003994	0.002306	1.792442
33A	2.011917	0.529888	0.300216
34A	-0.366735	0.848040	-0.599655
35A	-0.003993	-1.689162	-0.599656
36A	1.098118	-1.689162	-0.599655
37A	0.547062	-2.007315	0.300215
38A	0.547062	-0.952151	1.792442
39A	1.098118	0.002306	1.792443
40A	-0.917792	0.529888	0.300215
41B	0.547063	1.976458	-1.397566
42B	0.547062	-2.608150	1.844240
43B	2.532256	0.830305	1.844241
44B	-1.438131	0.830305	1.844240
45B	2.532256	-1.461997	-1.397567
46B	-1.438130	-1.461997	-1.397568
47B	0.547062	-0.315847	3.330210
48B	0.547062	-3.245034	-0.812290
49B	-1.989688	1.148748	-0.812288
50B	3.083814	1.148748	-0.812286

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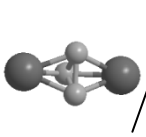
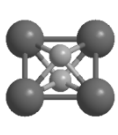
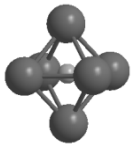
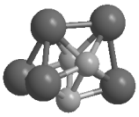
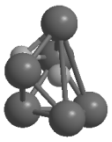
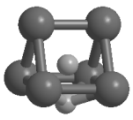
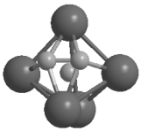
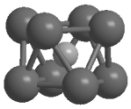
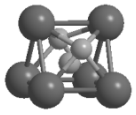
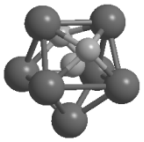
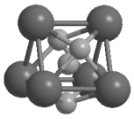
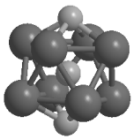
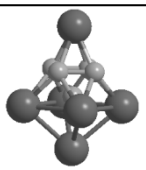
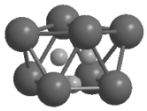
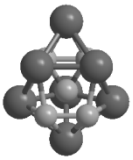
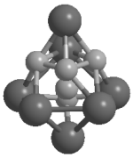
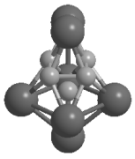
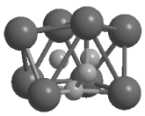
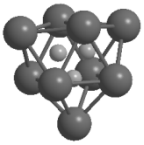
5/6						
7						
8						
9						
10						
11						
12						

Figure S1