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Supplemental Material for:

Global search for low-lying crystal structures using the artificial force induced reaction method: A case study on carbon

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CONTENTS:

S1. The full list of references on carbon crystal structures

S2. The derivation of Eq. (1)

S3. Initial structures

S4. Cartesian coordinate of all obtained MINs

S5. Primitive lattice of 3D-min10, 3D-min12, and 3D-min13

S6. Phonon dispersion curve of 3D-min10, 3D-min12, and 3D-min13

S7. Symmetry k-points of 3D-min10, 3D-min12, and 3D-min13

S1. The full list of references on carbon crystal structures

Carbon can take various forms,[1-247] such as diamond,[22-24] graphite,[25,47] lonsdaleite (hexagonal diamond),[27] fullerene[29,38] (or fullerite[44]) and related structures,[81-124] carbon nanotube (CNT)[41] and related structures,[125-139] graphene[60] and related structures,[140-172] graphene nanoribbon (GNR),[66,173-176] q-carbon,[77] carbyne,[79] graphyne[80] and related structures,[177-202] n-diamond,[203-214] and amorphous carbon.[215-247]

Furthermore, many stable structures have been predicted theoretically.[248-460] M-carbon,[313,324] 8-tetra(2,2) tubulane[127] (or bct C_4 [293,329]) or other names[132,288,305,308,332,334,348]) Cco-C_8[343] (or Z-carbon[345]), and so forth have been predicted recently from first principles.

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S2. The derivation of Eq. (1)[S1]

Suppose the unit cell h_0 with its volume $V_0 = \det h_0$. When an infinitesimal strain tensor (3×3) ε is applied to the system, the total energy E changes. The stress tensor (3×3) σ is defined as a conjugate intensive tensor to the strain. In this case, the energy change ΔE is described as,

$$\Delta E\big|_{h_0} = \mathrm{Tr}(\sigma\varepsilon)V_0 = V_0\sum_{i,j}\sigma_{ij}\varepsilon_{ji}$$

$$\sigma_{ij}\big|_{h_0} = -\frac{1}{V_0}\frac{\partial E}{\partial \varepsilon_{ij}}\bigg|_{h_0}$$

In the case, the unit cell matrix h with the strain ε is described as,

$$h = (\mathbf{I}+\varepsilon)h_0$$

where

$$h \equiv \{a_1, a_2, a_3\} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

$$\varepsilon = hh_0^{-1} - \mathbf{I}$$

$$\varepsilon_{kl} = \sum_m h_{km}(h_0^{-1})_{ml} - \delta_{kl}$$

$$\frac{\partial}{\partial h_{ij}} = \sum_{k,l}\frac{\partial \varepsilon_{kl}}{\partial h_{ij}}\frac{\partial}{\partial \varepsilon_{kl}} = \sum_{k,l}\sum_m \delta_{ki}\delta_{mj}(h_0^{-1})_{ml}\frac{\partial}{\partial \varepsilon_{kl}} = \sum_l (h_0^{-1})_{jl}\frac{\partial}{\partial \varepsilon_{il}}$$

$$\frac{\partial E}{\partial h_{ij}} = \sum_l (h_0^{-1})_{jl}\frac{\partial E}{\partial \varepsilon_{il}} = -V_0\sum_l (h_0^{-1})_{jl}\sigma_{il}$$

[S1] Y. Tateyama, Ph.D. thesis, The University of Tokyo, 1998.

S3. Initial structures

(i) 3D: random structure

C	0.137308413163	0.506599825145	-1.868353596046
C	0.454881030641	0.261893055938	-0.459650647353
C	-0.038572922682	-0.582719939072	1.856101415009
C	-0.553616521124	-0.185772942013	0.471902828391
TV	2.403797389080	0.633328610945	-0.618894291773
TV	-0.000000000000	2.485867546525	0.618802310954
TV	0.000000000000	-0.000000000000	4.655918444073

(ii) 3D: optimized structure from the random structure (i)

C	0.092861193378	0.549889344723	-1.863216378662
C	0.512456418314	0.219972286613	-0.457163965076
C	-0.092850046223	-0.549905060801	1.863215315444
C	-0.512467565473	-0.219956570536	0.457165028293
TV	2.421958222986	0.587673818868	-0.584585848161
TV	0.000000000000	2.492272339496	0.584417956901
TV	-0.000000000000	0.000000000000	4.640726338585

(iii) 2D: random structure

C	0.842413738951	-0.699941099220	-1.536504084107
C	-0.150809902139	0.330402959125	-0.417816714320
C	-0.668202549609	0.989342176372	0.929799430199
C	-0.023401287203	-0.619804036277	1.024521368228
TV	2.970616288560	0.000000000000	0.000000000000
TV	0.000000000000	3.149283275592	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

(iv) 2D: optimized structure from the random structure (iii)

C	0.980565465842	-0.000102994868	-1.199464635400
C	-0.326823115063	0.000028326091	-0.611024974393
C	-0.326844680284	0.689777160123	0.905223289939
C	-0.326897670489	-0.689702491349	0.905266319858
TV	2.614795654964	-0.000098341352	-0.000000000000
TV	-0.000000000000	2.724424929913	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

(v) 1D: random structure

C	1.156776368568	-0.019423438428	-0.006132277899
C	-0.000010435852	0.268348498411	-0.851570760546
C	0.000010488915	-0.229477135115	0.863831443902
C	-1.156776421628	-0.019447924867	-0.006128405456
TV	3.696192700632	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

(vi) 1D: optimized structure from the random structure (v)

C	1.144569087036	-0.069925312093	-0.020371337496
C	0.000009423911	0.310333337432	-0.807407316215
C	-0.000013133539	-0.170501186304	0.848170586744
C	-1.144565377405	-0.069906839033	-0.020391933034
TV	3.665894106167	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

S4. Cartesian coordinate of all obtained MINs

(i) 3D

Geometry of 3D-min0

C	1.147842342502	1.700352278037	-1.329375344457
C	0.428767591338	1.709003411360	-0.079152785827
C	-0.428741552599	-1.708991305308	1.320779273830
C	-1.147833049317	-1.700370464390	0.083533552347
C	1.147857918577	1.700402713041	1.158112265234
C	0.428725431963	1.708954131732	2.408313505717
C	-0.428762182926	-1.708981430634	3.808246706383
C	-1.147856499557	-1.700369333837	2.570996721426
TV	2.149992471718	-0.025740779877	1.238180962191
TV	0.000000000000	6.856836876772	-0.032611172401
TV	0.000000000000	-0.000000000000	4.974956273322

Energy = -45.570529730612 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min1

C	0.405369110385	0.552763705506	-1.824959361196
C	0.675571709636	0.112802143854	-0.362985362802
C	-0.405386411479	-0.550303999130	1.828868758790
C	-0.675439475849	-0.110274787025	0.366895068197
C	0.405366875369	2.977482038234	-1.095083402545
C	0.675573217955	2.537421249362	0.366863329458
C	-0.405465713987	1.874491466655	2.558520124925
C	-0.675589312031	2.314442884398	1.096520780613
TV	2.161987717042	1.326069148902	-0.000024381284
TV	-0.000000000000	4.849473585721	1.459415318269
TV	0.000000000000	0.000000000000	4.383515387665

Energy = -45.570244519236 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min2

C	0.605432750131	0.141260014007	-1.793105037990
C	0.605283799848	0.142115020721	-0.359307236904
C	-0.567227799250	-0.271446927687	1.792801566677
C	-0.567028465128	-0.272383616585	0.359017090652
C	2.950421925038	0.968718524912	-1.794263836776
C	2.950234725945	0.969685527814	-0.360475329362
C	1.777723039434	0.556044005542	1.791613250002
C	1.777904061989	0.555152929177	0.357810154968
TV	4.689891146422	1.654886230197	-0.002315819788
TV	0.000000000000	3.600048323482	-0.831403469444
TV	0.000000000000	0.000000000000	4.303045447497

Energy = -45.567833103166 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min3

C	0.444237167204	0.590494860246	-2.218197461915
C	1.168783875360	0.231477167647	-0.874471879349
C	-0.441555463037	-0.594171165173	2.214955959401
C	-1.166112077459	-0.235201547121	0.871237934065
C	2.377669225420	2.068775356942	-2.865652205534
C	3.102201319859	1.709782757150	-1.521916916538
C	1.491873792950	0.884095177567	1.567601360268
C	0.767307103894	1.243103620098	0.223896040019
TV	3.866840585532	2.956615427991	-1.294765113512
TV	0.000000000000	2.436282337615	0.650742739695
TV	0.000000000000	-0.000000000000	4.883867163692

Energy = -45.562067504289 hartree

Spin(**2) = 0.000000000000
Geometry of 3D-min4
C 1.212176941906 -0.093808709661 -2.578292416218
C 1.354923417360 -0.810307803587 -1.194246233594
C 0.415609237428 -1.044423141151 2.004990391184
C -0.266570247377 -0.398401440109 0.755815236717
C 2.833853349290 1.735814926358 -3.368451845660
C 2.151632854407 0.140290723453 -0.285570276543
C 2.631086628638 0.222339670170 2.302671035584
C -0.063993606487 1.115214185905 0.576680030028
TV 3.830369343544 3.094887565191 -0.489932551609
TV -0.000000000000 2.241509634113 1.159891031977
TV -0.000000000000 0.000000000000 5.491927687343
Energy = -45.531893603257 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min5
C 2.189149416060 0.158812099638 -2.205207354864
C 1.774908934721 -1.469191860881 -0.324506390126
C 1.578693141590 -1.186248053872 4.816780525732
C -0.626202822465 0.063223822916 -1.703057192653
C 1.939068526338 1.796314932780 -4.134613194723
C 1.828504905812 -0.377526071080 0.595686125444
C 1.992901858590 0.441898590256 2.936017891070
C 0.064046165099 1.281735018525 -1.446779463805
TV 4.329982939335 2.519475374174 0.079661162215
TV -0.000000000000 2.445925134671 0.468339829334
TV -0.000000000000 -0.000000000000 6.618565158163
Energy = -45.522840925808 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min6
C 0.680589377711 -0.097183438006 -2.501549746526
C 1.603626449773 -0.662811942458 -1.436053846654
C -0.117983997144 -1.069842914003 2.038212277085
C -0.085348797439 -0.288273288562 0.565584616178
C 2.525567010527 1.370316234592 -2.561680430851
C 2.493307330709 0.588595142802 -1.088932112058
C 1.726816246300 0.397666125054 1.978290573898
C 0.804237528095 0.963170724985 0.912537641614
TV 3.968769930673 2.775725591636 0.179254095906
TV 0.000000000000 2.240643224156 1.188579449957
TV -0.000000000000 -0.000000000000 5.412386335325
Energy = -45.521115656061 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min7
C 0.434642467764 0.585751164355 -1.434825044893
C 1.549272270506 0.166195014333 -0.402145817505
C -0.434650557144 -0.581237745477 1.435756324619
C -1.549338980702 -0.161679014351 0.403130446457
C 0.434681723552 2.919873158648 -0.485605182465
C 1.549334266881 2.500343251205 0.547036672146
C -0.434692757143 1.752911406671 2.384938981545
C -1.549345380370 2.172529667664 1.352314804705
TV 3.098717902982 1.167293055634 0.474647601280
TV -0.000000000000 4.668350826935 1.898463346967
TV -0.000000000000 -0.000000000000 3.345159985802
Energy = -45.515956494259 hartree
Spin(**2) = 0.000000000000

Geometry of 3D-min8

C	0.605676167110	0.469837520152	-0.943358510340
C	1.494772744147	-0.314941464229	0.087441235918
C	-0.618406249520	-0.315327711287	1.910379675544
C	-1.507296029662	0.469629257761	0.879417238687
C	-0.158458021227	2.662028019789	-1.829347067009
C	2.258920575785	1.877390037998	0.973090256569
C	0.145675601640	1.877228012310	2.796020710399
C	-2.271441196513	2.661861705837	-0.006400660672
TV	3.306325540160	0.000401636668	0.490518091109
TV	0.000000000000	4.384756331796	-0.000339110841
TV	-0.000000000000	-0.000000000000	3.342638348226

Energy = -45.512974765684 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min9

C	1.465203757298	0.274401334650	-1.774549946771
C	0.624092824785	-0.381044809390	-0.589518983294
C	-1.154779536211	-0.113085783197	1.325718607425
C	-0.313584947219	0.542320632303	0.140641769861
C	2.836813798386	2.002393744022	-0.161069549227
C	3.690280397451	3.091894663588	-0.808969774429
C	0.623984119444	-2.042322532815	1.189495364966
C	1.477301333208	-0.952474540542	0.542064827573
TV	4.003659608196	0.888512838190	0.829671302154
TV	-0.000000000000	3.454217430539	-0.236837359590
TV	0.000000000000	0.000000000000	3.462413900379

Energy = -45.512927947066 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min10

C	2.136402982649	0.158049361446	-3.679661372793
C	1.059492142464	-1.013887670602	0.179651657614
C	1.707645353553	-1.241523626776	5.234918810659
C	0.648861323044	-0.593531199539	-1.203533334750
C	1.568633011207	1.974670024174	-5.349054009244
C	1.217841304813	-0.013112750680	1.193179809833
C	1.726560586248	0.579092359354	3.551677618173
C	1.077746055289	0.806093454566	-1.503428624014
TV	3.221635236593	3.139231726558	-1.722025205550
TV	0.000000000000	2.396185854581	0.727728020202
TV	0.000000000000	0.000000000000	8.614812782519

Energy = -45.504929533754 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min11

C	1.341397852353	-1.048617893022	-1.379103125827
C	0.621256443074	-0.303606881619	-0.417575928865
C	-0.669589855731	0.866733232556	1.147959122773
C	-0.689048059087	-0.213070889066	0.107633232012
C	2.754173348843	-0.542565753572	-1.357148803440
C	2.773004226800	0.537628118631	-0.317239300477
C	0.743077023255	1.372647760513	1.169683904236
C	1.462743470544	0.627822236440	0.207758911948
TV	4.515656684151	1.570829793917	0.023211946237
TV	0.000000000000	3.430159178244	-1.485003379439
TV	0.000000000000	0.000000000000	4.812796978416

Energy = -45.500391031008 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min12

C	2.740750343098	-0.240644765646	0.118692092223
C	0.617790029518	-1.407088222927	-0.357738198707
C	1.994638403756	-1.407445391064	2.981734111647
C	-1.341759869145	0.181044590711	-0.916291536797
C	4.117709963704	2.092968988831	-2.268335426186
C	-0.188620663359	-0.240180526603	0.118041409142
C	4.924187464632	0.925997541698	0.595296915940
C	-1.341592095382	1.672097872761	-1.235206450355
TV	7.418989494500	3.500285722298	-1.910025935294
TV	-0.000000000000	2.333822584529	0.951787500582
TV	0.000000000000	-0.000000000000	3.339271987206

Energy = -45.496013269734 hartree

Spin(**2) = 0.015380859375

Geometry of 3D-min13

C	2.584713085332	0.150977112963	-1.309410765998
C	0.814647411994	-1.443118293242	-0.591913056108
C	1.680735538543	-0.990733068438	1.892935719528
C	-1.369639220483	-0.123232164825	-0.405316760588
C	2.895847437299	2.022064718831	-2.802570294938
C	1.369048141474	-0.490411762193	0.488080352588
C	3.450666033668	0.604043424293	1.175382552001
C	-0.684948302073	0.979428510880	0.087133199590
TV	6.320093595183	3.046124012115	-1.152437956193
TV	-0.000000000000	2.370732181092	0.844850425698
TV	-0.000000000000	-0.000000000000	3.743104937331

Energy = -45.494461750714 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min14

C	0.728394362085	-0.331222774423	-1.849159152283
C	0.728346011775	-0.331330819059	-0.436432927647
C	-0.640909513456	-0.330913305859	1.766418649283
C	-0.640931204532	-0.330946144533	0.193928852156
C	3.309667139158	-0.331773334279	-1.929009781441
C	3.309674698622	-0.331820006310	-0.356440293856
C	1.940370749067	-0.331603252200	1.686409465481
C	1.940272251733	-0.331691561442	0.273711510514
TV	4.719209632579	-1.303900273699	-0.000095664302
TV	-0.000000000000	2.606067978978	-0.000084629449
TV	-0.000000000000	-0.000000000000	4.245699041938

Energy = -45.491477155693 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min15

C	0.573286827500	0.443199188233	-2.196201804195
C	0.604863042491	0.396922609287	-0.620225346997
C	-0.036815094160	-0.935744413933	2.772099836616
C	-0.902134739025	0.350847444807	-0.320235206037
C	0.598731220642	2.690982893282	-1.472255955126
C	0.579820669481	2.719396739971	0.744122932962
C	-0.294357039749	1.733130249271	2.966849086054
C	-0.643971521577	2.252567793485	1.573240444753
TV	2.117230493444	1.424837361761	-0.000522063017
TV	0.000000000000	4.570322195256	2.088477607211
TV	0.000000000000	-0.000000000000	5.267894587602

Energy = -45.489765078948 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min16

C	1.206348012942	-0.207991239666	-2.597912466368

C	1.305932442615	-0.912468045678	-1.252108092004
C	0.374767200236	-1.161309200759	1.985622923566
C	0.275020470744	-0.457227046624	0.639807068184
C	2.831259180199	1.669681922014	-3.424829660771
C	1.685853419918	-0.134360943001	0.022580125878
C	2.635752762530	0.118957356527	2.299851864933
C	-0.104670555960	1.033655371066	0.552577082572
TV	3.885758268228	3.158236214823	-0.512852001163
TV	0.000000000000	2.269032612186	1.187431766168
TV	0.000000000000	-0.000000000000	5.523178162857

Energy = -45.487520026995 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min17

C	2.590099679054	-0.227559403549	-0.177796906202
C	0.409171770359	-1.469774978001	-0.448040995473
C	1.895887253886	-1.424808810435	2.924677959836
C	-1.320550876472	-0.056989900339	-0.619646690758
C	4.031040506129	2.168459310513	-2.896761743750
C	-0.266759141680	-0.500838997379	0.530401118905
C	4.725375329273	1.021914316906	0.074508893366
C	-0.644691070746	1.318152127689	-0.694001154880
TV	7.532618830826	3.468181931760	-2.008135941180
TV	0.000000000000	2.344004755483	0.904278236248
TV	0.000000000000	0.000000000000	3.489119091286

Energy = -45.487394454610 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min18

C	2.715860969186	-0.640915839647	-1.262438433536
C	0.545596387009	-1.692550773732	-1.963633814212
C	1.900596906294	-1.691999446727	2.585656686551
C	-2.226547365819	0.839029443807	-1.201655990337
C	3.825878541541	-0.019530820761	-2.192462192933
C	-0.269596398551	-0.641713227846	-1.260923945198
C	4.672794032258	0.839745587182	3.347165964496
C	-1.379543779984	2.081777686129	-0.786466743879
TV	6.052399165702	0.000483694551	2.273416153854
TV	-0.000000000000	2.102135599854	1.404476740296
TV	-0.000000000000	-0.000000000006	4.550185802624

Energy = -45.486786878307 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min19

C	1.964379883144	1.483350915231	-4.950862436638
C	0.798699974743	-2.716290515858	3.516703237648
C	1.964426326512	-0.067285443686	-0.398898641011
C	-0.804466597285	-0.618138797110	0.414820289192
C	3.228154426725	3.581376790695	-5.791607185985
C	0.798485612549	-2.161942307341	4.957712549722
C	3.228216991291	2.030941326544	-1.239747283497
C	-0.804432910472	-0.063731337462	1.855934184841
TV	5.198492389804	4.196082642127	-3.941274003988
TV	0.000000000000	2.098230371687	1.419551414208
TV	0.000000000000	0.000000000000	4.520612723925

Energy = -45.486323910529 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min20

C	2.847938174009	0.559537988219	-2.752698069453
C	1.846366945078	-1.053508944448	-1.108067369649

C	2.467653527630	-0.814676388937	4.004117407435
C	-0.686930795957	-1.306439856046	0.138545217937
C	2.045094005130	2.200054828127	-4.530582799973
C	1.466218719339	0.027960994627	-0.138420259849
C	2.270318347697	0.843472236302	2.138578172690
C	-0.030323176537	-0.041088822932	0.204031278998
TV	5.031619094293	4.391126326074	-2.733661860841
TV	0.000000000000	2.455850942775	0.499675023103
TV	-0.000000000000	-0.000000000000	6.287008656834

Energy = -45.483380070490 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min21

C	2.507964424628	0.093185196234	-1.168898393994
C	0.786022130730	-1.502478627921	-0.426527884847
C	1.648399488188	-1.037267765099	2.114585542030
C	-1.293961555618	-0.025103193656	-0.825889953770
C	2.807300673187	2.023674359936	-2.885186473100
C	1.349109896953	-0.539590117581	0.668087026344
C	3.666914033808	0.758622667438	0.789597007669
C	-0.730678966119	0.937975958919	0.268554075738
TV	5.260297298204	2.681362340601	-0.004660543439
TV	0.000000000000	2.395646971541	0.824880535436
TV	-0.000000000000	-0.000000000000	3.891582588991

Energy = -45.480509839315 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min22

C	0.183000306146	0.613787879244	-1.710696606777
C	2.016927839182	-0.288822135061	0.280022407723
C	-0.194566046712	-0.700332763906	2.130702660439
C	-2.028254165691	0.202132584447	0.140264155520
C	0.523755741524	2.875321105135	-0.668405337419
C	1.548675372160	2.239415912725	0.414851516399
C	-0.535178317797	1.851555370521	2.158919576283
C	-1.560206834139	2.487308447306	1.075682524851
TV	3.269828667321	0.608576126477	0.652917130555
TV	-0.000000000000	4.813418833090	1.070436107689
TV	-0.000000000000	-0.000000000000	3.389464345615

Energy = -45.480291879171 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min23

C	0.691946108924	0.088530948981	-3.668353467313
C	2.639460117258	0.087358332347	-1.720653424735
C	2.639291866389	-1.176266139231	2.725112524968
C	-0.668761615952	-2.438513746465	1.585877783247
C	1.500883956835	1.352113401376	-3.667978935711
C	2.639891277128	0.087359301898	-0.360157155830
C	2.639817620682	1.351249921539	0.448821662398
C	-1.477796503689	-1.174855421400	1.585603743356
TV	5.255595090023	2.526657615249	0.001620556440
TV	0.000000000000	2.527504520661	0.000021919636
TV	0.000000000000	0.000000000000	5.254828735573

Energy = -45.479469466415 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min24

C	-0.092137360674	0.524008224653	-1.775953012458
C	1.098337533188	0.159856279964	0.622057546612
C	0.089967029153	-0.318775348811	2.791036259311

C	-1.100542796086	0.045334625608	0.392868217483
C	0.551725479154	2.921407306422	-1.041226049143
C	1.742232771553	2.557136355640	-0.112943940288
C	-0.554168591537	1.915375899251	2.055975111151
C	-1.744565378761	2.279448481307	1.127525874028
TV	3.304819114453	1.120626937809	-0.000049812486
TV	-0.000000000000	4.631268966482	-0.000428347125
TV	0.000000000000	-0.000000000000	3.326383285654

Energy = -45.479159596253 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min25

C	1.487129926801	0.232847425251	-1.794637064327
C	0.568024701411	-0.347069448465	-0.631517051857
C	-1.607831082993	0.890596814404	0.513677976693
C	-0.218675852982	0.856465092747	-0.107375609132
C	2.739058557852	1.881022626857	-0.210296094391
C	4.128263665401	1.915510371856	0.410572219161
C	0.666207860375	-2.080112203454	1.151984030638
C	1.487133971285	-0.927177970576	0.531403909317
TV	4.346945383297	0.000385955644	1.710703300752
TV	-0.000000000000	3.465859130157	-0.144426062284
TV	0.000000000000	-0.000000000000	3.422616713523

Energy = -45.479030238690 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min26

C	0.630501536095	0.394760667460	-1.006540188534
C	1.537193961129	-0.348504192163	0.033313203476
C	-0.637069353365	-0.333509422278	1.976156719196
C	-1.563591103149	0.409746471650	0.953810363357
C	-0.225207143699	2.684484635233	-1.961268523078
C	1.873229850389	1.932980707700	1.400995432600
C	0.701211736717	1.941172583344	2.448132235161
C	-2.399753351004	2.699459372051	-0.018595342185
TV	3.366197411024	-0.023238675977	0.379635853287
TV	0.000000000000	4.420642892757	-0.032925980872
TV	0.000000000000	-0.000000000000	3.387020818595

Energy = -45.477590988805 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min27

C	0.613302864264	0.110325500959	-1.866158604252
C	0.751804716970	0.544259921552	-0.441560829345
C	-0.256685063835	1.195994778157	1.700729829669
C	-0.549919342676	0.760503727800	0.268331498401
C	3.169036343645	0.123471214235	-1.823950689156
C	3.307671180478	0.557326558353	-0.399254872742
C	1.943365324846	-0.124183702644	1.664688462849
C	1.977367548770	0.791716124593	0.371944037024
TV	4.727457594032	1.107921977282	-0.660770486370
TV	0.000000000000	2.396680539955	-0.728493260239
TV	0.000000000000	0.000000000000	4.302241985688

Energy = -45.475639931313 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min28

C	0.477633719501	0.512981629094	-1.483476008794
C	1.583789442287	0.141548099461	-0.437746381315
C	-0.438943074212	-0.621815804360	1.473396384943
C	-1.567098438478	-0.258803577613	0.448356169821

C	0.511321768061	2.982877679736	-0.437631810544
C	1.023388238282	2.386967915535	0.863211694354
C	-0.073376418128	1.973060657061	1.899556189734
C	-1.511142042234	2.219515779653	1.473344853342
TV	3.141565229032	1.185711341942	0.414771200136
TV	0.000000000000	4.754521713963	1.898828532381
TV	-0.000000000000	0.000000000000	3.383051400278

Energy = -45.470826800991 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min29

C	0.234133466259	1.428679246598	-1.260032013467
C	0.494977740141	0.658550622511	0.001265552220
C	-0.234146065517	-1.428691857142	1.262375168376
C	-0.495001060696	-0.658568586012	0.001036674620
C	0.234123101224	1.428689909809	1.262615129026
C	0.494992039055	0.658565951129	2.523912434384
C	-0.234097786070	-1.428680566590	3.785026456133
C	-0.494981434420	-0.658544720327	2.523703956450
TV	2.561772141209	0.832762127440	2.522413548399
TV	-0.000000000000	4.133578060858	0.000117248557
TV	-0.000000000000	-0.000000000000	5.045330412955

Energy = -45.470132643319 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min30

C	-0.377548437954	1.096206708388	-1.365193187687
C	1.271435326983	-1.635666260866	0.156172394759
C	-1.020865567380	0.256943455094	3.574212493927
C	-2.519480492506	0.587500016965	0.258755689901
C	1.721503581243	3.903925731690	-1.538174316097
C	0.768069233292	2.727323121531	0.292511655922
C	-1.373750217606	2.218611307941	1.916452043199
C	-0.730546980603	3.057847074708	0.708080882719
TV	2.372210676140	-0.523244115257	0.898769230464
TV	0.000000000000	5.638892114913	-0.449724796424
TV	-0.000000000000	-0.000000000000	3.730978854909

Energy = -45.468301021076 hartree
Spin(**2) = 0.066405687500
Geometry of 3D-min31

C	2.873964243882	0.398432626535	-1.925859375573
C	-0.136275802771	-1.833745488897	0.616306896254
C	2.045104735949	-0.718122366030	1.196672142523
C	-1.157335893449	0.062795281687	-0.758357635030
C	3.895021077617	2.294892843602	-3.300179537247
C	0.692635895918	-0.717245430215	1.195463607337
C	3.895043278319	0.735479814157	0.606407254690
C	-1.157332510329	0.737139296622	0.604385749928
TV	6.408287407878	2.231806031476	-0.691330058615
TV	0.000000000000	2.233506416522	1.157504787964
TV	-0.000000000000	0.000000000000	3.701678398173

Energy = -45.467700647637 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min32

C	1.098282583314	0.086617644207	-3.364009381248
C	2.290906372912	0.086354613919	-2.200457553289
C	2.899049445377	-1.172010256773	2.563429655111
C	-0.355932029159	-2.429548319271	2.280652050483
C	1.706733504885	1.344849037070	-3.987574078689

C	2.069354442312	0.086749759724	-0.740557030500
C	1.928836549907	1.345106893270	-0.060579170273
C	-1.032498041994	-1.171142773115	2.437368238798
TV	5.385683126789	-0.000567880776	-0.130922093111
TV	0.000000000000	2.516638142091	-0.000321587865
TV	0.000000000000	-0.000000000000	5.386945860513

Energy = -45.464469464761 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min33

C	0.296515563306	-0.660661137102	-1.174069665025
C	0.960513836814	0.319980935136	-0.173724663710
C	-0.085066384147	-0.126172697766	0.957816361512
C	-0.748977838769	-1.106738427340	-0.042647006441
C	0.296511491531	1.719368849039	-0.236203775538
C	0.960558373960	2.699998898047	0.764123036000
C	-0.085038016212	2.253869528974	1.895654094925
C	-0.748972043092	1.273281624519	0.895233339372
TV	3.207234794508	1.368069044752	0.017099844300
TV	-0.000000000000	4.760066681133	1.875721058391
TV	-0.000000000000	0.000000000000	3.487636197121

Energy = -45.463158139216 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min34

C	0.646248714271	-0.124881907718	-1.775871539520
C	0.646216348065	-0.280500521281	-0.331631165128
C	-0.573989113657	0.142946627780	1.771123293975
C	-0.574096087331	-0.547810732864	0.452458306017
C	3.074010856593	-0.549392949768	-1.713120351179
C	3.074129581403	0.141275493129	-0.394465786106
C	1.853780857203	-0.281263923710	1.833938735114
C	1.853767068154	-0.125473794046	0.389745789611
TV	4.641886589545	1.587791542579	-0.470755560274
TV	-0.000000000000	3.178564869059	-0.940758645119
TV	-0.000000000000	0.000000000000	4.331156453739

Energy = -45.462466076255 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min35

C	0.545673839836	-0.018637084190	-1.856891036026
C	0.679794426705	0.233508927215	-0.389388839827
C	-0.309128080364	1.085411489972	1.753357822179
C	-0.590044084804	0.566895537105	0.330006193937
C	3.035335018113	-0.387377990869	-1.868202666070
C	3.169469647162	-0.135221336487	-0.400668502578
C	1.866922158987	-0.112890759637	1.752295465156
C	1.848237513209	-0.040941512317	0.315460175405
TV	4.614135435429	0.788812367802	-0.679420082055
TV	-0.000000000000	2.595068684754	-0.663718592194
TV	0.000000000000	0.000000000000	4.325316904111

Energy = -45.458932630324 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min36

C	2.458814227963	1.124626494191	-2.568558553320
C	2.450976879806	-0.326834974994	-0.035069933983
C	2.457089282713	-0.327120372777	4.952236604278
C	-0.779225877394	-1.270396156337	-0.531340403716
C	2.442514154389	1.858458738942	-6.314946595017
C	2.444656737576	1.124439055999	-0.074994750143

C	2.446846485137	1.124534981925	2.418919602697
C	-0.867497567981	-0.078557341034	-1.044076392652
TV	6.553505776633	2.200926944046	1.199722023496
TV	-0.000000000000	2.185699711940	-1.292416869575
TV	0.000000000000	0.000000000001	7.481052821104

Energy = -45.456334785017 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min37

C	2.194872234520	1.738074619349	-5.669884913960
C	0.295296223551	-2.082501635772	3.233625223478
C	1.935210949085	0.255995799254	-0.710370114601
C	0.008354055676	-0.673288783682	0.856637357441
C	2.907490096463	3.879448526713	-6.823637210408
C	-0.069871081210	-2.091327955104	5.708223417094
C	2.647825422577	2.397812487165	-1.864742073122
C	-0.357843174017	-0.682690259217	3.331093255492
TV	4.904517733956	4.742813203042	-5.542486083632
TV	-0.000000000000	2.157013564481	1.278897745258
TV	0.000000000000	0.000000000000	4.917962792061

Energy = -45.456231298966 hartree
Spin(**2) = 0.015380859375
Geometry of 3D-min38

C	1.995608841000	1.719497301529	-1.770840216177
C	1.992809736273	-1.049882148420	-0.846712006629
C	1.996302488602	0.610843161692	3.857015034307
C	-1.400639172531	-1.708133604799	-1.844013563523
C	1.994338726153	2.269974164690	-4.569246032630
C	1.992611221754	0.058913234164	0.090172765455
C	1.995384923652	0.888684000252	2.442303557678
C	-1.242331408287	-0.483496106089	-1.483332488414
TV	6.629780105298	3.540030934128	0.845378535733
TV	-0.000000000001	2.490056411825	0.490878811877
TV	-0.000000000000	0.000000000001	6.564502716793

Energy = -45.456171213848 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min39

C	3.334984550256	0.314878455659	-1.887159829486
C	1.315319044850	-1.049006633129	-1.358631429970
C	2.673106734789	-0.975769096138	5.330422405602
C	-1.349329944848	-1.201751471478	-0.355892382912
C	1.954119969686	2.065176666491	-4.596422894403
C	0.653340011936	0.168694129071	-0.928205432855
C	1.950099391187	0.842304989809	2.183909608489
C	-0.692487134271	0.091142469654	-0.418234541369
TV	6.029624958036	4.102489051537	-1.658749865873
TV	0.000000000000	2.508380955366	0.383478063682
TV	0.000000000000	0.000000000000	7.170214817165

Energy = -45.456056225265 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min40

C	4.015555749826	0.813284338194	-2.439377455781
C	2.079806408921	-0.521820626980	-1.609937655750
C	3.382014009665	-0.475592051548	5.131459976980
C	-0.509697863266	-0.610701856911	-0.420747792765
C	1.130107033629	0.574385263373	-4.676061743095
C	1.439137601857	0.722127377077	-1.221901769158
C	1.192452895029	-0.683330567803	2.403111215351

C 0.127919208427 0.677401788256 -0.624453982521
TV 5.823452691892 4.002359805388 -2.454301201889
TV 0.000000000000 2.531411365309 0.190006949342
TV 0.000000000000 -0.000000000000 7.357752974787
Energy = -45.455930395635 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min41
C 2.384044636641 1.886152128172 -2.184186679076
C 2.377430784846 0.217397276396 -0.327486496044
C 2.383925451490 -2.005006123398 4.322532798492
C -0.818677925266 -1.454937475481 -1.473707322222
C 2.374527444993 1.051556706223 -4.536127675831
C 2.375027695225 -1.170839297672 0.113856552536
C 2.376997573521 -0.336625173917 2.466924885713
C -0.820218241477 -0.272159573903 -1.238493153256
TV 6.394783429002 0.814093971765 2.360168828075
TV -0.000000000000 2.502993838846 0.496152581474
TV -0.000000000000 -0.000000000000 6.561514434140
Energy = -45.455918525609 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min42
C 2.359348923297 0.905237881345 -3.131483259656
C 2.360949251264 -0.763423472117 -1.276133827491
C 2.360113256752 -0.483003556501 3.870442982096
C -0.865164515233 -1.616749830233 -0.020093799677
C 2.358727618803 2.574362597618 -4.986853299730
C 2.360534965789 0.351438717861 -0.338502115625
C 2.358315820837 1.186066612405 2.015188416103
C -0.865280566800 -0.433909829210 0.212678184577
TV 6.451797148388 2.477218601002 0.548833280284
TV 0.000000000000 2.502999939562 0.496443574799
TV 0.000000000000 -0.000000000000 6.560712521630
Energy = -45.455655400566 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min43
C 1.332666040747 -1.346985887596 -1.018635070647
C 0.621977873763 -0.484757900970 -0.183756320418
C -0.767394007742 0.939379128727 1.214041625950
C -0.813054251095 -0.266344062600 0.131069311909
C 2.836892203491 -1.055578052370 -0.872512843258
C 2.882887579692 0.149843285058 0.210635583200
C 0.736957680223 1.230710726740 1.359880716584
C 1.447877188092 0.367612151309 0.526045600629
TV 4.370994066379 1.777834748511 -0.305820836755
TV 0.000000000000 3.564216978271 -0.399471628937
TV -0.000000000000 -0.000000000000 3.566371783013
Energy = -45.454845629572 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min44
C 2.403203824661 0.087444843790 -1.770160094662
C 1.347272702931 -1.552778239122 -0.200084292626
C 1.659626972181 -1.237979842639 4.475461595557
C -0.293470874876 0.250722758326 -2.516139543482
C 1.661222566391 1.736954081015 -3.382290372015
C 1.347971950715 -0.426548912452 0.753666186011
C 2.404456423774 0.411297173192 2.864200492573
C 0.539555916854 1.488964604932 -2.245310555956

TV	4.018628337194	2.475462695431	0.543247856412
TV	-0.000000000000	2.477131547612	0.539706677082
TV	0.000000000000	0.000000000000	6.121679226638

Energy = -45.454149597685 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min45

C	1.952936732713	-1.330576676248	-3.549868594817
C	1.962200989100	-1.880533602625	-0.749926528897
C	1.949563881739	-2.708375653923	3.464736367337
C	-1.254742232741	1.666109866185	0.565407375669
C	1.967521317034	0.325159625967	-5.412919071396
C	1.956016768050	-0.502793814944	-1.198004841323
C	1.964868440883	-1.052668976971	1.601704466548
C	-1.251321349515	2.858880509466	1.056719918177
TV	6.412106318023	-0.796520262734	-2.362050631443
TV	-0.000000000000	2.483776600420	0.487749793457
TV	-0.000000000000	0.000000000001	6.566065623459

Energy = -45.453519751301 hartree
Spin(**2) = 0.312500000000
Geometry of 3D-min46

C	2.368818754859	-0.077274563779	-3.159914478276
C	2.371918429400	-1.734113519426	-1.296628468794
C	2.370189359873	-1.455486830154	3.855759280766
C	-0.860652961678	0.460973929557	0.688523116763
C	2.367840056920	1.578230511810	-5.022907764321
C	2.371090509405	-0.628049768136	-0.360460877515
C	2.367079214586	0.200302267645	1.991919329007
C	-0.854903458667	1.750564551771	0.689612190090
TV	6.452323315576	2.429836934135	0.625556790223
TV	0.000000000000	2.484260377706	0.487676632386
TV	0.000000000000	0.000000000000	6.566556064111

Energy = -45.453340341181 hartree
Spin(**2) = 0.312500000000
Geometry of 3D-min47

C	2.304492528556	-0.139214087953	-2.528749744310
C	2.304637596583	-1.799493853670	-0.668595044163
C	2.304814868928	-1.520759607832	4.480878281437
C	-1.082110595283	-1.573666937933	-1.402711815624
C	2.304161311946	2.630216124617	-3.452813843678
C	2.304598719606	-0.690432904688	0.268106954192
C	2.304327946465	1.521332598502	2.173627443141
C	-0.927918799353	-0.313050823573	-1.234489607400
TV	6.625817500084	1.109545188698	0.229800564127
TV	0.000000000000	2.490590366810	0.490692856810
TV	-0.000000000000	-0.000000000000	6.563896915275

Energy = -45.453090703134 hartree
Spin(**2) = 0.750000000000
Geometry of 3D-min48

C	2.529149305403	0.082068785694	-2.944725857443
C	2.526485825606	-1.578578531946	-1.083676926597
C	2.527704874888	-1.299838423036	4.064896187958
C	-0.854564336301	-0.183779192449	0.688978578164
C	2.531038850202	1.742667345880	-4.805098039467
C	2.527721034208	-0.469350974250	-0.147209651730
C	2.531220361396	0.360989774474	2.203909178820
C	-0.727812196830	1.084808499308	0.819710103725
TV	6.653867585728	0.118815679068	-0.194305089873

TV	0.000000000000	2.490901346543	0.490836578541
TV	0.000000000000	0.000000000000	6.563220582255

Energy = -45.453070380767 hartree
Spin(**2) = 0.750000000000
Geometry of 3D-min49

C	2.167378768917	0.753963638118	-4.223927846795
C	0.266298287607	-2.209760916002	0.413738834951
C	2.167225638547	-0.774183603353	-0.198362951383
C	-0.738895183841	-0.345515193012	-0.993494128007
C	3.494283481455	3.019288194313	-1.066170650992
C	1.162179391069	-1.109815695438	1.018538436102
C	3.494393085041	1.359324090882	2.898704393672
C	-0.739061526771	0.326197429285	0.407665463867
TV	5.560069810158	3.298905102563	1.814130599484
TV	-0.000000000000	2.199922764946	1.210035560601
TV	0.000000000000	-0.000000000000	3.834545754402

Energy = -45.452946609099 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min50

C	2.317782928818	-0.050678627345	-0.959490161544
C	0.632986002775	-1.700664010968	-0.050291199343
C	1.366995359088	-1.326508624720	3.769778271316
C	-0.657665030054	-0.068062945490	-2.101476320844
C	2.486533073274	1.322010218151	-3.007359632474
C	1.027177158263	-0.816174882557	1.231099826112
C	3.123018259282	1.666013373692	1.015975567692
C	0.293036801326	1.207935723509	-1.664451752628
TV	3.949759066775	3.106430497717	1.069510023749
TV	0.000000000000	2.398363795281	0.924942654468
TV	0.000000000000	0.000000000000	5.165695758192

Energy = -45.450188867554 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min51

C	3.035254898904	1.076385041895	-0.271416508313
C	1.604558620768	-1.446248511060	-0.734094557260
C	3.035310418044	1.076593886871	1.167009792362
C	-1.212159933006	-1.446461514238	-1.479399646916
C	0.782101961248	2.338608948624	-2.628770007116
C	0.781955075911	-0.184704736603	-0.328785168481
C	1.604606174687	1.077063461386	1.629890339025
C	-0.307541859956	-0.184836573875	-1.479087193245
TV	5.216440289919	2.522911921464	0.000501581829
TV	0.000000000000	2.523363679957	0.000144057144
TV	-0.000000000000	0.000000000000	3.853991062115

Energy = -45.449899466757 hartree
Spin(**2) = 0.015380859375
Geometry of 3D-min52

C	0.079285171884	0.430167229963	-0.563157913443
C	1.063785823509	-0.219265653546	0.454337684523
C	-0.078574229239	-0.219389663906	1.560336448239
C	-1.062931220314	0.430113575074	0.542840967947
C	-0.078714733977	2.647154321613	-1.914116800448
C	2.408303708315	1.997777318697	0.657342584666
C	0.079241919570	1.997597774856	2.911178247491
C	-2.407737068193	2.646873775682	0.339724457854
TV	3.471440615696	0.000402752233	0.114545756768
TV	0.000000000000	4.433868226694	-0.000064395953

TV	0.000000000000	0.000000000000	3.474345321287

Energy = -45.449508931864 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min53

C	0.340377671945	-0.779465303224	-1.942527474259
C	0.340333098066	-0.779388107330	-0.348424461840
C	-0.021149739346	0.544037246671	1.742151377402
C	-0.021082538685	0.544160068065	0.328359127039
C	2.180694505131	2.353740527432	-1.845309453757
C	2.180987922123	2.353956600183	-0.446078836726
C	1.780518786921	-1.116722636849	1.843291605389
C	1.780424339592	-1.116752993029	0.227516414307
TV	2.508840425509	0.681551703357	0.000051681539
TV	0.000000000000	4.936781646770	-2.181240768361
TV	0.000000000000	-0.000000000000	4.361760171908

Energy = -45.447974942264 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min54

C	1.802400226834	0.770341270804	-1.230071288045
C	1.108278619028	-0.140670610696	-0.356915053428
C	-1.062985702003	-0.836755621201	0.834025575069
C	-0.344149787006	0.153995390092	-0.114830369148
C	3.255197612591	2.203576132613	0.333250223173
C	3.973789908143	3.194429311471	-0.615711584768
C	1.108494731252	-1.973269878265	1.292590628287
C	1.802789066432	-1.062019536413	0.419751896845
TV	4.318067380490	1.834941957266	1.804499366943
TV	0.000000000000	3.560353480002	0.155254671315
TV	-0.000000000000	0.000000000000	3.564319639490

Energy = -45.447840403049 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min55

C	0.615862947842	0.236955199399	-1.825632215055
C	0.622716329785	0.372762971313	-0.411217607827
C	-0.577818121388	0.530103388180	1.756526899194
C	-0.725135807122	0.327287631984	0.282219423540
C	3.068622216794	-0.022255158153	-1.770325049283
C	3.204845575942	0.477315590205	-0.370413932727
C	1.837035238668	-0.166454308071	1.679539535555
C	1.855909782971	0.725574670123	0.397378364528
TV	4.821252270645	1.538861400389	-0.636779054395
TV	-0.000000000000	2.480729862850	-0.739297529069
TV	0.000000000000	-0.000000000000	4.285880495010

Energy = -45.446804476815 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min56

C	-0.453726031387	0.752156250575	-2.410241029025
C	2.575509895773	-1.147721743439	-1.224536925404
C	-0.453438379417	-0.363794451422	3.058153200165
C	-0.205948432537	0.681371968875	0.744958328424
C	-0.205961928428	2.693791329944	-0.781069922007
C	0.556336517152	1.828667582258	0.167999049538
C	-0.700648412888	2.145735580549	2.675602938379
C	-1.462897829695	3.011124608529	1.726770005568
TV	3.276180148284	-0.854969386752	-1.127452844947
TV	-0.000000000000	4.451143636059	1.246511845100
TV	0.000000000000	-0.000000000000	4.622054681802

Energy = -45.445323920709 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min57

C	-0.992080712678	-1.778575517484	-1.771768332765
C	0.847421971430	-0.155122780651	-0.416758065801
C	-0.443935048956	-0.545969140945	1.829883535627
C	-0.443828769859	-0.545959455209	0.278927515965
C	4.526043503027	-0.614846691819	-1.772083186013
C	2.686684941419	1.468263101377	-0.416590980176
C	2.138661166251	0.235536691946	1.829796069648
C	2.138758804116	0.235313769919	0.278881721492
TV	3.678635052333	3.246933699705	0.000023194043
TV	-0.000000000000	3.706541919990	0.000124781490
TV	0.000000000000	-0.000000000000	4.297218654262

Energy = -45.445252627052 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min58

C	0.610534267626	0.111046930830	-2.204622031744
C	1.365437008258	-0.265996640525	-0.902064472265
C	-0.243172823904	-0.887428343904	1.914886006445
C	-0.370395402003	0.024901662579	0.679867209283
C	2.650597018349	1.187908514891	-2.438140682747
C	2.778309076925	0.275547517062	-1.203329205507
C	1.796792045448	0.189324853637	1.681303938007
C	1.042307244180	0.566052713135	0.378475001755
TV	4.244804301969	2.432223881656	-0.084435732030
TV	-0.000000000000	2.360562612610	1.043295670858
TV	0.000000000000	0.000000000000	4.919467331913

Energy = -45.442832868889 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min59

C	0.642867024575	-0.021025578309	-2.133542469391
C	1.376571298234	-0.734648903323	-0.938073758633
C	-0.221006365580	-1.066233876513	1.985035227999
C	-0.463365565510	-0.310287600314	0.553444466279
C	2.628510071427	1.459698786875	-2.482723949094
C	2.871228075826	1.376209142352	-0.866173990543
C	1.764720940619	0.249341904809	1.590434593615
C	1.031285668930	0.248582768835	0.198008852444
TV	4.109048284086	2.760873783517	-0.615435751992
TV	0.000000000000	2.409109041524	0.663612085049
TV	0.000000000000	-0.000000000000	4.705966903985

Energy = -45.441430478560 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min60

C	1.722492981400	-0.280420566116	-1.986710102705
C	0.363328133833	0.372640192989	-1.879777112092
C	-1.250775066099	-0.238358424609	-0.093343806536
C	-0.390788287747	0.947818662808	-0.636802588986
C	3.254017171934	2.135095601597	0.600101345220
C	3.970898527243	2.705773058210	-0.641449090152
C	0.363369721303	-1.990593553893	0.613080373834
C	1.722582509848	-1.337240382019	4.281737933358
TV	4.504711454034	0.001398308165	1.779909211315
TV	0.000000000002	3.513448034195	-0.006910340079
TV	-0.000000000001	0.000000000000	3.562474359689

Energy = -45.440495098432 hartree

Spin(**2) = 0.000000000000
Geometry of 3D-min61
C 0.275163723372 0.632804847361 -1.834736113430
C 2.176629821890 -0.148343355404 0.339723316909
C -0.164419830733 -0.688989399648 1.960468414953
C -1.814741614886 0.025187305350 0.059152891080
C 0.052857682767 3.167370338884 -1.269983824065
C 1.749013697138 2.293630649004 0.763195463487
C -0.592099838645 1.753075019971 2.383898506748
C -1.592294482563 2.223933374200 1.134306571543
TV 3.123760734572 0.946722118368 0.834666737536
TV -0.000000000000 4.733130381360 1.639086838588
TV -0.000000000000 0.000000000000 3.663487738529
Energy = -45.439610101606 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min62
C 2.579180636400 -0.383503122872 -1.790523091199
C 0.438589885697 -1.452540304055 -2.481830761742
C 1.803848609376 -1.452413231060 2.201922280285
C -2.251688506489 1.087438603907 -1.718303571887
C 3.942157209945 -0.785634958008 -1.169616714900
C -0.366829505207 -0.383669434283 -1.789412010873
C 4.657563837846 0.047716439283 4.570804904937
C -1.536266979714 2.392430041230 -1.390536331707
TV 6.193516131950 -1.068477824968 3.990133474466
TV 0.000000000000 2.138166582091 1.384177522162
TV -0.000000000000 -0.000000000006 4.684337814829
Energy = -45.437334988718 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min63
C 1.122742942070 -0.762008634269 -2.426363577860
C 1.605346405070 -0.534715696533 -1.031784550540
C -0.141190826256 -0.614944551821 2.371262458567
C -0.623566542384 -0.842184442879 0.976610580344
C 2.335430006836 1.520401992402 -3.057444103309
C 3.459262063907 1.247623369742 -1.921907967666
C 2.369129489906 0.327126341055 1.066545152032
C 1.245357876474 0.599391826534 -0.069074452184
TV 3.722950536610 3.224029498273 -1.935686410361
TV 0.000000000000 2.569004258055 0.285174194867
TV 0.000000000000 -0.000000000000 5.171868368123
Energy = -45.435461325267 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min64
C 0.936486327358 -0.925451207559 -2.072328605690
C 0.936536248654 -0.925536122942 -0.494815872952
C -0.471995235092 -0.925465012674 1.701961721316
C -0.471854161061 -0.925473214390 0.111528106886
C 3.159129715685 0.364982473583 -2.698869047090
C 3.159293570951 0.364929210769 0.132063278117
C 1.603220134911 0.365068203636 1.721582735952
C 1.603365438236 0.365018044666 0.090633380127
TV 4.468731346593 -0.000138414057 -0.000078875516
TV 0.000000000000 2.580985204334 -0.000373451241
TV -0.000000000000 0.000000000000 4.380139363710
Energy = -45.433933656548 hartree
Spin(**2) = 0.000000000000

Geometry of 3D-min65

C	0.186700131315	0.620370826578	-1.762148526168
C	2.081483632632	-0.240453518828	0.278163375394
C	-0.206687736460	-0.640806130733	2.231113296278
C	-2.098540886448	0.220314711458	0.188198753434
C	0.145084899745	2.744691949502	-0.242733753259
C	1.510830971503	2.214470354442	0.259722620775
C	-0.634489262675	1.839120852906	2.090755305552
C	-1.040699011293	2.537004338048	0.769221449760
TV	3.338258734142	0.584314623670	0.590757873455
TV	0.000000000000	4.865365342065	0.997684032556
TV	0.000000000000	0.000000000000	3.439966376702

Energy = -45.432820446521 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min66

C	0.638361204664	-0.075126072082	-1.684575311217
C	0.638361996165	-0.331203443108	-0.289583359494
C	-0.607036149236	0.370158737162	1.632061414970
C	-0.606971259436	-0.776503937714	0.458271627166
C	3.106801247202	-0.776337527606	-1.573932307468
C	3.106914371297	0.370157576567	-0.400241411573
C	1.861783450302	-0.330789425387	1.742620542974
C	1.861853363743	-0.075457616309	0.347556087433
TV	4.884051136053	1.276512212482	0.213216279257
TV	-0.000000000000	2.553048272077	0.426540796263
TV	0.000000000000	0.000000000000	4.064390452498

Energy = -45.432445419836 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min67

C	0.582553974096	-0.140948041488	-1.850521119456
C	0.582515237553	0.308276146951	-0.477517948762
C	-0.667187261205	-0.175019657924	1.602883869850
C	-0.667222328827	0.341705876204	0.294334724185
C	3.081836191222	0.893194021465	-4.472291896261
C	3.081918661182	-0.726405919946	2.144155326406
C	1.832358119478	-0.174957258283	1.602885948245
C	1.832341618646	0.341718068666	0.294362041217
TV	4.998701900495	0.000067039003	-0.000084595517
TV	0.000000000000	2.884310026442	1.135165995175
TV	-0.000000000000	-0.000000000000	4.225305676904

Energy = -45.432169763280 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min68

C	2.596056362630	0.000841426918	-1.980389811183
C	1.091240940025	-0.506113730619	-0.554244798421
C	1.201305163847	0.000654048829	1.794184091076
C	-1.681014577845	-0.748818851874	0.131209029849
C	2.705738466993	1.875359012346	-3.483153074803
C	0.498350462248	0.448406421566	0.534263029020
C	3.298987225479	0.448402420536	0.534388460687
C	-1.012649835874	0.441614423834	0.554198376030
TV	6.491096845930	3.571859754009	-2.507093395343
TV	0.000000000000	2.381187666473	0.845666181903
TV	0.000000000000	0.000000000000	3.774857790486

Energy = -45.430825363358 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min69

C 0.174079878847 0.412046529604 -1.312513428418
C 1.353363106825 0.251231629030 -0.286958497915
C -1.231757452587 -0.176182901584 2.263058456802
C -1.944743519055 -1.128966410935 1.237470633662
C 1.231787676756 2.514848469058 -1.312795192725
C 1.944686485563 3.467562126449 -0.287297261440
C -0.174028588926 1.926667657310 2.262778870802
C -1.353418784761 2.087326334831 1.236982170896
TV 3.298093900405 1.380222611257 -0.000371407555
TV -0.000000000000 4.629025375724 1.787262057332
TV 0.000000000000 -0.000000000000 3.575358895254
Energy = -45.430018863052 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min70
C 0.885003377062 0.609950919129 -1.733197802115
C 0.929746645906 -0.418100901423 -0.566809863013
C -0.537894247488 0.609988522069 1.125606753463
C -0.582501115013 -0.418091885648 -0.040723989799
C 3.913188409769 -1.957283879663 -2.098745242493
C 3.177307552925 0.610062578037 0.378063355343
C 0.929765863762 -1.957366927148 2.846138991189
C 1.665784788713 0.609980609839 0.369108330537
TV 4.495676086891 -0.000025338633 1.354713462897
TV 0.000000000000 3.595582322841 -0.000120656015
TV -0.000000000000 -0.000000000000 3.412769579426
Energy = -45.429174216965 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min71
C 0.139775067062 0.398770395446 -1.412416989193
C 1.173404055318 0.175235408392 -0.245805713201
C -1.248684207101 -0.119485341803 2.077458556633
C -2.119681292635 -1.692636790938 -0.043430557463
C 1.248684490383 2.458211488182 -1.127159279277
C 2.119540525854 4.031304043205 0.993614078125
C -0.139707506322 1.940109649724 2.362610735167
C -1.173362329893 2.163024581551 1.195854920879
TV 3.180236144398 1.620919583302 1.286146998259
TV -0.000000000000 4.867940068650 3.145605799081
TV 0.000000000000 -0.000000000000 3.794293185023
Energy = -45.428752702406 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min72
C 2.798151697188 -0.286382575043 0.248562923610
C 0.676342363546 -1.304932518164 -0.506850244554
C 2.048769350555 -1.308575422431 3.791262356906
C -1.302078127136 0.330735252840 -0.596755711439
C 4.170678535947 1.758765749828 -2.546155087355
C -0.153174780885 -0.279842309891 0.239003385278
C 5.000142598314 0.734139574498 0.999904587066
C -1.302648990199 1.157880464404 -1.723749869960
TV 7.452048463668 3.061815999597 -2.036806305500
TV -0.000000000000 2.048068548371 1.494666450677
TV 0.000000000000 -0.000000000000 4.292550233070
Energy = -45.426721127181 hartree
Spin(**2) = 0.015869140625
Geometry of 3D-min73
C 0.175321425227 -0.728397564396 -1.940778821176

C 0.175439681775 -0.728603741159 -0.391090446147
C -0.322862220541 0.545671702792 1.663771216690
C -0.323030835676 0.545650056001 0.302793678674
C 3.003375412412 2.420257060529 -1.954087234235
C 3.003056504395 2.420498880466 -0.375464726603
C 1.497007928932 -1.028787041604 1.658504359552
C 1.497304737375 -1.028759650653 0.308466965363
TV 3.745568419384 0.601849795703 0.001117577864
TV -0.000000000000 3.735843147109 -2.149062221568
TV -0.000000000000 -0.000000000000 4.298844347918
Energy = -45.425760426780 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min74
C 0.760903317975 -0.278796594918 -1.544626202304
C 0.760775220802 -1.434592319810 -0.591961840324
C -0.627239517384 -0.658376976812 1.667257339161
C -0.627156463511 -1.055227976710 0.142953426543
C 3.314335861441 -0.657944803202 -1.830183706198
C 3.314559192112 -1.054667857611 -0.305944749052
C 1.926631526510 -0.278774720764 1.381106912242
C 1.926611905819 -1.434536635820 0.428488119480
TV 4.746099013209 -1.242840582990 -0.000054244447
TV -0.000000000000 2.486909123882 0.000290632449
TV 0.000000000000 -0.000000000000 3.946320180061
Energy = -45.422953367664 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min75
C -0.039447451217 0.500053299151 -1.716731735618
C 1.092078198710 -0.036516053784 0.859915628330
C 0.029724192214 -0.324866368345 3.028918410262
C -1.101512392085 0.211428909856 0.452946137147
C 0.274214502738 3.032778289936 -1.633536231612
C 2.144142029131 2.286957422075 0.223353382567
C -0.284070064498 1.852956153804 2.313533446961
C -2.153791276784 2.598774549712 0.456928128100
TV 3.424035119531 0.645677122127 0.326153127752
TV -0.000000000000 4.710826897863 -0.632717811744
TV 0.000000000000 -0.000000000000 3.458250711025
Energy = -45.422634604170 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min76
C 2.276768296203 -1.118279949360 -1.055387014076
C 0.007751905136 -1.399386294343 0.088348589354
C 1.653704359711 -0.769738958366 2.687573420209
C -0.545742140761 0.398114502572 -2.043352415021
C 2.123622295538 0.633945853165 -2.996430326356
C 1.500632662084 -1.415896751976 0.153414539924
C 3.633116490201 -1.739162417552 1.461118013494
C 0.144230102661 1.602964769506 -1.770060256108
TV 4.315361552792 0.865058821011 1.646314273716
TV 0.000000000000 2.398326857668 0.592803388383
TV 0.000000000000 0.000000000000 5.153388843226
Energy = -45.421988220597 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min77
C 2.810222139422 0.054098922873 0.247865789485
C 0.686847632528 -1.210656682351 0.250751437985

C	0.686960489953	-1.210685839610	2.766376421842
C	-1.146093562641	0.054498211616	-2.494528914530
C	2.141131320752	1.318898953180	-1.742981838042
C	2.141011844790	1.318948978326	0.756157415808
C	2.810392037833	0.054083628019	2.768433333204
C	-0.279777895040	1.319122144360	-2.494698675171
TV	5.286428777983	2.528715155111	2.000840161603
TV	0.000000000000	2.529682549843	-0.000078805378
TV	0.000000000000	-0.000000000000	4.003280435631

Energy = -45.419763454261 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min78

C	2.053810443891	0.435706352028	-2.238701867432
C	1.250152530070	-1.600604569908	-0.911432317256
C	1.785642050356	-0.960519784165	3.535461751588
C	-0.960408137669	-0.325766761136	-0.664043533728
C	2.781334323915	1.038123242730	-3.484744145244
C	1.695954236693	-0.762826669430	0.241378359205
C	3.596626843568	-0.042759314060	1.636741561936
C	-0.256771745388	0.764942684550	-0.034474670142
TV	5.966124838830	2.506182255021	-2.297747290929
TV	-0.000000000001	2.261752873610	1.092642570473
TV	-0.000000000002	-0.000000000000	5.771281223145

Energy = -45.419661070690 hartree
Spin(**2) = 0.015869140625
Geometry of 3D-min79

C	0.860873333888	0.050901050352	-1.541918462644
C	0.861147341623	0.050732043785	-0.158208290961
C	-0.184908802593	0.053153440333	0.886254268332
C	-1.567498546505	0.055786449320	0.885756926153
C	4.334408187853	0.042373859498	-1.541265395878
C	4.334370364886	0.042129866011	-0.157559362692
C	3.288676282699	0.044516211947	0.887170136421
C	1.906142002100	0.048347227379	0.886777141946
TV	6.947168839597	-0.015389324442	0.001315038207
TV	-0.000000000000	3.404646564231	1.712790028494
TV	0.000000000000	-0.000000000000	3.473373815611

Energy = -45.419280458111 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min80

C	0.028629911904	-0.529121662542	-1.558532033619
C	0.672980413195	0.038188932452	-0.317227931155
C	0.391736768808	0.636942689559	1.997620089803
C	-0.378455487654	0.419584593012	0.657656683558
C	3.026630604465	0.502159650538	-2.191767269497
C	3.176914594838	0.372717805661	-0.669296774775
C	1.883103181888	0.530257171511	1.578219783687
C	1.929650383530	0.358199490061	0.141411927265
TV	4.439758405986	1.225066188440	-1.182829780357
TV	-0.000000000000	2.614197492010	-0.374483177291
TV	0.000000000000	0.000000000000	4.561011609751

Energy = -45.418990212079 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min81

C	1.455475601004	-1.416211522576	-1.158872537840
C	0.618258960666	-0.462343106686	-0.282086049444
C	-0.743774798454	1.046967735760	1.092240035502

C	-0.745754538209	0.172679303522	-0.511665057858
C	2.827928334476	-0.722744180491	-1.301705570886
C	2.830058125877	0.151498870180	0.301977593071
C	0.628807790705	1.740460715811	0.949537960349
C	1.466014973989	0.786662115343	0.072541639489
TV	4.808440227254	0.830380155337	0.832499510580
TV	0.000000000000	3.459351007908	0.311603793703
TV	-0.000000000000	-0.000000000000	2.946629536580

Energy = -45.418469106897 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min82

C	0.094426546620	0.539217165450	-1.926798847941
C	0.512344663007	0.146128409825	-0.543425285250
C	-0.094516208653	-0.519047427439	1.808919440206
C	-0.512315464670	-0.126169983185	0.425514639944
C	0.094475637287	3.011413391732	-1.224508328393
C	0.512367158147	2.618344026789	0.158888400598
C	-0.094506557012	1.953148347539	2.511235355656
C	-0.512275774746	2.346055427278	1.127846452792
TV	2.429007273049	0.187297292973	-0.680731248711
TV	-0.000000000000	4.944427153733	1.404783231687
TV	-0.000000000000	0.000000000000	4.713009481162

Energy = -45.417873804862 hartree
Spin(**2) = 0.066406250000
Geometry of 3D-min83

C	0.002945751132	0.804722080816	-1.866277208734
C	1.348041052515	0.804024066686	-1.133840581793
C	0.237082641371	-1.778227678527	2.219458513493
C	-0.275014399600	-1.778012673415	0.894048215048
C	2.392273861810	2.095383441697	-3.177433174974
C	2.191490319037	2.095387693215	-1.592335043647
C	1.666849743461	0.804093194530	1.739364715740
C	1.028282910244	0.804264426012	0.329509436145
TV	3.811364282145	3.873347173036	-1.832759321648
TV	-0.000000000000	2.582788758996	0.000190023761
TV	0.000000000000	-0.000000000000	5.453140580068

Energy = -45.417279274563 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min84

C	-0.971156560542	-1.047471817350	-0.799608374333
C	0.237546374387	-0.595717660252	0.095912946633
C	-1.130411640629	0.279251343645	1.842324147151
C	-0.327196083315	0.625580897892	0.785787651647
C	4.387556612698	3.362635491491	-1.246277825550
C	3.147524385393	2.709236256846	-0.660686181126
C	1.938824293770	-1.972129099469	0.160277221178
C	1.422925252146	-0.943855710875	-0.905614593496
TV	3.634353687881	0.757098779099	-0.691421016644
TV	0.000000000000	4.229607699081	-1.716377214578
TV	0.000000000000	0.000000000000	3.396752146040

Energy = -45.416750746020 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min85

C	0.667319718170	-0.325993392002	-2.074220678020
C	-0.242540525187	1.995512694561	-0.961379056924
C	-0.254208339768	0.910621030672	1.715604415041
C	-0.548691250554	1.111130875986	0.241539024865

C	2.922894823140	-1.577330555332	-1.878550371436
C	3.217943640812	-1.778925879909	-0.404764053369
C	2.001246867923	-0.341018638555	1.912225301083
C	2.911185663409	-2.662483028721	0.798872324789
TV	4.581458234722	-1.854985585700	-0.267151971763
TV	0.000000000000	3.511008235217	1.371493228245
TV	0.000000000000	-0.000000000000	3.781237569020

Energy = -45.416589526807 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min86

C	-1.046860853522	0.243697047631	-1.604852411645
C	2.909257651510	-0.081574302575	2.054703286272
C	-0.466826270596	-0.556088038768	3.202639742131
C	-3.754353097466	-2.684228130223	0.245947076526
C	0.549350604925	3.698390920046	-2.296340457200
C	3.616307226283	4.542812036770	-0.529278980958
C	-0.450701099042	1.634276070825	1.780244703331
C	-1.120027413413	2.252753967610	0.756807515269
TV	3.087098699598	1.970970674395	0.646845155424
TV	0.000000000000	5.312087127730	-1.346962767044
TV	0.000000000000	-0.000000000000	3.641754656883

Energy = -45.416522900313 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min87

C	-0.719675862454	0.688308178481	-1.946041227894
C	1.297435440692	-2.190783248045	0.726284567996
C	-0.921396689340	-0.162850047895	3.137588116569
C	-3.461591241567	0.473913934299	-1.241958859416
C	1.297310006214	3.509801457625	-0.762442511773
C	2.293149915205	2.370044939995	1.130074061439
C	-0.444776640670	2.033603023259	1.912256738755
C	-0.247136246343	3.006743392967	0.764032218330
TV	2.540271691972	-0.636733054953	1.927634919430
TV	-0.000000000000	5.700675786189	0.000960466607
TV	0.000000000000	-0.000000000000	3.857962498031

Energy = -45.415595752030 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min88

C	2.694165086738	-0.229014769245	1.610756630483
C	0.230953567025	-1.850064183500	-1.263891496261
C	2.636024605614	-1.640502132402	5.606396685682
C	-1.311662570001	-0.216406575506	-2.147367484166
C	3.327194441646	2.591217634646	-2.632764713968
C	0.172582806049	-0.911782408374	-0.179278234287
C	4.178153307414	1.425294522550	0.667746047919
C	-0.460329196682	0.967229801807	-1.757620474597
TV	6.841910858873	3.997615911023	-0.113878762178
TV	0.000000000000	2.349662719836	0.829577724899
TV	0.000000000000	0.000000000000	3.740643013204

Energy = -45.415113417367 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min89

C	-3.486018589861	-1.716518069737	-0.290191142487
C	0.701635790887	0.082453326465	-0.267714257020
C	-0.346837915207	0.338787217271	2.092483990568
C	-0.326027475220	-0.308963326026	0.700322497755
C	6.348688250409	-0.968385747584	-3.017780944391

C	2.854711050352	0.672213862767	-0.954817044127
C	2.698493316692	-0.083175149819	1.405976845846
C	2.013081426681	0.282227863801	0.172008331852
TV	4.222254628610	1.913497120322	-1.473562578966
TV	-0.000000000000	3.146860058694	-0.599525756946
TV	-0.000000000000	-0.000000000000	4.818219350733

Energy = -45.412543060542 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min90

C	1.848908931088	-0.451381929104	-1.509355763929
C	0.571734424169	0.267958981571	-1.849818465982
C	-1.905771030754	1.842216708839	0.310731988578
C	-0.704526647542	1.135558729592	0.023453281901
C	3.050040677269	1.271892708713	-0.092648993752
C	4.250860821607	1.980573896183	0.191920535131
C	0.572089253051	-2.506934764365	2.118957563242
C	1.849371345504	-1.787672604202	1.778690415243
TV	4.955698721849	-1.783060028772	2.551343870883
TV	0.000000000000	3.568961154853	-1.302722198936
TV	0.000000000000	0.000000000000	3.804512941296

Energy = -45.410260891787 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min91

C	0.786293890101	0.612034320101	-1.537745376778
C	0.544543475761	0.218778637199	-0.088526355034
C	-0.563053323407	-1.528037508491	1.428829733022
C	-0.321058798973	-1.135013840099	-0.020365005830
C	3.296752430106	1.256543125700	-1.250042013802
C	3.777422596536	-0.155284925906	-0.899043497290
C	2.025415658846	1.358435241619	1.758447566809
C	1.544937316441	0.075900742774	1.041210171891
TV	5.099035763119	0.836524577338	0.251139940941
TV	-0.000000000000	2.694336962920	0.366302620480
TV	-0.000000000000	-0.000000000000	3.802919130231

Energy = -45.409799798224 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min92

C	2.715810338356	-0.677006754670	-1.120060216126
C	0.567305737688	-0.910330245443	-0.456740691319
C	1.339922569248	-0.468864872277	2.057941902050
C	-1.581300250500	0.531201665709	-0.778087968291
C	2.656518561820	2.574682578686	-2.806410010978
C	1.200052247157	0.023858907448	0.661187029784
C	4.032371024882	0.003672316684	0.717130592839
C	-0.948855618138	1.465621518798	0.339753832925
TV	5.753655115216	1.343009319180	-0.041862755113
TV	0.000000000000	2.363158731705	0.833164378031
TV	-0.000000000000	0.000000000000	3.767353676864

Energy = -45.408145858884 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min93

C	2.898236195605	-0.677187445065	-1.413832135050
C	0.793093036103	-1.495715591419	-0.655074314284
C	1.533151340820	-0.919114094524	1.860921406018
C	-1.383158617431	-0.227516501295	-0.306351418049
C	2.893425605994	1.911371323298	-2.921435909594
C	1.414393226295	-0.556007801176	0.421090628269

C	3.756915764159	1.953523264887	1.923019910135
C	-0.711295283357	0.954547734168	0.069908887024
TV	6.622190364029	4.681103174354	-0.706980634352
TV	-0.000000000000	2.458903697255	0.765279009044
TV	-0.000000000000	-0.000000000000	3.698969798611

Energy = -45.406717303048 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min94

C	0.432478230208	-0.786772606704	-1.410821616312
C	0.977852882084	0.271416681018	-0.303780501304
C	-0.052124290158	-0.313207104830	0.763104573403
C	-0.597187013304	-1.371603714460	-0.343830919339
C	0.142748762062	1.545842652982	-0.270989844229
C	1.146068695737	3.307315446077	1.663521441909
C	0.238291942849	2.791664548976	2.603744651279
C	-0.765399193160	1.030517371115	0.669034826859
TV	3.068810345311	1.742451361967	0.369261053639
TV	-0.000000000000	5.437556737943	2.980796818400
TV	0.000000000000	-0.000000000000	3.549212223703

Energy = -45.405867622305 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min95

C	2.562912726002	-0.982837961861	-0.667583264235
C	0.456246458951	-1.189788262651	0.090518118836
C	1.117095129084	-0.843531288140	3.569814487001
C	-0.721863248622	0.718997422025	-2.149220325138
C	2.506046001187	2.370898225737	-3.445394446596
C	1.026648547050	-0.165430875912	1.089324119254
C	3.532301352363	-0.319807510513	1.653954539857
C	0.285816730149	1.889326892855	-1.684144847756
TV	4.492874305296	0.974132634101	1.182752621119
TV	0.000000000000	2.414155091748	0.659422020781
TV	-0.000000000000	0.000000000000	4.746708585272

Energy = -45.405646869214 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min96

C	2.555176456627	0.082286609680	-0.703652714425
C	0.443541646911	-1.113146054685	-1.204516488286
C	1.816798822370	-1.113341083933	2.151403157434
C	-1.516078506008	0.514432803198	-1.734821594288
C	3.901280300368	0.082258194559	-0.703514546423
C	-0.352466898128	0.082595180928	-0.703962220473
C	5.207692461189	-2.307716970044	1.651321116236
C	-1.516200255251	2.042275400911	-2.027374057730
TV	7.774236495545	2.392019127186	1.002662511057
TV	0.000000000000	2.391215596546	1.001429491180
TV	-0.000000000000	-0.000000000000	3.355698331830

Energy = -45.405382604943 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min97

C	0.584787331243	1.250617096480	-3.693347498696
C	0.634457120687	-0.981779129726	1.748211566623
C	-0.765242609933	1.008505620588	0.650546175454
C	-0.704921535155	-0.373996306975	1.619853505872
C	3.209709252330	-0.331695272392	-1.784919736348
C	3.135769102652	0.519092617216	-0.467129388251
C	1.836292238372	-0.388999779627	1.302298933197

C	1.775819592675	0.493833652081	0.231333270886
TV	4.733087600259	0.752549581260	-0.860256805608
TV	-0.000000000000	3.470511968021	-2.349439589697
TV	0.000000000000	-0.000000000000	3.732775537689

Energy = -45.404875390999 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min98

C	0.214090185385	0.934887432320	-3.024142926430
C	1.301076085318	0.257810783634	0.012287117563
C	-0.623617673294	-0.329598339006	1.783452082159
C	-1.576047926340	0.102493251708	0.503992494166
C	2.577902593291	1.779770650447	-2.672099889412
C	3.114822691206	1.497661662858	-1.239114342635
C	1.734635029110	0.552142640690	1.600770517625
C	0.399810687703	1.452032994521	0.291770546129
TV	4.243890070865	2.497772388032	-0.762223911876
TV	-0.000000000000	2.484981359208	0.415790456863
TV	0.000000000000	0.000000000000	4.792053064800

Energy = -45.401001389234 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min99

C	0.007638249347	-1.279400104450	-2.452786909587
C	0.891479323300	0.611441268845	-0.126988965382
C	0.508063784198	0.142428968946	1.287682299684
C	-1.235601148829	-2.140589374783	-2.167640930827
C	0.032447744251	1.660157133343	-0.127059782842
C	0.865802450088	3.508169820358	2.117043755362
C	-0.225627967447	2.461281688937	2.402063513730
C	-0.503024417148	1.376716190611	1.287700774637
TV	2.861837293671	2.340078930161	0.789816811472
TV	0.000000000000	5.836959157104	4.569064724187
TV	-0.000000000000	0.000000000000	3.779975280373

Energy = -45.400266770574 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min100

C	1.279689289011	-0.471752273548	-2.571311519332
C	1.605120112363	-0.521052543104	-1.060254092118
C	-0.108712707801	-0.601645460178	1.701049300660
C	-0.809571573841	-1.896443233604	1.315882696613
C	2.507696479493	1.643749989820	-2.812584539576
C	3.714921938812	1.710608720990	-1.916685723089
C	2.010308284701	0.420117391556	1.269321627087
C	1.173059592912	0.657107612299	-0.017574210869
TV	3.967990660536	4.048245137590	-1.883702507597
TV	-0.000000000000	2.658972778146	0.510771188536
TV	0.000000000000	-0.000000000000	4.838043607155

Energy = -45.400077989381 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min101

C	2.835268634607	-0.423942368877	0.279942472900
C	0.695043104655	-1.597281368817	-0.242500137959
C	2.145434065260	-1.588263991957	3.839950791369
C	-2.084172524903	1.445472503780	-1.488524020321
C	4.312971393176	1.857743812215	-2.712837984988
C	0.005882802721	-0.448187250568	0.303425447922
C	5.093217965336	0.523506381156	1.240442387221
C	-1.475562443392	1.978867534371	-2.582934954282

TV	7.413595096304	2.504492887802	-1.245054662290
TV	0.000000000000	2.331937286768	1.042268828523
TV	-0.000000000000	0.000000000000	4.094180234333

Energy = -45.399103691736 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min102

C	1.496845817230	4.122212542851	-4.661755581734
C	0.311778522882	-2.269907757960	3.152512021210
C	1.496902665862	0.116588909684	-1.214616831115
C	0.311771551569	-2.663331143504	-0.420855040657
C	2.681930810847	6.119665730862	-5.984657186547
C	-0.934613939907	-3.210201657044	4.933905234041
C	2.681841671002	2.705133703352	-1.726262865669
C	-0.934489206764	-1.722134871859	2.736296195336
TV	4.862839860409	5.731861189768	-5.997191100525
TV	-0.000000000000	2.293072804536	1.551527819548
TV	0.000000000000	0.000000000000	4.938082179902

Energy = -45.397154618706 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min103

C	0.617256247588	-0.307060100204	-2.273943113744
C	-1.527862384756	-0.596546376649	-1.154826501555
C	-0.358612706622	0.595747023372	1.145868496578
C	-0.943462500921	-0.438826500877	0.222562875805
C	2.859182268710	-1.004245508897	-1.087510421864
C	3.443905879287	0.030089769857	-0.164275557143
C	1.883545126254	-0.101504214440	2.331877097659
C	4.028506389160	0.188098065422	1.213172682071
TV	4.387188805316	1.659235639170	-1.003392210306
TV	-0.000000000000	3.438075106318	-1.780820956939
TV	0.000000000000	0.000000000000	4.207729317391

Energy = -45.396370535478 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min104

C	3.197228118138	0.330280826446	-1.997043655144
C	-0.463318362876	-2.984272665967	-0.063640873666
C	1.719765318256	0.334419062231	1.733023213518
C	-1.358350412734	-1.067677968953	-1.429057270380
C	4.092183073754	2.242453017204	-3.363467703509
C	1.014212168526	1.413877746601	2.331499973736
C	4.092276762200	0.613848323980	0.566113321344
C	-1.358085311448	-0.494607525728	-0.029009377637
TV	6.851077428626	3.308974806571	-0.070610541819
TV	-0.000000000000	2.201197123871	1.198245765911
TV	0.000000000000	-0.000000000000	3.728030438551

Energy = -45.395203781710 hartree
Spin(**2) = 0.049072265625
Geometry of 3D-min105

C	1.399221898179	-0.341542701866	-1.946772394957
C	0.339180609607	-0.763899159541	-0.862751249274
C	-1.789428630279	0.314212677471	0.245415891604
C	-0.725158686886	0.358824062987	-0.876383313486
C	2.547920543159	2.583269799085	0.049215586761
C	4.499004817723	3.549751556317	1.043036970008
C	1.458101951166	-2.642515813532	2.107237953980
C	1.340095377206	-0.682204735997	0.345763197445
TV	4.248694118588	2.026388388818	2.084741326396

TV	0.000000000000	3.777266938694	0.106694311585
TV	-0.000000000000	0.000000000000	3.779007927425

Energy = -45.395198894052 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min106

C	1.877043465412	2.107172544649	-5.148088578979
C	0.882876171488	-2.473682648399	3.258114734152
C	1.877177690045	0.525571422417	-0.545043447656
C	-1.027217896894	-2.014649544503	0.379299617407
C	3.151119733240	3.991700723998	-5.805826880785
C	-0.011502562225	-1.525817104907	4.116289634809
C	3.151017941509	2.431135896959	-1.222699277708
C	-1.027010603637	-1.036599765842	3.083699436474
TV	5.500716442670	5.684578326110	-4.387268213929
TV	-0.000000000000	1.895122681148	1.716822240197
TV	0.000000000000	0.000000000000	4.769207011762

Energy = -45.394926361186 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min107

C	0.671210798956	1.570951766710	-1.616224543851
C	0.671235231813	1.570630800486	-0.205102460084
C	-0.646744685536	-1.281662085567	1.766576888570
C	-0.646692666091	-1.281341488235	0.246948643817
C	2.685853882980	0.738540496411	-0.910809112877
C	3.986469725991	0.140123661624	-0.911695308265
C	1.890270497250	1.064523564626	1.759629866974
C	1.890593403299	1.064413888963	0.300502206149
TV	5.382956104749	1.085185857879	0.022098069148
TV	-0.000000000000	3.458972509920	-1.917493760740
TV	-0.000000000002	0.000000000002	3.881238568057

Energy = -45.394879322072 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min108

C	-1.868455481491	1.662223490033	-1.844168749739
C	2.519515202723	-2.100077470327	-0.044147010244
C	-2.356027558408	0.572770798631	2.804825724235
C	-5.608999780871	2.530465206246	-0.973212819499
C	3.456649497806	2.257443359937	-0.720512902032
C	3.456780425915	0.590162587200	1.116699652935
C	-0.283989238293	1.458456368957	1.987695715757
C	0.203787081241	2.547718768312	0.982325844194
TV	4.064269776011	-1.481788990575	1.367796040290
TV	0.000000000000	3.632021704488	0.291848365142
TV	0.000000000001	0.000000000000	3.643640498845

Energy = -45.394748604785 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min109

C	0.429789846053	-0.746675554937	-0.887582252411
C	-0.004448398802	0.276251633271	0.160697340278
C	-0.003546344967	0.276595699701	1.507850598990
C	-0.437895763441	-2.090288598217	-0.888639470310
C	2.884130014562	0.329614527232	-0.885303435593
C	2.449926810089	1.352538681220	0.162985456323
C	2.450715547323	1.352834569969	1.510141820000
C	2.016442562571	-1.013991823370	-0.886340911314
TV	4.908579526877	2.152702114096	0.004558964060
TV	-0.000000000000	3.389638338136	0.001017161384

TV	-0.000000000000	0.000000000000	3.444630185935

Energy = -45.394747796300 hartree
Spin(**2) = 0.015380859375
Geometry of 3D-min110

C	0.482507114733	-0.643462916520	-2.584150364023
C	0.482311077426	-0.643775340216	-1.180139744979
C	-0.629726112834	-0.642146040034	1.266266265732
C	-0.629770305327	-0.641990786719	-0.137842062802
C	1.847548520579	1.764957581998	0.562174894926
C	1.848119516999	2.837786979954	1.649518346343
C	1.848726374683	0.427775893127	0.563054223009
C	1.848324378082	-0.644973745566	-0.524407140918
TV	3.843707101837	3.477630168976	2.443046579590
TV	-0.000000000000	3.482206912118	-0.001631473723
TV	0.000000000000	0.000000000000	4.891931581707

Energy = -45.394202473324 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min111

C	2.135129159767	0.406547784625	-1.870643506911
C	1.789573280486	-0.826919696490	-2.503376539703
C	1.089572826016	-3.293683373482	2.677571772606
C	-1.093406656706	0.406379903099	2.408777440699
C	2.119313201004	0.406612832302	-5.753436274700
C	2.835529123127	-2.060071973046	-0.564507943993
C	1.806254934499	-0.826841000203	1.379255285981
C	-0.385256884381	1.639810434568	2.525149098560
TV	5.403797278337	0.000154108500	-2.821320833193
TV	0.000000000000	2.466826243181	0.000026679177
TV	0.000000000000	0.000000000001	6.487604430883

Energy = -45.392644339429 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min112

C	0.274721597017	0.493017545398	-1.817489898697
C	0.320161637257	-0.141903283742	-0.407758512888
C	-0.565477313302	-0.593040670030	1.946007669382
C	-0.778758522759	-0.793837770801	0.445476945194
C	0.565549165795	3.020230561704	-1.212265168308
C	0.778618220061	3.220969634501	0.288077364306
C	-0.274488919199	1.934262117051	2.551195427741
C	-0.320329468223	2.569128666853	1.141399728271
TV	2.311292283644	1.087315603175	-0.007531940321
TV	0.000000000000	4.866590340297	0.953608282147
TV	-0.000000000000	-0.000000000000	4.435872971541

Energy = -45.392618063674 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min113

C	0.150141328325	0.408954590068	0.137139929443
C	2.487461805878	0.410337746530	1.263990416734
C	-0.085401856397	-0.730592368138	2.603574470443
C	-2.431153471182	-0.736028451929	-1.682127237178
C	1.107776440231	3.723348535560	0.097515909219
C	0.882168640008	2.334752975773	0.288528006104
C	-0.433385701356	1.751394709195	0.355690444140
C	-1.613940545240	2.516129571149	0.546492400141
TV	3.915978716800	1.736418191221	2.190749771245
TV	-0.000000000000	5.283111721559	1.094504756510
TV	-0.000000000000	-0.000000000000	3.221365461894

Energy = -45.391978258228 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min114

C	0.821784078867	0.716909197876	-1.209151483412
C	1.142117427587	-0.463787602635	-0.426341124412
C	-0.307908098166	-0.707293761346	-0.192776618343
C	-0.628170215439	0.473379445710	-0.975788050000
C	3.366990755019	2.600088131579	1.484629456289
C	4.352195844905	3.473756783508	0.848886288213
C	0.955694550584	-2.328573800451	0.834252234425
C	1.941110331923	-1.454851935825	0.198379325246
TV	4.794463127986	1.135702609487	3.085194027121
TV	0.000000000000	4.202642491583	1.265838143544
TV	-0.000000000000	-0.000000000000	4.091031071637

Energy = -45.391697530266 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min115

C	0.041727952972	0.517102991522	-1.672509472669
C	1.022247093979	-0.165100850602	0.812576171498
C	-0.030133913504	-0.337449001559	3.140686214086
C	-1.117755487043	0.199854137441	0.734358590942
C	0.299950023667	3.202769757811	-1.899704786177
C	1.359062432238	2.017330838599	-0.180474808806
C	0.457946159397	1.889817810419	2.277534231936
C	-2.111890343084	2.726611280039	0.847441936942
TV	3.243688273905	0.613400650919	-0.350771058973
TV	-0.000000000000	4.890067469027	-0.945233157881
TV	0.000000000000	-0.000000000000	3.494085246393

Energy = -45.389341973145 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min116

C	0.810119253864	1.729940822388	-0.193673705285
C	-0.187044046559	0.743333305200	0.501656233179
C	-0.406098351324	-1.846324509266	1.218862016385
C	-0.414873908081	-0.742557477587	0.054601182627
C	-1.361846635031	1.534398549548	1.220599011798
C	0.736105970162	1.703033511679	1.292624702782
C	0.359240902304	-1.516279477827	3.895913602138
C	-0.364352913662	-1.173587155771	2.549305063794
TV	2.472188915583	2.228031718595	1.941791396022
TV	-0.000000000000	4.537691542719	0.332322412200
TV	0.000000000000	0.000000000000	5.016981873471

Energy = -45.388925235996 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min117

C	1.403845393202	-0.235609144422	-1.961595376618
C	0.396862882117	-0.740887492283	-0.777266360851
C	-1.577108857288	0.620148206539	0.569491837536
C	-0.536615811185	0.389826084607	-0.515708725759
C	2.736620649118	2.515279448820	0.151724690531
C	4.042234764981	3.216227833579	0.691014910393
C	1.290260637487	-2.329561111026	1.503368682960
C	1.312838221464	-1.059528140887	0.443732983886
TV	4.053942188717	1.598254658061	1.841432780936
TV	-0.000000000000	3.646905937455	0.285927365405
TV	-0.000000000000	-0.000000000000	3.702750390274

Energy = -45.388718374143 hartree

Spin(**2) = 0.000000000000
Geometry of 3D-min118
C 0.636263902193 -0.400290770815 -2.451114416431
C 0.073623573520 -1.070069063724 -1.240536907313
C -0.141495905997 -0.214397333788 0.027976407948
C -1.204072294003 -1.254791423523 -0.317376775622
C 2.731525346207 -0.233306068217 -0.997103070291
C 2.516575507596 0.622505794712 0.271366797093
C 1.953742687258 -0.047347031870 1.481846543527
C 3.794156623982 0.807039494178 3.121497129073
TV 3.230173026571 3.271174048868 0.267956647276
TV -0.000000000000 4.749340939651 -2.923750518088
TV -0.000000000000 0.000000000000 3.773687590596
Energy = -45.388631168036 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min119
C 1.929062753543 -1.653717159999 -1.991412869314
C 0.300127123155 -0.749871053988 -0.704596193498
C -0.134962751225 1.337089346025 1.586842382529
C -1.170438151676 1.193990308823 0.320855247916
C 1.357341426454 -0.211438684122 -1.728649351887
C 2.419019551505 0.339279778300 -0.803948599193
C 1.124594119835 0.502111703488 1.470093671474
C 1.581746908173 -0.514262992636 0.344981815725
TV 3.493671836322 0.590789286863 -0.681325364217
TV -0.000000000000 3.386840335114 -1.478471700871
TV -0.000000000000 -0.000000000000 4.542233822813
Energy = -45.388333204650 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min120
C 0.751628667551 1.520206922118 -0.585914376392
C -0.100530476508 0.717793274859 0.333575220622
C -0.695602830580 -1.356687439964 1.289184526307
C -0.610795723988 -0.743293479757 -0.078760378660
C -0.756991643845 1.513343249926 1.483922999875
C 0.429058153719 0.701717985460 1.819494279171
C 0.348196920100 -1.310147786013 3.818790886863
C -0.193712794771 -0.610975158256 2.459594949624
TV 2.480534268691 2.066214254393 2.308281521351
TV 0.000000000000 4.327297766353 0.189574646619
TV 0.000000000000 -0.000000000000 4.997187046390
Energy = -45.388213438656 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min121
C 1.559984108898 -0.478623893758 -1.262100434306
C 0.251638611365 0.127536207819 -0.853323439475
C -1.205285825943 0.908839753703 0.874880265342
C -0.260496552896 1.441450166480 -0.336369485424
C 2.799598933101 1.304878244058 0.580478994077
C 3.153951821422 2.742236986674 0.373693567122
C 0.749798656555 -1.106856346131 -0.101814940516
C 1.789892604295 -1.202048870316 0.999707246262
TV 4.006533946069 -0.685713506825 2.108942957520
TV 0.000000000000 3.673450130508 0.023361768312
TV 0.000000000000 -0.000000000000 3.587014273784
Energy = -45.386725532688 hartree
Spin(**2) = 0.000000000000

Geometry of 3D-min122

C	3.000327313196	-1.584759065786	-1.830076325258
C	0.803669467885	-1.392494349708	-0.713762940097
C	1.528545654308	-1.148397574653	1.690756188851
C	-1.392820691704	-0.134503105313	-0.297652415229
C	2.902157252440	2.407886197161	-2.671540530130
C	1.431410802642	-0.402557194508	0.410540840484
C	3.625281357926	2.174347315399	2.319864882650
C	-0.703809888515	1.024378666275	0.070117353196
TV	6.518894124163	4.735619537455	-0.317139810615
TV	-0.000000000000	2.372527746385	0.789552929284
TV	0.000000000000	0.000000000000	3.696410951442

Energy = -45.385981836949 hartree

Spin(**2) = 0.084228515625

Geometry of 3D-min123

C	3.198072673393	-0.079785470795	-2.069766333587
C	-0.407973328481	-1.221328833234	1.040800907492
C	1.768234517435	-0.049568795191	1.498006608820
C	-1.358476361902	0.704908797437	-0.557726182629
C	3.876216596769	3.210983254064	-3.736056103310
C	0.442545123031	-0.040949955447	1.474439934019
C	4.013861531724	0.354045373270	0.397387860656
C	-1.385849803137	1.571863268946	0.731054722119
TV	6.774769910216	1.821446187832	-1.314850130329
TV	0.000000000000	2.361373386861	0.865956624064
TV	-0.000000000000	0.000000000000	3.650555112191

Energy = -45.385451323943 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min124

C	2.270300974467	0.562695207472	-2.297765378604
C	1.535204317129	-1.094166311132	-0.514409326595
C	2.132735889771	-0.822114313903	4.717934761142
C	0.020835268303	-1.029753175819	-0.839024837940
C	1.934052769154	2.238538066823	-4.177234064157
C	1.950383567346	0.018282376210	0.460534858072
C	2.436278545812	0.849990839908	2.856951271121
C	-0.409802017649	0.366297449405	-1.299202651142
TV	3.739541848053	4.565401335398	-3.298648149183
TV	0.000000000000	2.512092198003	0.496200515289
TV	-0.000000000000	-0.000000000000	6.611516956329

Energy = -45.385223147492 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min125

C	-0.853555807395	0.481219672570	-1.790129286699
C	1.732381554221	-1.740940875582	0.153365662219
C	-1.021614496855	-0.398733281637	3.189619107817
C	-3.559256035904	-0.399242514649	-0.506738848260
C	2.307887641746	4.116249218819	-1.099738090200
C	1.227589559729	2.773143061807	0.430211454578
C	-0.853065581547	1.893166595666	2.000006198161
C	-0.060715912851	2.772900307378	1.096429837177
TV	2.873458283399	0.000464276346	1.316982485621
TV	0.000000000000	5.856862737267	0.000465226227
TV	-0.000000000000	0.000000000000	3.790192832812

Energy = -45.385179268819 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min126

C 0.307283913561 -0.873911924707 -1.746519748718
C 0.356644179649 -0.887281409711 -0.262921440195
C 0.126953822283 0.478512307682 1.664995154881
C -0.325369539501 0.471784947367 0.259054295049
C 2.409541394348 0.074767103010 -1.083498392081
C 2.956704209503 -1.271199100067 -0.530211273791
C 1.536274906863 -0.159889585684 1.711435891354
C 1.798929758538 -0.617119858926 0.220126884651
TV 4.779348702933 0.961894800290 -0.426859535407
TV -0.000000000000 2.701060141817 -0.021154301995
TV 0.000000000000 0.000000000000 4.063557481722
Energy = -45.385091695219 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min127
C -1.471614779279 0.765240381012 -1.857162120785
C 2.231598379426 -2.349948254785 0.320066154433
C -0.661851320558 -0.280393197015 2.569204088866
C -2.688856976313 0.248899317361 -2.434231266104
C 2.502936063682 3.521257335439 -0.267684751204
C 2.008791511955 2.247866728424 1.616584174271
C -1.099536718088 2.187663517967 1.992391594026
C -0.870242391738 2.999889672687 0.795114499759
TV 2.909598050226 -0.759979082600 2.277047580593
TV -0.000000000000 5.942155718967 0.786302743255
TV 0.000000000000 0.000000000000 3.849884578065
Energy = -45.385051822220 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min128
C 3.054726570662 0.765662052514 -1.727644017218
C -0.436483996154 -2.626840983072 0.173808636903
C 2.223253101375 -0.364536503673 1.391202786675
C -1.350172764220 -0.683889829289 -1.166772453574
C 4.069898322424 2.682662146187 -3.068670328945
C 0.897463852168 -0.364147958093 1.388899768262
C 4.069946157199 1.109369376657 0.826529376828
C -1.350192027178 -0.048395847714 0.215521792507
TV 6.787863420619 3.392239594068 -0.038607029595
TV 0.000000000000 2.260936913174 1.213534999641
TV -0.000000000000 0.000000000000 3.726064458728
Energy = -45.383792055954 hartree
Spin(**2) = 0.015380859375
Geometry of 3D-min129
C 0.397082304369 -0.141951127396 -1.985691987295
C 0.668715940024 0.510934704395 -0.543563991853
C -0.362574258939 0.987280128713 1.798235418451
C -0.624926791426 0.711065311227 0.295337287800
C 2.835360919227 -1.730504428932 -1.577163150122
C 3.106819209878 -1.077205783915 -0.134947141888
C 1.934478846454 -0.509274725375 2.684904054765
C 1.569732275323 -0.710210355780 -0.286073656331
TV 4.491453716507 -0.452841425852 -0.271873480600
TV 0.000000000000 2.464548862825 -0.576639005696
TV 0.000000000000 -0.000000000000 4.519104249210
Energy = -45.382934878353 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min130
C 2.806278240910 0.230116150116 -0.736107057206

C 0.659723425052 -2.570138152807 -0.732957622955
C 1.508310243499 0.058858868524 2.600495582836
C -1.399890960885 -1.015905859637 -1.201057888248
C 2.950476622304 2.455676646674 -2.460596914240
C 1.502049805297 -0.062972256399 1.143566527263
C 3.854145875214 1.082707627067 1.213949226857
C -0.831142021760 -0.020261185717 -0.116599160530
TV 5.586918230049 4.043283652972 0.704933726919
TV -0.000000000000 2.519542148728 0.710624010668
TV -0.000000000000 -0.000000000000 3.830941978055
Energy = -45.382843409326 hartree
Spin(**2) = 0.015380859375
Geometry of 3D-min131
C 0.789943677918 0.340637942985 -0.967144879493
C 1.694420456868 -0.397621132987 0.162956759161
C -0.339511948436 -0.717368202995 2.693562819297
C -1.750218808083 0.588714039133 0.802986317051
C -0.113257563489 2.660996026074 -2.072886645988
C 2.140921608311 1.713188037064 1.810650194396
C 0.832872254190 1.921394482202 2.528415850601
C -2.916481704741 3.139641532829 -0.473875624561
TV 3.460870906971 -0.113750461472 0.551723575667
TV -0.000000000000 4.519922636688 -0.174471593550
TV -0.000000000000 0.000000000000 3.506584814254
Energy = -45.381512863893 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min132
C 2.648347629836 -0.798073673249 -1.192902354688
C 0.525089066923 -4.358002691393 -2.501752702155
C 1.940192861934 -1.984589681375 2.155065489787
C -1.370753575339 0.390861836817 1.128370743588
C 4.093459119762 1.574440653054 -4.103987463668
C -0.715539660354 2.321241016197 3.240762600312
C 4.798501369796 0.386227694687 -0.751986871308
C -0.715289597528 3.210737117689 0.754813142888
TV 7.665645704754 2.369324288902 -4.794026308697
TV -0.000000000000 2.374621488242 0.869071026347
TV 0.000000000000 0.000000000000 3.784558194628
Energy = -45.381188294008 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min133
C 0.744270717775 -0.197689194257 -2.411442066053
C 2.132975704092 0.038795417412 -2.955200438840
C 2.689027404274 -0.833136474108 2.178512776292
C -0.714992713850 -2.445574382364 2.755013331571
C 1.835235390610 1.737978785008 -6.860634557644
C 2.367819410008 -0.239061460590 0.813856327727
C 2.236830902804 1.176711790344 0.688846419490
C -1.406798024849 -1.305271129551 3.263317851041
TV 5.618171764125 0.468515320362 -1.076852647594
TV 0.000000000000 2.289930127308 0.996041154433
TV 0.000000000000 0.000000000000 6.259160837520
Energy = -45.380955229899 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min134
C 0.858512554916 0.545466720162 -3.907127373513
C 0.858873819758 0.133424839764 -1.881431944887

C	2.850072687603	-0.882143838047	2.687932390390
C	-0.290526835159	-2.103639019050	2.427887767813
C	2.008016977323	0.339412666627	-2.894478310161
C	0.858712446999	-0.160740420804	-0.452553095412
C	0.858507250213	0.840345305259	0.507562671278
C	-1.132683794166	-0.882136119700	2.689085594312
TV	5.337621948574	0.000023236735	-0.001389094712
TV	-0.000000000000	2.443122609343	0.521594063169
TV	-0.000000000000	-0.000000000000	5.843431096264

Energy = -45.380134985352 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min135

C	-0.007663028097	0.728813658754	-2.846511113329
C	2.462980835518	-0.616387877985	-1.103892572876
C	1.805118063556	-1.868822344221	3.517297571063
C	-0.292996575110	-1.815478797492	0.585984123553
C	0.350085545456	0.714819750539	-1.499599076623
C	3.864964061036	-0.657953192795	-0.726936543055
C	4.523101687248	0.594696534782	-0.408321903160
C	-0.652323839122	0.741986977197	-0.475924674367
TV	6.631259191840	-0.185697400506	0.424500870544
TV	-0.000000000000	2.544374066630	0.284332175563
TV	0.000000000000	0.000000000000	4.941278430149

Energy = -45.379931614683 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min136

C	3.019559765329	0.592308427892	-1.498713753373
C	0.405640293763	-1.789759134041	0.840774822046
C	1.747172245283	-1.792180051121	4.191664190479
C	-1.543256305439	-0.163317987409	0.313260552440
C	4.361121094665	2.978769895945	-3.839125439834
C	-0.398353462892	-0.594788671161	1.341518059823
C	5.165224512080	1.783694174263	-0.991364759471
C	-1.543524091353	1.362980215010	0.024432774378
TV	7.853322003466	4.767544687906	-4.678293032103
TV	0.000000000000	2.389191706595	1.002878474374
TV	0.000000000000	-0.000000000000	3.348158544502

Energy = -45.378148317780 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min137

C	-1.293330939924	-0.743377453186	-1.489355655705
C	-0.332657411454	-0.484829313674	0.938757936598
C	-0.333477302515	-0.481764175527	3.010691772773
C	-2.438131475319	-1.708646444231	1.979991682311
C	1.515823954682	4.005893639332	-1.893300058281
C	2.649983809566	4.048801009504	-0.857879951410
C	0.371107316166	3.040522197268	1.576220593359
C	-0.588914875040	2.779296466879	0.541181711662
TV	3.239655142563	1.266880513992	-0.005839586554
TV	0.000000000000	5.981690669398	-0.409916480859
TV	-0.000000000000	-0.000000000000	3.464784458849

Energy = -45.378121160042 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min138

C	-0.049233188496	2.153922326791	-4.908594379555
C	2.511355804037	0.119339750090	-0.293256429436
C	-0.017625308421	1.082115564864	0.360351875534

C	-0.986020491483	0.134975967075	1.141105098723
C	2.209817087401	0.540727762470	-1.701402935593
C	1.400231905149	-2.178578549931	3.271137059584
C	1.224395066999	2.836494550028	-0.608073113209
C	-2.097064947654	0.809196943225	2.121401172468
TV	4.651436618342	3.580688940340	-3.158295237200
TV	0.000000000000	2.903593781831	1.847863337942
TV	-0.000000000000	-0.000000000000	4.389570604410

Energy = -45.377207425256 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min139

C	0.629431547662	0.125113270901	-1.957329853611
C	0.629481752542	0.123076085100	-0.544487341368
C	-0.670114663131	0.123912822484	1.810645540961
C	-0.670065669056	0.125511273142	0.215280122953
C	3.282814781815	0.123520671393	-2.734446809465
C	3.282831587685	0.120789671092	0.232683174324
C	1.766810156859	0.125142703253	1.726090102248
C	1.766808202728	0.120443268061	0.299818724466
TV	4.794147271923	1.363118033230	0.000233097117
TV	-0.000000000000	2.731270765038	0.000503855668
TV	-0.000000000000	0.000000000000	4.527651467506

Energy = -45.376325662369 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min140

C	1.259222057370	0.792791334195	-2.143409752857
C	0.081253042642	-0.135368601127	-0.094104269112
C	-0.915787585211	-0.801305102450	2.168664476574
C	-0.608645050888	-1.014047614290	-1.038437854845
C	-0.259860674177	1.457437289154	1.882608848124
C	0.120971926449	1.581868488843	3.273251236496
C	-1.992034553170	-0.831955542554	4.433675364803
C	-0.335214589715	0.153112641623	1.223992427505
TV	3.268165471133	1.224919047147	0.760493053746
TV	-0.000000000000	3.490087170032	-0.760802153033
TV	0.000000000000	-0.000000000000	5.946553112966

Energy = -45.376277594274 hartree
Spin(**2) = 0.015380859375
Geometry of 3D-min141

C	0.328346364354	0.226205348413	-3.257745582149
C	2.301535920631	1.217413360578	-1.830071854688
C	2.588537587463	-0.992994146351	2.231587323892
C	-0.977842824940	-2.188289527658	1.717904544380
C	1.097806884651	1.431797968125	-2.793027407377
C	2.785359976169	0.916608724453	-0.477114959199
C	3.047636338203	2.031321162431	0.397129450406
C	-1.790861618877	-0.897659095071	1.798405931150
TV	5.471768169041	2.626309888628	-0.040103423559
TV	-0.000000000000	2.494255507213	0.553488941226
TV	-0.000000000000	-0.000000000000	5.889643596435

Energy = -45.375035724921 hartree
Spin(**2) = 0.109375000000
Geometry of 3D-min142

C	3.416781981591	0.466712874058	-2.254707528334
C	0.547209455951	-1.129989874855	-1.031029297600
C	2.901358458058	-0.577507422228	1.770598280812
C	-0.972792594550	0.457044075519	-2.202730678717

C	4.303151146620	2.612290808247	-0.647464163775
C	1.061031555041	-0.059350229969	-0.217039330437
C	2.015060583801	-0.320579166853	0.787439070173
C	-0.459344873598	1.527598713861	-1.388423644263
TV	6.229034664054	1.893946291178	2.560485124902
TV	-0.000000000000	2.402324912046	0.624138659592
TV	0.000000000000	0.000000000000	4.941458952184

Energy = -45.369236720922 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min143

C	2.901179271669	-1.070536229080	1.530272618206
C	0.237608937266	-1.164901105002	-1.645289911906
C	1.671476745291	-1.114985898136	1.705749602355
C	-1.488635741888	0.272328001186	-1.776654499125
C	4.315647674119	1.391631466162	-1.194700591638
C	-0.433627565969	-0.179807068752	-0.639467981715
C	4.977898787478	0.230667842944	1.730809095000
C	-0.822450935059	1.676858803039	-1.827932896891
TV	7.950864681312	2.409425580804	0.819124528541
TV	-0.000000000002	2.392034586131	0.948931324318
TV	-0.000000000002	-0.000000000003	3.487046011578

Energy = -45.368779375789 hartree
Spin(**2) = 0.140625000000
Geometry of 3D-min144

C	2.447408775740	-0.878932439799	-0.595146652158
C	0.445747400956	-2.238839667947	-0.019073515889
C	1.477935082004	0.892582056041	3.621942209066
C	-0.514099127651	-0.472376816971	-2.837763348802
C	2.151905417070	2.163652553195	-3.509376505075
C	1.193267793470	-0.963570059844	-0.108444374719
C	3.455695451112	-0.190589243419	2.600689894831
C	0.159579082275	0.798741446042	-2.903469139004
TV	4.264570540113	2.131968165625	2.133847002820
TV	-0.000000000000	2.446008285545	0.423945864902
TV	-0.000000000000	0.000000000000	7.065748299738

Energy = -45.368066292223 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min145

C	2.712181755221	0.944186345156	-1.633773308526
C	0.571429626452	-2.965421213275	2.272594849177
C	-0.465683230705	-2.965346419810	5.026319046636
C	-0.466161106859	-0.357708979594	-0.481077463995
C	4.025179510818	3.547335016397	-5.544517235044
C	1.386175122601	-1.661621541253	2.273970767377
C	4.992653740143	3.546002496748	-2.794764230528
C	-1.362774913814	0.946132762867	-0.476368570693
TV	6.354870023700	5.207552528491	-3.903428396706
TV	-0.000000000000	2.607604396953	0.000308431306
TV	0.000000000000	0.000000000000	3.913530007265

Energy = -45.367679064768 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min146

C	1.366424631482	0.218178091841	-5.248037829703
C	1.358083969742	-1.476784023720	-1.957335960383
C	1.366334083363	-1.297702835933	6.001000381858
C	1.343450915239	-3.184309480595	1.411294182236
C	1.372283782402	1.351026636954	-4.358667817105

C	1.356202570425	-0.354236029696	-0.989685425705
C	1.348716286505	1.926232505930	0.677550482298
C	1.349804343083	-2.051512385904	2.300561550942
TV	3.293925085429	-0.125228277536	0.988797917089
TV	-0.000000000000	2.460951372771	0.331916838501
TV	-0.000000000000	-0.000000000000	9.293877779156

Energy = -45.367665688020 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min147

C	0.612603358030	0.330351862840	-1.029437740136
C	1.488525392658	-0.646969980557	-0.206549387768
C	-0.559226047979	-0.460364501190	1.818630239469
C	-1.338593952104	0.829117433355	1.367841449722
C	-0.116344991675	2.677883311895	-2.111788968348
C	2.335115842235	1.892305230869	1.032928849627
C	-0.417040577337	1.543453189352	2.544761485326
C	-2.141457177557	2.885045239744	0.141120141972
TV	3.353514925392	-0.048594972258	0.672480316065
TV	0.000000000000	4.522639398644	0.209875158408
TV	-0.000000000000	0.000000000000	3.557967756383

Energy = -45.367174607022 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min148

C	0.920281527414	-0.528849090944	-1.602879305068
C	0.596769977033	-0.351115445898	-0.265718460408
C	0.596153913824	-1.745183606958	1.859856750180
C	-0.028467976112	-1.437040252945	0.541962096572
C	2.678440452064	1.187365558006	-1.995818064395
C	3.746441635119	1.763763982274	-1.611191984162
C	1.545530317979	0.557243935400	1.850055576536
C	0.920935868297	0.865256043580	0.532014141089
TV	4.907518996371	3.831132647553	-1.738038743103
TV	-0.000000000000	3.907686927582	-1.696508803189
TV	-0.000000000000	0.000000000000	4.260548981242

Energy = -45.367146310055 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min149

C	0.938695839223	-1.097184540940	0.181794903198
C	0.655738098262	-0.054401263153	-0.889300675813
C	-1.360871820351	1.271429332579	0.169264843512
C	-0.957301431037	0.223450803789	-0.894642128337
C	3.438258772945	-0.237949602820	-0.965152392761
C	3.019230761870	0.816647805745	0.069740812611
C	1.031071549177	-0.129454715859	1.153071441947
C	1.365999841175	0.943890089749	0.121225298816
TV	4.791442011957	1.945633244146	0.968428113454
TV	0.000000000000	3.452053671093	-0.012180483039
TV	-0.000000000000	0.000000000000	3.475240518667

Energy = -45.366174511364 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min150

C	2.360453498478	-0.037972793088	-1.097966150329
C	2.164531900360	-1.279933313802	-0.229444620896
C	1.320245572826	-2.519812409012	4.638723109989
C	-0.770394718288	1.206790595979	-1.571027587967
C	1.679857880914	1.200914144631	-4.368012493478
C	1.924193026606	-1.282778677760	1.074917652985

C	1.576441272262	-0.034897946961	3.189193702380
C	-0.109040083840	2.450508840033	-1.794355971342
TV	4.557651613688	1.239225907670	-0.054788307408
TV	0.000000000000	2.484818545528	0.001372575695
TV	0.000000000000	-0.000000000000	6.839964498533

Energy = -45.365976248849 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min151

C	0.630282639377	0.095712875392	-1.702158272316
C	0.658380757578	-0.171127639779	-0.194228849784
C	-0.011697601585	1.155696632485	3.718662537099
C	-0.767952895089	-0.234377383662	-2.203034412989
C	3.130386187958	0.445450458664	-1.725613829259
C	3.158452818284	0.178595142172	-0.217663184744
C	1.867954987837	0.210382758184	1.952508154726
C	1.920815977944	0.063816347631	0.588411705875
TV	4.568524373396	2.076766847386	0.303581318430
TV	-0.000000000000	2.723815888620	-0.721514281099
TV	-0.000000000000	-0.000000000000	4.460567299194

Energy = -45.365011359027 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min152

C	2.947241088099	0.506767103306	-1.958957920578
C	1.285513307062	-1.046376327699	-1.082407374132
C	2.163376633792	-0.784357368262	2.874823142046
C	-1.014405135132	-1.268211317458	-0.251943982170
C	2.681661686915	2.297622423774	-3.724219779800
C	1.169158329375	-0.023823577594	0.028222415704
C	3.298791290801	0.904714769740	1.490780877043
C	-0.305001454509	-0.171023670889	0.579206200017
TV	4.721454039730	3.871494913515	0.320134377956
TV	0.000000000000	2.462652996923	0.657740524430
TV	-0.000000000000	-0.000000000000	4.938542996144

Energy = -45.363620287485 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min153

C	0.035491455269	-0.516493874376	-2.202455918265
C	-0.635409224534	-0.516325227003	-0.803736753025
C	-0.099828574393	0.802763410738	1.333924830588
C	-0.500271899237	0.802683582658	-0.009427814634
C	3.651576848503	2.105810393288	-1.189499089466
C	2.844526240132	2.105869041422	0.188729246323
C	1.452361386471	-1.177054248549	1.849141177478
C	1.495713386589	-1.176988946521	0.476210491262
TV	3.548116480199	0.000145928110	1.002077427531
TV	-0.000000000000	3.683626347507	-2.164120256872
TV	-0.000000000000	-0.000000000000	4.329925393501

Energy = -45.360385503177 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min154

C	3.195586749584	-2.260260384229	-1.180560468085
C	-0.015806101059	-0.682270648472	-0.749555976056
C	-0.459565581613	1.108237085504	1.926478201732
C	-1.767927516895	0.354643991422	2.184256165314
C	2.446478654664	-1.068615407593	-1.795132613455
C	2.205471956010	0.134981317495	-0.879676847081
C	0.753295738085	0.917127991889	1.067136716008

C 0.983859938296 0.155916029465 -0.060730621794
TV 3.170638518493 1.779048137889 -0.511381010354
TV 0.000000000000 3.296119862611 -1.621973915692
TV -0.000000000000 -0.000000000000 6.194987294872
Energy = -45.358902080625 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min155
C 3.037687033632 0.626931971889 -4.956289693567
C -0.296847658256 -0.907533140889 2.058645860660
C 2.285111497933 -0.689501740728 -0.565957607478
C 1.530615442523 -1.350612798289 0.604469496749
C 2.117815622655 2.720872248168 -4.751564596231
C -0.991756956106 -0.912959073940 4.400757138512
C 4.781036939293 0.143604999447 -1.926703630530
C -0.016657852540 0.607272097897 2.106399881541
TV 5.541176433486 3.976333485511 -3.664224572725
TV -0.000000000000 2.220440859466 1.352406552090
TV -0.000000000000 -0.000000000000 4.638971930942
Energy = -45.357942850196 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min156
C 0.601112762207 -0.237885556448 -2.224179581589
C -0.664412677852 -0.833479354067 -1.496311810583
C -0.347988642767 0.294164515800 0.858038246667
C -0.689615910940 -0.921988881826 -0.001070761123
C 2.848331095487 -0.702631979947 -0.799870489667
C 3.190858748415 0.513226251714 0.059404469873
C 1.899123369509 -0.170395783914 2.282315233252
C 3.165049574651 0.424742946283 1.554600250971
TV 4.232286059588 2.617500203487 -0.511037261049
TV 0.000000000000 3.743074220459 -1.894960157101
TV -0.000000000000 0.000000000000 4.180107551803
Energy = -45.357754069003 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min157
C 0.909691192407 0.510086653465 -3.036450759863
C 1.933711158075 0.295234635560 -2.069429893901
C 2.980966961049 -1.945306575091 2.151584932469
C -0.556038192904 -1.975317413167 2.278994007751
C 1.959793026377 0.745947518373 -4.091994552575
C 1.945520633218 -0.023808349558 -0.638574405691
C 1.953724410033 1.065501815852 0.308272229213
C -1.243000397382 -0.739584933522 2.569868086182
TV 5.691854767968 -1.195831031161 -0.461357590735
TV 0.000000000000 2.477300459005 0.552775429119
TV -0.000000000000 0.000000000000 5.833300103952
Energy = -45.357112389342 hartree
Spin(**2) = 0.058593750000
Geometry of 3D-min158
C 2.014564646702 -0.303295898452 -2.158330450809
C 0.957188694683 -2.333770350811 -1.530243146627
C -1.558326882362 1.877532370802 1.085994007091
C -0.631131574317 4.042361400343 -0.075127407444
C 2.569725801265 1.761504989306 -0.212151773037
C 3.492068763059 1.003490375793 0.516302312976
C 0.702833976067 -2.281611445490 1.403620844917
C 1.472609508430 -0.848363729275 1.019759734871

TV	3.820052264099	-0.160057948488	1.713036700550
TV	-0.000000000000	3.150378450259	-0.396497954771
TV	0.000000000000	-0.000000000000	4.476237177905

Energy = -45.356488349349 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min159

C	1.932302003443	-0.097556906038	-0.798302249463
C	0.489145465224	-1.527660386701	-0.202438429001
C	1.310941781323	-1.227059059655	4.409232180163
C	-0.152696328772	0.338596043926	-2.814561442102
C	1.772156791763	1.787837938804	-3.511850265306
C	1.110784176245	-0.398208638599	0.577485326189
C	2.575232011455	0.516247663502	2.350272604746
C	0.650200500153	1.547798940094	-2.402047324167
TV	4.041326541368	2.594681333954	0.008115869444
TV	0.000000000000	2.480753864553	0.537324139421
TV	0.000000000000	-0.000000000000	5.987459211173

Energy = -45.355834101424 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min160

C	1.270014630702	1.060161662968	-2.390642246669
C	1.193085805323	0.519604350774	-1.008893322945
C	-0.168451212383	0.785608934211	0.982982402809
C	-0.151288352659	0.667716767600	-0.473523759352
C	2.393141325176	-0.126246645933	-0.382049300494
C	3.843960225111	0.231336033624	-0.470087112239
C	1.787249636122	-0.953754017248	2.257002979406
C	1.928518493377	-0.209558787245	1.024377444641
TV	4.828478518360	-0.426702644519	1.215437512242
TV	0.000000000000	3.418000808871	-0.994254454170
TV	-0.000000000000	0.000000000000	3.862802734016

Energy = -45.353303066359 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min161

C	-0.154217033540	0.496777028602	-2.081545220896
C	2.747469111293	-1.200494850518	0.509100517173
C	0.130804834873	-0.669511711747	2.529525637583
C	-2.771312609772	1.027189361963	-0.061060682178
C	0.614011262271	2.559927708985	-1.069937444434
C	1.215990542147	1.568078770497	0.117678734011
C	-0.637875612045	1.830523782161	2.401008457498
C	-1.239978838886	2.821898968686	1.213360280565
TV	3.008815805201	-0.557214203220	0.596694756259
TV	-0.000000000000	4.563368838716	0.883076387214
TV	0.000000000000	0.000000000000	3.982217488598

Energy = -45.353239710552 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min162

C	0.536986781411	-0.205968777563	-1.616303644132
C	0.489051401803	-0.459049453387	-0.142812309468
C	-0.436617510883	-0.008274898221	1.011332792102
C	-0.726853396114	-1.402551040670	0.469792542124
C	3.264774955201	-0.122529902059	-1.566827841391
C	2.997638846442	0.327116948165	-0.121847971995
C	1.830902280928	-0.247920685188	1.776146043149
C	1.839020062078	-0.221553497662	0.372174120293
TV	4.535424900426	2.211064952610	0.601669403264

TV	0.000000000000	3.643774928669	-0.727335032904
TV	0.000000000000	0.000000000000	3.865737530933

Energy = -45.351985897674 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min163

C	-0.475634898703	1.252571977835	-1.125774791050
C	-0.475653734977	0.729091396162	0.509049656884
C	0.772012475696	-1.384266398909	0.812887135669
C	-0.657177666667	-0.836849965503	0.784081848183
C	0.771953245974	1.286597354842	1.259162144326
C	0.771868603295	0.694973977711	2.610873312787
C	-0.657138426558	-1.360387322327	2.419058587455
C	0.771820766473	-0.813038837848	2.390002637510
TV	2.676752868477	2.089216163188	2.577096294128
TV	-0.000000000000	4.178863896734	0.667235679382
TV	0.000000000000	-0.000000000000	4.487137154133

Energy = -45.351697893350 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min164

C	1.960653321336	-0.122352613810	-3.969848278127
C	2.735708983288	-0.643658658667	-1.697593310938
C	3.104943245915	0.164275673932	3.379486082375
C	0.482701948122	-1.051289745210	0.475665620203
C	1.012882236975	1.451734312321	-2.671385810334
C	2.156773066900	0.775079339371	-1.883478496758
C	1.379859424553	1.246523257905	2.185064380565
C	0.119153087846	0.322753750809	0.205379934874
TV	3.505065480941	1.390561048266	-0.176138739834
TV	-0.000000000032	2.582085515716	0.561366790671
TV	-0.000000000001	-0.000000000502	6.350168307297

Energy = -45.351693814176 hartree
Spin(**2) = 0.015380859375
Geometry of 3D-min165

C	0.128862610717	-0.403688994805	-1.320737041045
C	0.128340118365	-0.405627253953	0.094762227424
C	0.128335688444	0.308288397691	1.329185342750
C	0.128061751663	-1.631607196577	-0.605908991923
C	0.128879383011	-0.403650200663	2.562354608752
C	0.128362440778	-0.405472953196	3.977843754701
C	0.128359121745	0.308376354036	5.212310424751
C	0.128101824056	-1.631511555277	3.277243251390
TV	3.242987658780	1.669279204533	-0.983366923892
TV	0.000000000000	3.365337471611	1.926008545644
TV	0.000000000000	-0.000000000000	7.766172870355

Energy = -45.351187886458 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min166

C	1.396406008738	-0.015297889783	-2.958202622311
C	2.250778313054	1.292215571962	-1.093445918308
C	-0.126460918354	-0.059631029601	1.239373734473
C	-1.248047989117	-0.071905562677	0.102518995526
C	0.126342186753	2.398558786977	-0.289134266189
C	1.247973606063	2.410619841543	0.847649330444
C	-1.396255909574	2.353800604107	3.908361494541
C	-2.250715850557	1.046208051792	2.043497577039
TV	3.444290401096	1.305759293606	0.356758133948
TV	-0.000000000000	3.906111944073	2.031464368436

TV	-0.000000000000	0.000000000000	3.880094853306

Energy = -45.351061064597 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min167

C	0.063600056611	0.533317493083	-1.797793332207
C	2.383127238772	-0.795871332055	0.854893650598
C	0.312514682892	-0.305048050564	2.996568369763
C	-3.582772146396	-0.653159661537	0.657871613751
C	0.839639320581	3.025168261971	-1.625461850005
C	1.995910711507	2.807745471316	-0.573926077784
C	-0.344866764343	1.983099782932	2.069472215844
C	-1.431006350942	2.454787606175	1.028245883792
TV	3.409596207783	0.448185876701	0.006710014179
TV	0.000000000000	4.794082861318	-0.684277728859
TV	0.000000000000	0.000000000000	3.739762406522

Energy = -45.350630289213 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min168

C	0.698185165680	0.045925131944	-1.640755467181
C	0.698484908900	0.042233834488	-0.222824865358
C	-0.010588626895	-0.021306921032	1.008393844428
C	-1.426955412306	-0.150888908005	1.009492821949
C	0.705057229443	3.481889832062	-1.219151814176
C	0.705205902027	3.479173039508	0.198727741280
C	-0.003851912891	3.417687499694	1.430118882750
C	-1.420299868003	3.287219755012	1.431154558402
TV	3.349262272852	0.303278509535	-1.942237315423
TV	-0.000000000000	6.847176150687	1.055432903126
TV	-0.000000000000	0.000000000000	3.880487182161

Energy = -45.349968581179 hartree
Spin(**2) = 0.032226562500
Geometry of 3D-min169

C	3.220521460977	0.468537851873	-2.438248449697
C	2.478355268359	-0.863006873210	-0.652949022405
C	2.741284722458	0.587714409923	3.785985152218
C	0.016831190481	-1.358472199857	-1.479124102761
C	1.948172823913	2.331636300543	-2.199039780936
C	1.464905670861	1.450396825048	-1.017172535748
C	2.214221107967	1.280974267779	1.504804717990
C	-0.636616309461	-0.203333844401	-0.982111300436
TV	5.296447960250	0.605686575738	2.929756896250
TV	-0.000000000000	2.557322787777	0.748360236371
TV	-0.000000000000	0.000000000000	4.750277351641

Energy = -45.349184497951 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min170

C	1.136407718274	-1.113813219438	-1.859027911616
C	2.096813807421	-2.762541407905	0.751942538502
C	2.966114257442	0.307863061540	5.326311468764
C	-1.036160758120	0.198307364364	-1.822468120141
C	1.544335270556	1.225216651622	-3.556275707013
C	2.144298380193	1.513013954167	-1.066742574193
C	1.718387875429	-0.112541642125	1.827320904918
C	-0.343287500459	1.451876587830	-1.986123662843
TV	5.490273217454	2.642714950064	0.917155531789
TV	-0.000000000000	2.518802238296	-0.281992202550
TV	-0.000000000000	-0.000000000000	5.928120694350

Energy = -45.348869813630 hartree
Spin(**2) = 0.187500000000
Geometry of 3D-min171

C	1.981342511870	0.641606156634	-3.076954939505
C	-0.003366469506	-0.700444668255	0.547978628662
C	-1.086274530519	1.666087683767	-0.431819161156
C	-0.061686584998	0.635119864793	-0.054866934373
C	2.640228895718	1.435873244422	-0.629850482044
C	4.046210898869	1.747990427549	-0.058479639536
C	0.910275008532	-1.579336379986	2.406685536739
C	1.434567067966	-0.783897068540	1.203257849080
TV	4.116755461292	-0.746351317804	2.558178528118
TV	-0.000000000000	3.226224482013	-1.697479451073
TV	-0.000000000000	-0.000000000000	4.163875594444

Energy = -45.348630575637 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min172

C	4.160069960960	-0.363130692005	-1.612178625473
C	-0.222862796923	-2.595789754979	-0.220741841423
C	3.094228581079	-1.297094699892	3.514783774236
C	1.227798336585	0.128210634661	-0.750853821079
C	1.266739641029	1.467851035016	-4.205595862603
C	-0.115060749032	-1.376532977339	0.717973688886
C	1.916512093839	0.232204007205	0.690027771100
C	1.530988742454	1.428218669593	-1.524061828141
TV	3.572611328583	2.975704059375	1.440337433513
TV	-0.000000000000	2.523490091953	0.116479100106
TV	0.000000000000	0.000000000000	5.558768952866

Energy = -45.348207701354 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min173

C	1.788967843465	1.410428699824	-3.938127723125
C	0.431762075288	-0.729385761759	-0.484375890175
C	-1.658206631014	0.711940821738	-0.412311732804
C	-0.330881092257	0.441534114048	-1.087642006318
C	2.906674125214	1.733742882849	-0.474738482686
C	4.282987997734	1.992557081750	0.183619555849
C	0.532447684011	-2.590253027841	2.143132343511
C	1.808787047994	-1.221204828131	3.408232466281
TV	4.582314717994	0.935443075018	2.715798484718
TV	0.000000000000	3.200874901286	-1.841986380200
TV	-0.000000000000	-0.000000000000	4.203968162044

Energy = -45.346427601641 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min174

C	2.116783380241	-0.606525593932	0.764850460666
C	0.145739802012	-1.500163470706	-0.468567016823
C	1.667244237233	-1.532842911664	3.414253422885
C	2.282954973861	1.279780987949	-0.840519771071
C	3.552116441376	1.526680494344	-1.547024049600
C	-0.562458608936	-0.310178953509	-0.081649458024
C	4.381664930113	0.374495374324	1.748857203893
C	-1.986877885682	2.049825436633	-3.042521446662
TV	7.700021116518	3.086448005959	-1.249933911247
TV	-0.000000000000	2.361579480581	0.825022711219
TV	0.000000000000	-0.000000000001	3.790066478105

Energy = -45.345455435456 hartree

Spin(**2) = 0.000000000000
Geometry of 3D-min175
C 2.437988597410 -0.104012455131 -1.278241668316
C 0.583200041902 -1.693471057712 -0.556687232593
C 1.551976024022 -1.269135855796 2.208611418755
C -1.779274022612 -0.368380394898 -0.645786246726
C 3.366546207359 1.613050842566 -3.263391544219
C 0.611376641020 -0.850446468000 0.878591879396
C 4.600368633463 2.132386585321 1.090516367749
C -0.838470955920 0.851101935055 -0.072566761767
TV 5.307645035084 3.329135000220 -0.381275985927
TV -0.000000000000 2.366368729588 1.099247152441
TV -0.000000000000 0.000000000000 4.061608078707
Energy = -45.345439192262 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min176
C 1.196919089528 -0.134147987969 -3.046575656007
C 0.974640318532 -1.441629587882 -2.237502234756
C -1.686730235917 1.626402559177 1.745743101293
C -0.484797690543 1.527027548414 0.864301856689
C 2.723208451126 2.279702507814 0.357757395391
C 3.889246238081 2.100717234757 1.224594658439
C 0.831933521530 -2.137639826890 0.805962642655
C 1.575113241199 -0.902584735217 0.335542358230
TV 4.177397588436 0.288636026197 1.746199429891
TV -0.000000000000 3.430671990079 0.844925266942
TV -0.000000000000 -0.000000000000 4.462379534906
Energy = -45.345401487472 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min177
C 2.404135796815 0.575239596453 -2.525278301898
C 2.847218897595 -3.080208271911 -1.328636474167
C 2.158571942436 -0.905581408889 2.454046977885
C -0.604588382284 0.606208959733 0.255737055603
C 0.779138195071 0.369601827222 -4.249030399323
C 2.151732902108 -1.647231380837 -1.201798919399
C 0.966991614962 -0.030766925504 2.075106141812
C -1.287360458814 1.726597966955 0.797585112609
TV 5.647485445819 -0.334902747390 0.410036184251
TV -0.000000000000 2.222309886118 1.282708829585
TV 0.000000000000 0.000000000001 4.992017416884
Energy = -45.344587931300 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min178
C 1.836325394891 -0.995859692252 -2.778251661351
C 0.911006379876 -1.600058790193 0.186991874737
C 3.125417593743 -1.171416385999 3.355613811987
C -1.441808616813 -1.194205933302 -1.343631615922
C 2.273254343290 1.585451889137 -3.856027006611
C 0.368760439997 -0.275939757655 0.063131148743
C 1.872847159745 0.536247426644 1.859765748960
C -0.827534987961 -0.068722514942 -0.712433623882
TV 5.961272650979 2.303257671500 -0.841936180541
TV -0.000000000000 2.410644137374 0.643674091463
TV -0.000000000000 0.000000000000 6.622030722094
Energy = -45.343659423292 hartree
Spin(**2) = 0.000000000000

Geometry of 3D-min179

C	0.845763048674	-0.184574813414	-2.516808976758
C	1.770520262376	-0.780098225812	-1.458130666460
C	0.047493584036	-1.586280386882	2.824733101007
C	0.390502346198	0.120583228640	-0.208985626416
C	2.360141053681	1.886657981264	-3.348032965562
C	2.017419101197	0.179884901995	-0.314521309270
C	1.561740995355	0.484902229705	1.993443481504
C	0.637230757010	1.080561728915	0.934711934634
TV	3.820180694661	3.315496026988	-0.191973010775
TV	0.000000000000	2.435907181997	1.369861171563
TV	-0.000000000000	-0.000000000000	5.700098590653

Energy = -45.342018529956 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min180

C	1.035610453910	-2.335756008394	-0.798152919274
C	3.683758204056	-1.421592540293	-1.029759429248
C	-0.858298803393	1.782944528982	0.655330483431
C	-1.939318767536	0.844933805195	1.094345556789
C	2.325759011294	-1.616428136350	-0.463313157380
C	1.937125182213	-0.430436682229	0.431011061485
C	0.621637218907	1.895365049972	1.052489192296
C	1.472537807722	0.814849371404	0.424817815848
TV	3.281392151154	1.254399465032	-1.412857000515
TV	0.000000000000	4.694125756353	-1.875881841498
TV	-0.000000000000	0.000000000000	5.078322152309

Energy = -45.341001603115 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min181

C	0.350447228981	-0.139565484380	-2.025733104855
C	0.321693609437	-1.100023955650	-1.041130378691
C	-1.077168814727	-1.693763336309	2.705615156031
C	-1.049309965576	0.472230241074	-2.231882631962
C	3.028004853907	1.997664965260	-0.526455254403
C	3.163599294676	3.094960670609	0.673204144140
C	1.614322849571	-0.297482526759	0.829476228968
C	1.546521245093	-1.167127617419	-0.228379094728
TV	4.859155011347	2.396247600155	0.662408072804
TV	0.000000000000	3.373574795879	-0.196857658103
TV	0.000000000000	0.000000000000	3.638255581381

Energy = -45.340621688773 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min182

C	2.568238461887	0.703292327833	-3.531866122859
C	1.512206463543	-0.971800875523	-0.360192341896
C	2.158768724717	-2.018947432848	3.272959365745
C	-0.575176563345	-2.400395516117	0.210859463323
C	2.584669183478	1.466347112249	-4.779957839909
C	1.738597889899	0.393486136150	-1.026630639966
C	3.399682212876	0.158634114178	1.173299334088
C	0.076284374281	-1.045802846963	0.164775201273
TV	5.436338918136	2.560747760721	0.703186104655
TV	-0.000000000000	2.558773392528	0.275555770555
TV	-0.000000000000	-0.000000000000	5.840274057060

Energy = -45.340588136655 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min183

C	3.661399409901	0.068367456804	-1.265375067748
C	0.830835440471	-1.186477570090	-1.223121330166
C	0.707872591468	-0.438616889722	1.265604430784
C	-1.286360714344	-0.743339191779	0.058866489611
C	3.035564863322	1.956912007199	-2.790564998083
C	1.497652626896	-0.266405593570	-0.048715242620
C	3.516720909880	0.516720640495	1.166183484602
C	-0.417338045070	0.420581964283	0.565761727701
TV	6.219403842438	3.369005489956	-1.030404373359
TV	-0.000000000000	2.302396772083	1.010061642715
TV	0.000000000000	-0.000000000000	3.785323474919

Energy = -45.339165717953 hartree
Spin(**2) = 0.140625000000
Geometry of 3D-min184

C	2.791872912606	-0.301669467087	0.093537176383
C	0.675134859497	-1.408226082130	-0.808051541649
C	2.211855023163	-1.353769196313	3.402856858174
C	-0.219380247033	0.799746823621	-1.714854852190
C	2.889019015886	1.568338249494	-1.866759287144
C	-0.019201788236	-0.189056681611	0.078479405293
C	3.728580040905	0.331885990890	2.120820756516
C	-0.534776239948	2.129500450900	-2.269835598476
TV	4.967523772745	2.517095370845	-0.926987410324
TV	0.000000000000	2.471444725472	0.473633339185
TV	-0.000000000000	-0.000000000000	4.231931235223

Energy = -45.339017324248 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min185

C	3.442512634518	0.760582663494	-1.605446248257
C	2.722058848726	-0.472318474204	-1.770332521804
C	1.240871257846	-2.888437352067	3.862520815798
C	-0.519530160243	0.492738598437	-0.285704608355
C	0.928705576917	1.197305202935	-3.736609234106
C	1.063653973569	-0.955240022788	0.602716841090
C	0.966811763005	-0.168952732529	2.952455319614
C	0.301204454954	1.737140556737	-0.177572722626
TV	5.346406843218	2.755474008948	-1.096908235045
TV	0.000000000000	2.431659610669	0.496751054810
TV	-0.000000000000	-0.000000000000	6.201317702180

Energy = -45.338733582844 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min186

C	0.847437792470	0.415285739245	-1.871409143808
C	0.848146932482	0.416261786770	-0.370266676809
C	-0.478602009312	0.976325632218	2.730342945856
C	-0.479447952461	0.976080635980	-0.377654956317
C	2.999937654965	-0.485965342000	-1.872994298606
C	3.000769876722	-0.484820688185	-0.371773421318
C	1.924591603995	-0.034564851971	1.895142799076
C	1.923788973413	-0.034453720941	0.455496600543
TV	4.805829052027	1.630586288229	-0.937809274644
TV	-0.000000000009	3.653598316588	-0.936388571736
TV	-0.000000000005	0.000000000007	4.593885891262

Energy = -45.337051787529 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min187

C	0.826955487759	-0.509553542262	-1.857594198649

C 0.826695803032 -0.509673170973 -0.238435440365
C -0.664354770103 -0.508528477252 1.610180365340
C -0.664775809574 -0.508839617727 0.052746686769
C 2.959122258926 2.364326721620 -2.929779895864
C 2.958986935645 0.232989721706 0.830740094994
C 1.443664726364 2.070884371939 0.830786427535
C 1.443592177682 0.526275957211 0.831298315406
TV 4.359636764276 1.807174300997 -0.001368468338
TV -0.000000000000 3.616788154496 -0.000990856307
TV -0.000000000000 -0.000000000000 3.759686675683
Energy = -45.336873920880 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min188
C 0.734155848102 0.219321515929 -2.395105651537
C 2.780997938458 1.350029817892 -1.452659914233
C -0.566534950694 0.219030000455 2.400400261076
C -2.760116660798 -0.586874064566 1.525307356443
C 2.781197198446 -0.911819977276 -1.452851854191
C 2.684284059265 0.219008584490 -0.514261216973
C 1.805247701939 -0.858065032559 1.764656473543
C 2.283613614868 0.219469745077 0.777532756515
TV 4.565324007983 1.883984177523 0.239486001120
TV -0.000000000000 3.768602185800 0.000462108127
TV 0.000000000000 -0.000000000000 4.478798510816
Energy = -45.334329215071 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min189
C 1.517798773030 0.563855239394 -2.586464895980
C 2.661022661741 1.252150577013 -0.527608164697
C -2.141651163644 0.214029637442 0.942789167762
C -0.728208199219 0.260434333414 0.395284467514
C 2.114256050233 2.503536905473 -1.102631550585
C 4.077111225467 1.507148874320 -0.017163805289
C 0.148728976678 -3.364385116228 2.587772416639
C 2.003363200682 0.091957163246 0.117234150472
TV 4.762297961072 1.191952913079 1.020433524485
TV -0.000000000000 3.735606494708 -0.936955433444
TV 0.000000000000 0.000000000000 3.968946951505
Energy = -45.333931183320 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min190
C 0.889287284288 0.440752245795 -1.832492757771
C 2.034108145127 -0.244467025913 -0.043142213971
C -0.700565991027 -0.679075320966 3.480261753762
C -1.511659201046 -0.009640042514 2.278313469871
C -0.593343077668 2.470357426419 -1.930208725096
C 2.077557096742 1.873770362432 1.221078185226
C 0.663219276676 1.787260729407 1.640173381954
C -3.005884350179 4.205013952690 -1.072752370246
TV 3.735165860738 0.287791364119 -0.908074048483
TV -0.000000000000 4.691929759000 -1.415574771912
TV 0.000000000000 0.000000000000 3.828771116015
Energy = -45.331808433062 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min191
C 2.732388860122 0.252323478089 -1.161951343431
C 1.354871405511 -2.231432200593 -1.735205703399

C	1.425141413426	-2.433733267924	1.812986708321
C	-0.802081234342	1.057781783915	0.111436475517
C	1.696317139062	0.679620955792	-2.128317282938
C	0.705446289338	-1.341924775898	-0.651661010253
C	0.980883000852	-1.929026747458	0.672999785566
C	-1.484695968027	2.256622277435	0.494769698015
TV	5.655610018804	0.164804952337	-0.371255462069
TV	0.000000000000	2.289566264674	1.012617483962
TV	0.000000000000	0.000000000001	6.185901418543

Energy = -45.331242567223 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min192

C	0.900232215224	-1.524726952513	-0.996772530522
C	0.535442417114	-0.397946872556	-0.233172539222
C	-1.819919873034	0.303816710662	0.862374837239
C	-0.844738094590	-0.024167149328	-0.204726889527
C	3.889808676848	-0.419263573626	-0.520855196725
C	2.914622494266	-0.091598668998	0.546170667754
C	1.169009464755	1.406921515505	1.339109954648
C	1.534353006583	0.280844379160	0.574640300301
TV	5.759427332504	3.493110581287	0.056253712449
TV	0.000000000000	4.042676598363	-0.680569324515
TV	-0.000000000000	0.000000000000	3.524178367192

Energy = -45.331133789272 hartree
Spin(**2) = 0.015869140625
Geometry of 3D-min193

C	0.031667370531	-0.645938188128	-0.919414904255
C	1.461451277868	-0.985564232909	-0.711981290615
C	-0.625854750951	-0.006065970669	1.567095198057
C	-0.755976470962	-1.020491890480	0.388987172333
C	0.631036297986	2.875497161042	-0.903018940455
C	1.191579199039	2.404077970755	0.387766176559
C	0.057467231287	2.485895089625	1.473707955189
C	-0.991353565308	1.331475975907	1.439014912245
TV	3.573830505578	0.543853028743	-0.758206671595
TV	0.000000000000	4.818920422801	0.591737163478
TV	-0.000000000000	0.000000000000	3.693899851781

Energy = -45.330658547226 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min194

C	0.750932282378	0.130978113864	-3.775239679908
C	2.146269692045	-0.346327231663	-1.502838042109
C	2.107642339930	-1.435678211324	3.668922798713
C	-0.151795239332	-2.072961131743	0.588718395879
C	1.619161284990	1.323339652367	-3.332512394625
C	1.832674429029	-0.647766810189	-0.073182619024
C	2.600403629252	1.569600647182	1.604685674398
C	0.385542959078	-0.707016233906	0.206626031110
TV	4.255404942032	3.659018369345	0.936588531485
TV	-0.000000000000	2.462019230868	0.518321542159
TV	0.000000000000	0.000000000000	6.105338688063

Energy = -45.328186421300 hartree
Spin(**2) = 0.066406250000
Geometry of 3D-min195

C	0.539461214532	0.869256816297	-1.491067579374
C	1.072692442847	0.234458819612	1.100653214771
C	0.087449448439	0.046529777771	3.686902257891

C	-1.381914143004	0.465656208499	0.145109683579
C	0.240189946831	2.844781557593	-1.260900422981
C	1.360311137462	1.981585165855	-0.756067557033
C	-0.701266980890	1.739845232552	2.114358370589
C	-1.674746268930	1.878552516552	0.937548370930
TV	3.212942552860	1.092353297901	0.422649005940
TV	0.000000000000	4.158098347764	-0.406292328715
TV	0.000000000000	-0.000000000000	3.878209024008

Energy = -45.328045267209 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min196

C	1.092823137021	0.501518781509	-1.415414371030
C	0.299630536545	-0.340380159064	-0.406505234132
C	0.190599331992	0.424463950038	0.945059818864
C	-1.223656146028	-2.739026345109	0.149737705058
C	3.315650452254	1.511714008299	-1.893451007561
C	2.522443791855	0.669831148577	-0.884551161481
C	2.413399926582	1.434668826154	0.467001088051
C	0.999199420388	-1.728829596579	-0.328326085698
TV	4.445669552909	2.020387099677	-0.956095627228
TV	0.000000000000	3.365487682317	1.467720705315
TV	0.000000000000	0.000000000000	3.663773647982

Energy = -45.326291002259 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min197

C	0.468603501265	-1.421885987802	-1.498395883962
C	0.601202289498	-0.195882399026	-0.714102749493
C	-0.655110365753	0.665433947184	1.010233919005
C	-0.765673749540	0.335584456650	-0.344341289133
C	3.779159530450	0.646029901641	-0.971371192394
C	3.039566694135	0.214086253385	0.183236196998
C	0.803238468419	0.841992218899	1.290537841013
C	1.590187503134	0.271940806180	0.259441986004
TV	4.709384334399	2.599684339960	0.673264617167
TV	0.000000000000	2.932853403995	-0.978862537708
TV	0.000000000000	-0.000000000000	5.028839567697

Energy = -45.325003747511 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min198

C	0.598798946713	-1.221444135114	-2.041243751232
C	0.485000305410	-0.670557548071	-0.685642589847
C	0.803264447878	1.003798784183	0.926338785248
C	-0.254777113737	0.354875345090	-0.114742366543
C	2.042171450933	0.768364067626	0.028644315927
C	2.635385381749	-1.964471257264	0.306220425126
C	1.053313060456	-0.346929566321	1.558810058887
C	1.803806165864	-0.707973211169	0.254076493578
TV	4.319152984121	1.110705661678	-0.960060096154
TV	0.000000000000	3.642858578248	-1.122696923040
TV	0.000000000000	-0.000000000000	4.560879169025

Energy = -45.322386829313 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min199

C	0.696421360069	-2.018874689812	-3.367217476785
C	0.745196650004	-0.156194669614	-1.457343872754
C	-0.301188850559	-1.160339520096	2.759928272373
C	-1.318521165292	1.239001943681	2.890979010636

C	2.997700425627	1.576955575516	-1.607583387748
C	2.858129168350	0.886881719211	-0.367869034996
C	1.587723507662	-0.922760786150	0.841885399697
C	1.528550562978	0.278329954483	-0.125503930153
TV	4.924951446059	-0.180195966830	-2.168530963135
TV	0.000000000000	3.143979917587	0.812254967671
TV	-0.000000000000	0.000000000000	3.519810551458

Energy = -45.320675597802 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min200

C	1.113039222498	-2.449863511733	-0.171682058411
C	3.832745650066	-1.965744605701	-0.186926210053
C	-0.871438276311	1.639697076717	0.080017449189
C	-2.073488942107	1.607860181312	0.951719150559
C	2.315453178050	-1.663829838008	0.205632090515
C	2.044616939274	-0.207817310744	0.261420895081
C	0.645831975894	1.846948921443	0.530283507420
C	1.272050559807	0.726628474997	-0.303696220337
TV	3.186795065262	1.599788241410	-0.966808297210
TV	-0.000000000000	4.074230392248	-2.463288109479
TV	0.000000000000	-0.000000000000	4.601749340038

Energy = -45.320241919222 hartree
Spin(**2) = 0.000000500000
Geometry of 3D-min201

C	1.658864099003	0.062652808376	-1.848357779155
C	0.695847039736	-0.473930724835	-0.528498726012
C	-1.564385368075	0.899613646336	0.105353058108
C	-0.074189360977	0.789422321671	0.000905708985
C	2.098744698459	1.739472463000	-0.470159594045
C	4.915118731042	1.680163185239	1.373260060935
C	0.774282484892	-2.381584939665	1.254484830305
C	1.566232559366	-1.053839984675	0.650008016331
TV	4.379981261617	-0.093995900061	2.352674950539
TV	0.000000000000	3.683786372252	-0.023230170700
TV	0.000000000000	0.000000000000	3.596963557440

Energy = -45.318305892197 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min202

C	0.957212898001	0.283528032369	-1.735158194903
C	0.475948897032	-2.543794774666	-1.275116251910
C	2.685393570891	-1.735204964011	0.590102950841
C	-1.152228492156	0.800019170470	1.140837474584
C	3.823447833631	0.900490999097	-3.873801275752
C	0.241604941056	-1.524833823339	-0.139128696709
C	1.342798289286	-1.839957403368	0.952479458480
C	-1.765907031760	1.969984266827	1.754841862770
TV	6.905817198178	-0.915549808836	-1.488849537538
TV	0.000000000000	2.486955823882	0.719134230808
TV	-0.000000000000	0.000000000001	4.670367941752

Energy = -45.317152441677 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min203

C	0.867140747734	-0.372849254412	-2.370095738944
C	0.727573884264	-0.065734653056	-0.968996652884
C	-0.534162980011	2.318185252767	1.944290165175
C	-1.405007737270	1.086500293828	2.140406519737
C	3.003486121821	-1.314578009842	-1.980522804358

C	2.878978878169	-1.116052374364	-0.449523976953
C	1.655400048657	0.769121616233	1.105457234813
C	1.953728735810	0.289432434015	-0.287114801932
TV	5.358714917196	0.243690407057	-1.722985800234
TV	-0.000000000000	2.489290141138	-0.387465251197
TV	0.000000000000	0.000000000000	4.071139051950

Energy = -45.316690980621 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min204

C	2.012402572941	-0.719374090980	-3.199153906733
C	2.647402219170	-0.940037941714	-0.017703423409
C	2.016374328876	-2.168756385857	2.949951142694
C	-0.102786279047	0.907888793922	0.424835632831
C	1.380881909965	0.654481606492	-5.421076114596
C	2.017298055468	0.108820982570	-0.860369468003
C	2.010437194687	-0.394463171753	1.209355313359
C	-0.741532729809	2.180562572778	0.715093930779
TV	4.872633343293	1.829257936037	0.408660391470
TV	0.000000000000	2.602803288011	0.597970498562
TV	-0.000000000000	-0.000000000000	5.788707239378

Energy = -45.316623876385 hartree
Spin(**2) = 0.015869140625
Geometry of 3D-min205

C	2.791737241648	-0.193891759709	-1.500471955122
C	1.410793855018	-1.756097244398	-0.150976185109
C	1.993098030950	-1.509024542118	4.341363272315
C	-0.054149942672	-0.068151270678	-2.146258764541
C	2.290299967157	0.952476669013	-4.278851063873
C	0.879635432085	-0.615248119253	0.623316044156
C	1.256649249885	1.390965001943	2.414247003632
C	0.752315416777	1.250264280242	-2.079689542541
TV	4.180454593512	2.480711141357	0.895850580191
TV	0.000000000000	2.563405066015	0.482531147561
TV	0.000000000000	0.000000000000	5.905544580874

Energy = -45.314977838146 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min206

C	-0.268836337830	0.660618347657	-2.384816889143
C	0.222967807830	-0.206742863581	-1.181535317980
C	-0.620094979339	1.281280707541	1.540989792162
C	-1.156384668583	-0.344821850489	-0.476933397947
C	0.287382432655	2.252027946692	-0.719602360134
C	0.567915970552	1.756940910999	0.693677193382
C	-0.895320077239	1.766817279938	3.753730082477
C	-1.247761340341	2.388174777718	2.430308914878
TV	2.206676656110	1.250370822470	-0.000253124704
TV	-0.000000000000	5.143499941641	3.536240442034
TV	0.000000000000	0.000000000000	5.320083802974

Energy = -45.314597152068 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min207

C	0.540991732416	0.611118583573	-1.930601719329
C	2.690690246069	-1.913707093872	1.206075722969
C	0.381827934522	-0.273010634263	3.346019457239
C	-1.981176527465	0.707593394998	-1.151609141044
C	0.009971879435	2.510984505308	-0.983737478759
C	2.262818389959	2.618438065512	1.923668890010

C	-0.835141298857	1.530557631509	2.174259968569
C	-1.575280958387	2.146981147088	1.014945902092
TV	2.933062480883	-0.350147973103	1.688632856527
TV	-0.000000000000	5.523524165766	-0.076351557011
TV	-0.000000000000	0.000000000000	3.943065736713

Energy = -45.314539455655 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min208

C	0.441097402038	-0.154051572072	-2.158481286267
C	1.829884304601	0.085662324366	-1.679631442055
C	-0.859697718550	-0.037391804451	1.960349837177
C	-2.248344398822	-0.276702871784	1.480879488673
C	3.201568903186	2.077453833832	-0.957568390284
C	2.482669843438	1.344247648510	0.210558687986
C	1.497459089868	-0.884434373587	0.935542537688
C	2.216466619998	-0.151217782902	-0.232671135373
TV	5.117610101935	1.384106959184	0.176535341598
TV	0.000000000000	3.459382735021	-0.784817948583
TV	-0.000000000000	-0.000000000000	3.813244100451

Energy = -45.313591103022 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min209

C	1.207822926678	0.301696415413	-0.981447596644
C	0.880208133619	0.502952726721	0.476338277183
C	-0.256775857899	-1.463879097191	1.396093636815
C	0.045792792421	-0.775102463715	0.241511568137
C	3.324945466514	0.506552202788	-2.451336184840
C	4.173811177972	-0.757939930724	-1.963456679483
C	1.917124716564	0.552713973688	1.625810122938
C	-0.316843640257	1.444447295535	0.964767606239
TV	4.303251255253	-0.324297650650	-0.747077328692
TV	-0.000000000000	4.315561694764	-0.744983214353
TV	-0.000000000000	-0.000000000000	3.761890081828

Energy = -45.312783242992 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min210

C	0.850166862133	-0.010954961544	-1.543649702278
C	0.697954112758	-0.532721232706	-0.136513620439
C	0.231047818888	0.463904635271	1.031619820806
C	-1.265536776954	-2.065204630204	0.137247760387
C	0.850314156686	2.503391345878	-0.609704746357
C	0.697824564188	1.981613181114	0.797387346217
C	0.231046217815	2.978200208150	1.965601306142
C	-1.265514016734	0.449075399186	1.071346062599
TV	3.243278895943	1.809852615665	-1.021752877336
TV	0.000000000000	5.028618730313	1.868026675224
TV	-0.000000000000	0.000000000000	3.853335859900

Energy = -45.312725546579 hartree
Spin(**2) = 0.015869140625
Geometry of 3D-min211

C	0.389963138698	0.561509322189	-0.824705898880
C	0.444100555932	-0.968011026502	-0.677811577401
C	-0.514313488796	0.717294206420	4.247429123142
C	-2.065110428923	0.350345357344	-0.021252905960
C	1.662743071619	3.843616558408	-2.302010765754
C	0.006803481401	2.241406740755	0.341421326329
C	-1.701313466777	2.739656745989	1.918775927293

C -1.140527926746 3.253684733406 0.585041729209
TV 2.278586915500 -0.856102986805 0.907742163819
TV 0.000000000000 5.812623097987 -1.394029107183
TV -0.000000000000 -0.000000000000 3.930348432636
Energy = -45.311541520636 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min212
C 2.633096491787 -0.283613818813 -2.675337369633
C 0.986508272442 -2.048623544809 -0.219163291118
C 1.316075943458 -2.245024389392 4.073599343052
C 0.017550836675 -0.407388581138 -2.018815762685
C 2.238681330870 1.120616857825 -3.180206940831
C 1.332363315366 -0.907820095538 0.636977496644
C 2.126159587852 -1.114197742676 1.770443021304
C 0.459630573278 0.723537620086 -1.089743172888
TV 3.832916239673 2.482339109160 0.708509454616
TV 0.000000000000 2.526553347048 0.489292825276
TV 0.000000000001 0.000000000000 6.848096121299
Energy = -45.311443179488 hartree
Spin(**2) = 0.244384765625
Geometry of 3D-min213
C -0.076974803774 -0.148277193344 -1.029355712047
C 1.049310057672 0.176401975816 0.053303916496
C 0.285591942099 -0.730878863396 1.069016162424
C -0.705978181028 -1.179378164021 -0.113068165887
C 0.030192585721 1.261367180820 -0.479879333401
C 1.070434449032 2.950518664811 0.849064689807
C 0.009516381278 2.308630739975 1.811693345292
C -0.812212950499 1.659681434730 0.705406750381
TV 3.269578367595 1.362818835541 0.086153037310
TV -0.000000000000 4.789953347165 2.477555421457
TV -0.000000000000 -0.000000000000 3.469161006842
Energy = -45.310247320268 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min214
C 1.936043609313 -0.821502172368 -3.099056881627
C 1.276192728215 -1.268929320634 -0.883291227286
C 0.896478222639 -0.786723193593 2.397078181571
C -1.321338487482 0.306148454443 -1.395774715798
C 3.375829094856 1.591504796073 -1.681775210821
C 1.484873600562 -0.363514135494 0.188434730679
C 3.929736548020 1.100932975263 4.122024269940
C -0.584664524931 1.671659371281 -1.261156695437
TV 5.463920124307 1.986945010223 3.070562244806
TV 0.000000000000 2.367327772283 1.130104668604
TV -0.000000000000 0.000000000000 4.579899372771
Energy = -45.309532693231 hartree
Spin(**2) = 0.097412109375
Geometry of 3D-min215
C 0.264621499503 -0.212521837629 -1.869176324181
C 0.660725310351 -0.579106079252 -0.663226397653
C -0.132887462211 0.151033845479 1.608520871906
C -0.378186646557 -0.908923154951 0.470861859428
C 2.832231996813 -0.003776564360 -2.643701222420
C 3.228337428557 -0.370222787782 -1.437686140156
C 2.434721021705 0.359871532686 0.834018299844
C 2.189394366931 -0.700043293573 -0.303597798611

TV	5.135243665740	0.417836799652	-1.548854844694
TV	0.000000000000	2.571600140500	0.774250598117
TV	0.000000000000	-0.000000000000	4.680006785416

Energy = -45.305751409970 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min216

C	1.669300263036	-1.242641090517	-1.256475573358
C	0.706107281559	-1.242929769208	-0.211067341797
C	-0.350990893771	0.637379808924	1.257241196983
C	-0.126870338348	-0.871675984948	1.006954870969
C	3.006151206373	-0.775780436151	-1.288794549664
C	3.712816502414	-0.119234054560	-0.250179267542
C	0.932918877308	1.490702191319	1.278452442607
C	0.148755178766	1.618936936814	0.204758371147
TV	4.319716878538	1.511884495372	-0.007992941099
TV	0.000000000000	3.273067595593	-2.041182301669
TV	-0.000000000000	-0.000000000000	5.713516059731

Energy = -45.305112780501 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min217

C	0.955364690940	0.421431393928	-1.492869711277
C	1.025609794870	-0.506380550197	-0.183251944351
C	-0.600274780152	-0.031094767218	1.671227281809
C	-0.403738956390	-0.595470151688	0.301677641833
C	2.906322242687	-1.058965985491	-1.650482028426
C	3.598902899061	0.126076329931	-1.075111550466
C	1.678403511944	-0.558573996630	4.805728495325
C	1.498223342111	1.802481832158	-1.485406988415
TV	4.672582012915	1.142582453775	-0.239107935369
TV	0.000000000000	3.350911634893	-0.290639266948
TV	0.000000000000	0.000000000000	3.611204754675

Energy = -45.304266554194 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min218

C	0.396922582946	-1.636987412006	-2.122148256044
C	-0.153774559420	-0.515460081872	-1.411943005797
C	1.207152662702	-0.963735636687	0.200918758703
C	-0.413248573208	-0.918329128066	0.035665533469
C	2.188994901758	-0.637384770958	-0.970127892714
C	3.382960572583	-0.923297580626	0.055459162969
C	1.933851306639	-1.618091013651	2.544068877253
C	2.254652367860	-1.217496036248	1.109590542861
TV	4.647894564830	-1.148518784590	-0.612262946227
TV	0.000000000000	2.448883554990	0.682001584689
TV	0.000000000000	0.000000000000	4.730527336273

Energy = -45.304074980053 hartree
Spin(**2) = 0.097412109375
Geometry of 3D-min219

C	2.805385266095	-1.996330704611	-4.835164042282
C	-0.036948042075	1.899557373091	2.753234726931
C	0.171490963659	0.641908131264	2.163725738698
C	-0.992732870210	0.026260894980	1.564255322771
C	2.575254748314	-0.126535711434	-2.195897061831
C	2.452814890732	-0.626139710592	-0.618080479854
C	1.306962685471	-0.084066391336	1.513648369269
C	1.111453929171	-0.588212580459	0.172918267650
TV	4.108578178815	0.698068429101	-1.928298126555

TV	0.000000000000	3.227885792657	-1.363493040930
TV	0.000000000000	-0.000000000000	4.610287006270

Energy = -45.302881325792 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min220

C	2.151019128692	-0.065873404575	-0.113951247384
C	0.413078217859	-1.951346021173	0.701686990766
C	1.393795886233	-1.386050538511	3.840539047388
C	1.152611829204	-0.235452588557	-1.224815070620
C	3.631018513798	2.305217345702	-3.288683526968
C	-0.452473454227	-0.756066624445	1.222814003907
C	4.325656524774	1.167342617211	0.285641313700
C	-1.781523959755	1.536211367656	-1.853588119005
TV	7.526845131410	4.268157916259	0.166348584094
TV	-0.000000000000	2.298289457440	1.136213904288
TV	0.000000000000	0.000000000000	4.192881448213

Energy = -45.301927019770 hartree
Spin(**2) = 0.312500000000
Geometry of 3D-min221

C	0.710414141370	-0.050287654960	-2.600835559607
C	2.265307666039	0.268811221639	-2.230853789919
C	3.490987205929	-0.743273746523	1.622414864533
C	-0.224825726916	-2.914416292034	1.462250567962
C	0.669597916936	1.463380266191	-2.972182840974
C	2.580772889022	0.503294726083	-0.774781078510
C	2.158448526512	1.353304696767	0.479292126986
C	-1.045969791367	-1.703836618141	1.942968439922
TV	5.882776412987	1.105204906629	-0.449523134680
TV	0.000000000000	2.422593737535	0.962686686924
TV	-0.000000000000	0.000000000000	3.797277883039

Energy = -45.301909269855 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min222

C	1.987739705565	-0.367699806850	-1.595240618424
C	1.586933433263	0.303651833645	-0.200296959841
C	-0.734791865506	0.681850093813	1.139131834354
C	0.222039627569	1.116826358945	-0.042749623984
C	2.947318722408	1.186602535235	-0.244844247685
C	2.859149952174	2.278950573969	-1.266830319324
C	0.377461534877	-1.612071408116	0.749339215412
C	1.330257099326	-0.648966413891	0.942502695845
TV	3.734987962641	0.084995859773	0.987106819075
TV	-0.000000000000	3.964397780826	0.055295426379
TV	0.000000000000	0.000000000000	3.872115395557

Energy = -45.299967620185 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min223

C	0.633818889548	-0.180061503331	-1.481894369557
C	0.391222045013	-0.480200198270	-0.065179404473
C	0.132856463573	0.297151135196	1.190656266192
C	-0.652273211103	-1.762401845642	-0.138312741035
C	3.069049495513	0.840375424842	-2.103550497626
C	2.826250651891	0.540438109666	-0.686816398347
C	2.568006151510	1.317742850880	0.569103479762
C	1.782843517230	-0.741902495662	-0.760228210635
TV	4.870179026903	2.041146059417	-1.243386536985
TV	0.000000000000	3.337084179743	1.343358450657

TV	0.000000000000	0.000000000000	3.856542529569

Energy = -45.299796699155 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min224

C	0.683996078134	-0.447264089761	-1.955313409411
C	0.466179650715	-1.669770688921	0.038514838441
C	-0.569805557095	0.281387563975	1.478250523624
C	-0.559959557564	-0.345128722626	0.087699343326
C	4.159979184789	5.246156057936	-1.180424954355
C	3.012791612106	2.919878895308	-0.235732972604
C	1.495251697946	-0.579837015013	0.544230762935
C	0.723377033133	-3.138274454698	0.310081405815
TV	4.336431797972	3.475300449232	1.004795380176
TV	0.000000000000	3.430754067110	-0.797795745570
TV	-0.000000000000	-0.000000000000	3.879750188568

Energy = -45.298805055837 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min225

C	0.967950318888	0.328752610853	-1.080991623227
C	2.183265061459	-0.104538549825	-0.075562018241
C	-0.433010719825	-0.272569570899	1.895623383392
C	-1.458803075306	0.511039739065	1.047868357181
C	-0.781453577512	3.138330753829	-2.254413336013
C	1.720006616224	2.324938958262	1.333146586662
C	0.752646242056	1.800618981531	2.418317489154
C	-3.103909569192	2.118555762657	0.466354488113
TV	3.563025824438	0.288776483959	0.073206992988
TV	-0.000000000000	4.635429908476	0.093846434692
TV	0.000000000000	-0.000000000000	3.224827531534

Energy = -45.298483866889 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min226

C	1.636441496866	-0.840787682277	-2.843927190266
C	1.685559276663	-1.267353006936	-1.423510448230
C	1.722077023536	-0.721677616623	0.905900221714
C	0.227323370990	-0.593317647616	0.458676406177
C	2.322751681449	1.258472163923	-3.278778981870
C	2.412386826968	-0.233439236617	-0.397896714460
C	2.900724184254	-0.162724784178	3.154695691656
C	0.288489363378	0.982501351024	0.052750605908
TV	3.671716036024	3.178337713022	-0.508829745424
TV	0.000000000000	2.415854786355	0.895195043100
TV	-0.000000000000	-0.000000000000	6.354423952024

Energy = -45.297173496826 hartree
Spin(**2) = 0.187500000000
Geometry of 3D-min227

C	0.426604104096	-0.512151817677	-0.914059747606
C	0.075805504584	-0.464885170823	0.506622432525
C	0.042658224030	0.229205489260	1.690342691675
C	-0.349834907324	-1.685289275594	-0.222179625570
C	2.494269969056	0.548046833184	-1.718534570931
C	2.845589994457	0.501126275341	-0.298144171584
C	2.461675347791	1.242395834418	0.955305043774
C	2.068858568265	-0.672289822436	-0.988862715846
TV	4.838114775075	2.025780047025	-0.002245159805
TV	-0.000000000000	3.352307858747	1.928423688802
TV	0.000000000000	0.000000000000	3.857497358677

Energy = -45.294662894375 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min228
C 0.124201810575 -0.849372766232 -1.372869454426
C 0.739490692598 0.375721735226 -0.344715138976
C 0.571063271802 0.160122862907 1.155419358323
C -1.143306955028 -1.560095605573 -0.910382884494
C 0.070312009280 1.822392054380 -0.209429806147
C 0.841858254065 2.856886995028 0.843111427778
C -0.233088766503 2.331622273441 1.940770518027
C -0.629352299024 1.202928042640 1.118109734704
TV 2.965917407133 1.913157968988 -0.490579976373
TV -0.000000000000 5.121490786749 2.416819247873
TV -0.000000000000 0.000000000000 3.563027573022
Energy = -45.294071561265 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min229
C 0.504097648865 0.435885784557 -2.035324685161
C 0.499759031159 0.389860833944 -0.611792250357
C -0.650095952948 0.866735314375 1.612384512646
C -0.774497517820 0.203761008183 0.249548547121
C 2.893729132809 -0.201720892964 -3.524939208213
C 3.799976093919 -1.298737315970 1.229743964251
C 1.587181045113 0.143497407310 1.595054778356
C 1.630536032674 0.232678521211 0.221952815667
TV 5.061619673798 -0.075872308734 1.316577221828
TV -0.000000000000 3.270704329169 2.021418750631
TV 0.000000000000 0.000000000000 4.478004459620
Energy = -45.293650120205 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min230
C 0.899634423926 0.531359426356 -1.168706797403
C 1.108714574855 -0.408853758583 -0.127513234667
C -0.417977742871 -0.551758179821 0.272338621999
C -0.530675889914 0.602494969155 -0.773309634739
C 3.425682939704 2.398310726812 0.846006759428
C 4.177820194271 3.450153981389 0.019649631813
C 1.033603321382 -2.322585095688 1.009072894104
C 1.947012853911 -1.389495611206 0.484551787450
TV 4.618884169301 1.815258552526 2.985936954088
TV 0.000000000000 3.730954796104 0.239920450032
TV -0.000000000000 0.000000000000 3.538424693032
Energy = -45.293527965507 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min231
C 0.514238020592 0.387660571816 -2.067354966767
C 0.762027068275 0.272936339283 -0.674376270426
C -0.466968180965 1.194890751986 1.734254225407
C -0.251500540588 0.271757056372 0.498217666107
C 3.469889872502 -1.927366022121 -0.578564095452
C 3.184503640934 -0.683843657867 -0.181565477690
C 0.941768146614 -0.252323886665 1.311508771642
C 1.778906783568 -0.313486363717 0.134491109812
TV 4.586089495082 0.061004791237 -0.532835262766
TV 0.000000000000 4.316413592408 -2.519042077086
TV -0.000000000000 -0.000000000000 4.586247838981
Energy = -45.285705030139 hartree

Spin(**2) = 0.000000000000
Geometry of 3D-min232
C 0.816190896705 0.235620992165 -1.670903133140
C 1.427967887500 -0.546284859546 -0.691870358541
C -1.440087867041 -1.018614268310 3.053247250632
C -1.751748442034 0.068944156215 1.985740455331
C -0.807862927584 3.562481489133 -2.078584723845
C 2.954075536453 1.922630921064 0.345025371581
C 3.069633345103 0.605888281308 4.111062223834
C -4.581641252686 5.202028850678 -0.919310135516
TV 3.519578312971 -0.371747740622 -1.239510805726
TV -0.000000000000 7.136291621432 -1.666011083039
TV 0.000000000000 -0.000000000000 3.525444696719
Energy = -45.285322065604 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min233
C 0.514620347407 -0.118810358386 -1.822287446687
C 0.514805608212 0.018331820384 -0.321561782952
C -0.536236883747 0.195568836304 1.993664834832
C -0.536043332259 -0.295924579132 0.596857469632
C 3.395629301371 -0.466364814901 -1.700485294525
C 3.395670663252 0.366799509670 -0.444643589774
C 1.955182433638 -0.295708354020 2.963841762990
C 1.955184607203 0.195612044874 -0.373874757493
TV 4.982252758887 1.483455081663 -0.522681070573
TV 0.000000000000 2.966117854002 -1.043704927492
TV 0.000000000000 0.000000000000 4.734289245687
Energy = -45.284715150788 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min234
C 1.165021821646 0.074956972092 -1.770256207704
C 0.735767703925 0.602444375330 -0.456992504176
C 0.141031163367 0.455502569307 1.821579592698
C 0.064475060375 -0.413269741526 0.583539071175
C 2.253862212314 -0.029067175400 -2.626908149922
C 4.148572661182 -0.306100780787 -1.042322069373
C -0.599828101071 1.578055733238 2.444904840222
C 1.357615620681 0.390842456995 0.873554857384
TV 4.165585582282 1.506013217056 -1.166420690667
TV 0.000000000000 3.652138842470 -1.101548052751
TV -0.000000000000 -0.000000000000 4.683666615078
Energy = -45.284318515510 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min235
C 0.131347276878 -1.815213823745 -1.406511871619
C 1.163408681304 -0.912372952190 0.232377735938
C -0.486428104732 -1.092747723749 2.256142941094
C -0.003677714726 -1.249669924361 0.875631756549
C 2.687133127721 0.504036500298 -1.697858710657
C 3.500557764359 1.926524873648 -1.502499068587
C 1.556450711015 -1.816170938934 3.714941249855
C 2.294771712251 2.717389055265 -1.972436578228
TV 4.303736914090 3.928766977063 -1.301350024195
TV 0.000000000000 3.201909477477 -1.369898748918
TV -0.000000000000 0.000000000000 4.674396363589
Energy = -45.282439376413 hartree
Spin(**2) = 0.000000000000

Geometry of 3D-min236

C	0.927256426851	-0.695152559353	-1.224574532971
C	0.395341967054	0.598185584910	-1.700800541270
C	0.395122978117	0.459535492392	0.759140211657
C	-0.673954464582	0.527835860268	-0.471055297036
C	1.459698166067	-0.538181207355	0.144441047798
C	2.529087650769	0.529465107650	-0.469753751981
C	0.927927273516	1.752614289326	0.283441285273
C	1.459746708653	1.596261734487	-1.085995933417
TV	4.575359444488	0.002228320379	0.002069078924
TV	-0.000000000000	3.601140897865	-1.813832503962
TV	-0.000000000000	-0.000000000000	4.032335632571

Energy = -45.282083459368 hartree

Spin(**2) = 0.000013000169

Geometry of 3D-min237

C	2.468354074589	-0.181541002746	-0.970957237130
C	0.216343367260	-1.039788349960	-2.389011436907
C	1.594111964023	-1.267647992981	3.244033846237
C	-1.696791481798	-0.457070909158	-0.735053043438
C	3.527769088574	0.458357834651	-2.046311380823
C	0.516187683733	-1.468433731702	-0.569038310570
C	4.546061848120	1.476102210522	3.743057393662
C	-0.294654413986	-0.361206800986	-1.098743584586
TV	5.002051919909	1.667107855788	2.279262443694
TV	-0.000000000000	2.160189181260	1.411853613298
TV	-0.000000000000	-0.000000000006	4.936075815536

Energy = -45.281986882188 hartree

Spin(**2) = 0.000000000000

Geometry of 3D-min238

C	2.041484001797	-0.332729491010	-0.948367778413
C	1.215359219698	-1.467835207387	1.095969373002
C	1.704070251292	-0.479011161366	4.301898821688
C	-0.292080989934	0.595557077785	-3.484400768003
C	2.174302196641	0.768732291979	-3.254011986030
C	1.435768364056	-0.237267375574	0.319321839116
C	0.978598992721	1.078355167911	2.350523159358
C	0.349485267663	1.916733657311	-3.211221269040
TV	3.992015492598	2.678018306281	-0.008760943600
TV	0.000000000000	2.568089218383	-0.184892719390
TV	-0.000000000000	-0.000000000000	6.674541465115

Energy = -45.279173649188 hartree

Spin(**2) = 0.084228515625

Geometry of 3D-min239

C	3.050603135571	0.591173817313	-4.372829583923
C	0.899635816346	-2.665194351004	3.724210665914
C	2.344821299192	-0.797837909280	0.514320909066
C	1.001224215299	0.273121765200	-1.312729355666
C	2.390469803770	2.774365509947	-5.619680822681
C	0.081451207811	-1.730429388740	4.621359476560
C	2.757075709329	1.343543209918	-0.661494752309
C	-1.230245801932	0.345273385151	1.057781651812
TV	5.744062533504	4.501825675180	-2.731982006734
TV	0.000000000000	2.175833275863	1.267727394546
TV	0.000000000000	0.000000000000	5.003701857771

Energy = -45.277744431864 hartree

Spin(**2) = 0.312500000000

Geometry of 3D-min240

C	0.710607153650	-1.593681485246	-0.151306121815
C	1.110828649421	-0.121946912471	0.035100613042
C	-0.982807544866	1.021594649547	1.105057453063
C	-0.139474334978	0.816584672476	-0.040467959647
C	3.008468615400	-0.922337319955	-2.443498576858
C	4.279867652635	2.064292925211	-2.601992488409
C	1.583156091448	-2.826688668933	3.448913134028
C	1.900523420786	-0.031099859707	1.402892990104
TV	4.897710328671	0.757542929128	-1.206936605920
TV	-0.000000000000	3.437807195002	-0.822914746701
TV	-0.000000000000	0.000000000000	3.884301013199

Energy = -45.276133452465 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min241

C	4.132431506986	0.334108568895	-4.352418213258
C	0.313854250775	-1.860739231158	2.472444942004
C	1.612541025496	0.563180088328	-1.372381948407
C	-0.946741421788	1.000672025386	-1.010222217432
C	2.952570229196	2.534834800831	-4.763751990146
C	-0.217649704402	-1.213215435985	3.762091327071
C	3.752232857373	1.350298853868	-0.315174115270
C	-1.214480684144	0.104464745769	1.349251351457
TV	6.104282294678	3.023794138777	-2.932038429386
TV	-0.000000000000	2.004328618494	1.685447605949
TV	-0.000000000000	0.000000000000	5.079480382632

Energy = -45.272851702542 hartree
Spin(**2) = 0.187500000000
Geometry of 3D-min242

C	0.641731304162	-0.742608897631	-1.691196603032
C	0.826230966042	-0.800152391785	-0.154490462575
C	-0.488598127167	-0.419798070304	2.051382441592
C	-0.485303356096	-0.833926046243	0.647652350566
C	3.311591312976	-0.185321628748	-1.795148583607
C	3.338122558948	0.726827783230	-0.615009996596
C	1.936941312746	-0.138923812327	2.630155065099
C	1.762847482459	0.655678130056	-0.573556757092
TV	4.875569121922	2.315270945042	-0.722773700364
TV	-0.000000000000	2.774713619428	-0.720721070402
TV	0.000000000000	-0.000000000000	4.513577781301

Energy = -45.270399457992 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min243

C	-0.194754022167	-1.301580412066	-1.600910968744
C	0.980308996813	0.843211231320	0.536970428989
C	-0.177212490964	-0.083977588172	0.708875612466
C	-0.818665015257	-1.123967370946	-0.123136462543
C	0.289701075325	1.923745089205	-0.267131515686
C	0.788110867144	3.089808502336	0.741322149456
C	0.267737309288	1.909854478861	1.557675278891
C	-0.889015971149	1.359324767960	0.621380401591
TV	3.232092911772	1.743411332734	0.434899428359
TV	0.000000000000	5.572897429129	2.422814187226
TV	-0.000000000000	-0.000000000000	3.265989048780

Energy = -45.270390895403 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min244

C	2.610518100299	0.006044452543	-1.807366373846

C	0.836631968210	-1.883813607007	-0.031690034339
C	1.327054847231	-0.183692586753	1.555257914373
C	-1.153712539965	-0.286268786277	0.245120035363
C	2.846772288228	2.359179302759	-3.862257461313
C	1.478362278932	-0.525766940170	0.148584609714
C	3.686214243324	0.896682183429	0.188318248668
C	-0.222266426931	0.111525026306	1.443263765971
TV	4.926960850905	3.537410787502	-1.966011983970
TV	-0.000000000000	2.747554647194	0.608047327033
TV	-0.000000000000	0.000000000000	4.050927951089

Energy = -45.268816702061 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min245

C	0.988397000317	-0.246581500896	-1.891101520571
C	0.059259082362	0.303960994033	0.493828015257
C	-1.303334418533	2.105054867935	1.819673088943
C	-0.869349232147	1.218448154325	1.039378985534
C	3.484630519776	-0.963086692764	-3.021206198286
C	4.768195706270	-0.592550266251	-2.476336993012
C	2.151143551970	-0.511067164773	2.170331798556
C	0.967318228799	-0.123431120815	1.501401435736
TV	4.816997032293	-0.394119769061	-1.593053761101
TV	0.000000000000	3.641845008894	-0.553489405130
TV	-0.000000000000	-0.000000000000	4.830653751423

Energy = -45.268656217834 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min246

C	0.822348227652	0.633437443050	-2.604731220830
C	0.573456056646	0.141393222947	-1.254485650927
C	0.834849578191	0.221640659827	0.840872266054
C	-0.207480474021	0.578093228444	-0.198954888165
C	1.674905982293	-0.523311732471	-0.345945518637
C	2.860752788416	0.415126923347	-0.027871862299
C	1.663361340759	1.753819022907	2.103687787701
C	2.090216283048	1.165864400289	0.843017688255
TV	4.460729126110	3.126509528319	-1.983128302423
TV	-0.000000000000	3.684535480893	-2.013201785640
TV	0.000000000000	-0.000000000000	4.938492058984

Energy = -45.267769677536 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min247

C	1.806370170469	-0.229600295403	0.815979156112
C	-0.249861647846	-1.206261096998	-0.010512311966
C	1.805148740475	-0.852034322055	2.134348557282
C	-0.251161571655	0.125149233744	-2.829105342966
C	4.008544740804	0.575929908550	-3.783856081751
C	0.441523897261	0.021045339171	0.284950923544
C	3.139749066271	1.694208677631	2.531986813495
C	0.440150407859	1.132754922481	-2.068105478583
TV	5.386102817144	2.233249362949	1.058634255576
TV	0.000000000000	2.235482944366	1.055430994682
TV	-0.000000000000	-0.000000000000	5.788913544279

Energy = -45.266950682466 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min248

C	0.461391621829	0.771465023660	-1.133079202507
C	0.448892444484	0.522305097407	0.462418819211

C -0.329734914612 -1.092277913148 2.226775880179
C -0.025504165262 -0.821351877914 0.934511792911
C 2.770979315420 1.200155842874 -2.975073047959
C 4.068570811153 1.408296794537 -3.432712140084
C 1.569458235688 0.849725634797 2.860449523889
C 1.538142839946 0.747862002798 1.486534554792
TV 4.699412617729 1.586208385827 -1.734721721122
TV 0.000000000000 3.010895926697 -1.700472488674
TV -0.000000000000 0.000000000000 5.033734930467
Energy = -45.265920856618 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min249
C 0.419090122723 0.388229188164 -2.126296205547
C 1.574375579631 -0.205655924689 -1.753661926307
C -0.851855008199 0.737334788817 2.563309096271
C -1.880286643346 -0.468137961040 2.542246811168
C 3.267578533540 -1.824563816824 -1.774682793621
C 2.827554682849 -1.556975316906 -0.400087818244
C 2.575741758417 -0.914549634669 2.144936758812
C 1.812950680417 -0.632344402820 -0.360728935079
TV 4.749497933518 -0.073322753402 -1.822647772178
TV 0.000000000000 3.811691838004 -1.906950271595
TV -0.000000000000 0.000000000000 4.741939290170
Energy = -45.265864630177 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min250
C 1.143826692147 -1.416444688701 -0.619962583444
C 0.976905021994 -0.057773761203 -0.108871678635
C -0.545018143739 1.470395603663 1.361489012856
C -0.641456247214 0.238688440047 0.332446298025
C 2.501209036650 -1.840445238308 -0.959403501673
C 3.156314846742 -0.726131040433 -0.145161154237
C 0.270504405950 2.295976064067 2.371298694475
C 2.351511106720 0.529940240087 -0.099147264362
TV 3.925505344444 1.586960621772 -0.759901663461
TV -0.000000000000 4.717867118225 -0.475553062021
TV 0.000000000000 0.000000000000 3.271940849308
Energy = -45.264370623824 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min251
C 0.725126486795 -0.095910399538 -2.205045354720
C 1.861143402062 0.870498735030 -1.562727051899
C -0.610621659935 -0.095212083037 2.364189379572
C -1.802466662137 -0.700054752634 1.616644023904
C 2.472879913071 -1.371301736857 -1.431243294325
C 2.418132601867 -0.155327397685 -0.598379740303
C 1.861843135219 -1.062017059930 1.724299740526
C 2.418854361602 -0.035857513345 0.759973147947
TV 4.275806310145 1.879892165880 -0.023370388452
TV 0.000000000000 3.761135731275 -0.051807646316
TV 0.000000000000 0.000000000000 4.570493184132
Energy = -45.264144174590 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min252
C 2.375129005714 1.216613079397 -3.476876941223
C 2.392397793955 -0.057642686173 0.046733333685
C 2.368814297581 -1.331234344706 4.950412239339

C	-0.758173212252	-0.077150498704	-0.512188122529
C	2.383744401887	2.490066523756	-5.619556287655
C	2.358626144810	1.216051704651	-0.715877083030
C	2.379117254253	-0.057290427669	2.807783691927
C	-0.540597473946	1.196572053505	-0.552329134164
TV	6.047100257408	0.006942343720	0.373847992892
TV	-0.000000000000	2.547566980453	-0.000419354240
TV	0.000000000000	0.000000000000	7.052117557570

Energy = -45.261317711840 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min253

C	1.992514085380	2.663013476171	-3.876267389652
C	1.197693547643	-1.864267783476	3.625903489456
C	1.955094412724	-0.899255763221	-0.191428926014
C	-1.314939740801	-0.956084267194	-0.797406059146
C	3.235926552876	5.044598884572	-4.194451481085
C	-0.254155988567	-1.920053545560	3.806043641627
C	3.235966721156	1.214562668937	-1.177882130758
C	-1.315672151361	-0.681766973948	0.640500862488
TV	5.709401050637	3.924434117242	-2.616327195287
TV	0.000000000000	2.194503599738	1.656685830953
TV	-0.000000000000	-0.000000000000	4.796515355499

Energy = -45.258118206868 hartree
Spin(**2) = 0.049072812500
Geometry of 3D-min254

C	1.476882544289	0.533636562715	-1.488516531517
C	0.504578386863	-0.251254150563	-0.591204711894
C	-1.798328250133	0.793002783793	0.493987841486
C	-0.363783490403	0.944376637342	0.067619696050
C	2.212028968101	1.538709109511	-0.567152758887
C	4.750405728849	2.153588945050	0.653258304509
C	0.545643841967	-2.237644506178	1.110914798960
C	1.232141393325	-1.384075109003	0.049122108667
TV	4.789797466196	0.008354832990	1.612138412356
TV	0.000000000000	3.746939948888	0.099582745515
TV	0.000000000000	-0.000000000000	3.448892101541

Energy = -45.258058268747 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min255

C	1.550747961206	1.642321472994	-3.379209161147
C	-0.332773795872	-1.757170729061	2.050103452019
C	2.731956238914	-0.043475246118	0.703073638168
C	1.147496381209	0.663230827763	-2.517370074646
C	3.583910218233	3.020905767327	-6.233851037094
C	-2.123854858017	-1.650256561417	4.524195800093
C	2.286674057232	2.241931770798	-0.440481704312
C	-1.063882414075	-0.406702402708	2.436575822918
TV	4.884102215848	4.692046957819	-3.682563850250
TV	0.000000000000	2.308662801561	1.419263968045
TV	0.000000000000	0.000000000000	5.785175088575

Energy = -45.257510667313 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min256

C	3.104553886886	0.150179978705	-1.696906369990
C	1.444156707042	-1.359763645937	-0.366918275857
C	2.583338364097	-1.250120737240	3.510950398748
C	-0.899111854817	0.041552798006	-1.412030105831

C	3.966622257449	1.797525139605	-3.615305750452
C	0.795006578340	-0.093951686958	0.223719059002
C	3.263121537363	0.367330301022	1.611464370027
C	-2.922944011858	1.259130754125	0.465912990735
TV	4.709155984836	1.886594089450	1.099314034157
TV	-0.000000000000	2.645525102264	0.360460072606
TV	0.000000000000	0.000000000000	4.826494315550

Energy = -45.256405174641 hartree
Spin(**2) = 0.000003999984
Geometry of 3D-min257

C	0.805676168233	1.057918439326	-1.702269890426
C	0.826514602223	0.025423975796	0.241255477604
C	-0.617310881762	-1.518289359274	1.757366268713
C	-0.205990326054	-1.171127475257	0.305447122956
C	3.303955681690	0.482560115558	-2.479852579272
C	3.881339648399	-0.893609941815	-2.030733800918
C	1.312602992832	2.367638920207	2.886930490757
C	1.784465359846	0.352841118375	1.454622133574
TV	5.054566410738	0.048034182396	-1.120363645063
TV	-0.000000000000	2.696672322423	0.081518117152
TV	0.000000000000	0.000000000000	3.991136391677

Energy = -45.247985871508 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min258

C	-1.187734683868	-1.800636813926	-2.851341928048
C	0.752883415104	1.153805719335	-0.504514852670
C	0.159731035250	-0.097245122764	2.769070685487
C	-1.342172228450	-0.249008037350	-0.030216131366
C	1.312257666489	3.956723269521	-0.431115918939
C	2.099094737063	2.855530942676	0.427833106703
C	-0.400475919680	2.090873813852	2.839527101182
C	-1.342779578453	2.246439691617	1.644573532315
TV	3.597338256761	1.553802634832	0.002872905097
TV	-0.000000000000	4.992026052012	0.002735760927
TV	-0.000000000001	0.000000000000	3.273665963452

Energy = -45.244819661409 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min259

C	0.519792839327	-0.353947274459	-3.010113210131
C	1.360018753318	-0.034439352964	-0.567889293100
C	-0.033122116680	0.737280252336	1.309586631072
C	-3.524361568637	-0.031230718623	1.931305610744
C	3.500239190328	2.177164025503	-2.032696635117
C	2.420119095986	1.258570865023	0.829581811316
C	1.694855049706	-1.370071899391	0.941193607612
C	2.623562802412	-0.379760495521	0.158009775151
TV	4.843487119253	1.116160117326	0.054538417637
TV	-0.000000000000	3.528291674677	-1.373354428514
TV	0.000000000000	-0.000000000000	3.496545704580

Energy = -45.244766742406 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min260

C	1.499468747973	-1.376870930526	-1.019124703668
C	0.581242004706	-0.526487761503	-0.308283822074
C	-1.250845694028	0.703204862216	0.795487161358
C	-0.929936062234	-0.374826547847	-0.319983964881
C	2.963738556057	-1.190015192130	-0.791173123233

C	2.695922663856	0.573044018428	0.999489541624
C	1.463561709512	1.209411839884	1.620791223686
C	1.269570156972	0.372983474913	0.535110321570
TV	4.543701365403	2.211256918054	0.712097706507
TV	0.000000000000	3.609398040432	-0.073096961801
TV	0.000000000000	0.000000000000	3.704384506524

Energy = -45.243375450367 hartree
Spin(**2) = 0.102539062500
Geometry of 3D-min261

C	3.584409294779	0.115464249928	-1.246374646201
C	0.907474339973	-1.264573257620	-1.157782519089
C	0.726523361402	-0.760225877368	1.148693250666
C	-0.679361478477	-0.557693482995	0.595029544770
C	3.105302871688	2.023597436872	-2.774758235260
C	1.530704734259	-0.318132128036	-0.060746864002
C	3.435775542218	0.563239027708	1.213766247963
C	-0.600284581000	0.902870310257	0.289468259684
TV	7.241196339064	3.089785937870	-0.921738002878
TV	-0.000000000000	2.377985622017	0.871318993884
TV	0.000000000000	0.000000000000	3.683566299190

Energy = -45.242765117866 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min262

C	2.515183614629	0.650578666257	-2.475510132160
C	2.290569434536	-0.754676746836	-0.386455406338
C	2.858947382344	-0.655128548364	2.345764950774
C	-0.740237675446	-1.413722542397	-0.672542225066
C	2.209123084998	1.678986868891	-4.392972837596
C	2.344273213477	0.575456878787	-0.998752907131
C	1.344422230398	1.063856054986	2.056970040931
C	-0.739517885311	-0.037286218741	-0.617389292687
TV	6.078410450544	2.626269613143	0.824496711409
TV	0.000000000000	2.617469005116	0.108371669233
TV	0.000000000000	-0.000000000000	5.555630210865

Energy = -45.231481059205 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min263

C	2.111807786410	0.768024920083	-2.625267872202
C	0.521607207748	-0.446122403140	-0.646293263797
C	-0.552574272317	0.936579467192	1.706970072740
C	-1.556955318079	-2.535952217180	0.751733602984
C	3.065862788514	0.740259692953	-1.493224491151
C	2.689984168088	0.649595852705	-0.137489741501
C	0.830899825930	0.749700861344	1.507766302039
C	1.226382263718	0.434883756893	0.097773403266
TV	4.744346054993	3.246535062103	0.460816630193
TV	0.000000000000	3.502988699376	-0.132757296452
TV	0.000000000000	0.000000000000	4.788608860179

Energy = -45.231422297062 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min264

C	1.328517220223	-0.059628060805	-3.368575156743
C	1.324678706285	-0.529373805626	-0.740377874465
C	1.310635276757	0.402784613717	1.558926134078
C	-1.901309861141	-1.067564396953	-1.625050387615
C	1.337754528423	-0.286265944017	-2.107538738885
C	1.319128170877	0.646833393552	0.191840083497

C	1.322067868858	0.173866521812	2.819523275532
C	-1.901362964871	0.315265125337	-1.379303894742
TV	6.455650052212	0.906527798677	2.341731655580
TV	-0.000000000001	2.601479876397	0.462408795869
TV	0.000000000004	-0.000000000000	7.487318029391

Energy = -45.231248472837 hartree
Spin(**2) = 0.140625000000
Geometry of 3D-min265

C	0.993166449334	1.492945093193	-1.543787936410
C	0.993119947902	1.492892647449	-0.239905639332
C	-0.947783359023	-1.489585525744	1.754127221722
C	-0.947872199787	-1.489626477669	0.450233175677
C	0.993141821332	1.492966728902	1.063968073367
C	0.993109603600	1.492928224189	2.367861161555
C	-0.947849216162	-1.489630060057	4.361924282455
C	-0.947860957070	-1.489631633220	3.058034995124
TV	3.235333982507	-0.000324160360	0.661083290412
TV	-0.000000000002	5.965753893999	-0.000767436168
TV	-0.000000000000	0.000000000002	5.215558128144

Energy = -45.228233927130 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min266

C	1.163882680956	0.489876962587	-3.246059812476
C	0.016474869294	0.043676941002	-0.000228042132
C	-0.022596273806	0.022255424793	3.246341398064
C	-1.169860082896	-0.424371763445	-0.000330625817
C	3.593743680898	1.448215189471	-3.245888810353
C	2.446332367120	1.002003990770	-0.000056333666
C	2.407268710442	0.980574218748	3.246522928455
C	1.259995563794	0.533985698222	-0.000160315638
TV	4.859681197486	1.916592953997	0.000344747357
TV	-0.000000000000	3.548697495058	0.016046322078
TV	-0.000000000001	-0.000000000000	6.492693509965

Energy = -45.223229332915 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min267

C	0.998876487753	-0.746460678014	-1.599940925772
C	0.595368610582	0.084330006556	-0.488320270043
C	-0.081514763527	-1.481595904341	1.698763552707
C	-0.412163777802	-0.373016950916	0.622166186618
C	3.239038061157	0.002886720574	-2.287741243564
C	3.666801804959	-0.804999852073	-1.164994918335
C	1.858955921297	0.018539357611	1.711355764011
C	0.809522150040	0.649016102487	0.858138176592
TV	4.506183271504	-1.124061598851	-0.569220617046
TV	-0.000000000000	3.301163475995	-0.036174722059
TV	0.000000000000	0.000000000000	4.205764214597

Energy = -45.212009401796 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min268

C	0.430880087353	1.029870027946	0.298477499025
C	-0.050028707907	0.839289477556	1.740108784205
C	0.145634660880	-1.660935429877	0.689834079011
C	0.581416548825	-2.116557370913	-0.810763164512
C	1.040531711608	1.241514540104	2.617665271752
C	0.781641768929	2.166062564792	3.652802530215
C	-0.332355416066	-2.057387393493	2.205064185414

C 0.205083864148 -0.249882233570 0.711608103090
TV 2.417481938459 -0.186497087718 0.763792397579
TV -0.000000000000 7.065189344670 -1.399614611553
TV -0.000000000000 -0.000000000000 4.087880086253
Energy = -45.197136883490 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min269
C 3.463934387906 -0.583573857573 -3.221799096937
C 1.495713667236 -2.215187650612 -1.370506422598
C 3.463923683968 -1.893173482342 4.344873519284
C -1.361898005863 1.495109536287 0.688297285503
C 1.500270239671 0.190990692324 -5.087713534678
C 1.495737285006 -0.905676883920 -1.318344367272
C 1.500450129761 -1.118603550335 2.478858541145
C -1.362251931183 2.804653926086 0.740148633348
TV 4.820272627981 0.752483209563 0.015472132983
TV -0.000000000002 2.619111480968 0.104305670903
TV 0.000000000005 -0.000000000001 7.618604893349
Energy = -45.192217400672 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min270
C 3.475283675316 1.192927410451 -2.078260715865
C 1.797766961507 -1.054745514316 0.112054031980
C 2.892541133021 -2.527153132820 1.437692726664
C -1.049573916444 1.303267745657 1.358717165490
C 3.258461086379 1.174098623558 -3.593635318548
C 1.078884031304 -2.303604823493 -0.416209175055
C 1.453145155569 -2.214828290292 1.056520195304
C -0.416663602764 2.642250213499 1.695108747424
TV 5.627092025453 0.035909225041 -0.557812538524
TV 0.000000000000 2.481038215854 1.032193774090
TV 0.000000000000 -0.000000000000 5.077437842301
Energy = -45.185992251702 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min271
C 1.837919224782 -0.189308501787 -1.714770731932
C 1.498855384775 0.925207415500 -0.794993976204
C -0.648872375956 1.397448128703 0.978173805556
C 0.300811046973 1.702683173760 -0.202983962892
C 3.061116035711 1.147371304814 -0.588559694101
C 2.403233344720 1.934553570112 -1.594795161049
C 0.854273793853 -2.566785932364 1.601272002996
C 1.268771754805 -1.412025391980 1.797669693972
TV 3.700697823983 -0.813174952977 0.822105964838
TV -0.000000000000 5.626876883058 -1.495568306686
TV 0.000000000000 -0.000000000000 3.877132939478
Energy = -45.176283452114 hartree
Spin(**2) = 0.000000000000
Geometry of 3D-min272
C 0.811584902730 0.620768139040 -3.551688966214
C 0.759914476174 0.190051341792 -1.535112657184
C 3.487379140338 -1.442775122847 0.280255763559
C -0.376007055235 -1.975381087583 2.762465245749
C 1.838781509734 0.401543117700 -2.523379024506
C 0.752785257367 -0.115340648034 -0.104137282199
C 0.827472393013 0.927932653022 0.855303570778
C -1.232425516623 -0.776808258899 2.993171049824

TV	6.060641613511	-0.674911759370	-2.671638294786
TV	0.000000000000	2.387000190524	0.508999088203
TV	0.000000000000	0.000000000000	5.845932019144

Energy = -45.170410545258 hartree
Spin(**2) = 0.312500000000
Geometry of 3D-min273

C	0.382117895944	2.590797650962	-1.302452895429
C	0.387508648866	1.695550457565	-0.056235199321
C	-0.421449264062	-1.698192278339	1.302312367234
C	-0.416140346100	-2.593282461256	0.056041651170
C	2.007881642387	2.600431338947	-1.182892200211
C	2.013272503441	1.705218299273	0.063331157253
C	1.204302690031	-1.688576912191	1.182832779878
C	1.209637725004	-2.583649251340	-0.063475507696
TV	3.251523888738	0.019294871870	-0.000101312035
TV	0.000000000000	8.574046608458	0.004635209481
TV	0.000000000000	-0.000000000000	2.492545319727

Energy = -45.067395327039 hartree
Spin(**2) = 0.000000000000

(ii) 2D
Geometry of 2D-min0

C	0.794607238981	-1.159235688860	-1.202580713854
C	0.077310880258	-2.401335677432	-1.202677110858
C	1.668979505105	2.513084207947	2.248482297837
C	0.951771324254	-1.213352661082	2.248424800309
C	1.298571278352	2.422682209350	-4.661104981301
C	2.015609308792	1.180534829466	-4.661090565340
C	2.548688265657	3.493892138629	5.714393783097
C	1.831595877732	-0.232522811396	5.714317334529
TV	2.151417439927	1.242046296272	-0.000000000000
TV	-0.000000000001	2.484306514885	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.570633400409 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min1

C	0.231083829933	-1.017328070195	-1.157871700331
C	-0.486413755634	-2.259443709729	-1.157951253228
C	1.195012709564	3.023194911362	2.305895771387
C	0.477514791269	-0.702687894817	2.306068505673
C	0.818034301526	2.590587319824	-4.605447802647
C	1.535508749540	1.348710243100	-4.605389952810
C	2.536883481894	3.329547850241	5.765083061546
C	1.819509401650	-0.396355835405	5.765099855205
TV	2.151773691282	1.242554143876	0.000000000000
TV	-0.000000000001	2.483952359776	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.570613408786 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min2

C	1.657896646263	-1.772785039980	-1.351181365506
C	0.223545565683	-1.773006365099	-1.351272078237
C	1.044635204865	2.008089314197	2.107507642156
C	1.761948721378	-1.718510807678	2.107461686699
C	2.662055518176	2.066979910605	-5.027273807855
C	1.944999460342	0.824663671204	-5.027260039805
C	2.156328803334	3.921836409887	5.599819715127

C	2.873443182455	0.195331858110	5.599851406296
TV	2.151512226910	1.242371888710	0.000000000000
TV	-0.000000000001	2.484426761957	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.570207475934 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min3

C	0.997871549326	0.203372854869	-1.713922812573
C	-0.433496324018	0.202006948431	-1.713670495789
C	-0.642005033614	0.418569112389	1.713672638095
C	0.077627511385	-0.832257977764	1.713919294241
C	0.997872736866	2.691387522843	-1.713930791689
C	-0.433498335043	2.690029262581	-1.713676768677
C	-0.642008032141	2.906575762798	1.713678665688
C	0.077635927255	1.655761891900	1.713930270710
TV	2.150997839334	1.238573056381	-0.000000000000
TV	-0.000000000000	4.976033373043	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.565357816800 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min4

C	0.611914782031	0.408449699927	-0.052493253764
C	-0.633210118704	-0.309029969989	-0.052407089042
C	0.612020797451	1.843786728711	-0.052372629488
C	-0.633126888877	-1.744368796799	-0.052401562648
C	3.102289981432	0.408735503208	-0.052400210921
C	1.857126449963	-0.308673214131	-0.052381866885
C	3.102383067002	1.844067350816	-0.052474689234
C	1.857199350555	-1.744019771977	-0.052439470772
TV	4.980603844039	0.000569303420	0.000000000000
TV	-0.000000000000	4.305133333682	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.558217867315 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min5

C	-0.983606969299	-0.173405473891	0.165824112192
C	-0.118642191995	-1.283991246983	0.165850109535
C	-0.240044043696	1.028973565524	0.165840560404
C	-2.328276560487	-0.602093601772	0.165826030228
C	3.776959342616	1.147050497340	0.165792312086
C	1.225883119825	-0.854867143748	0.165810728991
C	2.333672323164	1.526590499372	0.165846658645
C	5.842744157894	-0.505154233532	0.165870714793
TV	4.639508219811	-1.154822538653	0.000000000000
TV	0.000000000000	4.788126548050	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.489961577496 hartree
Spin(**2) = 0.066406812500
Geometry of 2D-min6

C	0.594308771001	0.389309299177	0.312436825388
C	-0.728046890655	-0.116339044903	0.312196771215
C	0.594259243727	1.803387254218	0.312544563069
C	-0.728008802889	-1.560662453971	0.312295792170
C	4.193309865306	1.096446749893	0.312378511015
C	1.916479193376	-0.116143858087	0.312440890726
C	2.799148912982	1.096877249394	0.312559691653
C	1.916503821542	-1.560425668977	0.312535690650

TV	5.803664682944	-0.000277457943	0.000000000000
TV	0.000000000000	3.869906441793	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.456726128394 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min7

C	-1.313613549241	-1.796060008645	1.105355313771
C	-2.018318987860	-3.065629851790	1.107543558782
C	0.833398810785	2.012158200471	1.096402558059
C	0.128160588648	-1.797089458572	1.098394135623
C	4.071210119142	3.849957542928	-2.251385586288
C	3.884142883319	2.573437248793	-2.238182791195
C	2.980295891695	3.280656155841	1.103171714477
C	2.275288473721	-0.528641464010	1.099120834602
TV	6.440314565248	3.805572379457	0.000000000000
TV	-0.000000000001	2.539681067472	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.452599916131 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min8

C	-1.799196788251	-1.251009911327	0.977436753758
C	-2.504469531789	-2.520679827410	0.981325812162
C	0.348424334730	2.557882979077	0.974470664519
C	-0.357175987685	-1.251090642898	0.973619276065
C	2.986376634112	1.238145342108	-2.386912251126
C	3.172254817505	2.508803084277	-2.347968688660
C	1.790361834639	5.097104130331	0.980283206669
C	2.495479011851	1.288124306885	0.983191698407
TV	6.441789592659	3.808783480314	0.000000000000
TV	-0.000000000001	2.539320492066	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.452592897013 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min9

C	-1.586557786291	-1.661090776183	0.525650186224
C	-2.292081578362	-2.930676569648	0.525892476178
C	0.560500613844	2.147930265606	0.532902725394
C	-0.144729044248	-1.660977018938	0.529799252017
C	1.318412495596	4.347701491351	-2.715989561290
C	1.322494254068	3.082665668126	-2.907620149898
C	2.707850787865	3.417364591052	0.530645732874
C	2.002655066598	-0.391243736473	0.533522398574
TV	6.441731644832	3.808805048472	0.000000000001
TV	-0.000000000001	2.539171473544	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.452583599438 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min10

C	-1.717924398546	-1.207259295868	0.976605395692
C	-2.423010907626	-2.476937878355	0.981066787543
C	0.428913049717	2.601616719829	0.977380392087
C	-0.276287307217	-1.207301904141	0.974867693746
C	2.849500239679	1.106285831786	-2.468542500594
C	2.824952214672	2.378309960234	-2.278871317432
C	1.870624063747	5.140817798895	0.985357162919
C	2.575287370682	1.331748228660	0.987582857835
TV	6.439791140336	3.808527023870	0.000000000000

TV	-0.000000000001	2.539260072879	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.452538177294 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min11

C	-1.800847190639	-1.287576267145	1.168280665526
C	-2.506357353769	-2.557211265554	1.172588368896
C	0.346634584095	2.521328040214	1.172465225121
C	-0.358936694201	-1.287592072403	1.168314384696
C	2.165696110511	0.849816899354	-2.191853764762
C	2.354810127928	2.120577060935	-2.190575323016
C	1.788456303643	5.060480072661	1.182173953922
C	2.493299338584	1.251442025134	1.182286105745
TV	6.441593864936	3.808458279634	0.000000000000
TV	-0.000000000001	2.539451708284	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.452511019556 hartree

Spin(**2) = 0.000000500000

Geometry of 2D-min12

C	-1.709082803123	-1.452970510008	0.767648003987
C	-2.412697034970	-2.729184581726	0.769241210703
C	0.436140381063	2.375718828253	0.771436544552
C	-0.267117713027	-1.453114550345	0.768693936446
C	3.084237336497	4.423545375688	-2.468132844057
C	3.087698728413	3.075775171995	-2.467524802387
C	2.580989093720	3.652558001346	0.775050540748
C	1.877847350789	-0.176419991395	0.775921661736
TV	6.436626976994	3.829173417539	-0.000000000000
TV	-0.000000000001	2.552498037297	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.451538706374 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min13

C	-0.730516991234	0.085551076315	0.485736438951
C	0.832544443278	-1.871414861604	0.485777385767
C	-0.125420462269	1.462381215352	0.485648199193
C	-1.918655818052	-0.661847555979	0.485776573029
C	3.710594081910	1.046067897248	0.485868958545
C	0.580337058361	-0.490650614334	0.485754121279
C	2.373593677352	1.633752902552	0.485892041043
C	5.273599712925	-0.910939937352	0.485719383573
TV	4.088283351128	-1.797205810297	0.000000000000
TV	-0.000000000000	5.546903217989	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.451243756430 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min14

C	-1.833569165883	-0.772701639121	1.346782881104
C	-2.536960646259	-2.049035302780	1.350520790504
C	0.311431557243	3.056444637498	1.350888608488
C	-0.391918112784	-0.772589762051	1.347077446037
C	2.171274624003	0.460372645163	-2.030980193471
C	2.173065454938	1.808845060743	-2.030584658283
C	2.455781942673	4.331808538274	1.359384599090
C	1.753029066433	0.503045748619	1.359464138262
TV	6.434344004130	3.828054292867	0.000000000000
TV	-0.000000000001	2.552808362877	0.000000000000

TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.450868141757 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min15

C	-1.730718612344	-0.477637124430	1.326230794634
C	-2.436568280724	-1.745269365259	1.330737352509
C	0.416895394782	3.325520030188	1.330419549145
C	-0.289021632510	-0.477046268422	1.325895123790
C	1.755246945019	-0.356129955098	-2.017295798228
C	1.962646511985	0.911679074753	-1.924940970486
C	2.564427825364	4.593860916524	1.341047281063
C	1.859226568805	0.791212618072	1.340460279324
TV	6.442451975548	3.804809521644	-0.000000000000
TV	-0.000000000001	2.534904307676	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.449220266052 hartree

Spin(**2) = 0.312500000000

Geometry of 2D-min16

C	-1.746602857685	-1.544072010089	0.737455608672
C	-2.453098396448	-2.806719057534	0.738857950370
C	0.401773999708	2.243815343978	0.734045196934
C	-0.304960309797	-1.544761830054	0.733431803819
C	3.345149990493	4.705131797095	-2.392883352324
C	3.043190827124	3.439654363089	-2.337144076294
C	2.549508810163	3.505756908903	0.739067298530
C	1.843053275805	-0.282897771568	0.739503822020
TV	6.447354892684	3.785898851406	-0.000000000000
TV	-0.000000000001	2.525996571117	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.447948482763 hartree

Spin(**2) = 0.312500000000

Geometry of 2D-min17

C	-1.423045475876	-1.439756041457	1.103894681505
C	-2.130821899506	-2.696156611773	1.104922573137
C	0.726889242315	2.329255880826	1.088836010920
C	0.018262217950	-1.440315728124	1.092654538403
C	3.650870307107	3.956723564638	-2.012520135002
C	4.053493097339	2.701334816129	-2.060899281841
C	2.876306293714	3.585066037829	1.094421854110
C	2.167693544984	-0.184209164048	1.090595943126
TV	6.450623926204	3.767219907267	-0.000000000000
TV	-0.000000000001	2.513037610963	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.444558983870 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min18

C	-1.427264228052	-0.946384254128	1.073717841715
C	-2.136016441754	-2.203020287025	1.080608458261
C	0.722359849816	2.822965017748	1.079494916421
C	0.013481477786	-0.946675102572	1.073090868727
C	1.976606069543	0.878299223200	-2.105545306308
C	2.381639550007	2.135392192865	-2.102944122723
C	2.164751780816	5.335776660274	1.096725137348
C	2.872309761658	1.565759046714	1.096855516520
TV	6.449768766236	3.768280989164	0.000000000000
TV	-0.000000000001	2.513233011050	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.444297218551 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min19
C 2.319910455984 -1.910400697617 -0.379145596685
C 1.588175089361 -3.177780971274 -0.869602916530
C 3.051147940137 1.891674367434 1.690331819217
C 2.319444744753 -1.910498813377 1.199728841887
C 1.587302650985 1.891491464033 -2.524672780658
C 0.855402050251 0.624037583743 -2.883423694146
C 3.783327282788 3.158701487692 3.705469522531
C 0.856097044906 0.624155717448 3.346026179171
TV 2.195335849506 1.267157731581 -0.000000000000
TV -0.000000000000 2.534920092907 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.428870888180 hartree
Spin(**2) = 0.058594187500
Geometry of 2D-min20
C -0.558849846292 -2.312131362928 -0.247042468906
C -1.289004821021 -3.577550385745 -0.737060780620
C -0.559451143757 2.750073233473 1.335892811468
C 0.170792797904 -1.045140688338 1.825949419243
C 0.902734490334 2.745633212751 -2.394946153176
C 0.172393059579 1.480564491401 -2.753196005556
C 2.361206931465 2.751020214545 3.527520321511
C 1.630815234911 -1.043986414442 3.886817136828
TV 2.191044375870 1.264629247985 -0.000000000000
TV -0.000000000002 2.530276088703 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.426794625796 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min21
C 1.354921388852 -1.393149540183 -0.733136632012
C 0.623800016801 -2.658629708339 -0.239773540881
C 0.623864990410 2.403200076981 1.366266949479
C 1.354977060055 -1.393257166073 1.859692725193
C 1.355288842607 1.138026814094 -2.385987878927
C -0.106447184380 1.138144089676 -2.746133360677
C 1.355847558353 3.668614225891 3.512277837239
C 2.086793250776 -0.127803083399 3.872295713740
TV 2.192635011493 1.265289440486 -0.000000000000
TV -0.000000000001 2.531107637556 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.426294026727 hartree
Spin(**2) = 0.058593750000
Geometry of 2D-min22
C -0.578820689181 -1.372833567053 -0.580531226716
C -1.308162782263 -2.635944337047 -0.087194685509
C -1.308087796266 2.419227758134 1.522553719631
C -0.578703810633 -1.371179991896 2.017268428849
C 1.609336469849 2.416056591527 -2.238562388214
C 2.338770696246 1.152554015994 -2.598843815288
C 1.609956735689 2.420989976744 3.714419009040
C 0.880634368680 -1.369292891268 4.076561120886
TV 2.188280003300 1.263540742195 -0.000000000000
TV -0.000000000002 2.526879395758 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.423610592282 hartree

Spin(**2) = 0.000000000000
Geometry of 2D-min23
C 0.122759868406 0.709137822613 -0.677046650975
C 0.122699437115 -0.672405797368 -0.677049716527
C 1.168116704651 1.754708955499 -0.677167315284
C -0.922757319718 -1.717797587265 -0.676937463107
C 0.122772051538 4.181493884414 -0.676991501485
C 0.122736122047 2.799954151101 -0.677086826875
C 1.168087711512 5.227125757932 -0.677023652625
C -0.922759927360 1.754626714372 -0.676948191737
TV 3.474589921437 0.000121168480 0.000000000000
TV 0.000000000000 6.944845015640 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.410265117958 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min24
C 0.498487988306 0.928584496722 -0.740442318314
C -0.400085549330 -0.209507506816 -0.740357326167
C 1.833786061711 0.362930157575 -0.740347916546
C -1.853943153489 -2.023734291956 -0.740561303523
C -0.519151395415 4.846251949177 -0.740686598550
C -0.170054873684 3.493072815989 -0.740783691140
C 0.380034549808 5.984047484809 -0.740452882725
C 0.147543288200 2.281427003395 -0.740643674219
TV 3.602688942403 0.922911931578 -0.000000000000
TV 0.000000000000 7.436184219595 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.396007489068 hartree
Spin(**2) = 0.312500000000
Geometry of 2D-min25
C -0.842644365971 -0.897945106798 -0.280439192593
C -0.990179990267 -2.152234408875 -0.948046682165
C 0.146766010597 2.865746328626 1.617313342311
C -0.588842881003 -0.896693801552 1.271291543165
C 2.999315598857 2.862161635812 -2.387295453919
C 2.849823146006 1.607851295752 -3.001075361658
C 2.270451553503 4.119153981635 1.638969900665
C 1.560656065088 0.356686743152 1.682947089925
TV 4.336236638547 2.506971830610 0.000000000000
TV 0.000000000000 2.508330780222 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.385276544236 hartree
Spin(**2) = 0.312500000000
Geometry of 2D-min26
C 0.517324181603 -0.160674310264 0.280503527866
C -0.304241574796 -1.338844335547 0.280539121422
C -0.304170331952 1.017501579466 0.280572012585
C -3.059455191810 0.575157798971 0.280448270910
C 4.131008634540 0.551272129639 0.280544442846
C 1.961461153181 -0.160164115709 0.280469744053
C 2.812626305213 1.054198448510 0.280486937972
C 4.131152656573 -0.871531331489 0.280530949590
TV 5.872312570356 -1.949387794277 -0.000000000000
TV 0.000000000000 3.900104483597 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.382580468030 hartree
Spin(**2) = 0.000000000000

Geometry of 2D-min27

C	-0.279462459033	1.342939957506	-0.052328429637
C	-0.599249966820	-0.073543221033	-0.052401003336
C	0.519513302272	2.515077511861	-0.052351148049
C	-0.465724521012	-1.470396251020	-0.052343346155
C	3.068278701418	0.173266339339	-0.052403347161
C	2.748484977494	-1.243204764988	-0.052259831547
C	2.935052303891	1.570149508780	-0.052301500408
C	1.949707759847	-2.415340836659	-0.052402032231
TV	4.801831903178	-1.502639360479	-0.000000000000
TV	0.000000000000	5.065492967532	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.382340678797 hartree
Spin(**2) = 0.066406250000
Geometry of 2D-min28

C	2.791478476918	-1.199960147017	-0.499082593540
C	1.710232142985	-3.167026446882	-1.223560255951
C	3.483688684371	2.661883207763	1.421457500280
C	0.555282808673	-0.062200612235	1.049079812510
C	1.343532925023	1.372380706900	-2.664837465446
C	2.070792194880	0.091817968437	-2.655975654250
C	2.130371546904	2.700082670435	4.557107306168
C	0.661610071916	0.027952961248	4.557780442681
TV	2.198088558872	1.395366966493	-0.000000000000
TV	-0.000000000001	2.603597964143	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.363830934516 hartree
Spin(**2) = 0.628906250000
Geometry of 2D-min29

C	-0.055783249780	-0.276490703477	-1.063928666588
C	-0.728140001838	-1.530237595220	-1.245990737614
C	1.286983088520	3.485751078651	0.552340781382
C	1.285743395867	-0.275506840174	-0.284475539639
C	3.299027255936	0.977539873535	-1.246745600928
C	2.626589953285	-0.276067768855	-1.065126239989
C	1.292141016112	4.740881868191	2.630680043910
C	1.290628662752	0.979715412690	1.972365224313
TV	5.481324228622	0.000482632390	-0.000000000000
TV	-0.000000000000	2.507282328807	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.363279621403 hartree
Spin(**2) = 2.000000000000
Geometry of 2D-min30

C	-0.745843175196	0.581072205834	-0.668946372257
C	-0.746664812081	-0.659072281070	-0.668925816108
C	1.866911089050	2.821945862118	-0.668925802727
C	-0.746920899992	-2.080694375576	-0.668975980293
C	0.418173385672	4.305617912045	-0.668941221860
C	0.418957798904	2.820987112512	-0.668892542601
C	1.866110177021	4.306468542771	-0.668962626849
C	-0.745632377053	2.002624829251	-0.668945577560
TV	3.777646294628	0.001685903204	-0.000000000000
TV	0.000000000000	7.203454696617	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.360871806765 hartree
Spin(**2) = 0.058593750000
Geometry of 2D-min31

C 1.313907544745 -2.955148363324 3.513846717752
C -0.159358621241 -1.703214039170 2.010988959557
C 1.125082524770 5.634445128254 -1.541356807018
C -0.646849435933 -0.451709576857 1.505045647620
C 3.090184536047 0.628233820577 0.463314536546
C 1.575552800943 1.879758831347 -1.090391689608
C 2.602222393066 1.879763397113 -0.042141530040
C 0.864818391927 -4.206511189958 3.061571662517
TV 4.740993090231 -1.422998992922 -0.000000000000
TV 0.000000000000 2.503098860476 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.357426412176 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min32
C -1.759409316638 -1.107674700610 0.332771792708
C -2.453238205105 -2.404453937801 0.333895458235
C 0.382181844300 2.782654365867 0.333406351194
C -0.311735213135 -1.107900945756 0.332295811037
C 3.200580031259 0.790261164469 -2.917504598807
C 3.200748893267 2.164197105540 -2.917245023703
C 1.112222135661 4.683927869435 3.583133805183
C 1.111405056514 0.870253572080 3.582926020270
TV 4.283027187446 2.592805521838 -0.000000000000
TV -0.000000000001 2.593817264486 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.350995834576 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min33
C -1.204453108208 -1.404880990310 0.485243288729
C -1.898598959851 -2.701651718123 0.485265276130
C 0.936342919439 2.485853006858 0.485702392035
C 0.242141699960 -1.404627867460 0.485724040705
C 1.664451630386 0.587950180115 -2.802409837237
C 1.662737504013 1.807416558791 -2.802354338663
C 1.701663629665 5.773984269327 3.763019619644
C 1.701743431690 1.806076906672 3.763274101805
TV 4.283529981166 2.594046635964 0.000000000000
TV -0.000000000001 2.593695390738 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.350811279553 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min34
C 2.363318761079 -0.399563638819 -0.625572231733
C 1.382006510500 -1.457815476887 -0.625641254093
C -0.797676504732 1.845016435165 -0.625784762769
C 0.080024062030 -1.951850114187 -0.625753619006
C -0.279130738147 3.832148729651 -0.626121800518
C -1.596490391308 3.123679438464 -0.625984769244
C 2.691224752849 5.353408871295 -0.625493460793
C -2.990078201267 3.482743245627 -0.626026991484
TV 3.514959723352 -0.908976573348 -0.000000000000
TV -0.000000000000 7.150210069054 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.348480748710 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min35
C 0.389627769977 -0.008400387939 0.478493531898

C	-0.929007645986	-0.588333812535	0.478089239417
C	0.389495461966	1.515744589527	0.478373090742
C	-0.929174491175	-1.986665376195	0.478112915434
C	3.877194014310	2.100087680287	0.477537979195
C	1.235608377375	-1.287404047685	0.478808294848
C	3.877063958505	3.489242867215	0.477743261617
C	2.641036310794	-1.287686393210	0.478136251292
TV	6.035648152994	2.041101506284	-0.000000000000
TV	-0.000000000000	4.082129145069	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.342367097139 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min36

C	1.985779480498	2.058695070475	-0.770478305800
C	-2.609131047347	-0.592870836799	-0.770311586521
C	1.276118799945	0.831266549689	-0.770557370208
C	-1.374785816348	-1.305191379797	-0.770512667894
C	-0.666793017166	4.196756919680	-0.770523117620
C	-0.666269200577	2.771905860985	-0.770302417994
C	0.042952378907	5.424109689130	-0.770577800130
C	0.568037333556	2.059503987274	-0.770511991145
TV	3.885939579301	-0.000722175598	0.000000000000
TV	-0.000000000000	6.730151359849	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.341110381066 hartree
Spin(**2) = 0.058593750000
Geometry of 2D-min37

C	-0.057835505493	0.136228908623	0.933758801377
C	-1.416095804946	-2.344431352866	0.374881608980
C	1.413592521944	2.612769835736	0.490853811744
C	-2.093444781924	-1.099975880684	0.226652049339
C	4.241540466814	0.116260471018	0.075749849208
C	2.107438299237	1.365026767369	0.289243046660
C	3.529853790859	1.363917785862	0.083038239871
C	0.636753324032	-2.682421018535	2.095735721183
TV	7.769531666498	-1.278752874926	0.000000000000
TV	0.000000000000	2.495548016250	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.337490831507 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min38

C	-0.891880003179	-0.023219719568	1.012511354420
C	1.071780172133	-1.983887538637	-0.303420225893
C	-0.086603226574	1.144028366438	0.668296763438
C	-3.746304335157	-0.377097205724	1.156014617347
C	3.382361249689	1.859482471864	0.308205467278
C	1.375934073766	-0.715260317360	0.544194603767
C	1.933871406950	1.899486021300	-0.160227084126
C	4.844996446532	0.000176623618	0.183619741374
TV	3.716452947880	-0.731812526544	-0.000000000000
TV	-0.000000000000	4.969252556307	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.335402258105 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min39

C	-2.165513445045	-0.528258377089	0.098369152837
C	-1.478969876229	0.679337263717	0.393583701453

C	1.569644127343	1.884637256770	-0.443294342194
C	0.980883388059	-1.737965782430	0.028616146860
C	4.029883538430	4.299781288366	-0.811803639006
C	4.716719920814	3.092261089872	-0.517323824537
C	-0.149023042738	0.678395763324	0.944350721526
C	2.698874328555	-0.530644648568	-1.359817682976
TV	8.175567002463	3.620896782298	0.000000000000
TV	-0.000000000001	2.415120712636	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.328605694151 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min40

C	0.358302979945	0.243134219727	0.478640567935
C	-1.120889368836	0.242910616042	0.478675228749
C	1.082133027847	1.454117656181	0.477963913160
C	-1.844808339330	-0.968234144978	0.478386520945
C	4.956694940860	1.455021363933	0.478172362013
C	1.081778915778	-0.968115236239	0.477915780193
C	3.716283884357	2.167990578448	0.477934860920
C	2.322347715124	-1.680239933667	0.477605330530
TV	6.801765627158	0.001066974180	0.000000000000
TV	-0.000000000000	3.847733900509	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.328297734953 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min41

C	2.263993373651	1.984152419643	0.893988656648
C	-0.953440943160	-2.236368284931	-0.110375848341
C	-0.264319518277	1.606600135741	-0.148508301345
C	-2.400940024357	-2.230873216108	-0.037360923292
C	4.629810806665	0.104504610753	-0.013995826076
C	1.906527368011	0.325411093301	-0.618491547842
C	3.189112974709	-0.016494516706	0.025339103654
C	1.207096351984	-0.937723388803	-0.280076523898
TV	7.720810465839	-1.509291421038	-0.000000000000
TV	-0.000000000000	2.563029417643	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.320675193560 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min42

C	0.660653708938	0.543613066187	-0.676310395009
C	-0.424553261494	-0.475980066859	-0.676240461773
C	0.283972276607	1.890443854084	-0.674178778120
C	-0.048595287328	-1.822989522628	-0.674255416515
C	3.199635981225	1.252708409112	-0.677928370848
C	2.114465600989	0.233083010319	-0.677936842900
C	2.822953271720	2.599531441369	-0.679697796871
C	2.490470726048	-1.113886351502	-0.679703256565
TV	5.077984113146	1.418091669615	0.000000000000
TV	0.000000000000	4.916721884596	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.308426502322 hartree
Spin(**2) = 0.066406250000
Geometry of 2D-min43

C	3.559712977086	-0.647642427213	-1.039370237975
C	-1.788313384683	0.646225479152	-0.310165608687
C	-0.491685483322	0.646373545254	0.679710151141

C	0.022342085804	-0.647443745965	1.280252304923
C	4.938082225925	-0.647531391152	-1.264844860807
C	0.491183235511	0.646332850419	-0.664139832955
C	1.788067244310	0.646346851026	0.325451869968
C	1.400619060441	-0.647467754721	1.054693366369
TV	4.960726095923	-0.000003106777	0.000000000000
TV	-0.000000000000	2.587585595889	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.303887742331 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min44

C	-1.828704672919	0.813483271101	0.989300427581
C	1.383874568189	-1.036641933901	0.990864947695
C	-0.782512262254	1.909727270695	0.988840746397
C	0.003024965304	-1.036559471027	0.991190275506
C	3.214910577032	0.822171145486	0.989359871765
C	0.691140215927	0.160641656304	0.990837955279
C	2.165999453979	1.911102879781	0.988888338255
C	5.113481754039	-0.989483005987	0.989101612144
TV	4.419191425819	-2.539702298986	0.000000000000
TV	-0.000000000000	5.096951560552	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.299087106774 hartree
Spin(**2) = 0.058593750000
Geometry of 2D-min45

C	-3.545274263322	-3.973347216051	0.076864662298
C	-0.972040137675	-1.207459276514	0.077564146515
C	2.266327065940	4.278505211627	0.074646305768
C	-3.376850596108	-0.839213263857	0.077201210262
C	4.081171643011	2.141899137651	0.076820957778
C	0.242742128811	-0.541696850602	0.079243239916
C	3.827992683995	0.747989753511	0.075571456310
C	6.740733098727	-0.714603358331	0.075116386230
TV	4.333717290908	-0.917197379024	0.000000000000
TV	0.000000000000	5.594626435395	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.298753680305 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min46

C	0.142544322437	0.601889236138	-0.568886063035
C	0.143696063019	-0.762235578772	-0.568483921526
C	1.190312528273	1.653935318232	-0.569080421922
C	0.142007514289	-2.036109953090	-0.568445065917
C	0.137882057536	4.066531148474	-0.568888878359
C	0.138634496796	2.701698224475	-0.569167007094
C	0.140221464381	5.340526425907	-0.568529374426
C	-0.909276475641	1.649865528833	-0.569104510252
TV	3.484963905430	0.007547000819	0.000000000000
TV	0.000000000000	8.708401743423	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.293821188232 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min47

C	3.901129880048	2.111056624859	-0.684014477925
C	-2.216818117127	-2.250281098343	0.845351776720
C	0.468294612197	1.285974643399	0.239342330270
C	-0.970001255623	-2.651744527386	0.177752162760

C	2.657762208896	0.518987104533	0.739164956908
C	1.337202407675	0.105759092742	0.413785421430
C	2.727423268760	1.966643108560	0.447836004897
C	1.301580999941	-1.335265534156	0.282276186917
TV	5.775026837435	1.631085440108	-0.000000000000
TV	0.000000000000	3.756360848865	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.292272168165 hartree
Spin(**2) = 0.058593750000
Geometry of 2D-min48

C	0.517817523413	0.522934239801	0.626010848619
C	-2.162137080012	-1.569494392782	-0.872762807467
C	0.556472513709	1.943471112173	0.634738800984
C	-0.321768721400	-0.635917851021	0.556667222368
C	4.207986647381	0.953772916651	0.217774181621
C	1.932330221531	0.083139078728	0.670251788040
C	2.818870927452	1.222082748715	0.664232060338
C	1.959899203929	-1.337215502237	0.684959992526
TV	5.934092423823	1.831151309610	0.000000000000
TV	0.000000000000	3.715476425954	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.291266707108 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min49

C	-0.368455141451	-1.021901614346	1.281839775737
C	-1.053710855034	-2.297636184595	1.352069121658
C	1.874772036066	2.843361798629	0.969961149252
C	1.073366549595	-1.003783883295	0.969802052092
C	1.471887683553	2.201398963806	-1.664194827669
C	1.473329554370	-0.359317283108	-0.355760061393
C	4.002003476646	4.137010033961	1.351879514184
C	3.316656853482	0.302194079212	1.281545313842
TV	6.504929403653	3.874764064124	-0.000000000000
TV	-0.000000000001	2.559117204143	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.287753877539 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min50

C	1.048415088498	1.056157952817	-0.778187631794
C	0.186497200923	-0.079580110148	-0.778176304568
C	2.502459810388	1.056175497926	-0.778175190077
C	-1.216492723509	-0.079552833921	-0.778147946093
C	-0.514981517438	3.460477789034	-0.778233474706
C	-1.216585013050	2.192106736363	-0.778169148580
C	-0.515015927827	4.835078035955	-0.778193630462
C	0.186433992563	2.192028606839	-0.778151844635
TV	4.580999960069	0.000030124901	-0.000000000000
TV	0.000000000000	6.183097828640	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.286673558142 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min51

C	0.630724469469	1.508551172919	-0.840714071435
C	-0.025092895356	0.235093519397	-0.836338950069
C	2.033879988610	1.247420307412	-0.571100814206
C	-1.226565443989	-1.580862853764	-0.103545928878
C	0.123866514679	4.043631619344	-0.152418943611

C	-0.068979788853	2.752361475621	-0.819176597036
C	0.963432690354	5.237458725672	-0.571080340314
C	-1.211491914016	3.317179574506	-1.458611942933
TV	3.384118794980	1.480984300502	0.000000000000
TV	0.000000000000	6.149485456692	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.280981531378 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min52

C	0.763320411979	1.028651165594	-0.778197872156
C	-0.073323824338	-0.175964406301	-0.778161116355
C	2.180655134545	1.029496109971	-0.778223323306
C	-1.412976132476	0.298120236229	-0.778283858136
C	0.245054810718	3.606847882223	-0.778067435366
C	-1.413895036321	1.757403109122	-0.778304487579
C	0.246449089493	4.855715935546	-0.777972058996
C	-0.074553543047	2.232621642486	-0.778225019018
TV	4.799006698371	0.002548882758	-0.000000000000
TV	0.000000000000	6.406151666827	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.277237622163 hartree
Spin(**2) = 0.066406250000
Geometry of 2D-min53

C	0.549074601188	-0.372564583559	-0.183644571629
C	0.668790202700	-1.778065842664	0.114552790453
C	-0.238880154358	0.805484323329	0.112334394831
C	-2.793548683321	0.322770648218	-0.537453927155
C	3.307673789283	0.887847862713	0.756901232147
C	1.828856617234	0.061688786017	-0.654668787488
C	2.135172763775	1.454526324098	-0.128232135770
C	3.944831371382	-0.207858925392	0.144223991285
TV	5.622495284788	-1.230394908096	0.000000000000
TV	0.000000000000	3.678733344248	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.275599448275 hartree
Spin(**2) = 0.312500000000
Geometry of 2D-min54

C	1.159252293585	-0.597173271122	-1.697512023977
C	-0.104005395550	0.196782007021	-1.698083558181
C	-0.530047752792	1.038305237375	1.482798113930
C	-0.528164832876	-0.162836557907	1.915365889242
C	1.159226895205	2.598124890289	-1.697576793283
C	-0.104044729899	1.804280484853	-1.697959781081
C	-0.525296002386	3.439841656219	1.478059088735
C	-0.526920475267	2.239715532953	1.914909064628
TV	2.527280011163	-0.000139627363	0.000000000000
TV	0.000000000000	4.802829499705	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.272020874195 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min55

C	1.039331134720	-0.007757200888	-1.971292832077
C	-0.161687031589	0.000098888922	-1.538531037490
C	0.170036896152	0.631524184309	1.754813607814
C	-0.622750251357	-0.632061973580	1.754929366789
C	3.441724547207	0.008039197905	-1.970925606334
C	2.240554846065	0.000156635449	-1.538719894744

C	1.779594948595	0.631596329074	1.754911426279
C	2.572377530075	-0.631989426577	1.754814969779
TV	4.804696707947	-0.000035827048	-0.000000000000
TV	-0.000000000000	2.527592425014	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.271244728817 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min56

C	-1.026104552542	0.643684869083	0.698467143855
C	0.447722411284	-1.482129830127	-0.635283316343
C	-0.118023871303	1.604059501865	0.188283669231
C	-1.585443766388	-0.477164453199	0.699216467496
C	3.828971638736	0.821192000341	-0.125618306344
C	1.007281648208	-0.361435835590	-0.635088310903
C	2.491084745420	1.482199322670	0.188000393405
C	5.509990869475	-1.176492163116	-0.125656775806
TV	4.289845531547	-2.119892356927	-0.000000000000
TV	0.000000000000	5.383153152049	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.268846175005 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min57

C	1.384150002792	1.292863910404	-0.036296838838
C	-1.236954902591	-1.868658131613	-0.035838995129
C	0.146415896092	2.000995879932	-0.035979261229
C	-2.493447520284	-1.870373419673	-0.035864092198
C	4.771689868874	0.073429696992	-0.036116487318
C	2.101333851430	0.065408457342	-0.036690266311
C	3.519640725617	0.068045470671	-0.036417842681
C	1.385012467288	-1.162503011170	-0.036277426767
TV	8.625104270865	-1.922965739920	-0.000000000000
TV	0.000000000000	3.870222121082	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.263926251195 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min58

C	-0.653415080519	-0.938327126415	0.788867214081
C	-1.347063534083	0.285754304874	0.978033718607
C	1.703651893473	1.499668014624	1.577875979702
C	0.807384249992	-0.939930189454	0.362870484183
C	1.497647260214	2.897082584012	-1.724657302598
C	1.105589343337	0.277517647012	-0.453542161173
C	3.848992284183	2.735841653452	1.308071134566
C	3.129206789713	-0.937079388543	1.410433998284
TV	6.600556568814	0.000165841378	0.000000000000
TV	0.000000000001	2.449165584953	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.260094070143 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min59

C	5.309019923481	1.102093923819	1.179968919670
C	-2.423854233614	-0.527360562013	-0.430545341972
C	-0.216090922094	1.838970092831	0.089617568444
C	-1.611370926900	-1.692696292190	-0.386459755466
C	3.491589126451	0.883649780761	-0.406513218948
C	1.994207261692	-0.560848248117	-0.387969071277
C	2.007551049726	0.885697853095	-0.364181211448

C	1.198478474459	-1.731009579524	-0.283361147697
TV	5.924333536391	-0.034045783478	-0.000000000000
TV	-0.000000000000	3.775277443238	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.259639003466 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min60

C	-0.731790744994	0.288406888174	0.506046804000
C	0.572657432289	-2.164815055179	0.441687652130
C	0.120337419649	1.439086421958	0.369861732431
C	-1.870814869493	-0.584931569794	0.531134732759
C	3.768880445378	1.428869576804	0.206213282703
C	-0.457577770131	-1.089944321218	0.493943607145
C	2.528872664783	1.544710755538	-0.384590467955
C	5.298021988102	-0.283551474153	-0.063235234178
TV	3.921550401849	-1.435546768507	0.000000000000
TV	-0.000000000000	6.278228369654	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.258816149718 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min61

C	0.554718949782	0.167845809157	0.392848477450
C	-0.418410162051	-0.976227946736	0.392830607628
C	0.504938143308	1.562234930768	0.392815693315
C	-1.720528034194	-0.626301819846	-0.323610563141
C	4.151122197857	1.243416588112	1.109326068942
C	1.927628674304	-0.301475885602	0.392801290256
C	2.850606904979	0.888343097128	0.392811966544
C	1.876628532964	-1.696422157967	0.392793869323
TV	5.871527528293	-1.860101779808	0.000000000000
TV	0.000000000000	3.729723568825	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.258220369943 hartree
Spin(**2) = 0.066406250000
Geometry of 2D-min62

C	-2.608354799570	-0.441196084822	-0.166940295494
C	-1.163975538906	-0.316550883105	0.092683601134
C	2.934364671366	2.129194247493	-1.030154559338
C	-0.262651806488	-0.872648773770	0.982976454655
C	0.660790768339	3.464057560468	-0.849722239103
C	1.546976578867	2.329885299028	-1.025294788442
C	-0.006276580255	5.890574879121	-0.661998511157
C	0.309117965936	1.463514318356	-1.048591863501
TV	3.496117122958	-0.522526060352	0.000000000000
TV	0.000000000000	5.730253563770	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.256588333190 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min63

C	-0.960471149023	-3.279288014340	1.050006933397
C	-2.335850883186	-3.278625485415	1.042725377648
C	1.183383539920	3.102855468263	1.044347944166
C	-0.193761373141	-2.002674766819	1.050728462798
C	3.006392414501	3.094828558720	-1.952827654963
C	3.121742979407	1.818120052927	-1.822834433913
C	3.330260484036	4.378750022103	1.020204447880
C	2.567716980956	0.548923043621	1.031144368677

TV	7.052455218860	5.103255462754	0.000000000000
TV	-0.000000000001	2.553486597781	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.256318189029 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min64

C	0.684269338213	0.732000296584	-0.721561353674
C	0.167573033491	-0.592643064405	-0.721519624931
C	2.154184123458	0.731811889623	-0.721561007675
C	-1.243789815994	-0.592653024104	-0.721525555114
C	-0.537714021361	4.242414906284	-0.721559950666
C	-0.537922711412	2.987250594710	-0.721614998651
C	-0.537949890027	5.623207534569	-0.721542596393
C	-0.538084848093	1.588920247145	-0.721579544262
TV	3.914770623799	-0.000206075421	0.000000000000
TV	0.000000000000	7.448077297712	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.254149244892 hartree

Spin(**2) = 0.222656250000

Geometry of 2D-min65

C	-1.754584567266	-1.045799740209	0.908904655526
C	-0.373201404547	-0.738016061017	0.908438784541
C	-3.007556497078	1.397798415001	0.908213850582
C	2.199483101264	-0.173057061870	0.907991741001
C	3.683076523315	2.104087076516	0.908874397019
C	0.847540843905	-0.467687851907	0.907976245776
C	4.073414035082	3.291724318223	0.908735720976
C	3.555001037627	-0.603811552580	0.908292409614
TV	6.266018922688	-0.610451403578	0.000000000000
TV	0.000000000000	6.293700250201	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.251324656356 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min66

C	1.099014278395	-1.100988868571	0.746952261216
C	-0.182122882872	-0.268432752896	0.746880034284
C	0.642773289817	0.930458139042	0.747094786707
C	-1.522622176525	-0.587346036323	0.746918895079
C	4.014158015176	1.704287330473	0.746791352475
C	1.392719311086	2.217789649220	0.746899870790
C	2.673782305515	1.385141773619	0.746702894582
C	1.849027209897	-4.469263327246	0.747043140420
TV	6.752258199959	-2.015527826015	0.000000000000
TV	0.000000000000	4.655470958049	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.248585179217 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min67

C	0.034932496102	1.313327093313	0.207073007442
C	0.034919165347	-0.075827213376	0.206641500252
C	1.262847541943	1.399212099896	-0.811171443439
C	-1.017532430366	-0.872439511371	-0.543013415094
C	0.210565996455	3.585178101885	-1.560957580253
C	0.210600572765	2.196040153848	-1.560723311003
C	1.262793656834	4.381606873654	-0.811020350770
C	-1.017472350910	2.109746303442	-0.543079725766
TV	3.584095814542	-0.000328131694	-0.000000000000

TV	0.000000000001	4.543973232939	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.243911990259 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min68

C	-1.068348462248	2.034123838050	-1.535667397069
C	-0.035744965969	1.028533407560	-1.114952541410
C	-1.017296676231	3.503953079616	-1.452578627918
C	-0.023705586176	-0.502467180018	-1.452024676219
C	2.827770889494	-0.223258784094	1.181192497650
C	2.245720773364	-1.193461056236	0.380049838978
C	5.622085736485	-1.973189266885	2.386778576310
C	1.290230029749	-1.797736352135	1.182060319879
TV	2.513097933381	-2.449856178322	-0.000000000000
TV	0.000000000000	5.022564770085	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.240845995522 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min69

C	0.442860618749	0.480644493187	-0.511795685879
C	-1.793266278641	-0.658837550104	0.152048570927
C	0.483702617163	1.926298913739	-0.535946639565
C	-0.393221107240	-0.705971362155	-0.485173057020
C	2.961439504432	0.060548235255	0.423350521740
C	1.791317441904	-0.044054947150	-0.422429177463
C	3.382451974040	1.193797850851	1.069630060353
C	1.842716042964	-1.419778931970	-0.542040419910
TV	5.070771674190	-0.822934118213	0.000000000000
TV	-0.000000000000	3.854556632424	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.239049983358 hartree
Spin(**2) = 0.187500000000
Geometry of 2D-min70

C	1.347007087348	1.654485469919	-0.205706100837
C	0.876951336352	0.287464414101	-0.212746359045
C	2.773715167696	2.090656749644	-0.630825619151
C	-0.940688496051	-0.906836152006	-1.512366434694
C	-1.300210701069	1.674985837528	-0.864920325300
C	-0.674042091789	2.930604893433	-0.938939900495
C	-1.307526131103	4.237436776491	-0.920034573107
C	0.752286896646	2.862577888915	-0.704472845716
TV	3.336746344150	1.805228754926	-0.000000000000
TV	-0.000000000000	6.373842623380	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.236948951941 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min71

C	1.143353702731	0.468443298861	-0.385878957896
C	-0.905690688118	-1.983253938657	0.222612970501
C	0.562784949731	1.614715697759	0.186073546351
C	-1.708900420613	-0.835999156095	0.219125782450
C	3.974835947545	1.280345668708	0.551493818745
C	2.308987703944	-0.110103707204	0.464688960401
C	2.648939104469	1.286313989001	1.065870817648
C	1.702394907242	-1.459049237353	0.818630472127
TV	5.591678293149	-3.052902869729	-0.000000000000
TV	0.000000000000	3.762707277194	0.000000000000

TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.236160311799 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min72

C	-0.715002321931	1.127471883789	-0.463607130912
C	0.200363539944	-0.095810105679	-0.463596822581
C	0.462428414942	1.970484518129	-0.464148963395
C	-0.120689601985	-1.369094081909	-1.295436617335
C	0.772162562353	3.432945563448	-0.464726522772
C	2.200740284783	3.703580993506	-0.465077707748
C	-0.120906915752	4.398239499313	0.366591451830
C	-2.124077048970	1.256518961072	-0.463664662962
TV	3.522480557018	-0.384950604833	-0.000000000000
TV	-0.000000000000	5.768037355652	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.231893570183 hartree

Spin(**2) = 1.312502500001

Geometry of 2D-min73

C	-0.914055022039	-0.255189731799	0.083365258362
C	1.198953080378	-1.962807211800	0.084752154308
C	-0.298297246603	1.140743033877	0.081407577196
C	-2.285597233687	-0.426052497250	0.084697492703
C	3.549100381616	0.212770139599	0.080910350816
C	0.399951036865	-0.835465085992	0.083449384358
C	2.387543190674	0.731904583952	0.080952494323
C	5.662040658659	-1.495232887796	0.081332624847
TV	4.646146959539	-2.055755940899	-0.000000000000
TV	0.000000000000	6.113639176004	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.229097131617 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min74

C	-0.910277837687	-1.014873229657	0.216239508436
C	-2.298375222052	-3.657470448452	0.221921101087
C	1.691334524306	1.629283475292	0.216866343661
C	0.371538225787	-1.014473554281	0.215646278856
C	3.736201426344	0.976825714214	-3.039425490034
C	3.736941243762	-0.259873628988	-3.039444172482
C	4.361424476433	1.629706283424	0.223232638079
C	2.972790279679	-1.012935217395	0.224178398979
TV	7.372493242951	3.965577463452	0.000000000000
TV	-0.000000000001	2.642891149598	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.227398982860 hartree

Spin(**2) = 0.140625000000

Geometry of 2D-min75

C	-1.344128764022	-0.297377170313	0.407903253012
C	-0.521754768195	-1.221524345960	0.407898985578
C	0.246354767492	1.279668994951	0.411002485014
C	-3.588534175356	-2.078756320778	0.411258376505
C	3.656180549105	0.547803056790	0.409987712276
C	0.901982419303	-1.286637150557	0.410045839819
C	2.345190441314	1.113166599117	0.411203450439
C	6.127945355091	-0.402677920850	0.411024860241
TV	4.898208319178	-0.576425966722	-0.000000000000
TV	-0.000000000000	4.933359895947	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.226821210245 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min76

C	-0.746160414338	-0.364793946755	0.697690586119
C	0.985126959707	-1.910970061936	0.273670936915
C	0.289420156996	0.649470404485	1.215525845006
C	-1.252943361215	-1.699362849406	1.215312051558
C	3.245229532993	1.984233937694	0.697848687759
C	0.478347501382	-0.576246106966	-0.243937491468
C	2.020763271016	1.772530036403	-0.243816642401
C	4.976292055737	0.438038708699	0.273879127882
TV	3.462514731630	0.000166070225	0.000000000000
TV	-0.000000000000	4.697755445003	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.221952037229 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min77

C	1.810991743095	-0.352174884139	-1.548626344913
C	0.533304109321	-0.614906741686	-1.548546284355
C	-0.361815437132	2.572608744623	1.528671740647
C	-1.639511161186	-0.948991805106	1.528626591603
C	4.366337273141	0.173252806702	-1.548631961785
C	3.088661570302	-0.089502937589	-1.548492623554
C	2.193559361728	3.097935313072	1.528793406722
C	0.915863008039	-0.423644536139	1.528688250538
TV	5.110739098345	1.050721859639	0.000000000000
TV	0.000000000000	3.258900462329	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.221689794170 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min78

C	3.139446959407	-0.906811297921	-1.452783490246
C	-3.252561498678	1.059397779111	-1.452801888549
C	0.583843077831	1.818841952634	1.628157656165
C	-0.694526472290	-1.704117350275	1.627958323712
C	5.696129599484	-0.387400681956	-1.452445827275
C	-0.695769792380	1.578206162276	-1.453019872033
C	3.140509238236	2.338047325574	1.627996390332
C	1.862252287835	-1.185136060629	1.627950456539
TV	5.113427909952	1.038368236958	-0.000000000000
TV	-0.000000000000	3.263507059496	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.221687478963 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min79

C	-0.781788899641	-1.426660448351	-0.306481817488
C	0.505259070930	-1.594447689628	-0.834548812783
C	-0.381055955660	1.161772525631	0.460304464216
C	-1.038240641063	-0.020569486932	-0.073879625067
C	2.173232239853	0.442207984112	0.026294001947
C	1.658575347931	-0.903932908635	-0.628313700855
C	2.105277576440	1.931649991228	-0.134994064099
C	4.810717148486	-0.262557794033	0.530767017111
TV	3.796864764269	-1.605468538153	-0.000000000000
TV	-0.000000000000	6.014168690180	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.218914523205 hartree

Spin(**2) = 0.140625000000
Geometry of 2D-min80
C 0.821423714962 0.836196775376 0.541405340458
C 0.821477421923 -0.468413344751 0.541465821167
C 0.821491537389 2.140872873396 0.541455397584
C 0.821420921032 -1.773087708463 0.541400020614
C 2.701521730702 -0.794320337809 -1.895442103762
C 2.701619269108 -2.098934486463 -1.895548715783
C 2.701624001416 0.510365982686 -1.895541505176
C 2.701500183616 -3.403621100679 -1.895445573758
TV 3.761939762044 -1.968963299404 0.000000000015
TV 0.000000000001 5.218623510078 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.218578708032 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min81
C -0.727580149191 -0.716838619875 -0.194751064572
C -0.082950877570 -1.440133684886 -1.139446546239
C -0.321848607722 0.701327553385 0.094089358657
C -2.183101547256 -0.956508685576 0.094206297134
C 3.145459227279 0.796051566660 0.172958492555
C 2.078022411479 -0.154502559940 0.172818783908
C 2.194184092798 1.928794643093 0.202679390070
C 5.817352906509 0.369070944567 0.202536018988
TV 4.755137765133 -0.551855275220 0.000000000000
TV 0.000000000000 4.786197534987 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.218393712017 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min82
C 0.716691753370 1.328435836115 -0.324783450379
C -1.232817316491 -0.534005872695 -1.427852463915
C 0.980629665467 0.110115080804 -1.134951397774
C -2.504205066749 -1.900864450065 -0.455141664046
C -1.093299927571 4.473576236122 -0.592072424221
C 0.219574882343 3.941184517915 -0.246086985883
C -0.224648094249 6.368682612585 -2.034110585410
C 0.480814769228 2.543778263524 -0.191085684432
TV 3.736756221900 0.601096146898 -0.000000000000
TV 0.000000000000 6.200706635727 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.217044203941 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min83
C 0.107960149700 1.053916292372 0.238646767856
C -1.350653028422 1.055793895784 0.276037265711
C 0.884275974392 2.166699841312 0.698770911484
C 0.901008850197 -0.180297124249 0.076708801806
C 2.191003367132 0.090172036143 -0.382952300291
C 2.487936784116 -0.595658088407 2.272084435502
C 2.612398540984 0.616057643609 1.700750791286
C 1.991150367762 -1.744331361018 1.720079676976
TV 4.656503318415 -0.628828823098 0.000000000000
TV -0.000000000000 3.710910176548 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.216455222788 hartree
Spin(**2) = 0.000000000000

Geometry of 2D-min84

C	0.535031319666	0.285907582943	0.168506215254
C	0.164062810947	-1.008037294575	0.947573016077
C	0.989271690458	1.734887265348	0.554494144385
C	-1.162433037033	-1.338197527337	0.966966729203
C	2.407730430483	1.784705285550	0.868734996949
C	2.048424263455	-0.174579805854	-0.219019338084
C	2.960263289807	1.076049318782	-0.385790852490
C	1.943355064763	-1.693818961264	-0.657369904059
TV	3.976042737811	0.587864596688	-0.000000000000
TV	0.000000000000	3.937977420991	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.211726285130 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min85

C	0.675075892268	0.052427582721	-0.055008744413
C	-0.675918787209	0.051994298972	-0.055045185897
C	0.637232936876	3.324776548479	-0.049823630648
C	-0.628597228038	-3.221730284849	-0.049827866951
C	3.291823570073	0.052560917503	-0.054988323033
C	1.940804461526	0.052140364009	-0.055034122531
C	3.254062621529	3.324882725483	-0.049819246800
C	1.988225057430	-3.221573339734	-0.049823652453
TV	5.233615225243	0.000303459679	-0.000000000000
TV	0.000000000000	6.547454691726	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.210699987215 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min86

C	-0.847804481711	-1.402542024925	0.592007320205
C	0.506850512169	-1.616603138333	0.821728779206
C	0.653593946992	1.492453770222	-0.699378281515
C	-1.479729610392	-0.126006122169	0.596825711133
C	4.174312478517	1.470242997749	0.423620608735
C	1.571540503092	-0.715919897702	0.597096467275
C	-0.428552700061	0.898726732643	0.710852120680
C	5.412202689186	-0.308228554918	0.307231645992
TV	4.465559101084	-0.862256235866	0.000000000000
TV	0.000000000000	5.129013275521	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.210618991741 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min87

C	-1.184473757212	2.114086435815	-0.370180846408
C	0.677765506864	0.077638780811	0.302823775568
C	0.369831232481	2.813909372855	-0.572076181960
C	-0.030464597807	-0.818128082489	-0.537280869895
C	2.039402224903	0.153742274297	0.060677236874
C	3.566539827760	-3.143899754499	1.186020448286
C	2.594606555612	1.487791195076	-0.048565819814
C	1.843393105452	-2.286191978051	-0.440208381156
TV	3.945673418312	-3.079547848148	0.000000000000
TV	-0.000000000000	5.024195363738	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.207501731719 hartree

Spin(**2) = 0.000000000000

Geometry of 2D-min88

C	0.879025892239	-0.026384057263	-0.337090914971
C	-0.003102611234	-1.235954156245	-0.517240880106
C	0.915559087416	1.420853899203	-0.532163569397
C	-3.661023235001	-0.169270406511	-0.533126482420
C	4.582275462495	0.746293906018	-0.513564348350
C	2.329988751717	-0.485704010317	-0.337449791268
C	3.212251169332	0.723594261029	-0.517176142888
C	1.604474969484	-0.259429666390	1.038060561447
TV	5.955389174061	-1.763535976714	-0.000000000000
TV	-0.000000000000	3.774117452333	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.207075035508 hartree
Spin(**2) = 0.750000000000
Geometry of 2D-min89

C	0.101453215806	-0.296535124925	-0.121575400708
C	-1.268442892249	-0.331633616937	-0.108788858130
C	3.099697279013	0.508663120169	1.467509497060
C	-3.566189103981	0.354036999094	-0.067746546242
C	3.818522794684	0.475746071268	0.088012028208
C	1.470485083630	-0.273606632445	-0.093158186548
C	2.358913143783	0.923171129820	0.117625162970
C	3.776189075106	-0.968095297779	-0.131691156486
TV	5.962628596650	-1.745858205887	-0.000000000000
TV	0.000000000000	3.764763149169	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.207002455625 hartree
Spin(**2) = 0.515625000000
Geometry of 2D-min90

C	0.104270477873	-0.081822885784	1.119876620384
C	-0.787129802821	-1.216632253429	1.174170041188
C	0.104700610623	1.326003052135	1.118457118804
C	1.079070812367	0.622929205188	-0.434203896112
C	3.826659766602	0.619270353039	1.222852773839
C	1.506604920887	1.702380984954	0.732868196684
C	2.477642065823	0.622359515645	1.156336717635
C	1.505893976394	-4.134881446526	0.733311421396
TV	6.003645551916	-1.838446189353	-0.000000000000
TV	-0.000000000000	3.677440870042	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.205295303288 hartree
Spin(**2) = 0.750000000000
Geometry of 2D-min91

C	-0.834276040169	-0.596090796493	0.214306371041
C	0.025395955553	-1.614116654658	0.212905154748
C	-0.404837807670	0.821618636623	0.214613642437
C	-2.302352551600	-0.780921155694	0.214627161129
C	3.146595726049	0.709521458382	0.214735954020
C	2.018524086826	-0.238810705107	0.214824470762
C	2.147820793601	1.865089244436	0.214722516153
C	5.842652960290	0.117266508769	0.214755743500
TV	4.799992919504	-0.810840097980	-0.000000000000
TV	-0.000000000000	4.863595011779	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.203372910255 hartree
Spin(**2) = 0.066406250000
Geometry of 2D-min92

C	0.864655751395	2.553924766371	-0.713525146529

C	-0.277691348132	-0.296590897563	-1.710928817370
C	1.535153352112	1.503198788134	-1.410520239453
C	-2.395430250588	-1.647265061912	-1.710627884844
C	0.375833412780	4.583469246627	0.391172546062
C	-0.768121920162	3.854550140671	0.392836115689
C	1.433029038901	3.837434776474	-0.276013050324
C	-0.538984189383	2.581509918598	-0.275450480752
TV	3.164929945602	2.014996446376	-0.000000000000
TV	-0.000000000000	7.100414418073	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.202034022730 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min93

C	-2.027379121001	0.369699706111	1.447087932859
C	-1.277650180686	-0.368194370163	0.037118581369
C	0.940707558434	2.296050405831	0.138052958817
C	-0.433977757951	-1.541821383828	0.129838880249
C	4.646875489960	1.110002760433	0.122727804212
C	3.172405506828	-0.355979299002	0.122976121291
C	3.159157916503	1.115109140628	0.037626100283
C	2.315523632558	-1.557200033212	0.130354685369
TV	5.937719663675	0.007159487922	0.000000000000
TV	-0.000000000000	3.845930915402	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.201117164253 hartree
Spin(**2) = 0.750000000000
Geometry of 2D-min94

C	0.048123385801	0.603780682011	-0.509359584925
C	-0.433188073994	-0.782593112004	-0.612487081773
C	1.243869051290	1.361718841403	-0.511369096450
C	-1.402913700552	-3.851875563880	-0.848459323760
C	-0.362668416026	5.924139309682	-0.849691965251
C	0.952024193165	2.770772926199	-0.355400593270
C	0.354185154079	7.126639386212	-0.778113026550
C	-1.107173399324	1.500333366819	-0.353509283895
TV	3.144650877941	2.062945488077	-0.000000000001
TV	-0.000000000000	9.096938972631	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.200759078999 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min95

C	0.597479579474	0.982923053672	-1.413147526281
C	0.605550453879	-0.319687672907	-1.457778462663
C	0.589306143750	2.285378885690	-1.457149575565
C	0.599126632663	-1.561269382219	-0.836859013343
C	2.282353140123	0.350117996231	1.306522329739
C	1.415980242320	-0.622593148298	1.350351156796
C	3.149039434345	1.322706244609	1.352134131365
C	0.601876111909	-1.561078290925	0.730784950140
TV	3.359612850978	-1.265889147817	0.000000000000
TV	-0.000000000000	5.088661347704	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.195220113102 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min96

C	-1.083497667595	-0.765392252902	0.552883890813
C	0.054435768557	-1.171415753119	-0.158246355233

C -0.591561575847 -0.205697899990 1.879296422532
C -2.399172016206 -0.863667469646 0.126876372930
C 3.242342859185 -0.124051796398 2.651161098038
C 1.238333381022 -0.935759989303 0.553969061039
C 1.978398923877 -0.033193572434 2.651993608377
C 5.759899266189 -0.670312622330 1.879863265585
TV 4.925688481845 -0.358889827925 -0.000000000000
TV 0.000000000000 3.683736023179 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.190603407829 hartree
Spin(**2) = 2.000000000000
Geometry of 2D-min97
C -0.394538234106 -0.333583288041 1.225906359429
C 0.424531665765 -1.569412818472 0.720392234622
C 0.313109647095 0.974812531906 1.219750723997
C -1.567646030909 -0.911671443552 1.899435951708
C 4.647399381232 4.854156463653 -0.760336769207
C 0.565032311122 -3.737176001486 2.019596280027
C 2.221787008944 1.896992378072 -0.299797673620
C 3.321155169984 -0.262811788581 -0.233257565840
TV 2.459446673708 -1.525530125545 -0.000000000000
TV -0.000000000000 5.762637231693 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.190062641767 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min98
C 0.851418482768 0.945827497286 -0.591362384880
C 0.427899823117 -0.350464113501 -0.276730072474
C 2.349632222722 0.502946889483 -0.561420700028
C -1.280069722114 -2.439727761695 -0.092574092002
C -0.450394831656 4.724670566585 -0.929313204586
C -0.126282447701 3.367498781303 -0.995595480109
C -0.506036695080 5.891592609173 -1.696581146282
C 0.261326235968 2.189031409390 -0.846435077980
TV 3.145466045540 1.601132196726 -0.000000000000
TV 0.000000000000 8.061814837966 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.188935246507 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min99
C -0.525186236964 0.310468604430 -0.662167909889
C -0.324440014989 -0.993763202395 -0.662328187067
C 2.067715518664 2.520906277581 -0.661915140138
C -0.103203056020 -2.204249051874 0.110598535575
C -0.267834141213 3.791948045010 -0.662029308529
C 0.705745958621 2.619137365360 -0.661951643428
C -0.103323225183 5.066055248409 -1.435291398060
C -0.428278881538 1.653157347358 -0.661972726947
TV 3.477026818162 -0.254016836900 -0.000000000000
TV 0.000000000000 7.270420526592 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.183476688095 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min100
C -1.955542423458 1.587701547089 -1.031187690061
C 2.508805257369 -3.810466894243 1.744638841314
C -0.552617014544 1.356241675210 -0.207242195772

C	-1.527954483911	0.764905145073	0.920250645120
C	3.232175968670	0.760707730496	0.524318636176
C	0.841962344803	-0.688498356720	0.188908025241
C	1.898215332734	1.391902922523	0.887958536494
C	4.492029545445	-1.088197889101	-0.174771521580
TV	3.592656816159	-1.874267583641	-0.000000000000
TV	0.000000000000	4.052128993773	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.177904500824 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min101

C	-0.587589563701	-0.231286445790	-0.294684980848
C	0.163521994473	-1.455419210982	-0.373270303071
C	0.168640664225	1.173682478200	-0.175279171039
C	-1.997486524543	-0.041845806909	-0.150662235801
C	2.206310316768	0.346549508566	0.247209385826
C	1.619925985831	-1.659420259437	-0.541579973412
C	1.539977378842	1.251431898192	-0.696928029659
C	5.938675635369	-0.056229988452	1.024342770971
TV	4.754465059820	-0.886901956986	0.000000000000
TV	0.000000000000	4.341994702457	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.176331777453 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min102

C	0.013338588254	-0.034570332503	1.037814371221
C	-0.310463872642	-1.479914790871	0.821629782816
C	0.649215439361	1.054820937407	0.307131694443
C	-1.668814539749	-1.512675605432	0.279168107736
C	4.636000055128	1.456148646229	0.081130219266
C	2.032073280468	1.242200304530	0.082526201906
C	3.273422658045	1.359709015226	-0.003058492575
C	-0.262969298328	-2.618342658051	1.963571243561
TV	7.534303921631	-0.594753528117	0.000000000000
TV	-0.000000000000	3.588250714737	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.174954744146 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min103

C	-0.297826058478	-0.157635598294	0.682046298466
C	0.573698809992	-0.924146822236	-0.037047200360
C	-0.319772709098	1.229938435906	0.461098542903
C	-2.463369001641	-1.760116740611	0.623756686874
C	3.483526086683	1.572904152242	-0.182763536350
C	1.735634623625	-0.065571434090	-0.091049329549
C	1.891554420088	1.444208434772	-0.214323540567
C	4.028763410670	0.356309214342	-1.017563044549
TV	3.251656970208	-1.813434127741	-0.000000000000
TV	-0.000000000000	5.767729375881	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.173341155546 hartree
Spin(**2) = 0.058593750000
Geometry of 2D-min104

C	-0.127914321794	1.077293595434	0.071136430486
C	0.246597057817	-0.318010307096	-0.387075613699
C	0.042057272768	0.443300808105	1.261007576104
C	-2.128835149556	-1.672220870069	-0.618086909485

C	-1.132410973142	4.841321620115	-0.786541877301
C	-0.774434515467	3.494023422331	-0.775852795898
C	-0.761137513013	6.201145731054	-0.618721328801
C	-0.459516227849	2.321216701106	-0.484221429285
TV	3.742779130604	0.993574592842	0.000000000000
TV	-0.000000000000	7.510934903629	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.173051644500 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min105

C	-0.740023452230	1.785143034431	0.474169546269
C	-0.888103725187	0.281963447684	0.570757310807
C	0.745623929474	1.877293028604	0.037269670980
C	-1.607164955601	-0.862685536957	-0.102032342953
C	0.889654701678	5.728797532451	-0.724435044326
C	-0.047772118375	-0.473671237019	-0.250884013315
C	1.230262647914	4.424227623882	-1.023978995305
C	-1.818497170102	2.689210438696	0.318303929042
TV	3.918360857192	-0.206550184851	0.000000000000
TV	-0.000000000000	4.979932222649	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.172877893774 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min106

C	0.620684976823	0.128089815392	-0.903293760389
C	0.565731644344	-1.259242559733	-0.714369602882
C	1.767575445802	1.129821716667	-1.069919189237
C	-0.833281879137	2.367059596279	-0.139565377590
C	0.092191223745	3.231937410878	-0.790017087779
C	0.665942198281	2.138139468331	-1.589259308323
C	0.398982504257	4.588630495730	-0.613543979722
C	-0.312647319235	1.055227164290	-1.464628488982
TV	3.458282139059	-0.355495202201	0.000000000000
TV	0.000000000000	7.082347596492	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.168421084739 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min107

C	0.470902640732	0.544829593266	0.728490326904
C	-0.617829489201	-0.485780623844	0.680599413447
C	-0.618674582466	1.571542108439	0.664887421675
C	-1.614937306612	0.538906479719	0.523833026962
C	2.984288754747	-0.086529993632	-1.473923782663
C	1.785367568137	0.507272992372	0.538848212556
C	2.973573392398	0.292825202207	-0.062735526595
C	2.996087557756	-1.161148523909	-2.215138188696
TV	5.947977331532	-3.633416178600	0.000000000000
TV	0.000000000000	3.439573269725	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.166548523767 hartree
Spin(**2) = 0.312500000000
Geometry of 2D-min108

C	0.880058463895	0.516322963488	0.174210803872
C	-0.584574162927	-0.967539948933	-1.092428224648
C	0.590499585304	1.772775639913	0.620382840247
C	-0.815863041934	-2.066747046476	-0.119623276292
C	3.726022971778	1.808010830418	-0.087077252935

C	2.209246079905	-0.018513780171	0.699059067685
C	2.760876867914	1.400323805211	1.106087942082
C	1.791687350446	-1.412182936703	1.198776835887
TV	4.321822989761	1.650717716888	0.000000000000
TV	0.000000000000	3.824157648321	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.163530891119 hartree
Spin(**2) = 0.000000999999
Geometry of 2D-min109

C	0.308239314197	0.617560059264	-1.147424618170
C	-0.849958701761	-0.398259759960	-1.147738926960
C	1.198516221330	-0.404519707637	-0.331733533267
C	-2.123364557447	-0.390141210948	-1.963552236851
C	0.361379007373	4.600275333054	-1.148390032817
C	0.343867911771	3.307356980433	-1.147575739330
C	0.301119242235	5.997233769139	-1.148315674097
C	0.367282619834	2.014573568208	-1.147099618714
TV	3.321819619242	-0.013664724720	-0.000000000000
TV	0.000000000000	7.418222681386	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.162516720476 hartree
Spin(**2) = 0.140625000000
Geometry of 2D-min110

C	-2.431070681225	3.134266308699	-1.182397113795
C	3.160464355985	-4.537492876723	1.895274107252
C	-0.553285511161	1.382892544345	0.515966878553
C	-1.852204944579	0.708671249163	0.324881091533
C	3.290664182299	0.634662715126	0.546411264648
C	0.761565836531	-0.824238452916	0.389464408134
C	2.015428210071	1.382898077659	0.168126259540
C	4.545513079178	-1.607363685022	0.195146381077
TV	3.829560671128	-2.245777362874	0.000000000000
TV	0.000000000000	4.388663811075	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.161623161060 hartree
Spin(**2) = 0.066405687500
Geometry of 2D-min111

C	0.557259467858	-0.225808220701	-0.758514636655
C	-0.052700025470	-1.480358850026	-0.250249334514
C	-0.350226506500	0.814477721891	-0.859678354218
C	-1.620929787443	-0.018563199531	0.853837619601
C	3.622781691045	0.857696401123	1.328000023261
C	1.989999907952	-0.008194047338	-0.257733652067
C	2.491706349955	1.288662338506	0.420213890628
C	3.247814735156	-0.560996280349	1.768219451207
TV	3.895738015836	-0.958681579570	0.000000000000
TV	-0.000000000000	3.628843088297	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.158098571712 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min112

C	0.839476094602	0.147911934024	0.495032650606
C	-0.385367947807	-0.251244262679	0.922228621416
C	1.712155220414	1.376026274337	0.674439791716
C	-1.611478411876	-0.626001361363	0.894056690607
C	3.193060231743	1.105512624151	0.520273293640
C	1.615295371578	-0.408808784296	-0.595743089021

C	2.514364153961	0.865459713808	-0.810596316697
C	1.779275304873	-1.782598390801	-0.587843040661
TV	6.043152779646	-1.873092437270	-0.000000000000
TV	0.000000000000	3.965976185232	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.154453848878 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min113

C	0.141519099312	0.297534151429	0.318106328812
C	0.142180629179	-0.521607401855	-0.938128376371
C	1.243923193402	1.357785865081	0.256533438830
C	0.141051180808	0.714262799350	-1.536011055687
C	0.139621687599	3.380559844138	-1.109750424509
C	0.139920315110	2.013919751537	-0.612109688782
C	0.141446593885	4.618346989239	-1.185384066065
C	-0.963640728206	1.355298351273	0.256158601232
TV	3.554611903309	0.003878295226	0.000000000000
TV	-0.000000000000	6.523001190701	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.133523243955 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min114

C	0.890106999910	-0.040198996897	0.362510435939
C	-0.142272158753	-1.063553955738	-0.045700550903
C	0.176705115408	1.085098444409	-0.276266900227
C	-0.132120475889	0.066413018329	-1.150031880411
C	3.465831288794	0.839829873424	0.362534048882
C	2.433474424042	-0.183527193799	-0.045677642787
C	2.752505232441	1.965159592316	-0.276269682463
C	2.443702984079	0.946473238155	-1.150047360446
TV	5.151474106636	1.760111086623	-0.000000000000
TV	-0.000000000000	3.577826811061	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.130707952995 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min115

C	-0.547885448301	1.092978806796	0.374702650991
C	-0.759120920813	-0.237315784507	0.903813402920
C	0.690939455680	0.980939728064	-0.563298669958
C	-0.329736479703	-0.194794921038	-0.563104116575
C	1.051398022174	3.453792471399	-1.477070975342
C	0.246903192426	2.383060764877	-1.061834393103
C	1.902073343161	4.379529899802	-1.458859989344
C	-0.954626485825	2.357116688269	-0.309424730114
TV	3.013836130548	-1.871849787800	-0.000000000000
TV	-0.000000000000	7.237767112715	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.123337511852 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min116

C	-0.447944386502	1.228730542297	0.905172699535
C	-0.715735674009	-0.107695948349	1.122059676207
C	0.756478123318	1.526674255134	-0.021955061046
C	-1.523729756360	-0.905429830262	0.308945869042
C	0.309530626259	5.157513752364	-1.428063159767
C	-0.378144843586	1.904256385792	-1.093380979282
C	1.223470518975	4.583442627101	-0.624291740256

C	-1.459944750510	2.062786547697	0.130682756755
TV	3.525342316604	0.243911129295	0.000000000000
TV	-0.000000000000	4.468671513725	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.112367329028 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min117

C	0.624363103945	-0.463287320254	-0.741608423815
C	0.897887361256	-1.725785145349	-1.586511659577
C	0.551955729992	0.838398461575	-0.741378514522
C	-0.063106983795	-2.653845058082	-0.740571718968
C	0.265491831220	3.419949044466	-0.740400931826
C	0.392497356363	2.161572309990	-0.740851065301
C	2.102118390717	5.421299523199	-0.740479150280
C	-2.724604866453	5.409099907055	0.104505054510
TV	3.622248386425	0.340750081186	0.000000000000
TV	0.000000000000	7.475051183389	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.110808496896 hartree
Spin(**2) = 1.312500000000
Geometry of 2D-min118

C	0.326803778268	0.723164307417	-0.117685417362
C	0.311374336373	-0.673336823539	-0.112546906051
C	1.085908623664	-0.027441339938	-2.674198415447
C	0.191033426301	-1.942829841167	0.332152061954
C	0.154831565363	4.592527101916	0.462347609418
C	0.164500587279	3.265135523119	0.463084307605
C	0.678064037615	7.828720520005	-1.401082500008
C	0.200555997600	1.994168870790	0.327544488797
TV	3.388799790831	1.452321689193	0.000000000000
TV	-0.000000000000	7.807273372153	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.089269984926 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min119

C	0.100156016909	0.636016683725	-0.228354764327
C	0.100177462210	-0.602914001227	-1.125688611003
C	0.100175328120	1.875095537981	-1.125709263515
C	0.100160640443	-1.841974353950	-0.228365701526
C	1.735831242607	0.635345569911	-0.228362106993
C	1.735831433800	-0.603598567353	-1.125718280987
C	1.735827919735	1.874405674004	-1.125694029008
C	1.735815025627	-1.842676716744	-0.228358561272
TV	3.271317914581	-0.000104767692	-0.000000000000
TV	0.000000000000	4.956018242823	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.067428805658 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min120

C	0.697443145126	-1.680146781476	1.009396095004
C	-0.565517427688	-1.228650756775	0.890247087682
C	1.389955169133	1.071393794461	-0.218159526465
C	-1.738698523487	-0.668744324236	0.909494165488
C	4.024626028744	1.079117426122	0.881795500288
C	1.922649009681	2.523300480319	0.138504591908
C	2.820734238192	1.678847590128	1.008230820602
C	1.415537710773	-2.963471521251	1.355774501039

TV	6.947146436433	-2.970718015806	0.000000000000
TV	0.000000000000	4.191641763917	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.027487159149 hartree
Spin(**2) = 0.000000000000
Geometry of 2D-min121

C	0.669587700790	-0.050698647903	-0.567390036457
C	-0.838979396389	0.058180030492	-0.567388222501
C	-0.258818277950	0.738915474970	0.576374603717
C	0.089273123227	-0.731452635010	0.576331416025
C	3.577491771086	0.409178093017	-0.567399550126
C	2.068938253690	0.518067241300	-0.567401025045
C	2.649079834569	1.198760138396	0.576414484479
C	2.997177063129	-0.271603605427	0.576286379003
TV	5.815739542565	0.919712926046	0.000000000000
TV	0.000000000000	2.941527428595	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.016896412926 hartree
Spin(**2) = 0.000000000000

(iii) 1D
Geometry of 1D-min0

C	2.891042989071	0.701818141079	-3.557332854326
C	0.387262348708	0.267467337245	-0.783810798590
C	0.387018232677	0.043712112914	0.646788250093
C	-0.866300652734	-0.292085959162	2.791448988908
C	1.638947029935	0.603093424701	-2.928347984056
C	1.639552118269	0.376061393800	-1.478507642723
C	1.639161608760	-0.064953730528	1.341534396204
C	0.385792713988	-0.390878468077	3.420635038419
TV	2.504591976667	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.350787612999 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min1

C	0.696065406265	1.277849340382	-0.197517829562
C	0.695909299923	-1.024321818143	-1.076326653755
C	0.696102447199	-1.520798291445	0.223743594402
C	-0.614411031468	0.088951908237	1.412064622337
C	2.006540997280	0.967818848688	-0.889573647457
C	2.006429707850	-0.332221621613	-1.386179064328
C	2.006641209303	-1.211237259137	0.915950214730
C	0.696027727364	0.781183260863	1.102562725369
TV	2.620936152757	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.245668827661 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min2

C	0.732257185204	1.340938147373	-0.222283374576
C	0.732329113148	-1.040883450610	-1.147922703322
C	0.732313608343	-1.581584841856	0.243783441354
C	-0.519165162437	0.112413591032	1.471839863226
C	1.983589784802	1.038485037695	-0.909898322687
C	1.983601161926	-0.353263607628	-1.450449438480
C	1.983675208404	-1.279174687674	0.931311594050

C	0.732108108876	0.799940363300	1.169177828394
TV	2.502749085648	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.243958698629 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min3

C	0.070055521701	0.366029145703	-1.692367261759
C	0.069875948129	0.502698243374	-0.225777380314
C	-0.295674096334	-2.841926025277	-0.462129656172
C	0.068383952029	0.727556112339	2.547981868389
C	1.346660826606	0.304834722876	-2.309497218093
C	1.347499652557	0.561172544518	0.461863007685
C	0.987888559283	-2.931094959269	-0.339875894430
C	1.346499607503	0.679032613513	1.929709634017
TV	2.555935378103	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.242730904260 hartree

Spin(**2) = 2.812500000000

Geometry of 1D-min4

C	1.501808094029	1.002566011488	-2.287803747039
C	-0.377912219453	-0.777409588864	0.483541248656
C	-0.377801265770	-1.835752051220	-0.543245581143
C	-0.377812252804	1.231244118940	2.404767858796
C	2.857563502014	1.003142765899	-2.288705696362
C	0.904881799865	-0.281241916661	0.961520518014
C	0.905029751327	-2.277858818931	-0.973338063655
C	0.904942649229	0.784206511156	1.978958200534
TV	2.565599475123	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.242250370314 hartree

Spin(**2) = 2.812500000000

Geometry of 1D-min5

C	0.160366410908	0.395104963947	-2.378918713492
C	0.160383973477	0.531437800355	0.401270275839
C	-0.464410858984	-2.921247740017	-0.188068855944
C	0.160380678622	0.583292807650	1.873377795275
C	1.438588513894	0.428275066694	-1.759387413282
C	1.438620015913	0.502682725085	-0.288245648274
C	0.813967289757	-2.914886943494	-0.307323277890
C	1.438651424640	0.603753695095	2.493509459034
TV	2.556496724004	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.239232590668 hartree

Spin(**2) = 4.812500000000

Geometry of 1D-min6

C	2.899525732260	0.181374039383	-1.481323127134
C	0.562594993007	-0.225555718739	-0.455401982023
C	-2.566533103379	-1.091743235326	1.727062421719
C	-0.229606691941	-0.684844674496	0.701453220257
C	4.160794789080	0.181348938803	-1.481402258429
C	2.012873551905	-0.225600043760	-0.455441986208
C	0.656989893465	-1.091836882951	1.727264304246
C	2.805025690594	-0.684883628082	0.701431335695

TV	4.484762034603	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.232865148379 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min7

C	0.747692308829	0.017707230694	0.362231297585
C	0.747460245448	-1.125127745090	-2.295684304123
C	-1.706967419454	-1.683287024047	-3.596382028095
C	-0.479386382758	0.877579395635	2.349380273011
C	1.974622013330	-0.270343969582	-0.306213646185
C	1.974424366131	-0.833574892099	-1.616727052442
C	4.427341406574	1.443649160532	3.646414355670
C	0.747595338938	0.583604341704	1.671519139497
TV	2.453806078632	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.224610298398 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min8

C	1.203727853780	-0.345696092056	-0.780221070858
C	-0.071953203113	-0.847034279313	-4.045795206581
C	-0.069573081668	-0.023357982039	1.305245752279
C	-1.342763491090	0.296792613670	3.371604839205
C	1.202150231203	-0.536419786395	-2.026342805517
C	1.202255005807	-0.751516455853	-3.425327696568
C	1.204559359446	-0.130126365601	0.615790845717
C	-0.068648572902	0.201557268316	2.756191217284
TV	2.548614710538	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.220903138490 hartree

Spin(**2) = 2.812500000000

Geometry of 1D-min9

C	2.014502455142	0.363690234162	-1.514861844970
C	0.665715178294	0.363871730923	-1.514700015642
C	-3.256737166416	-0.369352860366	1.515965440908
C	0.708586503188	-0.369184059289	1.516155191167
C	4.631029053233	0.363703831968	-1.514901722644
C	3.282248845614	0.363877940430	-1.514710662768
C	-0.640216837357	-0.369350107830	1.515966460277
C	3.325109793041	-0.369188788458	1.516156305673
TV	5.233074008551	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.206679465961 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min10

C	2.967806621789	0.791159912630	-3.697308382301
C	-0.992541980087	0.442568192320	-1.654646109434
C	0.326736007353	0.094617346445	0.416809522257
C	-0.349198937001	-0.453269388562	2.974171352829
C	1.647739324574	0.690055333806	-3.106860061539
C	0.327509090690	0.326883527149	-0.969979122698
C	2.963419930278	-0.112923991372	1.695216041638
C	0.995714125243	-0.195435679886	3.017698886052
TV	2.640202911540	0.000000000000	0.000000000000

TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.200839523234 hartree
Spin(**2) = 0.750000000000
Geometry of 1D-min11
C 0.182397458429 0.752145346653 -0.404459905391
C 1.395022348972 1.106929996001 -1.005208255924
C -2.332272323406 -0.354549627089 1.470991793520
C 1.397444278823 -0.376964174445 1.509403221007
C 2.698203888872 1.083153873010 -0.965364978150
C 4.001157152786 1.105909042917 -1.003302178653
C 0.183726711557 -0.023664301549 0.910062569588
C 4.003537392387 -0.377892623106 1.510664443489
TV 5.032675336679 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.185124086058 hartree
Spin(**2) = 2.000000000000
Geometry of 1D-min12
C 0.941429922627 1.201221460350 -1.111333375043
C -0.316824560072 -1.331928521705 0.270449237723
C -0.317100994599 -2.792355983211 0.049778864408
C -0.316424086386 1.429481724045 1.111241534357
C 2.199073411438 1.294550080469 -1.654335731166
C 0.940886533725 -0.651015296486 0.361399261747
C 0.940506158807 -3.415518574005 -0.035726512106
C 0.941170068593 0.871084049546 0.580939424844
TV 2.515330879387 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.184533561434 hartree
Spin(**2) = 2.000000000000
Geometry of 1D-min13
C 0.928610906378 -0.610202343133 -1.857046128303
C 0.268679196364 1.792536211045 -0.573355528482
C -0.367626803066 0.504101245135 1.829050851818
C 0.361346802215 -1.899327797162 0.543073595098
C 2.239457257742 -0.610181164839 -1.856951531521
C 1.579521398260 1.792680126202 -0.573334698795
C 0.943221120101 0.504073785378 1.829068600520
C 1.672192896881 -1.899268231905 0.542983134406
TV 2.621687565394 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.181246482862 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min14
C 1.038443369110 1.858203220305 -0.248359213547
C 1.041159459873 -0.358039377626 -1.866186096205
C 1.038718183898 -1.974272283441 0.349391208100
C -0.264474023761 0.241086565106 1.966950212530
C 1.047217043800 0.242076150412 1.966536164249
C 2.352848257228 -0.356809659784 -1.866104365233
C 2.350396890311 -1.974126493815 0.350276696261
C -0.273228700271 1.857904505113 -0.249642055089
TV 2.623367432226 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000

TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.180840072268 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min15

C	0.871132850028	1.653253161140	2.905759443448
C	0.871057921488	-0.678838000255	-1.633354267087
C	0.871187628068	-0.508250490509	-0.225405971967
C	-2.822535241048	-0.250774779508	1.921390583560
C	4.564680934213	-0.955135457858	-3.762642837956
C	2.102274160372	-0.779431638565	-2.366944337545
C	2.102450000271	-0.406527576919	0.512001721667
C	-0.360098938344	0.992431542024	2.631929094826
TV	2.462516195205	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.173015997672 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min16

C	0.391396751783	-0.214581510452	-1.489682295363
C	-0.356513235432	-0.777450005448	1.168203642083
C	-0.262249152198	-2.927783543508	-1.603880188199
C	-0.373602946776	1.962600044578	1.314899176590
C	1.703522204430	-0.214628528059	-1.489905676281
C	0.955594442179	-0.777458055246	1.168055740899
C	1.049886001916	-2.927662573792	-1.603895580642
C	0.938572829256	1.962552986791	1.314822129884
TV	2.624266931608	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.172666034015 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min17

C	1.253667705717	2.592780571816	-0.910794309517
C	0.378559320455	-0.987411249491	-0.990879170575
C	0.259153146251	-2.824702892814	1.043132384175
C	-0.301893531170	0.739888161178	1.100126515841
C	2.565931855924	2.592730897726	-0.910817241139
C	1.690812201295	-0.987899494275	-0.990669152367
C	1.571463473946	-2.824567745756	1.043067165845
C	1.010371873058	0.739884354024	1.100378251873
TV	2.624546641243	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.172645674899 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min18

C	0.734744221165	0.901239477887	-0.859519313526
C	0.703990355184	-1.223075875505	-2.596678894881
C	0.561538794237	-1.157758303158	0.938836988024
C	-0.715158488103	1.002956563775	2.626461107067
C	2.047337152537	0.901011975264	-0.858494661314
C	2.016673525978	-1.223312750231	-2.596626214512
C	1.874197177652	-1.158406613386	0.937066183927
C	0.597536309321	1.001725308497	2.626003308482
TV	2.625254368597	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.172538624165 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min19
C 1.073290245835 1.192692380957 -0.400801948956
C 0.291250802696 -1.225422989291 -2.611194552707
C 0.787910302774 -1.325566777374 0.658263264203
C -1.029998092714 0.854835955770 2.318668299683
C 2.388090169613 1.216137789811 -0.391521838289
C 1.683132742029 -1.224946067187 -2.611503078683
C 2.100877770475 -1.334597540849 0.680612664232
C 0.274757716950 0.857956391167 2.318333839462
TV 2.627457383660 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.172134492029 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min20
C 1.152811984108 -0.599319454522 -2.701777277562
C -0.017913920082 1.310598285706 -0.054200454593
C 1.224080613841 0.469441489335 2.576074357885
C -0.709001204335 -1.361691645102 0.540936684356
C 2.388476845363 -0.598841758771 -2.701456278595
C 1.292921336004 1.317959107753 -0.045960628796
C 2.527755951497 0.465416355258 2.577150608977
C 0.605180075954 -1.353902634072 0.525564047566
TV 2.627879843477 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.172112148450 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min21
C 1.682822518705 2.673246889256 0.366184580120
C 0.372927938480 -0.278077700711 -1.421657002044
C 1.679372838298 -2.556755696425 0.061158451636
C -0.938280191380 -0.158324018222 1.357713319588
C 0.369087072979 0.053572294850 1.348948858171
C 1.680327676784 -0.284671472838 -1.418752583689
C 2.986760351967 -2.649742343739 -0.042853246947
C 0.375591012533 2.527210289497 0.429405696628
TV 2.614783956253 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.171536397047 hartree
Spin(**2) = 0.312500000000
Geometry of 1D-min22
C 2.797631542086 0.939777649894 -2.833493241772
C 0.206828897941 -1.070923955049 -0.942653961454
C 0.183222759450 1.032944516031 0.852213808295
C 0.227938089203 -1.002405590825 2.722298182379
C 1.539779496106 0.939496938667 -2.833181103257
C 1.493778876175 -1.070563287694 -0.943070984196
C 1.527490858751 1.032953739078 0.851951277556
C 1.485606933601 -1.002340070106 2.722190525764
TV 2.631040962338 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.171229466830 hartree

Spin(**2) = 0.000000000000
Geometry of 1D-min23
C 0.705759238083 -0.877156734125 -3.726513230358
C 0.384125587184 2.306174674685 1.033027946507
C -1.771304004581 0.043929161696 -0.497259002910
C -1.461577180313 -0.132416502479 2.242539339072
C 4.565972087603 -0.877096085505 -3.726647889425
C 1.696490848351 2.305196458223 1.033431182541
C -0.455915680792 0.046640733433 -0.495595920726
C -0.149392969312 -0.134266131139 2.242736946077
TV 2.628084478367 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.170358103996 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min24
C 2.403754295022 0.531318105509 -2.924862671548
C -1.482493356310 1.632217727083 0.657507452478
C -0.178124998489 -0.967394433609 -0.362987577591
C -1.477084939989 -1.594307415755 2.544451642917
C 3.795746166092 0.531445038515 -2.924717924670
C -0.226869887292 1.632259085241 0.657411775095
C 1.101467986970 -0.967234794289 -0.363066068115
C -0.232942124242 -1.594391239369 2.544468330891
TV 2.636395974925 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.166048328941 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min25
C 1.120529897718 -0.518268532226 -1.287547559313
C -0.121210133347 -0.434915244977 -0.682813804028
C -2.664557005542 -0.219031032028 0.884812800871
C 1.120150498955 -0.134357686786 1.501126235760
C 3.631634580077 -0.514349941565 -1.262764955642
C 2.362184493873 -0.435098474376 -0.682840884514
C -0.117406142011 -0.219464588773 0.884988612044
C 3.631207953289 -0.143497302387 1.433958709950
TV 5.022258996992 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.152935661480 hartree
Spin(**2) = 2.000000000000
Geometry of 1D-min26
C 0.580354657881 1.287385246463 -0.289418661559
C 0.854801970859 -1.111954517134 -1.349882601899
C 1.172339833209 -1.718068135386 -0.048261791246
C 0.160773567115 -0.188292945400 1.356310953418
C 1.852567473877 0.965586355609 -0.960963075583
C 2.051115447027 -0.392262180327 -1.537650667513
C 1.369255253875 -0.897807073310 1.101268136943
C 0.378171741287 1.244257487658 1.203687938550
TV 2.467553018319 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.137873994488 hartree
Spin(**2) = 0.000000000000

Geometry of 1D-min27

C	1.024547441574	1.257344882011	-2.095586653232
C	-0.762857371643	-0.549576044265	-2.083090736203
C	1.101540960136	0.082628509425	0.408897535366
C	-0.196517779607	-0.239194450431	2.538927416702
C	1.240387149888	0.310334224975	-1.022881098679
C	0.543962555535	-0.107676229070	-2.488509828847
C	2.410097691582	-0.013120951977	1.080971972219
C	1.110809460090	-0.331447783120	3.134693626499
TV	2.613659675798	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.137533144660 hartree

Spin(**2) = 1.312500000000

Geometry of 1D-min28

C	0.666624422606	1.488740836960	-2.013513957345
C	-1.655336958994	-1.459652373999	0.490462783821
C	-0.938235940528	-2.634641958535	0.125892150248
C	0.434050260208	1.046742573378	1.243982315112
C	1.950230312556	1.488515544478	-2.011355890451
C	3.948378648032	-0.137836513093	0.904502446232
C	0.428165503486	-2.634017531634	0.124238306045
C	1.863878390009	1.041609841549	1.254682706563
TV	2.800280285988	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.133607987859 hartree

Spin(**2) = 0.312500000000

Geometry of 1D-min29

C	2.695715958980	-0.611300837541	-2.641530535274
C	0.104263254903	0.151199641963	0.090179728178
C	1.003977766966	-1.332197138912	0.547812756629
C	-2.276346765199	-0.258546204981	2.865808781439
C	1.403981898686	-0.512444594210	-2.052593837183
C	0.444110031910	-0.404346142701	1.414193647117
C	1.382072178487	-0.246062569387	-0.567690138110
C	-0.979436827661	-0.197508139645	3.458483918680
TV	2.592852185276	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.117984350454 hartree

Spin(**2) = 2.812500000000

Geometry of 1D-min30

C	0.048938920536	-0.258119427390	-1.554227988412
C	0.048940791191	1.066395080820	-1.154242140988
C	0.049068562445	0.264906867786	1.502796988519
C	0.049082897737	-1.059516668570	1.102561435882
C	1.489729433947	-0.509470819779	-1.021776080962
C	1.489710816810	0.981546457600	-0.571482252824
C	1.489841967826	0.516360733802	0.970334496258
C	1.489838594783	-0.974666606843	0.519856475758
TV	2.881537246498	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.112260204796 hartree

Spin(**2) = 0.000000000000

Geometry of 1D-min31

C 0.604007075609 0.000292197549 0.259123700270
C -1.159842251268 0.528986610894 -1.557871364979
C 1.054615654074 -0.390838110118 1.604182461856
C -0.703773896970 0.143033916630 -0.230458742847
C 2.984188816361 -0.063935724662 0.480199843153
C 2.492580479331 0.563834564464 -1.678135913518
C 2.368031515884 -0.425065481069 1.724711105235
C 1.863232057151 0.203170681317 -0.439214682405
TV 4.959934960967 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.083608643834 hartree
Spin(**2) = 0.312499250000
Geometry of 1D-min32
C -0.135124607231 -0.080338482951 0.323207141737
C -0.811765223234 0.232889271671 -0.968060673807
C 3.607140541236 -0.352596635323 1.445456661486
C -2.182980473091 0.232924429945 -0.968073503810
C 2.894943075418 -0.080442756975 0.323312950164
C 2.069651877019 0.189855721311 -0.798028073640
C 4.907526348266 -0.352655977635 1.445648904436
C 0.690157186321 0.189831202626 -0.798121708489
TV 5.754449870098 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.077255938017 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min33
C 0.497499652126 -0.184147007945 -2.166702375324
C 0.497450030733 1.008248551227 -1.231296377716
C -0.533504568127 0.962172838710 2.407459844449
C -0.433987254797 -1.651031130878 1.045268396920
C 1.878593257067 -0.193153691871 -2.157624672704
C 1.878678257541 1.000641150766 -1.221471745822
C 0.943938977356 0.962196449428 2.407498739046
C 0.850772073557 -1.651268372448 1.045283702174
TV 2.761891836041 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.073377416088 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min34
C 1.104887492701 -0.413528119593 -3.297444289058
C 0.064699370805 0.696807926248 0.005846350164
C 0.180364030767 0.351144271297 3.478613392411
C 0.064712649276 -0.809173540449 0.174940997927
C 2.598508523357 -0.413546205434 -3.297392821449
C 1.447694372422 0.697460956679 0.001874103959
C 1.674013298676 0.351146866569 3.478694143143
C 1.447720585379 -0.810652409710 0.171199182151
TV 2.765897067529 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.070419574563 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min35
C 0.413691926892 -1.468410597573 -2.426184329733

C	0.295938105411	2.160434200743	-0.724297492080
C	-0.395529585890	0.059283502779	2.139743251135
C	-0.395693461995	-0.890212566739	0.959871973756
C	1.907700376053	-1.468352243273	-2.426270746640
C	1.789615279335	2.160425286031	-0.724311879758
C	0.987180742466	0.072740168470	2.127794433283
C	0.987076715341	-0.878749105713	0.943682284833
TV	2.765863608602	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.070316419256 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min36

C	0.185678609261	0.821520094097	-4.054247027619
C	0.064250896298	-0.128762220200	-0.845739391604
C	0.064447618160	-0.501448853940	0.626508784061
C	-0.738038640294	-1.277882724655	3.855333177618
C	1.679648941816	0.821525329871	-4.054226921570
C	1.447596141864	-0.126898180911	-0.852472471363
C	1.447597956326	-0.499152500039	0.617604278219
C	0.755903678437	-1.277933086929	3.855455393868
TV	2.765865470295	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.069336315221 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min37

C	-0.981375191357	-0.100884076537	-1.006759595567
C	0.203907372411	-0.239304105843	-0.423319682827
C	-3.752151783490	-0.733829873600	1.716507207684
C	1.319569207998	-0.386567930937	0.210288949269
C	5.277234750712	0.115984594045	-1.930882731420
C	4.815368205471	-0.182402723959	-0.642387416224
C	2.505645722911	-0.519964751020	0.793271826777
C	4.025541634575	-0.432320433359	0.429134405981
TV	7.315584944861	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.068908222536 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min38

C	1.201026917415	-0.409164865346	-3.283387435444
C	-0.062323890481	0.695991880457	-0.006130423568
C	0.401313064811	0.346705867757	3.472317479444
C	-0.062391231012	-0.810427237899	0.158867786144
C	2.580339657023	-0.409156380460	-3.283284815957
C	1.317182717230	0.698660989024	0.010236076554
C	1.889600159267	0.346714926001	3.472280529827
C	1.317132620004	-0.809665433936	0.175431862249
TV	2.758650470461	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.063199511587 hartree
Spin(**2) = 0.750000000000
Geometry of 1D-min39

C	1.437719931215	0.366180433782	-2.400163245443
C	-1.677479266679	1.287953945757	1.859344651152

C -0.275793526200 -0.667015729693 -1.095491069209
C -0.598756047496 -1.413221960474 2.085196824341
C 0.134222952860 -0.411837675518 -2.537210778911
C -0.373151163353 1.255714520149 1.916643498126
C 1.027436439499 0.108171333076 -0.956793838847
C 0.704162569789 -1.455887230463 2.077043080242
TV 2.606962120495 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.062256928595 hartree
Spin(**2) = 0.312500000000
Geometry of 1D-min40
C 0.544681175496 1.885932709240 1.480530813575
C 0.722432042000 -0.732453948619 -1.597825707395
C 0.707137025683 -0.646191039945 -0.078039803805
C -0.543292251270 -0.170075618277 1.879268345788
C 0.746733312430 0.484604363753 2.129603364257
C 2.029968142546 -0.760709822490 -2.174966019716
C 1.999242047354 -0.979679353055 0.633550039604
C 0.232307681831 0.653097472573 0.661203295662
TV 2.621737226984 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.061135817466 hartree
Spin(**2) = 2.000000000000
Geometry of 1D-min41
C 0.438551457086 -0.265839977312 -2.179363319890
C 0.438524860304 1.036221653870 -1.394471045463
C -0.430182328500 0.265381198478 2.180116896483
C -0.430184352268 -1.035779564667 1.393743218405
C 1.887946678787 -0.265834499879 -2.179368710010
C 1.887917668897 1.036244695574 -1.394511916189
C 1.019215447070 0.265382507116 2.180115711386
C 1.019212208496 -1.035776013170 1.393739165259
TV 2.898789726788 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.048768499464 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min42
C 1.024752983902 -0.075459496274 -2.733769117617
C 1.024717050710 0.491587637373 -1.322403480692
C -1.009130726637 0.306488084612 2.065543607653
C -1.009147869477 -1.194172934840 1.822818704397
C 2.474176637159 -0.075476770843 -2.733785535961
C 2.474144007656 0.491538593573 -1.322360873932
C 0.440300919689 0.306508804869 2.065616907665
C 0.440283686527 -1.194155626504 1.822881049602
TV 2.898855787103 0.000000000000 0.000000000000
TV 0.000000000000 20.000000000000 0.000000000000
TV 0.000000000000 0.000000000000 20.000000000000
Energy = -45.048338385567 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min43
C 2.119255712971 1.493139488708 -2.152811072129
C 0.327097180029 -1.188924520775 0.773707801756
C -2.430990786612 -3.506864800780 -0.210439447774

C	-1.804198274833	1.447353239639	0.954048644364
C	3.371705077569	1.493971991672	-2.150678382368
C	2.878251135780	0.119778086432	0.919441893467
C	-1.023312173093	-3.612758257374	-0.256147102832
C	2.198115816766	1.409276620132	1.084947165410
TV	2.683783061699	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.045217818108 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min44

C	1.141409085045	-0.089291191744	-0.026055189104
C	0.024575792770	0.339261707575	-0.836855946565
C	0.024661525591	-0.161882597264	0.888553512671
C	-1.092057439292	-0.089352755819	-0.025939977475
C	4.757595539625	-0.089096953740	-0.026058102978
C	3.641155499372	0.340423956702	-0.837034239000
C	3.641291003722	-0.160927791436	0.889253201559
C	2.524945417835	-0.089134374268	-0.025863259113
TV	7.233195624983	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.043942470135 hartree
Spin(**2) = 1.312500000000
Geometry of 1D-min45

C	1.717985303690	-0.058311615794	-2.697227352965
C	-0.534092192949	1.586063614256	1.910680662052
C	0.777021641421	-0.356863883439	-1.014670974953
C	-1.878360099768	-1.179473991679	1.583309810229
C	1.146284035159	-1.249955191107	-2.171481797121
C	0.862315889098	1.586599215514	1.911164429138
C	2.084821679555	0.166716743885	-1.254392614481
C	-0.494393419563	-1.191703247467	1.642764114458
TV	2.662215926306	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.031346755185 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min46

C	0.050028847026	-0.172127380411	-0.697254342777
C	1.581190332177	1.135318617100	-1.440217068840
C	0.050065242435	0.069616876851	0.906294342510
C	0.050004763585	-1.237697073091	1.649251788574
C	1.581153984726	-0.172076009828	-0.697146109863
C	3.112327743638	1.135350393497	-1.440142851749
C	1.581181768988	0.069561319363	0.906216127143
C	1.581144970757	-1.237698703480	1.649353464324
TV	3.062232743499	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -45.020105766712 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min47

C	0.575290462216	1.842237266073	0.627802388458
C	1.342275705841	1.216747988658	1.677577817118
C	-2.243749095189	-0.487030207735	0.175335166181
C	1.636143624624	0.218354212225	0.596418030365

C	3.099748658669	-1.912748667655	-0.187619710147
C	3.866427234996	-1.288031117710	-1.238029890633
C	0.280536806182	0.416503064293	0.263832892073
C	4.160501468892	-0.288817806317	-0.157549207127
TV	5.048730560828	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -44.983490924777 hartree
Spin(**2) = 0.000000000000
Geometry of 1D-min48

C	-0.026941410595	-0.013917459464	-0.607089237520
C	1.258730098631	0.665918990341	-0.175020107225
C	-2.170017139804	-0.794563997768	0.622220065217
C	1.687170189738	-0.114895941606	1.054337809994
C	2.544548365520	-0.013847034279	-0.607053952345
C	3.830235682204	0.665869384442	-0.174973451484
C	0.401449120933	-0.794650647095	0.622180467798
C	4.258713039021	-0.114886376228	1.054369798562
TV	5.143007614367	0.000000000000	0.000000000000
TV	0.000000000000	20.000000000000	0.000000000000
TV	0.000000000000	0.000000000000	20.000000000000

Energy = -44.945851879637 hartree
Spin(**2) = 0.000000000000

S5. Primitive lattice of 3D-min10, 3D-min12, and 3D-min13

(i) 3D-min10

C	1.250950276601	3.270843977735	2.832280962946
C	1.250825723173	2.511724973444	5.310415652655
C	0.001354814204	4.045870867698	3.102057891869
C	1.250862398251	1.949943009581	3.907906053659
C	0.001333550039	2.424151712098	0.794161598300
C	0.001210527711	2.796934896068	5.945908429379
C	1.250933928561	2.709298298849	1.429740061031
C	0.001267865449	1.174900546518	3.638046518164
TV	2.499224040018	0.000000000000	0.000000000000
TV	0.000030949010	4.115314703300	0.000000000000
TV	-0.000048640214	0.958254132540	6.492354517796

(ii) 3D-min12

C	3.606079713321	0.878697180841	6.094636497566
C	3.606438206722	-0.236048286936	7.248407229588
C	2.345589090485	1.738863241087	6.094755242897
C	2.345346252297	2.853988862186	4.941029283803
C	2.345644352010	2.850649777299	2.009481654887
C	3.605657320068	2.853854030597	4.133030638564
C	3.605914978791	2.851792517737	2.757958312723
C	2.345730174310	2.848828648194	0.634322546979
TV	2.520604640221	0.000000000000	0.000000000000
TV	1.259643447297	3.089747409611	0.000000000000
TV	1.260069396348	0.005258234985	7.422033107613

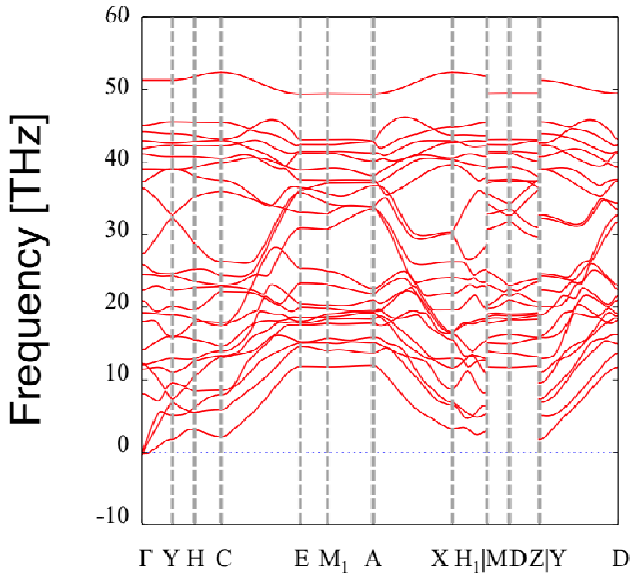
(iii) 3D-min13

C	2.216469437277	2.445974962274	4.952644826501
C	3.470135930818	2.348804909729	5.631818701658
C	2.216912616819	2.621215209839	3.451454307489
C	2.217644108191	1.283280268100	2.586440092207
C	3.470552096590	3.321207530547	2.896200777500
C	2.216999906055	3.603728289169	0.814237851500
C	3.471272259753	1.410665257136	1.679153656691

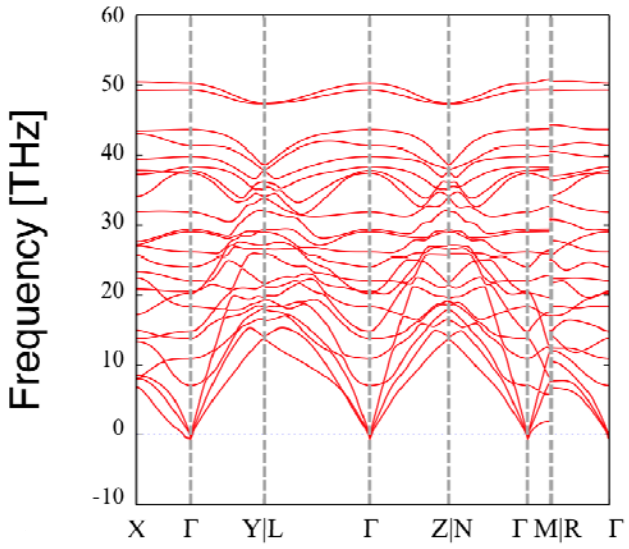
C	3.470818671036	2.903607568159	1.369307102559
TV	2.507324625909	0.000000000000	0.000000000000
TV	1.253188423812	3.530916143473	0.000000000000
TV	2.506440011809	2.100736841762	6.318499246203

S6. Phonon dispersion curve of 3D-min10, 3D-min12, and 3D-min13

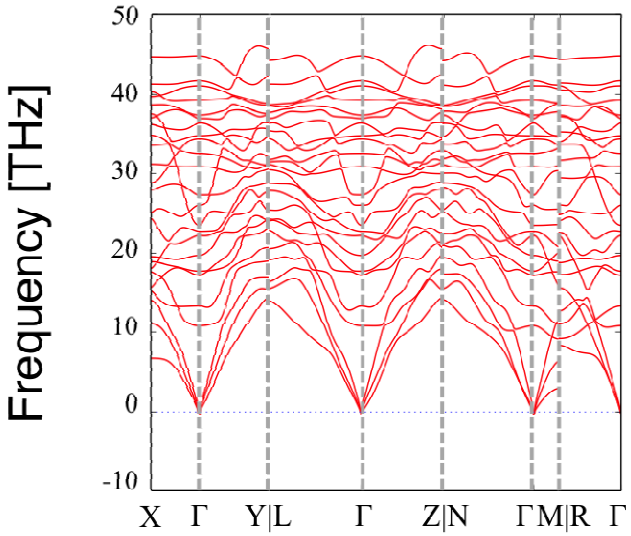
(i) 3D-min10



(ii) 3D-min12



(iii) 3D-min13



S7. Symmetry k-points of 3D-min10, 3D-min12, and 3D-min13

(i) Symmetry k-points of 3D-min10 (*P*2/m). The coordinates of symmetry k-points are given in fractions of the primitive reciprocal lattice vectors b_1, b_2, b_3.

$\times b_1$	$\times b_2$	$\times b_3$	
0.00000000	0.00000000	0.00000000	Γ
0.00000000	0.00000000	0.50000000	Y
0.00000000	0.23113863	0.55672762	H
0.00000000	0.50000000	0.50000000	C
0.50000000	0.50000000	0.50000000	E
0.50000000	0.23113863	0.55672762	M_1
0.50000000	0.50000000	0.00000000	A
0.00000000	0.50000000	0.00000000	X
0.00000000	0.76886137	0.44327238	H_1
0.50000000	0.23113863	0.55672762	M
0.50000000	0.00000000	0.50000000	D
0.50000000	0.00000000	0.00000000	Z
0.00000000	0.00000000	0.50000000	Y
0.50000000	0.00000000	0.50000000	D

(ii) Symmetry k-points of 3D-min12 and 3D-min13 (*P*1). The coordinates of symmetry k-points are given in fractions of the primitive reciprocal lattice vectors b_1, b_2, b_3.

$\times b_1$	$\times b_2$	$\times b_3$	
0.00000000	-0.50000000	0.00000000	X
0.00000000	0.00000000	0.00000000	Γ
0.50000000	0.00000000	0.00000000	Y
0.50000000	-0.50000000	0.00000000	L
0.00000000	0.00000000	0.00000000	Γ
-0.50000000	0.00000000	0.50000000	Z
-0.50000000	-0.50000000	0.50000000	N
0.00000000	0.00000000	0.00000000	Γ
0.00000000	0.00000000	0.50000000	M
0.00000000	-0.50000000	0.50000000	R
0.00000000	0.00000000	0.00000000	Γ