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Professional paper

CALCULATING THE SYMMETRY OF HEXAMETHYLCYCLOHEXANE

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An Euclidean graph associated with a molecule is defined by a weighted graph with adjacency matrix. Balasubramanian (1995) computed the Euclidean graphs and their automorphism groups for benzene, eclipsed and staggered forms of ethane, and eclipsed and staggered forms of ferrocene. It was shown by Balasubramanian that the molecular symmetry groups can be obtained as the automorphism groups of edge-weighted Euclidean graphs. In this paper we calculate the atom centers of hexamethylcyclohexane molecule using the chemistry package HyperChem and then compute its symmetry group.

Key words: symmetry group; hexamethylcyclohexane; automorphism of groups

ПРЕСМЕТУВАЊЕ НА СИМЕТРИЈАТА НА ХЕКСАМЕТИЛЦИКЛОХЕКСАН

Евклидов граф на молекулата е дефиниран преку тежински граф и матрица. Баласубраманиан (Balasubramanian) во 1995 година ги пресметал Евклидовите графови и нивниот групен автоморфизам за бензен, за еклипсната и sвездестата форма на етан и на фероцен. Баласубраманиан покажал дека молекуларната симетрија на групите може да се добие како автоморфизам на групите на гранично тежинските Евклидови графови. Во овој труд ги пресметавме атомските центри на молекулата на хексаметилциклохексанот со помош на софтверскиот пакет HyperChem, а потоа и неговата симетриска група.

Клучни зборови: група на симетрија; хексаметилциклохексан; автоморфизам на групите

INTRODUCTION

The symmetry of a graph through the automorphism group of the graph has been studied in Refs. [1–15]. The symmetry group of a molecule depends on the relative positions of the atoms in a three-dimensional space, that is the actual coordinates of the various centers in the three-dimensional space.

As shown by Randic [6], a graph can be depicted in different ways such that its point group symmetry or three dimensional preception may differ, but the underlying connectivity symmetry is still the same as characterized by the automorphism group of the graph which by definition comprises permutations of the vertices of the graph that leave the adjacency matrix invariant. However, the molecular symmetry depends on the coordinates of the various nuclei which relate directly to their three dimensional geometry.

By symmetry we mean the automorphism group symmetry of a graph. The symmetry of a graph, also called a topological symmetry, accounts only for the bond relations between atoms, and does not fully determine molecular geometry. The symmetry of a graph does not need to be the same as (i.e. isomorphic to) the molecular point group symmetry. However, it does represent the maximal symmetry which the geometrical realization of a given topological structure may posses.

In this paper, we investigate the automorphism group of weighted graphs. By definition, a

weighted graph is a graph whose edges and vertices are weighted with different weights. The adjacency matrix of a weighted graph is defined as: $A_{ij} = w_{ij}$, if $i \neq j$ and vertices i and j are connected by an edge with weight w_{ij}; $A_{ij} = v_i$, if $i = j$ and weight of the vertex i is v_i, and, $A_{ij} = 0$, otherwise. Note that v_i can be taken as zero if all the nuclei are equivalent. Otherwise, one may introduce different weights for nuclei in different equivalence classes and the same weight for the nuclei in the same equivalence classes.

Graph theory provides an elegant and natural representation of molecular symmetry and the resulting group expressed in terms of permutations is isomorphic to the permutation-inversion group of Longuet-Higgins. We apply our method to the hexamethylcyclohexane. Throughout this paper, all groups considered are assumed to be finite. Our notation is standard and taken mainly from Refs. [16–18].

RESULT AND DISCUSSION

In Ref. [19–21], the authors computed the non-rigid and symmetry group of some molecules. So it is natural to ask about automorphism group of the Euclidean graph of such molecules. The aim of this section is solving this problem.

Symmetry operations on a graph are called graph automorphisms. They affect only the labels of vertices by permuting them so that the adjacency matrix of the graph remains unchanged. The graph symmetry is completely determined by all the automorphisms it has, i.e. by specifying all the permutations which leave the adjacency matrix intact.

The automorphism group of a graph depends only on the connectivity of the graph and does not depend on how the graph is represented in three dimensions. That is, a graph, in general, can be represented in different ways in three dimensions such that two representations could yield different three-dimensional symmetries and yet their automorphism groups are the same since the latter depends only on which vertices are connected in the graph.

A permutation of the vertices of the Euclidean graph under consideration belongs to the permutation representation of an operation in the point group if and only if the corresponding permutation matrix P satisfies $P^tDP = D$, where P^t is the transpose of permutation matrix P and D is the adjacency matrix of the graph. All such permutations of the nuclei which preserve the connectivity of the Euclidean graph of the molecule form a group which we call the Euclidean distance group. Consider the hexamethylcyclohexane molecule to illustrate its automorphism group.

It suffices to measure the Euclidean distances and then constructs the Euclidean distance matrix D. It should be mentioned that one does not have to work with exact Euclidean distances in that a mapping of weights into a set of integers would suffice as long as different weights are identified with different integers. In fact the automorphism group of the integer-weighted graph (Figures 1–2), is identical to the automorphism group of the original Euclidean graph. The resulting atoms centers and distance matrices are shown in Tables 1–3. We continue Balasubramanian's result to compute the automorphism group of the Euclidean graph of hexamethylcyclohexane molecule.

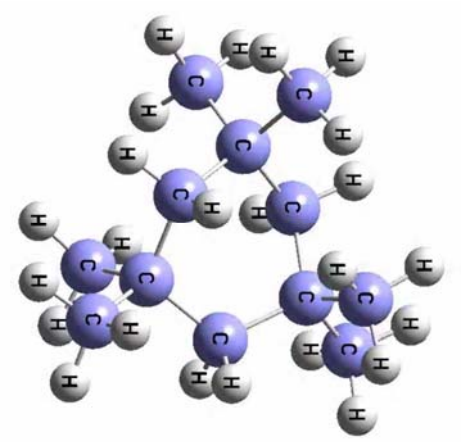

Fig. 1. 3D structure of hexamethylcyclohexane

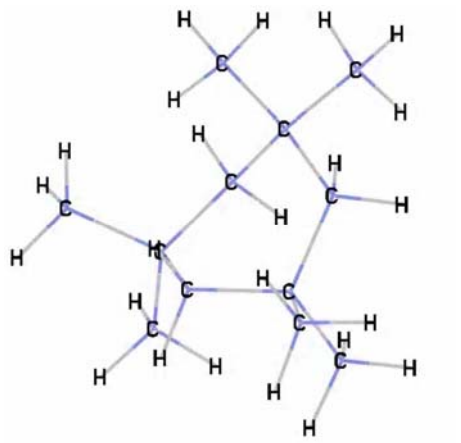

Fig. 2. The molecular graph of hexamethylcyclohexane

Suppose G is the set of all permutations which preserves the Euclidean connectivity. It is useful to mention that our calculations were done by a MATLAB program. Using such a program, we can recalculate all the examples of Balasubramanian [7].

For the sake of completeness we write below our MATLAB-program for computing the automorphism group of the Euclidean graph of the mentioned molecule.

A MATLAB Program for Computing the Symmetries of Molecules

```
n=length(a);
  for i=1:n-1
       for j=i+1:n
            b(i,j)=norm(a(i,:)-a(j,:));
       end
  end
b(n,n)=0;
b=b+b';
  function y=halat(s,a)
       t=1:length(a);
       m=length(s);
       t(s)=[];
       j=0;
            for i=t
                 if min(min(a(1:m+1,1:m+1)==a([s,i],[s,i])))==1
                      j=j+1;
                      y(j)=i;
                 end
            end
  function s=hazf(s)
       m=size(s);
            for i=m(1):-1:1
                 if min(s(i,:))==0
                 s(i,:)=[];
            end
  end
  function s=jaigasht(a)
       m=length(a);
            for i=1:m
                 s(i,1)=i;
            end
            for j=2:m
                 n=size(s);
                 k=0;
                      for i=1:n(1)
                           y=[halat(s(i,:),a)];
                                for r=1:length(y)
                                    b(r+k,1:n(2)+1)=[s(i,:),y(r)];
                                end
                           k=k+length(y);
                      end
                 s=b; s=hazf(s);
          end
b=0;
n=size(s);
  for i=1:n(1)
       for j=1:n(2)
```

```
                b(i,s(i,j))=j;
            end
        end
    s=b;
```

Table 1

Band order of hexamethylcyclohexane

H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}
H_7-H_6	1.764221	H_{14}-H_6	3.647971	H_{17}-H_6	5.901676	H_{21}-H_6	3.732236
H_8-H_6	1.767165	H_{14}-H_7	2.177500	H_{17}-H_7	4.587409	H_{21}-H_7	4.349868
H_8-H_7	1.765666	H_{14}-H_8	3.714603	H_{17}-H_8	4.851174	H_{21}-H_8	3.716691
H_9-H_6	5.035104	H_{14}-H_9	5.364456	H_{17}-H_9	6.250501	H_{21}-H_9	2.632028
H_9-H_7	5.474546	H_{14}-H_{10}	5.068589	H_{17}-H_{10}	6.240946	H_{21}-H_{10}	1.765738
H_9-H_8	5.622249	H_{15}-H_6	5.298823	H_{18}-H_6	6.550160	H_{22}-H_6	5.057166
H_{10}-H_6	2.477817	H_{15}-H_7	3.731586	H_{18}-H_7	5.233968	H_{22}-H_7	5.099642
H_{10}-H_7	3.717171	H_{15}-H_8	5.011860	H_{18}-H_8	5.913647	H_{22}-H_8	5.072215
H_{10}-H_8	2.956054	H_{15}-H_9	6.159501	H_{18}-H_9	5.966285	H_{22}-H_9	1.767193
H_{10}-H_9	3.598579	H_{15}-H_{10}	6.431746	H_{17}-H_{10}	6.859707	H_{22}-H_{10}	3.712259
H_{11}-H_6	3.123014	H_{16}-H_6	4.317072	H_{19}-H_6	6.215215	H_{23}-H_6	6.109570
H_{11}-H_7	3.731554	H_{16}-H_7	2.627126	H_{19}-H_7	5.245429	H_{23}-H_7	6.068017
H_{11}-H_8	2.476730	H_{16}-H_8	3.598926	H_{19}-H_8	5.431505	H_{23}-H_8	6.434041
H_{11}-H_9	4.321395	H_{16}-H_9	6.309920	H_{19}-H_9	5.116424	H_{23}-H_9	1.766897
H_{11}-H_{10}	1.767068	H_{16}-H_{10}	5.620800	H_{19}-H_{10}	5.940464	H_{23}-H_{10}	5.010852

Table 1 (continued)

H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}
H_{25}-H_6	5.010840	H_{29}-H_6	5.829742	H_{33}-H_6	4.277047	H_{14}-H_{11}	5.056017
H_{25}-H_7	4.678840	H_{29}-H_7	5.095482	H_{33}-H_7	3.856473	H_{14}-H_{12}	1.089308
H_{25}-H_8	5.938907	H_{29}-H_8	5.755198	H_{33}-H_8	3.578790	H_{14}-H_{13}	3.470413
H_{25}-H_9	3.778965	H_{29}-H_9	3.592639	H_{33}-H_9	3.721507	H_{15}-H_{11}	6.109319
H_{25}-H_{10}	5.433897	H_{29}-H_{10}	5.540054	H_{33}-H_{10}	3.596198	H_{15}-H_{12}	1.093247
H_{26}-H_6	5.174617	H_{30}-H_6	5.354183	H_{35}-H_6	2.662182	H_{15}-H_{13}	2.665538
H_{26}-H_7	5.382393	H_{30}-H_7	4.397526	H_{35}-H_7	2.414090	H_{15}-H_{14}	1.758695
H_{26}-H_8	6.240025	H_{30}-H_8	5.548063	H_{35}-H_8	3.596112	H_{16}-H_{11}	5.036299
H_{26}-H_9	2.561172	H_{30}-H_9	4.265377	H_{35}-H_9	3.727987	H_{16}-H_{12}	1.092861
H_{26}-H_{10}	4.853814	H_{30}-H_{10}	5.759434	H_{35}-H_{10}	3.579472	H_{16}-H_{13}	2.785539
H_{27}-H_6	6.144073	H_{32}-H_6	3.655125	H_{36}-H_6	2.792029	H_{16}-H_{14}	1.767224
H_{27}-H_7	5.878966	H_{32}-H_7	2.791163	H_{36}-H_7	3.456631	H_{16}-H_{15}	1.766718
H_{27}-H_8	6.859507	H_{32}-H_8	2.454249	H_{36}-H_8	3.906521	H_{17}-H_{11}	5.176408
H_{27}-H_9	3.172165	H_{32}-H_9	5.085068	H_{36}-H_9	2.524315	H_{17}-H_{12}	2.720043
H_{27}-H_{10}	5.914462	H_{32}-H_{10}	3.907012	H_{36}-H_{10}	2.454737	H_{17}-H_{13}	1.093298

Table 1 (continued)

H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}
H_{17}-H_{14}	3.763414	H_{21}-H_{14}	5.095625	H_{25}-H_{14}	3.492831	H_{29}-H_{14}	3.797695
H_{17}-H_{15}	2.958288	H_{21}-H_{15}	6.065644	H_{25}-H_{15}	4.228817	H_{29}-H_{15}	3.500200
H_{18}-H_{11}	6.144472	H_{22}-H_{11}	3.650567	H_{26}-H_{11}	5.904664	H_{30}-H_{11}	5.831867
H_{18}-H_{12}	2.749025	H_{22}-H_{12}	4.736615	H_{26}-H_{12}	5.284690	H_{30}-H_{12}	2.520075
H_{18}-H_{13}	1.093202	H_{22}-H_{13}	3.988945	H_{26}-H_{13}	6.001169	H_{30}-H_{13}	3.021635
H_{18}-H_{14}	3.726572	H_{22}-H_{14}	4.885055	H_{26}-H_{14}	4.754384	H_{30}-H_{14}	2.625294
H_{18}-H_{15}	2.461439	H_{22}-H_{15}	5.356194	H_{26}-H_{15}	5.638391	H_{30}-H_{15}	2.419417
H_{19}-H_{11}	5.011099	H_{23}-H_{11}	5.301465	H_{27}-H_{11}	6.551264	H_{32}-H_{11}	2.792519
H_{19}-H_{12}	3.466063	H_{23}-H_{12}	5.294181	H_{27}-H_{12}	4.898712	H_{32}-H_{12}	2.773831

H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}
H_{19}-H_{13}	1.092623	H_{23}-H_{13}	4.661949	H_{27}-H_{13}	5.201393	H_{32}-H_{13}	2.731159
H_{19}-H_{14}	4.345396	H_{23}-H_{14}	5.352239	H_{27}-H_{14}	4.647404	H_{32}-H_{14}	3.241333
H_{19}-H_{15}	3.696653	H_{23}-H_{15}	5.638564	H_{27}-H_{15}	4.961856	H_{32}-H_{15}	3.735642
H_{21}-H_{11}	1.764482	H_{25}-H_{11}	6.215668	H_{29}-H_{11}	5.344224	H_{33}-H_{11}	2.662130
H_{21}-H_{12}	5.145360	H_{25}-H_{12}	4.081344	H_{29}-H_{12}	3.387705	H_{33}-H_{12}	3.485685
H_{21}-H_{13}	4.961626	H_{25}-H_{13}	5.228954	H_{29}-H_{13}	2.506697	H_{33}-H_{13}	2.636201

T a b l e 1 (continued)

H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}
H_{33}-H_{14}	3.914813	H_{19}-H_{16}	3.778705	H_{23}-H_{18}	4.971436	H_{27}-H_{18}	5.164900
H_{33}-H_{15}	4.293286	H_{19}-H_{17}	1.769269	H_{23}-H_{19}	4.245020	H_{27}-H_{19}	5.265984
H_{35}-H_{11}	4.276914	H_{19}-H_{18}	1.768058	H_{23}-H_{20}	1.093258	H_{27}-H_{20}	2.748662
H_{35}-H_{12}	3.016551	H_{21}-H_{16}	5.474021	H_{25}-H_{16}	5.102432	H_{29}-H_{16}	4.267066
H_{35}-H_{13}	4.599021	H_{21}-H_{17}	5.385038	H_{25}-H_{17}	6.086932	H_{29}-H_{17}	3.585083
H_{35}-H_{14}	2.228215	H_{21}-H_{18}	5.879399	H_{25}-H_{18}	5.259475	H_{29}-H_{18}	2.598830
H_{35}-H_{15}	3.735811	H_{21}-H_{19}	4.681235	H_{25}-H_{19}	5.604862	H_{29}-H_{19}	2.405130
H_{36}-H_{11}	3.655505	H_{21}-H_{20}	2.736545	H_{25}-H_{20}	3.466077	H_{29}-H_{20}	2.517085
H_{36}-H_{12}	4.450061	H_{22}-H_{16}	5.371411	H_{26}-H_{16}	6.240668	H_{30}-H_{16}	3.595127
H_{36}-H_{13}	5.409476	H_{22}-H_{17}	4.769105	H_{26}-H_{17}	6.903072	H_{30}-H_{17}	3.946563
H_{36}-H_{14}	3.858785	H_{22}-H_{18}	4.658159	H_{26}-H_{18}	6.222329	H_{30}-H_{18}	2.874348
H_{36}-H_{15}	5.241903	H_{22}-H_{19}	3.508998	H_{26}-H_{19}	6.093969	H_{30}-H_{19}	3.504643
H_{17}-H_{16}	2.560517	H_{22}-H_{20}	1.089389	H_{26}-H_{20}	2.720441	H_{30}-H_{20}	3.385144
H_{18}-H_{16}	3.172294	H_{23}-H_{16}	6.162197	H_{27}-H_{16}	5.959147	H_{32}-H_{16}	2.527711
H_{18}-H_{17}	1.768123	H_{23}-H_{17}	5.650425	H_{27}-H_{17}	6.222875	H_{32}-H_{17}	2.544944

T a b l e 1 (continued)

H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}
H_{32}-H_{18}	3.748527	H_{36}-H_{18}	6.015668	H_{27}-H_{21}	5.235558	H_{32}-H_{21}	3.456948
H_{32}-H_{19}	3.056484	H_{36}-H_{19}	5.571693	H_{27}-H_{22}	3.726181	H_{32}-H_{22}	3.867476
H_{32}-H_{20}	4.456081	H_{36}-H_{20}	2.771481	H_{27}-H_{23}	2.461104	H_{32}-H_{23}	5.247979
H_{33}-H_{16}	3.730065	H_{22}-H_{21}	2.175884	H_{27}-H_{24}	1.093185	H_{32}-H_{24}	5.408845
H_{33}-H_{17}	3.003202	H_{23}-H_{21}	3.732546	H_{27}-H_{25}	1.768041	H_{32}-H_{25}	5.568216
H_{33}-H_{18}	3.645196	H_{23}-H_{22}	1.758563	H_{29}-H_{21}	4.385887	H_{33}-H_{21}	2.413947
H_{33}-H_{19}	2.393509	H_{25}-H_{21}	5.247494	H_{29}-H_{22}	2.618105	H_{33}-H_{22}	2.238018
H_{33}-H_{20}	3.024017	H_{25}-H_{22}	4.345410	H_{29}-H_{23}	2.418969	H_{33}-H_{23}	3.742916
H_{35}-H_{16}	3.713240	H_{25}-H_{23}	3.696615	H_{29}-H_{24}	3.026745	H_{33}-H_{24}	4.600560
H_{35}-H_{17}	5.144642	H_{25}-H_{24}	1.092623	H_{29}-H_{25}	3.510352	H_{33}-H_{25}	5.081681
H_{35}-H_{18}	5.047972	H_{26}-H_{21}	4.592492	H_{30}-H_{21}	5.094723	H_{35}-H_{21}	3.856829
H_{35}-H_{19}	5.082654	H_{26}-H_{22}	3.763911	H_{30}-H_{22}	3.795547	H_{35}-H_{22}	3.915421
H_{35}-H_{20}	3.485208	H_{26}-H_{23}	2.958803	H_{30}-H_{23}	3.494688	H_{35}-H_{23}	4.292982
H_{36}-H_{16}	5.079214	H_{26}-H_{24}	1.093309	H_{30}-H_{24}	2.505708	H_{35}-H_{24}	2.634525
H_{36}-H_{17}	6.015380	H_{26}-H_{25}	1.769284	H_{30}-H_{25}	2.406590	H_{35}-H_{25}	2.392385

T a b l e 1 (continued)

H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}	H_x-H_y	R_{Hx-Hy}
H_{36}-H_{21}	2.792435						
H_{36}-H_{22}	3.238787						
H_{36}-H_{23}	3.733724						
H_{36}-H_{24}	2.732330						
H_{36}-H_{25}	3.059411						

Table 2

Distance matrix of hexamethylcyclohexane

		1	2	3	4	5
1	C	0.000000				
2	C	2.654839	0.000000			
3	C	2.671530	2.654301	0.000000		
4	C	3.486746	1.550136	3.904970	0.000000	
5	C	3.905515	1.550104	3.486518	2.484446	0.000000
6	H	4.273061	2.185489	4.406242	2.737269	1.093598
7	H	4.054213	2.205624	3.279115	3.462623	1.089111
8	H	4.769299	2.187048	3.963644	2.682808	1.093169
9	H	2.192786	3.525898	4.441448	3.358541	4.921065
10	H	3.963516	2.187227	4.768783	1.093189	2.683211
11	H	4.406703	2.185292	4.272784	1.093579	2.736668
12	C	3.536902	3.240576	1.549352	4.727271	3.409139
13	C	3.892531	3.960872	1.547861	4.962298	4.779793
14	H	3.331485	3.028805	2.208677	4.578866	2.973715
15	H	4.040730	4.260476	2.177837	5.739911	4.474167
16	H	4.437844	3.523800	2.192938	4.920567	3.355729
17	H	4.765503	4.278535	2.191832	5.239831	4.830937
18	H	4.284206	4.810723	2.188308	5.913085	5.583914
19	H	3.981050	4.191440	2.191459	4.896415	5.245937
20	C	1.549355	3.242851	3.541593	3.410480	4.728882
21	H	3.279165	2.205556	4.053215	1.089143	3.462591
22	H	2.208683	3.031817	3.338776	2.974053	4.581801
23	H	2.177965	4.262577	4.045792	4.475294	5.741586
24	C	1.547935	3.960997	3.889928	4.781348	4.961539
25	H	2.191495	4.190781	3.975280	5.247217	4.895080
26	H	2.191992	4.279034	4.763520	4.833997	5.238366
27	H	2.188262	4.810976	4.282756	5.584941	5.912790
28	C	1.566486	3.111977	1.566148	4.224916	4.226900
29	H	2.167631	3.869582	2.182491	4.734760	5.129484
30	H	2.183263	3.874819	2.167517	5.132011	4.743956
31	C	2.895881	1.561254	1.553188	2.530621	2.565113
32	H	3.969251	2.180873	2.171175	2.974496	2.596159
33	H	3.056881	2.172754	2.147744	2.525021	3.426876
34	C	1.553265	1.561274	2.894661	2.565420	2.530576
35	H	2.147832	2.172648	3.055211	3.427167	2.524997
36	H	2.170981	2.180876	3.968191	2.596804	2.974042
		6	7	8	9	10
6	H	0.000000				
7	H	1.764221	0.000000			
8	H	1.767165	1.765666	0.000000		
9	H	5.035104	5.474546	5.622249	0.000000	
10	H	2.477817	3.717171	2.956054	3.598579	0.000000
11	H	3.123014	3.731554	2.476730	4.321395	1.767068
12	C	4.285100	2.735193	3.932072	5.552491	5.412937
13	C	5.783224	4.576790	5.014846	5.420032	5.951729
14	H	3.647971	2.177500	3.714603	5.364456	5.068589
15	H	5.298823	3.731586	5.011860	6.159501	6.431746
16	H	4.317072	2.627126	3.598926	6.309920	5.620800
17	H	5.901676	4.587409	4.851174	6.250501	6.240946

18	H	6.550160	5.233968	5.913647	5.966285	6.859707
19	H	6.215215	5.245429	5.431505	5.116424	5.940464
20	C	5.064434	5.147551	5.415160	1.092761	3.931079
21	H	3.732236	4.349868	3.716691	2.632028	1.765738
22	H	5.057166	5.099642	5.072215	1.767193	3.712259
23	H	6.109570	6.068017	6.434041	1.766897	5.010852
24	C	5.107904	4.960302	5.951094	2.785714	5.016445
25	H	5.010840	4.678840	5.938907	3.778965	5.433897
26	H	5.174617	5.382393	6.240025	2.561172	4.853814
27	H	6.144073	5.878966	6.859507	3.172165	5.914462
28	C	4.897642	4.104296	4.950539	3.510742	4.949333
29	H	5.829742	5.095482	5.755198	3.592639	5.540054
30	H	5.354183	4.397526	5.548063	4.265377	5.759434
31	C	3.516686	2.822275	2.827648	4.057305	3.491428
32	H	3.655125	2.791163	2.454249	5.085068	3.907012
33	H	4.277047	3.856473	3.578790	3.721507	3.596198
34	C	2.739920	2.818516	3.491293	2.771607	2.828021
35	H	2.662182	2.414090	3.596112	3.727987	3.579472
36	H	2.792029	3.456631	3.906521	2.524315	2.454737
		11	12	13	14	15
11	H	0.000000				
12	C	5.064261	0.000000			
13	C	5.108538	2.495912	0.000000		
14	H	5.056017	1.089308	3.470413	0.000000	
15	H	6.109319	1.093247	2.665538	1.758695	0.000000
16	H	5.036299	1.092861	2.785539	1.767224	1.766718
17	H	5.176408	2.720043	1.093298	3.763414	2.958288
18	H	6.144472	2.749025	1.093202	3.726572	2.461439
19	H	5.011099	3.466063	1.092623	4.345396	3.696653
20	C	4.287916	4.762438	4.407335	4.732379	5.293728
21	H	1.764482	5.145360	4.961626	5.095625	6.065644
22	H	3.650567	4.736615	3.988945	4.885055	5.356194
23	H	5.301465	5.294181	4.661949	5.352239	5.638564
24	C	5.784578	4.397404	5.068231	3.975930	4.650575
25	H	6.215668	4.081344	5.228954	3.492831	4.228817
26	H	5.904664	5.284690	6.001169	4.754384	5.638391
27	H	6.551264	4.898712	5.201393	4.647404	4.961856
28	C	4.895481	2.550066	2.534822	2.775880	2.820598
29	H	5.344224	3.387705	2.506697	3.797695	3.500200
30	H	5.831867	2.520075	3.021635	2.625294	2.419417
31	C	2.739896	2.570422	2.509341	2.917415	3.509034
32	H	2.792519	2.773831	2.731159	3.241333	3.735642
33	H	2.662130	3.485685	2.636201	3.914813	4.293286
34	C	3.516773	3.380720	4.371516	2.883693	4.180191
35	H	4.276914	3.016551	4.599021	2.228215	3.735811
36	H	3.655505	4.450061	5.409476	3.858785	5.241903
		16	17	18	19	20
16	H	0.000000				
17	H	2.560517	0.000000			
18	H	3.172294	1.768123	0.000000		
19	H	3.778705	1.769269	1.768058	0.000000	
20	C	5.554618	5.295219	4.906686	4.095403	0.000000
21	H	5.474021	5.385038	5.879399	4.681235	2.736545

22	H	5.371411	4.769105	4.658159	3.508998	1.089389
23	H	6.162197	5.650425	4.971436	4.245020	1.093258
24	C	5.410845	5.999777	5.199752	5.233803	2.495931
25	H	5.102432	6.086932	5.259475	5.604862	3.466077
26	H	6.240668	6.903072	6.222329	6.093969	2.720441
27	H	5.959147	6.222875	5.164900	5.265984	2.748662
28	C	3.510873	3.500225	2.750485	2.802311	2.549959
29	H	4.267066	3.585083	2.598830	2.405130	2.517085
30	H	3.595127	3.946563	2.874348	3.504643	3.385144
31	C	2.772633	2.776450	3.475378	2.730110	3.386521
32	H	2.527711	2.544944	3.748527	3.056484	4.456081
33	H	3.730065	3.003202	3.645196	2.393509	3.024017
34	C	4.051714	4.976836	4.961955	4.632398	2.570128
35	H	3.713240	5.144642	5.047972	5.082654	3.485208
36	H	5.079214	6.015380	6.015668	5.571693	2.771481

		21	22	23	24	25
21	H	0.000000				
22	H	2.175884	0.000000			
23	H	3.732546	1.758563	0.000000		
24	C	4.579272	3.470465	2.665623	0.000000	
25	H	5.247494	4.345410	3.696615	1.092623	0.000000
26	H	4.592492	3.763911	2.958803	1.093309	1.769284
27	H	5.235558	3.726181	2.461104	1.093185	1.768041
28	C	4.100538	2.775416	2.820464	2.535234	2.802572
29	H	4.385887	2.618105	2.418969	3.026745	3.510352
30	H	5.094723	3.795547	3.494688	2.505708	2.406590
31	C	2.818348	2.891740	4.185797	4.371467	4.629911
32	H	3.456948	3.867476	5.247979	5.408845	5.568216
33	H	2.413947	2.238018	3.742916	4.600560	5.081681
34	C	2.822707	2.917443	3.508899	2.509309	2.730578
35	H	3.856829	3.915421	4.292982	2.634525	2.392385
36	H	2.792435	3.238787	3.733724	2.732330	3.059411

		26	27	28	29	30
26	H	0.000000				
27	H	1.768155	0.000000			
28	C	3.500703	2.750741	0.000000		
29	H	3.950701	2.881648	1.094276	0.000000	
30	H	3.584567	2.593925	1.094292	1.744642	0.000000
31	C	4.977838	4.962475	2.564165	3.101829	3.432945
32	H	6.015720	6.015788	3.508115	4.016317	4.264751
33	H	5.148168	5.049762	2.809965	2.980222	3.840288
34	C	2.775897	3.475332	2.565363	3.431451	3.108206
35	H	2.999675	3.644239	2.813375	3.842638	2.990857
36	H	2.545610	3.749026	3.508930	4.262662	4.022232

		31	32	33	34	35
31	C	0.000000				
32	H	1.095632	0.000000			
33	H	1.094624	1.746227	0.000000		
34	C	2.564469	3.459249	3.065806	0.000000	
35	H	3.065258	3.804022	3.810570	1.094561	0.000000
36	H	3.459486	4.307666	3.805051	1.095666	1.746095

		36
36	H	0.000000

Table 3

Atoms centers of the hexamethylcyclohexane

Center number	Coordinates (Angstroms) X	Y	Z
1	–1.332207	–0.785656	0.119137
2	0.003802	1.505439	0.000227
3	1.328568	–0.791470	–0.120268
4	–0.669410	2.434525	–1.042129
5	0.681144	2.430807	1.043167
6	–0.070211	3.033830	1.560646
7	1.233641	1.868652	1.794760
8	1.378544	3.114437	0.551942
9	–2.912890	–0.058770	–1.215551
10	–1.364161	3.120721	–0.550685
11	0.084781	3.034900	–1.558519
12	2.012104	–0.699787	1.267127
13	2.297822	–1.542840	–1.064654
14	1.351011	–0.292782	2.031258
15	2.316790	–1.696760	1.596369
16	2.906991	–0.074065	1.222449
17	3.261129	–1.029513	–1.126584
18	2.480270	–2.558414	–0.703524
19	1.885573	–1.612944	–2.074090
20	–2.021289	–0.688624	–1.265151
21	–1.223931	1.875134	–1.794341
22	–1.361516	–0.283408	–2.031484
23	–2.331727	–1.683648	–1.594952
24	–2.300638	–1.534707	1.066325
25	–1.884084	–1.608923	2.073698
26	–3.261358	–1.017227	1.133818
27	–2.489204	–2.548629	0.703753
28	–0.003759	–1.606525	–0.004469
29	–0.095913	–2.262421	–0.875531
30	0.085211	–2.271991	0.859657
31	1.058473	0.612740	–0.726596
32	2.006006	1.158942	–0.791811
33	0.731750	0.460467	–1.760166
34	–1.054504	0.616658	0.726613
35	–0.727872	0.461856	1.759769
36	–1.999472	1.167198	0.793139

Rotational constants (GHZ): 0.9494785 0.9222698 0.6553439

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