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Article

Electronic Nature of the Aromatic Adamantanediyl Ions and its Analogues

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A estabilidade relativa do dicátion 1,3-desidro-5,7-adamantanediila é atribuída a sua aromaticidade tridimensional. Contudo, sua natureza eletrônica não é bem conhecida. A fim de entendê-la melhor, os di- e monocátions do adamantanodiil e alguns de seus análogos foram estudados utilizando a teoria de átomos e moléculas (AIM). Eles foram comparados com análogos de adamantano não-aromáticos. Os resultados de AIM indicam que a densidade eletrônica no centro da estrutura em gaiola e a média de todos os índices de deslocalização, envolvendo seus átomos cabeças-de-ponte são maiores em compostos aromáticos do que em não-aromáticos. A degenerescência energética dos átomos cabeça-de-ponte, a uniformidade e magnitude da carga compartilhada entre estes, distingue os dicátions 1,3-adamantila e 1,3-desidro-5,7-adamantanediila. Contudo, ambos são aromáticos, assim como o 1,3-desidro-5,7-diboroadamantano. O cátion 1,3-desidro-7-adamantila tem uma homoaromaticidade planar característica.

The relative stability of the 1,3-dehydro-5,7-adamantanediyl dication is ascribed to its tridimensional aromaticity. However, its electronic nature is not well known. In order to improve its understanding, dicationic and monocationic adamantanedyil species and some key analogues were studied by atoms in molecules (AIM) theory. They were compared to non-aromatic adamantane analogues. AIM results indicate that the density in center of the cage structure and the average of all delocalization indexes involving its bridged atoms are higher in aromatic than in non-aromatic compounds. Degeneracy in energy of the bridged atoms, uniformity and magnitude of their shared charge distinguish the dications 1,3-adamantyl and the 1,3-dehydro-5,7-adamantanediyl**.** However, both are aromatic as well as the 1,3-dehydro-5,7-diboroadamantane. The 1,3-dehydro-7-adamantyl cation has a characteristic planar homoaromaticity.

Keywords: adamantyl dication, adamantyl cation, degeneracy, delocalization index, ring density, aromaticity, tridimensional aromaticity, 1,3-dehydro-5,7-adamantanediyl dication

Introduction

Some cationic adamantanediyl species are relatively stable intermediates, e.g., Schleyer's 1,3-dehydro-5,7-adamantanediyl dication (Scheme 1). The adamantanediyl monocation is a stable species and can be synthesized from the 1-adamantanol and fluorosulfonic acid-antimony pentafluoride.[1] The adamantanediyl dication has not been observed as persistent long-lived species so far.[2] Ionization of 1,3-difluoroadamantane in superacids afforded only the monocation complex[3] $C_{10}H_{14}F$-SbF_5 (Scheme 1). Attempts of obtaining other adamantane-1,3-diyl dications were not successful.[4] However, the 1,3-dehydro-5,7-adamantanediyl dication (or 1,3,5,7-bisdehydroadamantane dication) is a stable species.[5] It exhibits shielded bridgehead carbons at δ 6.6 ppm with methylene carbon resonances appearing at δ 35.6 ppm which is characteristic of hypercoordinate carbocations.[5] Despite that 1,3,5,7-tetrasilaadamantane (Scheme 1) is easily obtained[6] from the 1,3,5-hexamethyl-1,3,5-trisilacyclohexane and $AlBr_3$, the 1,3-dehydro-5,7-tetrasilaadamantanediyl dication is not observed experimentally. However, it has a spherical homoaromaticity[7] which is another name for the tridimensional aromaticity.

A series of isoelectronic analogues of the adamantane and its dehydroadamantanes containing boron, nitrogen, and phosphorus atoms at bridgehead were studied and the three-

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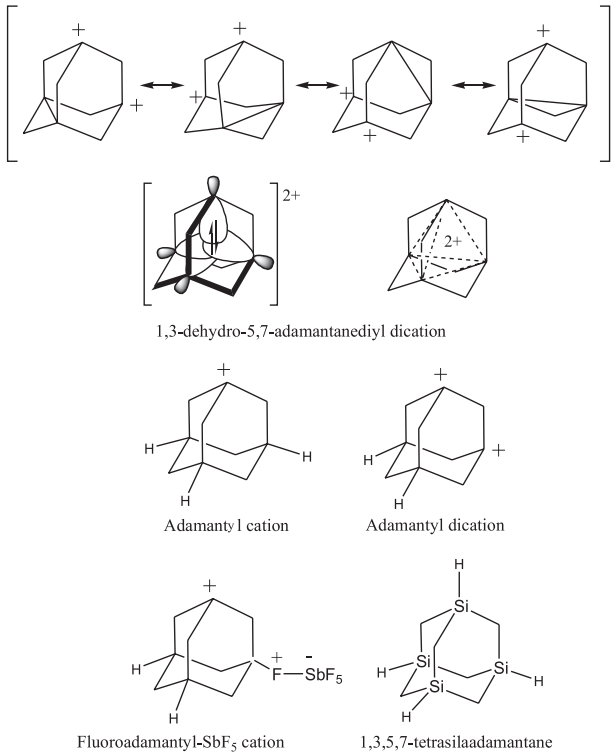


Scheme 1.

dimensional aromaticity is found to be general for 4c-2e electron systems.[8] The calculations of the isoeletronic boron and diboron analogues of the 1,8-dehydrohomoadamantanediyl-3,6-dication, $BC_9H_{12}^+$ and $B_2C_8H_{12}$, respectively, indicate that both have three-dimensional aromaticity.[9]

Despite that 1,3-dehydroadamantane undergoes addition reaction easily,[10] it is stable at low temperature and inert conditions. Hitherto, the 1,3-dehydro-5-adamantyl cation is not a long–lived stable ion but it is an intermediate in solvolysis of the 5-bromo-1,3-dehydroadamantane.[11] The density functional theory (DFT) study showed that the 1,3-dehydro-5-adamantyl cation has 20.0 kcal mol^{-1} stabilization due to trishomoaromatic interaction.[9] The 1,3-dehydro-5-boroadamantyl analogue has the same type of stabilization.[9]

The three-dimensional aromaticity of 1,3-dehydro-5,7-adamantanediyl dication is explained in terms of overlap among four p-orbitals in a tetrahedral fashion (Scheme 1) and its ^{13}C NMR spectrum has a single absorption ($\delta^{13}C$ 6.6 ppm) assigned for bridgehead carbons.[12] In order to understand the electronic nature of these systems we have performed AIM calculations of the 1,3-dehydro-5-7-adamantanediyl dication and its analogues.

Computational Methods

Geometry optimization, vibrational analysis and the generation of the electronic density were obtained with GAUSSIAN 03 package.[13] The geometries were optimized in DFT level employing Becke three-parameter interchange functional[14] (B3) in conjunction with Lee-Yang-Parr[15] correlation functional (LYP) and the split valence basis set[16] 6-311++G**. Dehalogenation calculations were performed at the same level. All geometries were characterized as stationary points after vibrational analysis.

The AIM 2000 software[17] was used for charge density calculations from the electronic densities (ρ) obtained at B3LYP/6-311++G** level. NICS[18] (nucleus independent chemical shift) calculations were performed at GIAO/B3LYP/6-311++G** level at the geometric center of the cage.

Rationale

Within the molecular orbital theory (MO) the aromatic character of benzene is explained through delocalized orbitals. Nevertheless by using spin coupled from valence bond theory (SC), Gerratt and co-workers[19] established that all six ω electrons of benzene are localized and distorted symmetrically towards neighboring carbon atoms on each side and possess same energy and shape. Furthermore, from a more rigorous quantum mechanical standpoint,[20] benzene has no resonance[21] since there is not intersection of degenerate point group states. It means that benzene (D_{6h} symmetry) cannot be related to Kekulé (D_{3h} symmetry) or Dewar (D_{2h}) structures. In this case, benzene stability is ascribed to maximum overlap among six degenerate single-electron states.[22] Then, in modern valence bond theory (VB), the idea of aromaticity is based on the overlap and degeneracy of the single-electron states.[22]

The index used to study the aromaticity of adamantanediyl ions and its analogues in this work, D_3BIA, is inspired to the modern VB idea of aromaticity. The modern VB parameters of aromaticity can be associated with topological parameters. Then, it is possible to quantify aromaticity by AIM theory inspired on modern VB ideas of aromaticity. In the case of adamantanediyl ions and its analogues, the aromaticity from modern VB theory can be associated with the energy of atomic basins of the bridged atoms, the charge density in the cage critical point and the delocalization indexes involving the bridged atomic pairs of the cage (from AIM). The use of Kohn-Sham orbitals for the calculation of delocalization indices is a good approximation, although not strictly correct.

It is important to emphasize that the calculus of energy of an atomic basin is an one-electron integration over the whole atomic basin. Then, the AIM provides the energy value of the total energy of each atomic basin. Since degeneracy in Quantum Chemistry means same energy, the AIM can provide the information whether some atomic basins in a given molecular system are degenerate or not (see Electronic Supplementary Information for more details).

Results and Discussions

The studied species are depicted in Scheme 2. The AIM theory[23] is based on the analysis of the electronic density distribution, ρ(r), obtained from a quantum mechanical wavefunction. Although DFT does not generate a wave function, it yields a density matrix similar to that from a post-HF method such as MP2. Much information can be obtained from AIM such as the bond, cage and ring critical points and their respective eigenvalues (see electronic supplementary information).

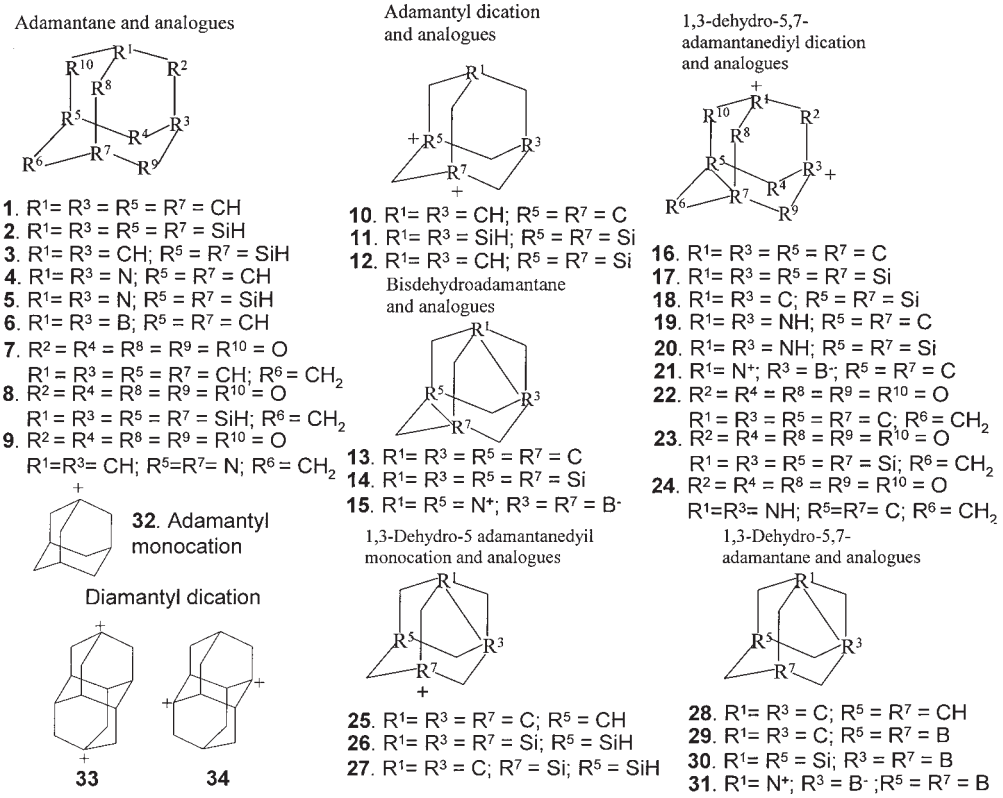
Table 1 contains the delocalization indexes and energy of bridged atoms (R^1, R^3, R^5 and R^7) of the species **1** to **32**, obtained from AIM theory. Their analysis allows the investigation of the electronic differences between aromatic and non-aromatic tridimensional systems. Table 1 also contains the point group symmetry of each studied species.

The delocalization index (DI) is a measure of number of electrons that are shared or exchanged between two atoms or basins. The integration of the Fermi hole density through a pair density matrix leads to the localization index (LI) and the delocalization index[24] (DI). Although DFT does not yield a pair density matrix, the delocalization indexes from B3LYP are close to those from MP2 (see electronic supplementary information). It is important to emphasize that the delocalization index does not measure the delocalization of valence electrons over the whole molecular system.

In a previous work on benzene-like compounds it was shown the importance of some electronic parameters to determine their aromaticity.[25] These parameters were degeneracy of the atoms in the ring, density inside the ring and uniformity of delocalization index between atoms of the ring. All of these parameters are also analyzed in this work.

The bridged atoms of the adamantane **1** and the 3-dehydro-5,7-adamantanediyl dication **16** are degenerate and the delocalization indexes (or amount of shared charge density) among them are uniform in both molecules (0.039 in **1** and 0.280 in **16**). However, the delocalization indexes in **16** are seven-fold higher than those in **1**. As a consequence, the species **16** has 1.70e among the bridged atoms while the species **1** has only 0.23e.

The delocalization indexes among bridged atoms in adamantyl dication **10** are not uniform (0.079, 0.147 and 0.143) and the energy of its bridged atoms is not degenerate (Table 1). The degeneracy of bridged atoms, uniformity and magnitude of their delocalization indexes are the electronic features that distinguish the species **10** and **16.** They can be regarded as determinant factors for the relative stability of the 1,3-dehydro-5,7-adamantanediyl dication. One simi-



Scheme 2.

Table 1. Delocalization index among bridged atoms, energy of bridged atoms and point group symmetry of the species **1** to **32**

Entry	Delocalization index						Energy / au				Point group symmetry
	R^1-R^3	R^1-R^5	R^1-R^7	R^3-R^7	R^3-R^5	R^5-R^7	R^1	R^3	R^5	R^7	
1	0.039	0.039	0.039	0.039	0.039	0.039	-38.06	-38.06	-38.06	-38.06	Td
2	0.007	0.007	0.007	0.007	0.007	0.007	-288.81	-288.81	-288.81	-288.81	C_1
3	0.038	0.016	0.016	0.016	0.016	0.008	-37.91	-37.91	-289.04	-289.04	Cs
4	0.107	0.068	0.068	0.068	0.068	0.041	-55.21	-55.21	-38.07	-38.07	C_1
5	0.119	0.034	0.034	0.034	0.034	0.009	-55.06	-55.07	-289.04	-289.04	Cs
6	0.026	0.033	0.033	0.033	0.033	0.045	-24.10	-24.10	-38.01	-38.01	Cs
7	0.022	0.023	0.023	0.023	0.023	0.045	-37.18	-37.18	-37.50	-37.50	Cs
8	0.008	0.006	0.006	0.006	0.006	0.006	-288.55	-288.55	-288.46	-288.44	Cs
9	0.049	0.045	0.045	0.045	0.045	0.091	-37.54	-37.55	-54.37	-54.37	C_1
10	0.079	0.147	0.147	0.147	0.147	0.143	-38.01	-38.01	-38.13	-38.13	Cs
11	0.023	0.023	0.024	0.023	0.023	0.011	-288.89	-288.82	-288.90	-288.82	C_1
12	0.056	0.061	0.061	0.061	0.061	0.033	-37.92	-37.92	-289.10	-289.10	C_1
13	0.825	0.081	0.082	0.082	0.082	0.829	-38.12	-38.12	-38.12	-38.12	C_1
14	0.102	0.070	0.086	0.106	0.146	0.091	-288.99	-289.15	-289.16	-288.99	C_1
15	0.073	0.144	0.073	0.031	0.069	0.069	-55.14	-24.11	-55.15	-24.11	C_1
16	0.280	0.280	0.280	0.280	0.280	0.280	-38.09	-38.10	-38.09	-38.09	C_1
17	0.097	0.096	0.096	0.097	0.097	0.096	-288.97	-288.97	-288.97	-288.97	C_1
18	0.153	0.140	0.140	0.140	0.140	0.183	-289.22	-289.22	-38.02	-38.02	Cs
19	0.065	0.085	0.085	0.085	0.085	0.836	-38.13	-38.13	-55.21	-55.21	Cs
20	0.010	0.019	0.019	0.019	0.019	0.068	-288.99	-288.99	-55.07	-55.07	Cs
21	0.147	0.254	0.253	0.107	0.107	0.184	-55.20	-24.12	-38.10	-38.10	C_1
22	0.137	0.158	0.158	0.158	0.158	0.248	-37.03	-37.03	-37.41	-37.41	C_1
23	0.151	0.119	0.118	0.118	0.119	0.057	-288.55	-288.55	-288.66	-288.66	C_1
24	0.046	0.060	0.060	0.060	0.060	0.804	-54.47	-54.47	-37.61	-37.61	C_1
25	0.410	0.071	0.410	0.410	0.071	0.071	-38.12	-38.12	-38.04	-38.12	C_1
26	0.155	0.019	0.155	0.155	0.019	0.019	-289.03	-289.03	-288.82	-289.03	C_1
27	0.217	0.034	0.217	0.217	0.034	0.028	-38.03	-38.03	-289.03	-289.33	C_1
28	0.855	0.062	0.062	0.062	0.062	0.036	-38.15	-38.15	-38.04	-38.04	C_1
29	0.319	0.113	0.113	0.113	0.113	0.041	-38.12	-38.12	-24.12	-24.12	C_1
30	0.228	0.055	0.055	0.055	0.055	0.026	-289.28	-289.28	-24.04	-24.04	C_1
31	0.103	0.103	0.103	0.029	0.029	0.029	-55.19	-24.11	-24.11	-24.11	C_1
32	0.112	0.112	0.112	0.053	0.053	0.053	-38.16	-38.04	-38.04	-38.04	Cs

larity between the species **10** and **16** is that their positive charge is distributed among the hydrogen atoms, as one can see in Figure 1.

The relative stability of the 1,3-dehydro-7-adamantyl cation **25** is experimentally known.[3] It is suggested that the species **25** (Figure 1) has homoaromaticity among R^1, R^3, and R^7 bridged atoms (see Table 2) since they are nearly degenerate. Besides, the delocalization indexes among these atoms have high magnitude and uniformity.

When bridgehead carbon atoms are substituted by silicon atoms, such as in **2**, **11**, **17** and **26**, it is noteworthy that their respective delocalization indexes decrease significantly (Table 2). All other electronic features remain the same when comparing the silicon derivatives with their carbon analogues **1**, **10**, **16** and **25**, respectively. Bridged silicon atoms in **17** are nearly degenerate and the delocalization indexes among them are nearly uniform. However, the magnitude of these delocalization indexes is almost three-fold smaller than that from **16**. The same occurs with **26** in comparison to **25**.

In **3**, **12**, **18** and **27**, only two carbon bridged atoms are replaced by silicon ones. This change decreases

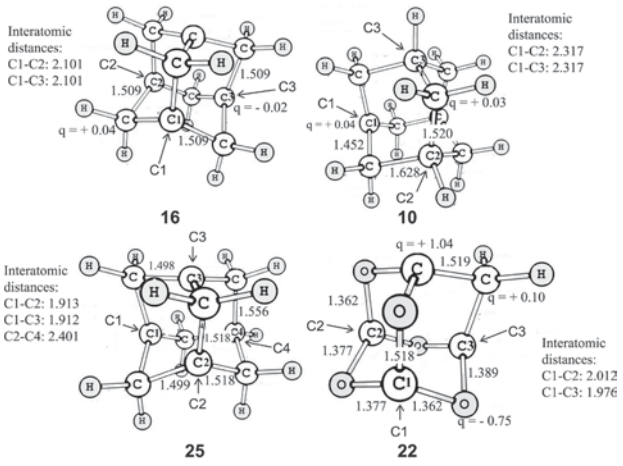


Figure 1. Bond lengths, interatomic distances (Å) and atomic charge (in atomic units) of 1,3-dehydro-5-7-adamantanediyl dication **16**, 1,3-adamantyl dication **10**, 1,3-dehydro-7-adamantyl cation **25** and oxy-species **22**.

degeneracy of their bridged atoms due to a decrease on the symmetry of their respective species. In **3** and **18** there is no uniformity of delocalization indexes involving the bridgehead atoms. The exception is the species **27**. As to the magnitude of delocalization indexes, **3**, **12**, **18** and **27** have higher values than those from their respective analogues **2**, **11**, **17** and **26**.

From AIM electronic analysis, bisdehydro-1,3,5,7-adamantane **13** and the 1,3-dehydro-5,7-adamantane **28** do not have tridimensional aromaticity since the delocalization indexes among their bridged atoms are not uniform. Moreover, they are smaller than those from **16** (except for the DI´s between C-C bonds). The non-stability of bisdehydro-1,3,5,7-adamantane[8] is probably due to its anti-aromatic 4n-electron character. The bridged silicon analogue of **13**, bisdehydro-1,3,5,7-tetrasilaadamantane **14**, has no Si-Si bonds (Figure 2b). However, its delocalization indexes are not so much different than those from **18** which has only 2 electrons among bridged atoms.

In oxy-species **7**, **8**, **22** and **23** there is no degeneracy of bridged atoms and uniformity of delocalization indexes among them. By comparing oxy-species with bridged carbon atoms (**7** and **22**) with their analogues **1** and **16**, one can see that the magnitude of the DI´s decreases significantly in **7** and **22** due to the higher electronegativity of the oxygen atom. However, this does not happen with oxy-species with bridged silicon atoms (**8** and **23**) when comparing to their analogues **2** and **17** (Table 1). The effect of oxygen atoms in **22** can be seen in Figure 1 where its bridged carbon atoms are positively charged while in **16** the corresponding bridged carbon atoms are negatively charged. Likewise, it is expected that **22** and **23** have smaller aromaticity with respect to their respective analogues **16** and **17**.

The dicationic diazo-analogues **19** and **20** have very small delocalization indexes values among bridged atoms in comparison to **16** and **17**, respectively. The species **19** and **20** probably do not have tridimensional aromaticity since their delocalization indexes among bridged atoms are equivalent with those from neutral analogues **4** and **5**, respectively (Table 1). However, in **19**, there exists a bond between bridged carbon atoms, while in **20** no similar bond exists between bridged silicon atoms. The diazo-oxy-derivative **24** has the smallest delocalization indexes values within the dicationic aromatic oxy-analogues (**22**, **23** and **24**) and it is probably the least aromatic one.

The dicationic **21**, containing one boron, one nitrogen and two carbon bridged atoms, has delocalization indexes among bridged atoms higher than those from **19** and **20**. Then, **21** is probably more aromatic than **19** and **20**, as it is confirmed by its NICS value in Table 2.

The molecular graphs of **14** and **19** show interesting aspects. In **14** (Figure 2a) both σ bonds between silicon atoms are broken after its optimization. Moreover, the delocalization indexes among R^1, R^3, R^5 and R^7 are not uniform. In **19** (Figure 2b) the two sp^2 carbon atoms make a bond after geometry optimization as it can be seen in the delocalization index between them (DI=0.836, in Table 1) and the density of this bond critical point (ρ=0.21a.u.). All other delocalization indexes among R^1, R^3, R^5 and R^7 are just little higher than those from **4**, which agrees with the small NICS value of **19** (Table 2). Nevertheless, no bond is made between silicon atoms in **20**.

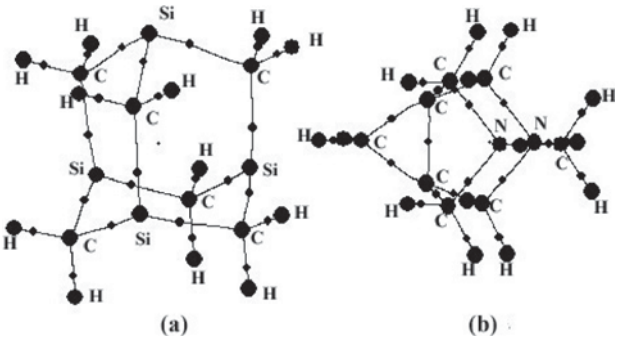


Figure 2. Molecular graph from AIM of the species **14** (a) and **19** (b).

Interestingly, in the neutral compound **29**, electropositive boron atoms attract electrons from bridgehead carbon atoms and generate reasonable delocalization indexes among bridged carbon and boron atoms. By comparing with compound **6**, where DI´s among bridged carbon and boron atoms is only 0.033, it is possible to see how effectively boron atoms distribute electrons from bridged carbon atoms in **29** (Table 1). This can be verified by comparing C-C atomic distances between **28** (1.562 Å) and **29** (2.110 Å) in Figure 3. The latter has a much larger distance which represents a delocalization

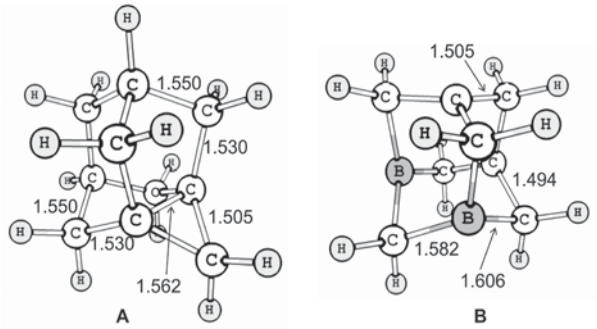


Figure 3. Selected atomic and interatomic distances (Å) of the species **28** (A) and **29** (B).

of this σ C-C bond. Then, **29** can be regarded as tridimensional aromatic species, as supported by its NICS value of -38.80 (Table 2). Although less effectively, boron atoms also provoke distribution of the electrons of the bridged silicon in **30**. Optimized structures of the species **1, 2, 4, 6, 7, 10, 11, 13, 15, 16, 17, 19, 21, 22, 25** and **26** are shown in the electronic supplementary information.

Another important analysis from AIM theory is the Laplacian of the charge density, $\nabla^2\rho$. It is defined as the sum of the three principal curvatures of the function at each point of the space. However, it is a convenient convention to use the negative of the Laplacian, L(r), rather than the Laplacian itself. Then, $L(r) = -\nabla^2\rho$. The density is a locally concentrated in those regions where L(r)>0, since $\nabla^2\rho(r)<0$ when ρ(r) is a local maximum. Likewise, the density is a locally depleted in those regions where L(r)<0, since $\nabla^2\rho(r)>0$ when ρ(r) is a local minimum.[24]

In Figure 4, it is depicted the negative of the Laplacian curves in a plane that passes through three bridged carbon atoms of **10** and **16**. It is possible to see that the negative of the Laplacian distribuition region in the 1,3-dehydro-5,7-adamantanediyl dication (**16**) where L(r)<0 encompasses the three bridged carbons atoms. This represents a uniform charge density distribution over these atoms and indicates

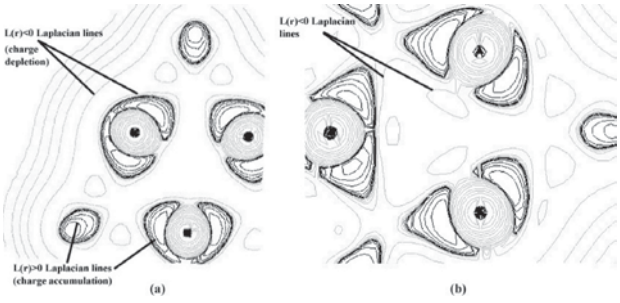


Figure 4. Contour maps of the Laplacian distribution of the electronic charge density for the 1,3-dehydro-5-7-adamantanediyl dication (a) and 1,3 adamantyl dication (b) in the plane that contains three bridged carbon atoms. The gray curves are related to charge depletion, while the black lines are charge concentration.

an interaction among them. In case of the 1,3 adamantyl dication (**10**), there exists no L(r)<0 Laplacian distribution region encompassing the three bridged carbons and it indicates absence of significant interaction among them.

The AIM study of the diamantyl dications **33** and **34** provides a different electronic nature between them (see Figure 5). The former was prepared and characterized but the latter was not obtained.[26] In the 4,9-diamantyl dication **33** there are three considerable delocalization indexes (DI= 0.117) linking each positively charged carbon atom (C1 and C8) and its corresponding bridgehead carbon atoms (C2 to C7). In the 1,6-diamantyl dication **34**, there exists just one considerable delocalization index (DI=0.168) and two delocalization indexes immediately inferior (DI=0.085) For **33**, the delocalization indexes are uniform and for **34** the delocalization indexes are not.

In Figure 6, one can see that the atomic distances between each positively charge carbon atom and its vicinal carbon atom is uniform in **33** (1.462 Å) and non-uniform

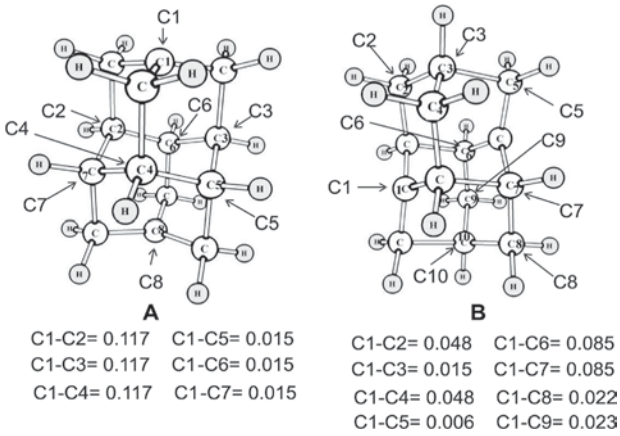


Figure 5. Delocalization indexes between positively charge carbon atoms and non-vicinal carbon atoms in the species **33** (A) and **34** (B)."

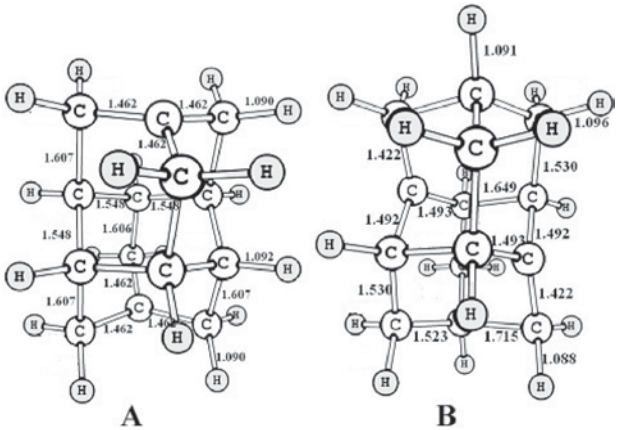


Figure 6. Atomic distances (Å) of the species **33** (A) and **34** (B).

in **34** (1.492, 1.493 and 1.422 Å). These results are in consonance with the uniformity of the delocalization indexes of each corresponding species mentioned above.

We proposed the D_3BIA index which is based on the density in the ring, the degeneracy and the delocalization index of atoms in the ring[21] and it is inspired to the modern VB idea about aromaticity as mentioned before. (see Electronic supplementary information).

The rationale on the index D_3BIA was influenced by modern VB studies on the aromaticity and the particularities of some aromatic compounds.[21] The similarities of the results between AIM and spin coupled wave function (SC) encouraged us to use the former since it provides important and complementary information. The coherence between the AIM and SC can be noticed from their results for benzene (see Electronic supplementary information).

There are some multi-center delocalization indexes proposed to measure aromaticity, for example, the six-center delocalization index[27] (SCI) and Fermi hole density delocalization index[28] (FDDH). However, it is important to emphasize that these multi-center indexes are based on MO approach of aromaticity, *i.e.*, the delocalization of orbitals in the aromatic molecules.[29] On the other hand, the D3BIA index is inspired to a different approach - the spin-coupled (SC) of the modern VB theory. The focus of SC study on the aromaticity is not the delocalization of the molecular orbital over the aromatic molecule since it was demonstrated that π single-electron orbitals are localized in each sp^2 carbon atom in the case of benzene.[19] The focus of modern VB study on aromaticity is the degeneracy and the overlap of the single-electron orbitals and these are the VB paremeters that inspired the formula of D3BIA index in atoms in molecules theory.

The electron density in the aromatic site can be understood in terms of the density in the region involving the bridged atoms. Then, the density factor is the density in the center of the cage structure and the magnitude of the delocalization indexes among bridged atoms or mean delocalization index $\overline{DI}$.

The degree of the degeneracy (δ) is derived from the energies of the atomic basins of the bridged atoms (from AIM theory).

The uniformity of delocalization indexes among bridged atoms is another important electronic feature found in the tridimensional aromatic species (Table 1).

The proposed D_3BIA formula is:

$$D_3BIA = \rho(3,+3) \bullet (\overline{DI}) \bullet DIU \bullet \delta \qquad (1)$$

The degree of degeneracy is regarded to be maximum (δ=1) when energy difference is smaller than 0.009 a.u.

The AIM provides a delocalization index for each bond between vicinal atoms.[19] The mean delocalization index ($\overline{DI}$) can be related to the magnitude of the single-electron states interaction (or overlap).

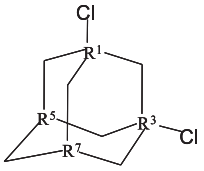
The delocalization index uniformity (DIU) among bridged atoms is given by equation 2:

$$DIU = 100 - \frac{100\sigma}{(\overline{DI})} \qquad (2)$$

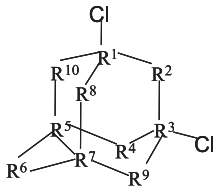
Where σ is mean deviation and ($\overline{DI}$) is mean DI of the ring.

In Table 2, one can see the D_3BIA values for all aromatic and non-aromatic species (**1** to **32**). It was also performed NICS of the species **1** to **32**. Their NICS values are depicted in Table 2 and it is calculated from a probe (berkelium) in the center of adamantyl cage.[7,5] Since all the studied species do not have π orbitals, the use of a dissected NICS, e.g. CMO-NICS method, is unnecessary.[30] Because the species **33** and **34** are structurally different from other species, their D_3BIA´s have not been calculated.

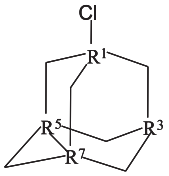
From the 1,3-dehydro-5,7-dichloro-adamantane, the 1,3-dichloro-adamantane, the 1,3-dehydro-5-chloro-adamantane and their analogues (Scheme 3) it is possible to calculate the stability of the species **10**-**12**, **16**, **18**, **21**-**23** and **25**-**27** by means of the equations 3 and 4.



35. R^1=R^3=CCl; R^5=R^7=CH
36. R^1=R^3=SiCl; R^5=R^7=SiH
37. R^1=R^3=SiCl; R^5=R^7=CH



38. R^1=R^3=CCl; R^5=R^7=C
39. R^1=R^3=Si; R^5=R^7=Si
40. R^1=R^3=SiCl; R^5=R^7=C
41. R^1=R^3=CCl; R^5=N^+ ;R^7=B^-
42. R^2=R^4=R^8=R^9=R^{10}=O
R^1=R^3=CCl; R^5=R^7=C; R^6=CH_2
43. R^2=R^4=R^8=R^9=R^{10}=O
R^1=R^3=SiCl; R^5=R^7=Si; R^6=CH_2



44. R^1=CCl; R^3=CH; R^5=R^7=C
45. R^1=SiCl; R^3=SiH; R^5=R^7=Si
46. R^1=SiCl; R^3=SiH; R^5=R^7=C

Scheme 3.

Table 2. Density of (3,+3) critical point [ρ (3,+3)], mean delocalization index ($\overline{DI}$), delocalization index uniformity (DIU) among bridged atoms, degree of degeneracy (δ), D_3BIA, NICS and free energy variation of the dehalogenation reaction ($\Delta G_{(dehalogenation)}$) of the species **1** to **32**

Entry	ρ (3,+3) / au	$\overline{DI}$	DIU	δ	$D_3BIAx10^2$	NICS	$\Delta G_{(dehalogenation)}$ / (kcal mol^{-1})
1	0.012	0.039	100	1	4.68	-0.38	-
2	0.007	0.007	100	1	0.49	-0.63	-
3	0.009	0.018	64.24	0.5	0.52	-0.90	-
4	0.014	0.070	82.38	0.5	4.04	2.38	-
5	0.010	0.044	43.18	0.5	0.95	1.78	-
6	0.015	0.034	88.99	0.5	2.27	-12.62	-
7	0.018	0.026	76.73	0.5	1.79	3.27	-
8	0.012	0.006	91.23	0.5	0.33	0.24	-
9	0.017	0.053	76.45	0.5	3.44		-
10	0.020	0.135	86.17	0.5	11.63	-19.31	384.97
11	0.011	0.021	83.99	0.5	0.97	-6.42	397.59
12	0.013	0.055	86.49	0.5	3.09	-9.07	419.74
13	0.044	0.330	0.32	1	0.46	1.91	-
14	0.012	0.100	82.19	0.5	4.93	23.53	-
15	0.020	0.076	70.59	0.5	5.36	-12.70	-
16	0.046	0.280	100	1	128.8	-46.47	355.34
17	0.021	0.096	99.48	1	20.05	-36.35	365.37
18	0.024	0.149	91.67	0.5	16.39	-29.08	375.27
19	0.023	0.207	1.39	0.5	0.33	-10.90	-
20	0.009	0.026	45.02	0.5	0.53	-0.87	-
21	0.033	0.175	68.63	0.5	19.82	-37.52	364.20
22	0.053	0.169	84.56	0.5	37.87	-36.81	513.71
23	0.015	0.114	83.38	0.75	10.69	-19.55	491.86
24	0.030	0.182	14.19	0.5	3.87	-6.31	-
25	0.031	0.240	29.52	0.75	16.47	-29.76	110.83
26	0.014	0.087	21.84	0.75	1.99	-15.93	127.35
27	0.018	0.124	25.70	0.5	2.87	-22.30	131.17
28	0.023	0.190	16.79	0.5	3.67	-9.90	-
29	0.030	0.135	54.76	0.5	11.09	-38.80	-
30	0.021	0.079	37.13	0.5	3.08	-29.32	-
31	0.027	0.066	43.94	0.75	5.87	-27.85	-
32	0.015	0.082	64.24	0.75	5.93	-8.58	-

$$Cl–R–CL \rightarrow R^{+2} + 2Cl^- \quad (3)$$

R= Adamantyl or its analogues; or 1,3-dehydroadamantyl or its analogues

$$R–Cl \rightarrow R^+ + Cl^- \quad (4)$$

R= 1,3-Dehydroadamantyl or its analogues

The energetics of all studied species are depicted in Electronic supplementary information. The free energy variation values of the dehalogenation of the species **10**-**12**, **16**-**18**, **21**-**23** and **25**-**27** are shown in Table 2.

From Table 2 one can see that the non-aromatic species **1** to **12** have the same electronic characteristics: small density in (3,+3) critical point (the density in centre of the cage structure) and small values of mean delocalization index among bridged atoms. One exception is the 1,3-adamantyl dication **10**, for not having two electrons distributed among bridged carbon atoms and still having a reasonable mean delocalization index value (0.135) and density in (3,+3) critical point (0.020 a.u.).

All non-aromatic species (**1** to **15** and **28** to **32**) have low D_3BIA. However, **10** and **29** have reasonable D_3BIA´s (Table 2) because their density in (3,+3) critical point and their values of mean delocalization index among bridged atoms are not small. There exists an apparent tendency for interaction between bridged atoms. In the 1,3-adamantyl dication **10**, there is no available electrons as it happens in its parent the 1,3-dehydro-5,7-adamantanediyl dication **16**, but it uses sigma electron density to generate interaction among its bridged atoms. On the other hand, **29** has two electrons between bridged carbon atoms but it has no positive charge as the aromatic species **16**. However, its bridged electropositive boron atoms draw the electron density towards them and this provokes a reasonable distribution of electron density among all bridged atoms (Tables 1 and 2). Then, **29** has tridimensional aromaticity.

The species **19** and **20** are not regarded aromatic ones since their D_3BIA´s are very low. The species **19** has quite small delocalization index uniformity and **20** has small density in (3,+3) critical point and small values of mean delocalization index among bridged atoms (Table 2).

In spite of not having tridimensional aromaticity the 1,3-dehydro-7-adamantyl cation **25** has a high D_3BIA (16.47). The species **25** has a characteristic planar homoaromaticity.

When analyzing its planar aromaticity, by exclusion of methine bridged carbon and the density in (3,+3) critical point, it is considered a three-membered planar ring among the other bridged carbons where its $\overline{DI}$ = 0.410, its DIU = 100 and its δ = 1. Then, its planar D_3BIA is higher than that shown in Table 2.

Free energies of dehalogenation reactions of **10**-**12**, **16**-**18**, **21**-**23** have been used to confirm the coherence of the D_3BIA values (Table 2). Despite there is no good correlation between them, it is possible to verify that the smaller the free energy of dehalogenation the higher is the D_3BIA. The smallest $\Delta G_{(dehalogenation)}$ value is for the 1,3-dehydro-5-7-adamantanediyl dication **16**. $\Delta G_{(dehalogenation)}$ values of **10** to **12** are higher for than those from **16**, **17**, **18** and **21**. All of these $\Delta G_{(dehalogenation)}$ values fit to their relation with D_3BIA. For example, **10**, with D_3BIA=11.63, has $\Delta G_{(dehalogenation)}$ value (384.97 kcal mol^{-1}) higher than those from the species **18** (D_3BIA=16.39, $\Delta G_{(dehalogenation)}$=375.27 kcal mol^{-1}) and **21** (D_3BIA=19.82 , $\Delta G_{(dehalogenation)}$= 364.20 kcal mol^{-1}). However, $\Delta G_{(dehalogenation)}$ value of **22** does not fit in the analyzed group, according to its D_3BIA. Moreover, one can see that NICS values somewhat support all of these tendencies described above (Table 2).

Within monocationic species **25** to **27**, there seems to be a reasonable relation between D_3BIA and $\Delta G_{(dehalogenation)}$ values, where the 1,3-dehydro-7-adamantyl cation **25** (D_3BIA=16.47) has the smallest $\Delta G_{(dehalogenation)}$ value (Table 2).

Conclusions

The electronic interaction among bridged atoms is decisive in tridimensional aromaticity, along with uniformity of the delocalization index involving bridged atoms and their degeneracy. The density in the center of the cage [(3,+3) critical point] and the mean delocalization index values among bridged atoms are distinguished between tridimensional non-aromatic and aromatic species: non-aromatic species have small ρ(3,+3) and $\overline{DI}$ values while aromatic ones have high ρ(3,+3) and $\overline{DI}$ values. The degeneracy of the bridged atoms, the uniformity and the magnitude of their delocalization indexes are the electronic features that distinguish the dications **10** and **16.** However, the 1,9 diamantyl dication **10** has tridimensional aromaticity as well as the 1,3-dehydro-5,7-diboroadamantane **29**.

The positive charge is mainly distributed among the hydrogen atoms and the bridged atoms remain negatively charged in the dicationic and monocationic aromatic species.

Supplementary Information

This supplementary material shows the atoms in molecules theory, the rationale on D_3BIA, benzene and resonance, delocalization index and basis set dependence, the quantum atom, similarities between NICS and D_3BIA, comparison of the delocalization indexes between MP2 and B3LYP computed energy values of the species **1** to **46**, optimized structures of the species **1**, **2**, **4**, **6**, **7**, **10**, **11**, **13**, **15**, **16**, **17**, **19**, **21**, **22**, **25** and **26** and their bond lengths, and internal coordinates of optimized structures. This material is available free of charge at http://jbcs.sbq.org.br, as PDF file.

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Electronic Nature of the Aromatic Adamantanediyl Ions and its Analogues

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Atoms in Molecules (AIM) Theory

Bader's Atoms in molecules (AIM) theory[1] is based on the condition defining the quantum subsystem in terms of a property of the gradient vector of the charge density ($\nabla\rho$). The quantum condition of the subsystem states that the surface bounding the subsystem shall not be crossed by any gradient vectors of ρ. Since the gradient vector of ρ always points at the direction of greatest increase in ρ, it must always be perpendicular to lines of constant density. Let n be a unit vector normal to the surfaces, if the scalar product $\nabla\rho.n$ vanishes, then $\nabla\rho$ has no component through the surface. This surface, where $\nabla\rho.n = 0$, is called zero-flux surface, and it is the borderline between subsystems. The point, within the zero-flux surface, where gradient vectors are pointed at, and therefore where $\nabla\rho=0$, is called a bond critical point.

Inside the nucleus charge density exhibits local maxima. Outside the nucleus, charge density decreases as it moves away from the nucleus in any direction. Knowing that gradient path is a junction of gradient vectors at a given direction, then all the gradient paths within a subsystem will terminate at the nucleus. A nucleus is said to behave as an attractor in the gradient vector field.

The critical points[1] are classified according to their spectrum, which is a set of eigenvalues of the Hessian matrix $\nabla\nabla\rho$. The Hessian is a matrix of second derivatives of some function with respect to all possible coordinates. The eigenvalue equation of $\nabla\nabla\rho$ has three solutions (λ_1, λ_2, λ_3) corresponding to each eigenvector $\vec{u}i_{(i=1,2.3)}$ which coincides with the principal axes of curvature. The Laplacian of the electron density ($\nabla^2\rho$) is the sum of the eigenvalues of the Hessian, or $\nabla^2\rho = \lambda_1 + \lambda_2 + \lambda_3$. The nuclear attractor is denoted by (3,-3) because it is a maximum in all the principal axes. The bond critical point (BCP) is denoted by (3,-1) because it is a minimum in the direction of the nucleus but it is a maximum in another main direction. The ring critical point (RCP) is denoted by (3,+1), where is minimum in two principal axes.

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The Laplacian of the charge density, is defined as the sum of the three principal curvatures of the function at each point of the space (equation 1), which is also the trace of the Hessian of the density at the corresponding point.[2]

$$\nabla^2\rho(r) = \frac{\partial^2\rho(r)}{\partial x^2} + \frac{\partial^2\rho(r)}{\partial y^2} + \frac{\partial^2\rho(r)}{\partial z^2} \quad (1)$$

It is a convenient convention of using the negative of the Laplacian, L(r), rather than the Laplacian itself. Then, $L(r) = -\nabla^2\rho$. The density is a locally concentrated in those regions where $L(r)>0$, since $\nabla^2\rho(r)<0$ when $\rho(r)$ is a local maximum. Likewise, the density is a locally depleted in those regions where $L(r)<0$, since $\nabla^2\rho(r)>0$ when $\rho(r)$ is a local minimum.

Rationale on D_3BIA

The coherence between AIM and SCVB can be noticed from AIM results of benzene. The DI between carbon atoms in benzene is 1.39. Since DI between carbon atoms in ethane is 1.0, it is established that 0.39e. from π system is delocalized in each C-C bond of benzene ring. This means that 0.61e. from each $2p_z$ electron is localized in each carbon atom in benzene. This result matches with spin coupled (SC) one where a $2p_z$ electron of benzene is localized and distorted symmetrically towards neighboring carbon atoms on each side.[3] Moreover, Gerratt and co-workers[4] remarked that distortion effects of $C(2p_z)$ orbitals are not larger than those in C-C π bonds in conjugated systems. From AIM calculations, DI´s in hexatriene are 1.74 (for double bond) and 1.14 (for single bond). That brings another convergence of results between SC and AIM theories since it shows that delocalization in acyclic conjugated systems is greater than that in benzene.

Pauling and Wheland[5] stated that benzene is represented by a linear combination of five independent canonical structures. This view is emphasized by SC theory,[6,8] where spin coupling two electrons allows the description of the different possible resonance structures and generates the stability of aromatic systems.

From a more rigorous quantum mechanical standpoint,[8] benzene has no resonance[9] since there is not intersection of degenerate point group states. Resonance is only possible when the superposition of the hybrids can recover the full symmetry of the system. Resonance is related to degeneracy or near-degeneracy effects. Degeneracy may be due to the existence of symmetry groups that commute with hamiltonian.[9]

It means that benzene (D_{6h} symmetry) cannot be related to Kekulé (D_{3h} symmetry) or Dewar (D_{2h}) structures since it is forbidden by point group symmetry rules.[10] In this case, benzene stability is ascribed to maximum overlap among six degenerate single-electron states.[11]

Benzene and Resonance

Resonance is related to degeneracy or near-degeneracy effects. Degeneracy may be due to the existence of symmetry groups that commute with hamiltonian.[9] The eigenfunctions of the exact hamiltonian must transform as irreducible representations of the commuting symmetry groups. When a given group has degenerate representations, some or all eigenstates of the hamiltonian of the system will reflect its degeneracy.

The real Hilbert space is always partitioned into a direct sum of subspaces, each representing a different energy eigenvalue of the spectrum of the hamiltonian operator. The direct product decomposition is the mathematical tool to analyze the symmetry of the allowed individual states. It is related to the "ascent in symmetry" method[12] for decomposition of tensor spaces in independent parts and justified by the Littlewood-Richardson rules.[13] These rules define the only allowed decompositions of a tensor space (e.g. point group space), providing us with the possible symmetries of the resonance hybrids, which reproduce the total symmetry of the system. Only invariant subgroups of some larger group can accommodate coherent states.

The possible forms of decomposing D_{6h} point group in direct products[14] are:

$$D_{6h} = D_6 \otimes Ci,\ D_6 \otimes C_s,\ C_{6v} \otimes C_s$$

The ground state of benzene is not degenerate, and there is no theoretical or experimental evidence of a near-degenerate electronic state with same geometry as the ground state. If there is no intersection of degenerate point group states one cannot follow the symmetry descent path in this case. The only alternative would be that of an accidental symmetry, but this is not possible since there is not direct product decomposition[8] from D_{3h} (Kekulé structure) and D_{2h} (Dewar structure).

However, in SC study of benzene, Gerratt and coworkers[15] stated that spin coupling two electrons (within same D_{6h} symmetry) allows the description of the different possible resonance structures and generates the stability of aromatic systems.

Then, existence of resonance in benzene depends on the rigor of theory applied to it. By spin coupling ω electrons, within same D_{6h} symmetry in SC, it is possible to associate the obtained stability with resonance of hybrid structures.[15] Otherwise, benzene molecule cannot be represented by "hybrids" of symmetries D_{3h} and D_{2h} since it is forbidden by point group symmetry rules.[8]

Delocalization Index and Basis Set Dependence

As stated by Popelier:[16] "since AIM charges are obtained directly from electron density, they depend less on the basis set used compared with methods which separate charges on the Hilbert space of the basis set." In addition, atomic charge is related to charge transfer between atomic basins. And since the delocalization index is related to the interaction between atomic basins, we can assume that the rough value of the delocalization index is not so sensitive to a basis set.

The Quantum Atom

Bader´s AIM theory defines atomic subsystems within a molecular system from its density matrix calculated by a specific *ab initio* or density functional method. Then, AIM divides the molecular system into atomic subsystems.[17] AIM is based on quantum subsystem in terms of a property of gradient vector of charge density ($\nabla\rho$). In AIM it is possible to define all average properties of an atom. The definition of these properties is reduced to the quantum-mechanical definitions of the corresponding properties for a isolated atom. The summation of the atomic values of a given property over all atoms of the molecule yields the average property for the molecule.

Therefore, AIM provides the energy of an atom inside a molecule. The total energy of an atom is the sum of the kinetic energy and the potential energy. The kinetic energy an atom is obtained by the kinetic energy density. This means that the kinetic energy is evaluated locally at a point just like the electron density. Integration over the kinetic energy density gives the integrated kinetic energy over a given volume. There are two types of kinetic energies denoted by K(r) and G(r), defined in equations 2 and 3, respectively.[16]

$$K(r) = -\frac{1}{4} N \int d\tau' \left[\psi^* \nabla^2 \psi + \psi \nabla^2 \psi^*\right] \quad (2)$$

$$G(r) = \frac{1}{2} N \int d\tau' \nabla\psi^{*}.\nabla\psi \quad (3)$$

where **r** represents the coordinates of a position vector and $N\int d\tau'$ summarizes the one-electron integration mode.

After some mathematical treatment, it is possible to obtain the following relation between K(r) and G(r):

$$K(r) = G(r) - \frac{1}{4}\nabla^2\rho(r) \quad (4)$$

If we integrate equation 4 over the full space then we obtain that K(full space) = G(full space) since the last term of equation 4 vanishes. That is a consequence of Gauss´divergence theorem (equation 5).

$$\iiint_{\Omega} dV\nabla^2\rho = \iiint_{\Omega} dV\nabla.\nabla\rho = \iint_{S} dS\nabla\rho.\mathbf{n} = 0 \quad (5)$$

where S is an interatomic surface (IAS) for which $\nabla\rho.n = 0$.

Then, the kinetic energy of an atom is unambiguously defined and it is commonly called T(full space), as defined bellow (equation 6).

$$T(\Omega) = K(\Omega) = G(\Omega) \quad (6)$$

The potential energy is obtained from kinetic energy by using the virial theorem. The roots of the concept of virial theorem lie in the development of thermodynamics in the nineteenth century, when it was realized that internuclear forces in real gases induce deviations in ideal gas behavior. Soon after the mathematical formalism of quantum mechanics was established, Slater derived the quantum analogue of the classical virial theorem (equation 7).

$$2\int d\tau\psi^{*}\hat{T}\psi = -\int d\tau\psi^{*}\left(\sum_j \hat{r}_j\hat{F}_j\right)\psi \quad (7)$$

In equation 7, the sum runs over all the particles (both electrons and nuclei) and the integration is over the total space in which the system exists. The right-hand side of equation 7 is the potential energy of the system of particles because it is the expectation value of the position and force operators. We conclude that the kinetic energy of a system is always related to its potential energy.

Within the Born-Oppenheimer approximation, equation 7 becomes the molecular virial theorem shown in equation 8. The term on the right-hand side of equation 7 falls into two terms in equation 8, namely the expectation value of the electronic potential energy and a term depending on the forces on the nuclei.

$$2\int d\tau\psi_{el}^{*}\hat{T}\psi_{el} = -\int d\tau\psi_{el}^{*}\hat{V}_{el}\psi_{el} - \sum_{\alpha} r_{\alpha}\frac{\partial E}{\partial r_{\alpha}} \quad (8)$$

where ψ_{el} is the electronic wave function, $\hat{V}_{el}$ is the electron-electron repulsion and electron-nucleus attraction potential energy operator, E is the total energy of the molecule and r_{α} are the nuclear coordinates.

For a geometrically optimized molecule, all forces on the nuclei vanish and the term $\sum_{\alpha} r_{\alpha}\frac{\partial E}{\partial r_{\alpha}}$ in the molecular virial theorem vanishes. By simply restricting the integrals of the expectation values in equation 8 to the atomic subspace rather than full space, we obtain a relation between potential energy and kinetic energy inside an atomic basin (equation 9).

$$2T(\Omega) = -V(\Omega) \quad (9)$$

Historically, the roots of the theory of AIM lie in the observation that the kinetic energy of a molecular fragment bound by a zero-flux surface in $\nabla\rho$ could be transferred from one molecule to another.[18] The further development of AIM has been driven by the desire to formulate an atomic virial theorem which could render the atom into an energetically meaningful fragment.

Table S1 illustrates the calculation of atomic energies of all atoms in methanal.[16]

Table S1. The energies of the atoms in methanal (in a.u.)

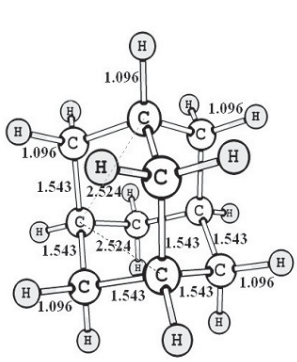
Atom	E / Ω
C	-37.4332
O	-75.9020
H	-0.6052
Total	-114.5456

Similarities Between NICS and D_3BIA

Table S2. D_3BIA and NICS of some aromatic compounds

Compound	D_3BIA x10^3	NICS
Benzene	10	-8.06
Pyridine	8.1	-6.8
Pyrazine	6.6	-5.34
Tryazine 1,4,5	2.57	-3.77
Tryazine 1,3,5	4.4	-4.07
Cycloheptatriene cation	4.0	-6.29
Anthracene (central ring)	6.0	-7.46

Optimized Structures of the Species **1**, **2**, **4**, **6**, **7**, **10**, **11**, **13**, **15**, **16**, **17**, **19**, **21**, **22**, **25** and **26** and their Bond Lengths.



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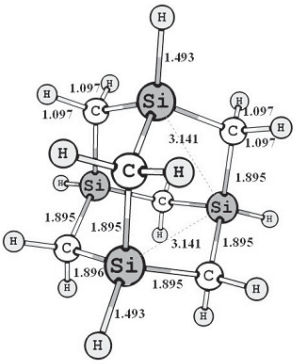

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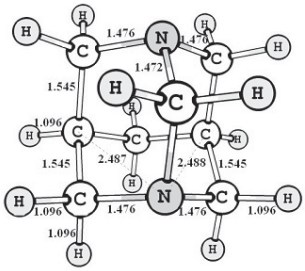

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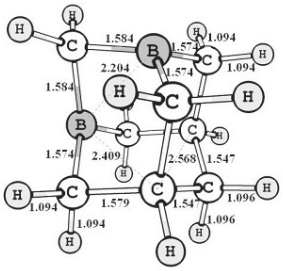

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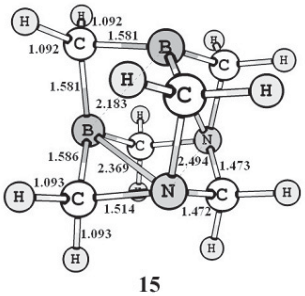

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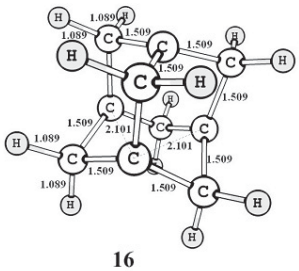

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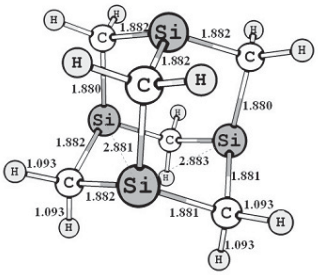

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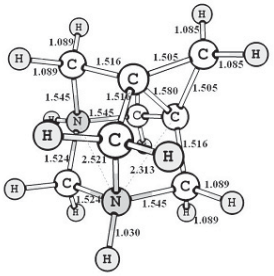

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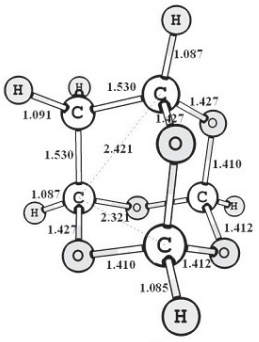

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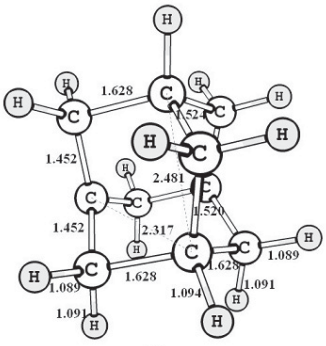

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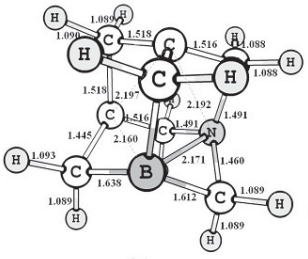

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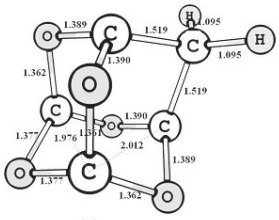

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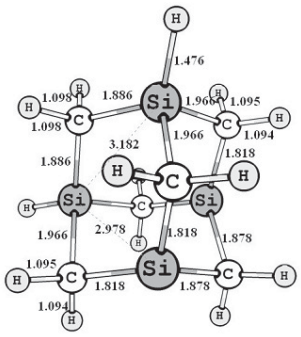

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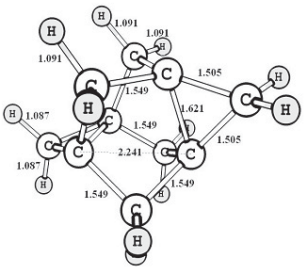

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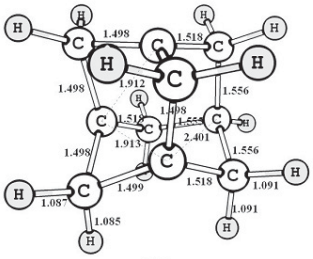

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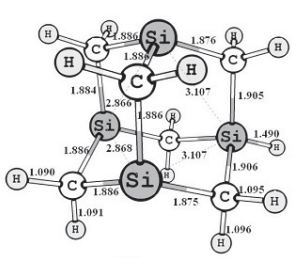

26

Table S3. Computed energy values of the species **1** to **46**

Entry	H / Hartree	S / (cal mol^{-1} K^{-1})	G / Hartree
1	-390.573479	76.061	-390.609618
2	-1396.321449	102.685	-1396.370238
3	-893.423903	92.051	-893.467640
4	-422.649468	80.494	-422.687713
5	-925.484387	91.575	-925.527897
6	-394.942092	84.722	-394.982346
7	-570.269011	77.465	-570.305817
8	-1576.414808	91.994	-1576.458517
9	-602.098577	78.616	-602.135930
10	-388.606446	82.909	-388.645838
11	-1394.438573	101.325	-1394.486715
12	-891.504397	91.702	-891.547967
13	-387.979284	80.885	-388.017715
14	-1393.769261	105.313	-1393.819298
15	-394.942074	84.529	-394.982236
16	-387.391465	80.422	-387.429676
17	-1393.241920	99.677	-1393.289280
18	-890.337262	89.828	-890.379942
19	-421.951412	80.549	-421.989684
20	-926.067598	91.992	-926.111307
21	-390.818886	81.693	-390.857701
22	-566.780090	77.250	-566.816794
23	-1573.080219	91.742	-1573.123808
24	-601.173938	79.207	-601.211572
25	-388.457228	81.045	-388.495736
26	-1394.223763	101.974	-1394.272214
27	-891.349536	91.400	-891.392963
28	-389.308420	80.737	-389.346781
29	-361.653560	83.127	-361.693056
30	-864.545577	92.935	-864.589734
31	-365.084394	84.080	-365.124343
32	-543.464416	91.392	-543.507839
33	-543.454349	92.974	-543.498523
34	-389.692107	82.262	-389.731192
35	-1309.851695	94.995	-1309.896831
36	-2315.701894	117.704	-2315.757819[a]
35	-1812.803290	107.493	-1812.854364
37	-1308.588536	94.510	-1308.633441
39	-2314.435291	118.636	-2314.491658
40	-1811.564830	106.588	-1811.615473
41	-1312.029887	96.184	-1312.075588
42	-1488.230438	89.453	-1488.272940
43	-2494.494200	107.219	-2494.545143
44	-848.949457	87.661	-848.991107
45	-1854.741158	111.039	-1854.793916
46	-1351.873878	98.644	-1351.920747
Cl^-	-460.301367	36.586	-460.318750

[a]Basis set 6-311++G(d,p)

Comparison of Delocalization Indexes Between MP2 and B3LYP

DI (C-C) = 1.379 (B3LYP)
DI (C-C) = 1.364 (MP2)

DI (C-C) = 1.437 (B3LYP)
DI (C-C) = 1.432 (MP2)

Internal Coordinates of Optimized Structures

Species 1

Charge = 0 Multiplicity = 1
C,0,1.4538527257,-0.0000000002,1.0280291215
H,0,1.4777495417,-0.0000000002,2.1241313909
H,0,2.4952334612,-0.0000000003,0.685191833
C,0,0.7285249617,1.261842248,0.5151449408
H,0,1.2452114793,2.156769548,0.8804974811
C,0,0.7285249614,-1.2618422482,0.5151449408
H,0,1.2452114788,-2.1567695483,0.8804974811
C,0,-0.7269263632,-1.2590733938,1.0280291212
H,0,-0.7388747715,-1.2797686438,2.1241313905
H,0,-1.247616731,-2.1609355657,0.6851918324
C,0,-0.7269263629,1.259073394,1.0280291212
H,0,-1.2476167305,2.160935566,0.6851918324
H,0,-0.7388747712,1.2797686439,2.1241313905
C,0,-1.4570499234,0.0000000002,0.5151449404
H,0,-2.4904229585,0.0000000003,0.8804974805
C,0,-1.4538527257,0.0000000002,-1.0280291215
H,0,-1.9864915016,-0.8811669218,-1.4046616119
H,0,-1.9864915013,0.8811669222,-1.4046616119
C,0,0.7269263632,1.2590733938,-1.0280291212
H,0,1.7563586907,1.2797686436,-1.4046616113
H,0,0.2301328119,2.1609355658,-1.4046616116
C,0,0.7269263629,-1.259073394,-1.0280291212
H,0,1.7563586903,-1.2797686441,-1.4046616113
H,0,0.2301328114,-2.1609355659,-1.4046616116
C,0,0.0000000003,0.,-1.5454348219
H,0,0.0000000004,0.,-2.6414924428

Species 2

Charge=0 Multiplicity = 1
C,0,0.3309365799,-0.0000057743,0.2409960137
H,0,0.3447185424,-0.0001367713,1.3375767505
H,0,1.3790158076,-0.0000224094,-0.0816308457
C,0,-2.3270485686,-1.5351006846,0.2070352342
H,0,-2.354642093,-1.5609532464,1.3029869641
H,0,-2.844874889,-2.4383817973,-0.1373459519
C,0,-2.3268811455,1.5353545108,0.2074481865
H,0,-2.8446331383,2.4387848969,-0.1366519002

H,0,-2.3544495774,1.5608834121,1.3034085709
C,0,-3.1819722706,0.0005007121,-2.3086530586
H,0,-3.7132156957,-0.8775908858,-2.6951569277
H,0,-3.7130996173,0.8787665901,-2.6949215454
C,0,-0.5225005491,1.535449125,-2.2773869725
H,0,0.5107807057,1.5607235336,-2.6438150473
H,0,-1.0099942468,2.4391257903,-2.6624155028
C,0,-0.5225929626,-1.5346941482,-2.2777667516
H,0,0.5107145451,-1.5598472136,-2.644133601
H,0,-1.010048567,-2.4382597575,-2.6631008381
Si,0,-0.5259663764,1.5706888655,-0.3830251718
H,0,0.1711096937,2.789325876,0.124249023
Si,0,-3.2469899947,0.0002584865,-0.4152359673
H,0,-4.6606347619,0.0002812524,0.0641708732
Si,0,-0.5261261512,-1.5704525642,-0.3834191633
H,0,0.1708067515,-2.789298869,0.1235489751
Si,0,-1.401091567,0.0004883583,-2.9581732472
H,0,-1.3824413292,0.0006563689,-4.4507792304

Species 3

Charge = 0 Multiplicity = 1
C,0,0.3925971753,-0.0000160839,0.2859839583
H,0,0.3949768083,-0.0001589627,1.3813310605
H,0,1.4364992315,-0.0000212484,-0.045349412
C,0,-2.3649939338,-1.2872070985,0.1104364631
H,0,-2.4787399278,-1.2569845715,1.2000467067
H,0,-2.9325370309,-2.1606220147,-0.2334927019
C,0,-2.3648702896,1.2874741581,0.1107785692
H,0,-2.9323349831,2.1610334543,-0.232912863
H,0,-2.4786103399,1.2569708588,1.2003818228
C,0,-2.9692592105,0.0002457483,-0.5194508685
H,0,-4.0441450443,0.000268385,-0.2984033547
C,0,-2.8474188554,0.000446043,-2.066059506
H,0,-3.3810048114,-0.8761787407,-2.4532673253
H,0,-3.3809121668,0.8772310897,-2.4530321386
C,0,-0.6270582254,1.2872930667,-2.2839515131
H,0,0.3741194892,1.2551866368,-2.7287478493
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H,0,-1.5382021955,0.0005989138,-3.7539486232
Si,0,-0.5506062956,-1.4892174594,-0.4012216199
Si,0,-0.5504683958,1.4894489858,-0.4008360402
H,0,0.0202304427,2.8036727378,0.0138333475
H,0,0.0199626977,-2.8036063746,0.0131025468

Species 4

Charge = 0 Multiplicity = 1
C,0,-0.000671011,-0.005653273,-0.0046293704
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H,0,1.037397622,-0.0366865286,-0.3535319547
C,0,-0.7148021438,1.2700016934,-0.5045620575
H,0,-0.2151673422,2.1643176524,-0.1144702673
C,0,-2.090121894,-1.1826987169,-0.0146278892
H,0,-2.0920443903,-1.1813405559,1.078875598
H,0,-2.5963668154,-2.0887243804,-0.3590792156
C,0,-2.1781914037,1.2139200379,-0.0102261052
H,0,-2.7457454393,2.0817565505,-0.3636280545
H,0,-2.217670208,1.2226655984,1.084635339
C,0,-2.8639825166,-0.0203477628,-1.9638316027
H,0,-3.404612975,-0.9133270677,-2.2966441448
H,0,-3.4295935579,0.8509322723,-2.3119241082
C,0,-0.7111365226,1.2687469789,-2.0471789537
H,0,0.317256019,1.2990306846,-2.4273285198
H,0,-1.2209791633,2.1606937014,-2.4312864543
C,0,-0.6868385889,-1.2401943103,-1.9584285358
H,0,0.3530236226,-1.2689054554,-2.302043111
H,0,-1.1656542159,-2.1681407972,-2.2899942839
C,0,-1.4264672594,-0.0099688113,-2.5303844338
H,0,-1.4483097952,-0.053594425,-3.6254916234
N,0,-0.6944266784,-1.2174289996,-0.4828171715
N,0,-2.8474123228,-0.0120636331,-0.4877836445

Species 5

Charge = 0 Multiplicity = 1
C,0,-0.0047409372,-0.0000000005,-0.0025900496
H,0,-0.0029312772,-0.0000000005,1.0929568337
H,0,1.0396892558,-0.0000000007,-0.3328969445
C,0,-2.7824242651,-1.2408857961,-0.2165963029
H,0,-2.9541567301,-1.1839316079,0.8630542985
H,0,-3.3891889705,-2.0807222064,-0.5762517905
C,0,-2.782424265,1.2408857959,-0.2165963033
H,0,-3.3891889698,2.0807222065,-0.5762517921
H,0,-2.9541567306,1.1839316085,0.863054298
C,0,-3.1726471321,-0.0000000005,-2.3061425037
H,0,-3.6928053994,-0.8851940976,-2.6842775398
H,0,-3.6928053997,0.8851940963,-2.6842775403
C,0,-1.0634248925,1.2406024723,-2.5814880322
H,0,-0.0890270442,1.1823587065,-3.0771360977
H,0,-1.5912701155,2.0811374503,-3.0479617296
C,0,-1.0634248925,-1.2406024732,-2.5814880321
H,0,-0.089027044,-1.1823587071,-3.077136097
H,0,-1.5912701152,-2.0811374512,-3.04796173
N,0,-3.3104653117,-0.0000000002,-0.8430863254
N,0,-1.8230315772,-0.0000000005,-2.891039445

Si,0,-0.9459796324,1.4932590504,-0.6893596166
H,0,-0.3891582029,2.8185371547,-0.284302923
Si,0,-0.9459796328,-1.4932590512,-0.6893596165
H,0,-0.3891582034,-2.8185371555,-0.284302923

Species 6

Charge = 0 Multiplicity = 1
C,0,0.1552060994,0.0000148161,0.1121862883
H,0,0.1173074784,-0.0001243276,1.2036514854
H,0,1.1805026193,0.0000211278,-0.264023778
C,0,-2.2076089656,-1.2953511095,0.0440664558
H,0,-2.2693514926,-1.2792472564,1.1362507596
H,0,-2.7418828727,-2.1776392183,-0.3198633481
C,0,-2.2074917682,1.2956177894,0.0444062962
H,0,-2.7416837995,2.1780491997,-0.3192953644
H,0,-2.2692364977,1.2792355994,1.1365863683
C,0,-2.9081316675,0.0002392173,-0.5246670404
C,0,-2.8512167995,0.0004415326,-2.0702902208
H,0,-3.3797865814,-0.8793930956,-2.4539804655
H,0,-3.3797095871,0.8804237785,-2.4537478345
C,0,-0.6412478384,1.2959855009,-2.1122075522
H,0,0.3783464046,1.2798000725,-2.508524806
H,0,-1.1528551135,2.1782340583,-2.5072651422
C,0,-0.6413660312,-1.2952875975,-2.1125501979
H,0,0.378230886,-1.2790904786,-2.508860434
H,0,-1.1530517318,-2.1773846507,-2.5078445295
C,0,-1.398844897,0.0004471076,-2.6028483278
B,0,-0.7655683722,1.1019991887,-0.5555576137
B,0,-0.7656669052,-1.1017084081,-0.5558461208
H,0,-3.9529253933,0.0002437105,-0.1964272317
H,0,-1.4095638244,0.0005931085,-3.697915519

Species 7

Charge = 0 Multiplicity = 1
C,0,0.020294489,0.0000000005,0.0144463801
H,0,0.0117524416,0.0000000017,1.1055666045
H,0,1.0490052857,-0.0000000003,-0.3492275759
O,0,-2.0864742065,1.1659975665,-0.0532258855
O,0,-2.086474208,-1.1659975647,-0.0532258848
O,0,-2.7252924221,0.0000000007,-1.9410580574
O,0,-0.7319825404,1.166062285,-1.9547923505
O,0,-0.7319825413,-1.166062284,-1.9547923499
C,0,-2.7214833343,0.0000000015,-0.5288066526
H,0,-3.7477135162,0.0000000014,-0.1778926953
C,0,-1.3893037538,0.,-2.3992349474
H,0,-1.3928208582,0.,-3.4837939472
C,0,-0.7413680279,-1.2104218096,-0.5284008423
C,0,-0.7413680253,1.2104218111,-0.528400844
H,0,-0.3319635456,-2.1741392378,-0.2366243691
H,0,-0.3319635437,2.1741392395,-0.2366243702

Species 8

Charge = 0 Multiplicity = 1
C,0,-0.034557691,0.,-0.0231669637
H,0,-0.0288574632,-0.0000000001,1.0721110167
H,0,1.0052267584,0.0000000002,-0.3672669699
O,0,-2.54649347,1.3263686386,-0.1746154398
O,0,-2.5464934698,-1.3263686388,-0.1746154401
O,0,-3.2980520048,0.0000000002,-2.3457877369
O,0,-0.9986174289,1.3252105227,-2.3513281951
O,0,-0.9986174288,-1.3252105224,-2.3513281953
Si,0,-0.9569018485,-1.5103163014,-0.6830384506
Si,0,-0.9569018488,1.5103163014,-0.6830384503
Si,0,-1.7646176061,0.0000000002,-3.0091410691
Si,0,-3.4200211232,-0.0000000001,-0.6795131167
H,0,-0.4529913557,-2.8447981923,-0.3253429232
H,0,-4.7992132346,-0.0000000006,-0.2020287542
H,0,-1.7667344112,-0.0000000006,-4.468696546
H,0,-0.4529913562,2.8447981922,-0.3253429225

Species 9

Charge = 0 Multiplicity = 1
C,0,0.006220515,-0.0112292987,0.0121197936
C,0,0.0145909097,-0.0256515165,1.5320015032
H,0,1.0370959966,-0.0139354624,1.9114477466
H,0,-0.5175799407,-0.898390246,1.9123512822
C,0,-0.7128195065,1.254496389,1.9099295044
O,0,0.6921585573,1.1505647389,-0.4603181023
O,0,-0.0064378933,2.3805647895,1.3842323278
O,0,-1.3024967974,2.2936918607,-0.5134531379
O,0,-1.3431878632,-0.0049289716,-0.460626109
O,0,-2.0417001359,1.2251145974,1.3838474966
N,0,-2.0417675114,1.1615601621,-0.0385595969
N,0,0.0484664069,2.3480255669,-0.0379018044
H,0,0.4882757519,-0.8604179171,-0.4672988323
H,0,-0.816313872,1.43653803,2.9774050658

Species 10

Charge = 2 Multiplicity = 1
C,0,1.4765072652,-0.0003529608,1.0720443757
H,0,1.4384137397,-0.0005485228,2.1615336502
H,0,2.500669351,-0.0004036998,0.6985070387
C,0,0.6282669413,1.100222305,0.4562738162
C,0,0.6283288465,-1.1007802742,0.4561004967
C,0,-0.6661970338,-1.335541726,1.0696439487
H,0,-0.6748326809,-1.3060902985,2.1600309818
H,0,-1.1927514051,-2.2131534766,0.6963951381

C,0,-0.6660563955,1.3354714049,1.0699055373
H,0,-1.1923769867,2.2132571282,0.6967368976
H,0,-0.6747122405,1.30587985,2.1602861346
C,0,-1.4097608294,0.0000887505,0.5093932062
H,0,-2.3975224033,0.0001206478,0.9807653771
C,0,-1.3973240983,0.0001413008,-1.0145524876
H,0,-1.9274883707,-0.8763492788,-1.3995753271
H,0,-1.9276868206,0.8765222274,-1.3995430785
C,0,0.8109918825,1.3356764011,-0.9644054198
H,0,1.8451185435,1.3062284725,-1.3102310899
H,0,0.293121691,2.2134628003,-1.3492136028
C,0,0.8109494096,-1.3353341811,-0.9648096316
H,0,1.8450840805,-1.3057432205,-1.3106073536
H,0,0.2930994144,-2.212946052,-1.3500441068
C,0,0.0478911161,0.0002891489,-1.4982051105
H,0,0.1902814617,0.0004824082,-2.5833730473

Species 11

Charge = 2 Multiplicity = 1
C,0,0.3447731878,0.0000074159,0.2507152789
H,0,0.3218514842,-0.0001330782,1.3447378234
H,0,1.3783927876,0.000009471,-0.1083631378
C,0,-2.3067654706,-1.5839297168,0.2567203566
H,0,-2.3259308223,-1.5658288222,1.3507064848
H,0,-2.8496046694,-2.4682225079,-0.0916466791
C,0,-2.3066290072,1.5841537738,0.2571487904
H,0,-2.8493999139,2.468587138,-0.0909670432
H,0,-2.3257835701,1.5657497368,1.3511300943
C,0,-3.1488352368,0.0004958676,-2.2869202294
H,0,-3.6874136223,-0.8725427877,-2.6779683144
H,0,-3.6873195859,0.8737031709,-2.6777220442
C,0,-0.4701589809,1.5849455774,-2.2728959681
H,0,0.5637911063,1.5688714574,-2.6309655608
H,0,-0.971083174,2.4687801296,-2.6802502735
C,0,-0.47027353,-1.5841834515,-2.2733109589
H,0,0.5636850652,-1.5680590244,-2.6313552476
H,0,-0.9712320964,-2.4678779442,-2.6809259224
Si,0,-0.6482998375,1.4211553492,-0.4708796486
Si,0,-3.2642076594,0.0002416149,-0.4046872197
H,0,-4.6110913225,0.0002200411,0.1990752994
Si,0,-0.6484182396,-1.4208709632,-0.4712535331
Si,0,-1.3945338505,0.0005067091,-2.9791610228
H,0,-1.2368633267,0.0006839543,-4.4466937513

Species 12

Charge = 2 Multiplicity = 1
C,0,0.3773029533,-0.0000129297,0.2759258299
H,0,0.3436560113,-0.0001543492,1.3696248044
H,0,1.4080378514,-0.0000088078,-0.0914340709
C,0,-2.3864418553,-1.3484324514,0.1663814733
H,0,-2.4796521641,-1.3091558792,1.2531528907
H,0,-2.9772165318,-2.1898288381,-0.2020502893
C,0,-2.3863204022,1.3486816931,0.1667409598
H,0,-2.9770225897,2.1902284771,-0.2014632039
H,0,-2.4795291454,1.3091220767,1.2535024535
C,0,-2.9246235762,0.0002369121,-0.5028032745
H,0,-3.9851198662,0.0002480364,-0.2193154397
C,0,-2.8191843377,0.0004384431,-2.0471628321
H,0,-3.3532343831,-0.8723682009,-2.4337645467
H,0,-3.3531516509,0.8733997854,-2.4335295665
C,0,-0.5809415169,1.3478958281,-2.3217119941
H,0,0.4236037947,1.3086918557,-2.7469233353
H,0,-1.1131615673,2.190557253,-2.7683030029
C,0,-0.5810593054,-1.3471459546,-2.3220675808
H,0,0.4234893365,-1.3079170348,-2.7472688119
H,0,-1.1133533297,-2.1896415688,-2.7688833247
C,0,-1.3843050404,0.0004505507,-2.6285277389
H,0,-1.4442074168,0.0005981005,-3.7245171847
Si,0,-0.6570165088,-1.3709464442,-0.4779669298
Si,0,-0.6568963196,1.3712126514,-0.4776060265

Species 13

Charge = 0 Multiplicity = 1
C,0,0.0421487693,-0.0142324884,0.0051609631
H,0,0.065455425,-0.1227864846,1.0902391188
H,0,1.0708112968,0.0857557937,-0.343385662
C,0,-0.8640549651,1.111718338,-0.5518390886
C,0,-0.8044302707,-1.1259043629,-0.6632039038
C,0,-2.0907238333,-0.9204346652,0.1759599343
H,0,-1.8829234747,-0.9510827453,1.2462941178
H,0,-2.9132972087,-1.6077471912,-0.0255324955
C,0,-2.0081686637,1.847243927,0.0928225124
H,0,-2.4161696811,2.7101972114,-0.4278502202
H,0,-1.9819412809,1.987019417,1.1708730766
C,0,-2.3521193712,0.4795684686,-0.4326529304
C,0,-2.6510068071,0.0086138696,-1.8780036523
H,0,-3.4247891974,-0.7598330849,-1.8998948738
H,0,-2.930645126,0.7846508267,-2.5917776418
C,0,-0.5188934756,0.9164638382,-2.0493658572
H,0,0.5579751895,0.9366733756,-2.2214968767
H,0,-0.9825507572,1.6153672427,-2.7467265899
C,0,-0.6005101965,-1.8515449643,-1.9657632658
H,0,0.4196736018,-2.0005798411,-2.3114148945
H,0,-1.2396555933,-2.7052225241,-2.1777952216
C,0,-1.1961196582,-0.4761418167,-2.0986395409

Species 14

Charge = 0 Multiplicity = 1

C,0,-0.3778964947,-0.0168070476,-0.2477657395
H,0,-0.3880021051,-0.0341933652,0.8429021434
H,0,0.6617664439,0.0007173593,-0.582696739
C,0,-3.0864972558,-1.4909759381,-0.305674471
H,0,-3.0785077738,-1.450372493,0.7840294972
H,0,-3.6091671236,-2.3839461132,-0.6483063916
C,0,-3.117331226,1.5951403001,-0.2810616087
H,0,-3.6005601532,2.5059763128,-0.6413547762
H,0,-3.1482046818,1.5911119353,0.8087767164
C,0,-4.0152430293,-0.0212513071,-2.8662347991
H,0,-4.5388366044,-0.9219161276,-3.1915281825
H,0,-4.534397739,0.8468920288,-3.278864631
C,0,-1.333827753,1.4204837895,-2.7614454327
H,0,-0.2959293679,1.448478972,-3.1361484096
H,0,-1.7715423371,2.3432636444,-3.1784273269
C,0,-1.3011684082,-1.6282722388,-2.8287732597
H,0,-0.2866544131,-1.6835756056,-3.2296059275
H,0,-1.844779847,-2.5188262214,-3.1508867742
Si,0,-3.7802250824,0.0855592549,-1.0639166678
Si,0,-1.3435125452,-1.3628731454,-1.0240792471
Si,0,-1.1954620563,1.7100764425,-0.8655763125
Si,0,-2.1786815743,-0.03469047,-3.7184778558

Species 15

Charge = 0 Multiplicity = 1

C,0,-0.2926793558,-0.0350223746,-0.1964615944
H,0,-0.3124840212,0.0068648134,0.8949729534
H,0,0.7489680025,0.0233614066,-0.5211773775
C,0,-2.625652422,-1.3839426114,-0.296338409
H,0,-2.6515487843,-1.4193755755,0.7949413958
H,0,-3.1553870798,-2.2267499566,-0.7458720864
C,0,-2.415198387,1.302295718,-0.2034210016
H,0,-2.8107631487,2.266490034,-0.5317205428
H,0,-2.3744782386,1.3042717336,0.8882454662
C,0,-3.1532094649,0.1119412152,-2.4802901819
H,0,-3.6380634068,-0.72483402,-2.9885575956
H,0,-3.5762124877,1.0391851495,-2.8748870972
C,0,-0.9845750259,1.2098367845,-2.1956638286
H,0,0.0572056754,1.1980239209,-2.5250063852
H,0,-1.4440680452,2.1431600361,-2.529805456
C,0,-1.0359352594,-1.2212064723,-2.4728903655
H,0,-0.0144276683,-1.2020873325,-2.8608900329
H,0,-1.577487755,-2.0216947585,-2.9821831748
B,0,-3.0288210873,0.0198372649,-0.902348987
B,0,-1.1818785311,-1.1444681974,-0.8956367111
N,0,-1.6850568511,0.0935939925,-2.8515575328
N,0,-0.9977851589,1.1962715013,-0.7232330134

Species 16

Charge = 2 Multiplicity = 1

C,0,0.0532371438,0.0000288549,0.0380406627
H,0,0.019665738,-0.0001176823,1.1261663249
H,0,1.0770444598,0.0000345803,-0.3319842953
C,0,-0.8236750735,1.0502730405,-0.5980744474
C,0,-0.8237685934,-1.049965951,-0.5983595516
C,0,-2.1838837556,-1.2906758733,0.0096244553
H,0,-2.1877442417,-1.2731267941,1.0980517762
H,0,-2.6876797234,-2.1741009872,-0.3788465071
C,0,-2.1837703437,1.2909412141,0.0099722878
H,0,-2.6874852728,2.1745155765,-0.3782642079
H,0,-2.1876336875,1.2731006171,1.0983949911
C,0,-2.6436825079,0.0002384109,-0.6215862772
C,0,-2.9036272163,0.0004483554,-2.1077895917
H,0,-3.3982638307,-0.9001030724,-2.467511509
H,0,-3.3981855833,0.9011385459,-2.4672716323
C,0,-0.6665722904,1.2914068409,-2.0790495286
H,0,0.3674925865,1.2734770651,-2.4188211223
H,0,-1.1918970593,2.174737921,-2.4380121502
C,0,-0.6666864497,-1.2907142911,-2.0794003324
H,0,0.3673799269,-1.2727858372,-2.4191673702
H,0,-1.192091044,-2.1739016981,-2.4385993257
C,0,-1.4091652097,0.0004111607,-2.320907649

Species 16 triplet

Charge = 2 Multiplicity = 3

C,0,-0.011806405,-0.0001417383,-0.0087496061
H,0,-0.0274627186,0.0985818692,1.0786626299
H,0,1.0172441828,-0.0985582546,-0.3601695611
C,0,-0.7708469345,1.1404881378,-0.6762383537
C,0,-0.8822392086,-1.1404577487,-0.5239178784
C,0,-2.2394486057,-1.3862467089,0.0872763638
H,0,-2.240334542,-1.3631560337,1.1777145694
H,0,-2.7442911664,-2.2696851698,-0.3057245528
C,0,-2.1503060173,1.2347908558,-0.035554074
H,0,-2.7433012912,2.0730005783,-0.4071160132
H,0,-2.0777633107,1.2814242493,1.0529589698
C,0,-2.6941297869,-0.0940873668,-0.547001537
C,0,-2.837996713,0.0004552915,-2.0610235873
H,0,-3.2868679512,-0.8884469041,-2.5091232097
H,0,-3.4030501495,0.8893015453,-2.3492951973
C,0,-0.6101064737,1.3872697355,-2.1558156728
H,0,0.4264650058,1.3656917573,-2.4944967693
H,0,-1.1417055809,2.2700438071,-2.5133112265
C,0,-0.6998712523,-1.2346410978,-2.0340607403
H,0,0.3576632647,-1.2828525312,-2.3018815312
H,0,-1.2375776466,-2.0723126353,-2.4827463424
C,0,-1.3532587268,0.0947983587,-2.3937816798

Species 17

Charge = 2 Multiplicity = 1
C,0,0.3782779497,-0.0000038695,0.2761524457
H,0,0.3651883656,-0.000150492,1.3689072705
H,0,1.4156146984,-0.0000010158,-0.0671249642
C,0,-2.3500013557,-1.5760140625,0.2390937091
H,0,-2.3659979968,-1.5821685085,1.3317233287
H,0,-2.8617567485,-2.4691372847,-0.1280371846
C,0,-2.3498657954,1.5762415005,0.2395373619
H,0,-2.8615508986,2.4695164216,-0.1273218216
H,0,-2.3658480546,1.5820736529,1.332169104
C,0,-3.2292751558,0.0005036096,-2.3413087141
H,0,-3.7433092827,-0.888411688,-2.7153750293
H,0,-3.7432205673,0.8895705826,-2.7151367175
C,0,-0.4990035968,1.5756027555,-2.3101229554
H,0,0.5347404247,1.5793234736,-2.6645799361
H,0,-1.0048147837,2.4698406254,-2.6824366472
C,0,-0.4991007172,-1.5748179352,-2.3105511441
H,0,0.5346587229,-1.5784548946,-2.6649668138
H,0,-1.0049137485,-2.4689357049,-2.6831480194
Si,0,-0.5997407348,1.4405716783,-0.437333786
Si,0,-3.0968138128,0.0002459123,-0.4658861062
Si,0,-0.5998637815,-1.4403001318,-0.4377287138
Si,0,-1.4044078941,0.0004856723,-2.7997199131

Species 18

Charge = 2 Multiplicity = 1
C,0,0.4066037246,-0.0000148132,0.2956636452
H,0,0.3950393034,-0.0001623224,1.3895296159
H,0,1.4442755814,-0.0000136737,-0.0502722391
C,0,-2.4501274294,-1.277018396,0.1259647339
H,0,-2.5183937145,-1.2500384726,1.2136145209
H,0,-3.0063273793,-2.1166143098,-0.2920858046
C,0,-2.4500159675,1.2772800648,0.1263067508
H,0,-3.0061436262,2.1170367507,-0.2915168579
H,0,-2.5182826341,1.2500126786,1.2139493583
C,0,-2.6784856954,0.0002301799,-0.5435857137
C,0,-2.8317254384,0.0004377687,-2.0556739356
H,0,-3.3375033068,-0.8917967646,-2.4230734759
H,0,-3.3374230035,0.8928159587,-2.4228351399
C,0,-0.6385595815,1.2775837315,-2.3692220379
H,0,0.3742754109,1.2509384458,-2.7716682323
H,0,-1.2085247631,2.1175023704,-2.7675983439
C,0,-0.6386697166,-1.2768157424,-2.3695643068
H,0,0.3741677925,-1.2501512548,-2.7720028444
H,0,-1.2087076867,-2.1165787323,-2.7681645916
C,0,-1.3458649444,0.0004154447,-2.3790403543
Si,0,-0.5853728187,-1.4237350618,-0.426251428
Si,0,-0.5852481212,1.4239842205,-0.4258686138

Species 19

Charge = 2 Multiplicity = 1
C,0,0.2422301853,-0.0000005684,0.1761665819
H,0,0.1877181839,-0.0001349975,1.2595761557
H,0,1.2565673149,0.0000084396,-0.2083461064
C,0,-0.7941348007,0.7900856845,-0.5771760635
C,0,-0.7941988299,-0.7898066208,-0.5773777649
C,0,-2.1505919062,-1.1786085199,-0.02263621
H,0,-2.2501055091,-1.1457178734,1.0615269959
H,0,-2.543821709,-2.1250732641,-0.3915424973
C,0,-2.1504813562,1.1788855141,-0.0223251721
H,0,-2.5436195489,2.1254864125,-0.3909803354
H,0,-2.2499924313,1.1457157514,1.0618296328
C,0,-2.9215328029,0.0004512233,-2.1206499942
H,0,-3.4252932667,-0.8941571685,-2.4865624766
H,0,-3.4252121528,0.8952008104,-2.4863288645
C,0,-0.6870170068,1.1790035041,-2.038394133
H,0,0.3130337778,1.1454696016,-2.4687913245
H,0,-1.1590941036,2.1258217045,-2.2974606365
C,0,-0.6871229998,-1.1783281268,-2.0387060966
H,0,0.312929659,-1.1447691187,-2.469096998
H,0,-1.1592843809,-2.1250344767,-2.2980274665
N,0,-2.9678392572,0.0002534894,-0.5973264281
N,0,-1.4873490663,0.0004535959,-2.6374093093
H,0,-3.9567269093,0.0002634826,-0.3105708003
H,0,-1.5212379916,0.0005921575,-3.666471579

Species 20

Charge = 2 Multiplicity = 1
C,0,0.0069151753,0.0000000018,0.0055121619
H,0,0.0175435117,0.000000001,1.1013918349
H,0,1.0541998196,0.0000000023,-0.3169511709
C,0,-2.7617280837,-1.2789575652,-0.2147587068
H,0,-2.9481428574,-1.1899149353,0.8567991677
H,0,-3.3674513039,-2.1111728311,-0.5829141796
C,0,-2.7617280843,1.2789575685,-0.2147587055
H,0,-3.3674513043,2.1111728348,-0.5829141781
H,0,-2.9481428584,1.189914938,0.8567991688
C,0,-3.2445365581,0.0000000024,-2.3597144975
H,0,-3.7499776383,-0.8932630631,-2.727520726
H,0,-3.749977638,0.8932630685,-2.7275207246
C,0,-1.0539163969,1.2787740371,-2.562409878
H,0,-0.0915129391,1.1885820551,-3.0690708664
H,0,-1.5894916192,2.1114591454,-3.0257422867
C,0,-1.0539163964,-1.2787740305,-2.5624098797
H,0,-0.0915129385,-1.188582047,-3.0690708676
H,0,-1.589491618,-2.1114591384,-3.0257422899
N,0,-3.3242317528,0.0000000019,-0.855576198
N,0,-1.8372604725,0.0000000034,-2.90003919

H,0,-4.3328261513,0.0000000017,-0.6631301343
H,0,-1.9652945852,0.0000000042,-3.9187722402
Si,0,-0.9011601519,-1.5000467781,-0.6570356993
H,0,-0.4398567095,-2.8565107976,-0.3210485538
Si,0,-0.9011601524,1.5000467822,-0.6570356974
H,0,-0.4398567103,2.8565108015,-0.32104855

Species 21

Charge = 2 Multiplicity = 1
C,0,1.3777603827,-0.0001780658,1.1661523206
H,0,1.302906398,-0.0048190181,2.2538238734
H,0,2.4171657275,0.0045457897,0.84066106
C,0,-0.76221375,-1.4077928532,1.0463246383
H,0,-0.8439801498,-1.3705016037,2.135429363
H,0,-1.2413523168,-2.2871706732,0.6191866645
C,0,-0.7713988068,1.3940121807,1.057902138
H,0,-1.2567282534,2.2735838206,0.6381922647
H,0,-0.8527321631,1.3471454194,2.1466626393
C,0,-1.4168684136,0.0002015205,-1.2084032219
H,0,-1.8277180941,-0.9001380579,-1.6617167765
H,0,-1.833710858,0.9014629037,-1.654351581
C,0,0.7599840062,1.2660686647,-0.9574731689
H,0,1.7967173908,1.2160378309,-1.284081606
H,0,0.2490951173,2.1221012866,-1.3943581214
C,0,0.7685517557,-1.2530494189,-0.9675815149
H,0,1.8049703918,-1.1929241996,-1.2935103115
H,0,0.2639884793,-2.1090215492,-1.4118890281
B,0,-1.3092347337,-0.0060214945,0.4001732904
N,0,0.0406226232,0.0054356987,-1.3003221041
C,0,0.5420754132,1.0979332767,0.533278143
C,0,0.549308352,-1.098569366,0.5243573052

Species 22

Charge = 2 Multiplicity = 1
C,0,0.0667140278,-0.1533810693,-0.0142931676
C,0,-0.1321167465,-0.0529087018,1.985136643
C,0,1.3325125794,0.0410520951,2.3757294364
H,0,1.824968706,-0.9350178246,2.4314894811
H,0,1.5066204937,0.700679081,3.2318137833
C,0,1.5343078649,0.7335797542,1.0390932709
C,0,-0.2732585892,1.5954793869,0.8395604618
O,0,-0.4633984549,-0.9362763169,0.964193501
O,0,1.4210097501,-0.0455092641,-0.1055185393
O,0,-0.6484246516,0.9789155365,-0.3329342508
O,0,-0.8656430002,1.126494942,1.9726059393
O,0,1.0188765566,2.0174539326,0.9028462235

Species 23

Charge = 2 Multiplicity = 1
C,0,0.126607065,-0.0000156583,0.0920042963
H,0,0.0996187347,-0.0113885155,1.1880609004
H,0,1.1648466141,0.0113390447,-0.2598853842
O,0,-2.4650424703,1.3241228917,-0.1300657676
O,0,-2.4450794264,-1.3591958867,-0.1571994747
O,0,-3.208812926,0.0000602266,-2.3368196325
O,0,-0.8981032677,1.3584829995,-2.283761436
O,0,-0.8783146546,-1.3231204559,-2.3109013111
Si,0,-0.8628757889,-1.4451451394,-0.6549456543
Si,0,-0.8850005331,1.4448909726,-0.6249854678
Si,0,-1.6550763306,0.0192428356,-2.9442456976
Si,0,-3.309459994,-0.0192732845,-0.6706189794

Species 24

Charge = 2 Multiplicity = 1
C,0,-0.0426783197,0.1094778764,0.06311146
C,0,0.0139905988,-0.032563268,1.5678278695
H,0,0.9971840679,0.0269646741,2.0340597546
H,0,-0.7025601106,-0.7119052897,2.0288804496
C,0,-0.5367199924,1.2378008168,0.9594845257
O,0,0.9531286269,0.7124773665,-0.7481120009
O,0,0.2302215943,2.3650836647,0.563822759
O,0,-0.8696880363,2.0223441839,-1.5054578715
O,0,-1.1588997232,-0.205353357,-0.7559391752
O,0,-1.8812298558,1.4462846482,0.5576264361
N,0,-1.7509871404,1.0660159932,-0.7885166383
N,0,0.4265780543,2.0143119734,-0.7801569273
H,0,1.038822467,2.6919352172,-1.296139588
H,0,-2.6615238834,1.081499632,-1.3090283436

Species 25

Charge = 1 Multiplicity = 1
C,0,0.0060621513,-0.0499433977,0.0044366137
H,0,-0.0011833628,0.0515271476,1.0908328413
H,0,1.0367703484,0.0522331281,-0.3387649184
C,0,-0.8935190824,0.983778798,-0.6485995125
C,0,-0.6265436516,-1.3943719721,-0.4557201234
C,0,-2.1165146922,-1.2751571174,-0.0224796501
H,0,-2.2217112214,-1.2297324835,1.0625958905
H,0,-2.7129579027,-2.1131324298,-0.3865583751
C,0,-2.2032556551,1.3253916524,-0.005725577
H,0,-2.7102475794,2.2132477751,-0.374732347
H,0,-2.1892318369,1.2762833706,1.0782064614
C,0,-2.5495400671,0.0275742208,-0.669815923
C,0,-2.9216601604,0.035986009,-2.1210370087
H,0,-3.3912336668,-0.8810706988,-2.4617169607

H,0,-3.4292744179,0.9236951875,-2.4895348446
C,0,-0.6875294149,1.3254026392,-2.0928789276
H,0,0.3477413523,1.2762033262,-2.414347516
H,0,-1.195409274,2.2131333084,-2.4608646805
C,0,-0.676365938,-1.2748583945,-2.0059047565
H,0,0.3228342048,-1.2294163336,-2.4419159745
H,0,-1.207210483,-2.1130380975,-2.4599637623
C,0,-1.4263034478,0.0275209623,-2.2176331211
H,0,-0.1166362697,-2.2862820693,-0.0853994958

Species 26

Charge = 1 Multiplicity = 1
C,0,0.3207531931,-0.0220275158,0.2349531227
H,0,0.328853021,0.0195128483,1.32966769
H,0,1.3670415705,0.0211724447,-0.08651691
C,0,-2.3005196362,-1.5385721189,0.1995878996
H,0,-2.3645633348,-1.54119824,1.2931454894
H,0,-2.8535378199,-2.4180684491,-0.1479134607
C,0,-2.3710513993,1.6122424085,0.2209874878
H,0,-2.8822238033,2.5048833104,-0.1390254993
H,0,-2.3819302656,1.6081236957,1.3121386397
C,0,-3.2493812594,0.039711026,-2.3555299124
H,0,-3.7544417895,-0.8549039648,-2.7235572798
H,0,-3.7660143828,0.9229475982,-2.7303925562
C,0,-0.5223217186,1.6114454529,-2.3238151624
H,0,0.5119999612,1.6027486412,-2.6718752106
H,0,-1.0190104561,2.5058412445,-2.6989544118
C,0,-0.5226309122,-1.5366462858,-2.2525656127
H,0,0.4967785967,-1.5385273654,-2.6535588295
H,0,-1.0238824048,-2.4170160031,-2.6693249719
Si,0,-3.0976556646,0.0185199347,-0.4772736632
Si,0,-1.4158951943,0.0201054664,-2.798283186
Si,0,-0.4789786122,-1.6494237204,-0.3510054359
H,0,0.217095132,-2.8656847992,0.1545644765
Si,0,-0.6145398738,1.4535039211,-0.4471471481

Species 27

Charge = 1 Multiplicity = 1
C,0,0.3423499755,-0.0334119266,0.2496116264
H,0,0.3533242938,0.0089645141,1.3446550691
H,0,1.3893250303,0.0092661631,-0.0710643337
C,0,-2.3461106776,-1.2467698301,0.11448213
H,0,-2.4393588982,-1.184842193,1.2003160724
H,0,-2.9848619392,-2.055328408,-0.251933064
C,0,-2.5097006549,1.3030902546,0.0989794231
H,0,-3.0386468219,2.148960501,-0.3335546356
H,0,-2.552602127,1.2921453591,1.1861050005
C,0,-2.8306218689,0.0195462834,-2.0545507986
H,0,-3.3149619524,-0.8906090491,-2.4061710821
H,0,-3.3540393884,0.8964280149,-2.4341685539
C,0,-0.6832468345,1.3031953949,-2.4188871826
H,0,0.3365962594,1.2924010481,-2.7979579554
H,0,-1.2586856571,2.1495429467,-2.7861639135
C,0,-0.6178828441,-1.2464102187,-2.2670320685
H,0,0.3856683343,-1.1842477226,-2.6922470297
H,0,-1.1637538494,-2.05514051,-2.7610165185
Si,0,-0.5143448663,-1.5959771658,-0.3751326623
H,0,0.0084651369,-2.9347868427,0.0040606476
Si,0,-0.5736336935,1.4853666282,-0.418185479
C,0,-1.3482552378,0.0389002411,-2.3606597349
C,0,-2.6610787761,0.0384060479,-0.5511793944

Species 28

Charge = 0 Multiplicity = 1
C,0,-0.0077113029,0.0525352374,-0.0480516597
H,0,-0.0145929572,-0.1539866623,1.0252282309
H,0,1.0359734406,0.0521789231,-0.3790126323
C,0,-0.7127476269,1.3775144793,-0.4366579528
H,0,-0.2273544133,2.2818153339,-0.0501301024
C,0,-0.8943559334,-0.9229590501,-0.8248729571
C,0,-2.196785802,-1.2112236949,-0.0754747626
H,0,-2.0351743083,-1.3189337646,1.0001103821
H,0,-2.711092061,-2.1116966777,-0.4263139212
C,0,-2.2034327676,1.3244598047,0.0375800469
H,0,-2.720217122,2.2277265257,-0.3064051767
H,0,-2.2312029954,1.3475861108,1.1330350383
C,0,-2.9849088653,0.065528738,-0.4658943444
H,0,-4.0179516616,0.092983152,-0.0986680804
C,0,-2.8525706015,-0.033457588,-2.0071677543
H,0,-3.3784483873,-0.9141660804,-2.3900723953
H,0,-3.2362104374,0.8396861049,-2.5411183977
C,0,-0.6640211468,1.2301906728,-1.9792507857
H,0,0.3688780589,1.2489666285,-2.3418466948
H,0,-1.2182262318,2.0047922771,-2.5152856007
C,0,-0.577831855,-1.442319432,-2.2018536344
H,0,0.4571792692,-1.4092722978,-2.5332084503
H,0,-1.1193506035,-2.3178132185,-2.5519514953
C,0,-1.3295328791,-0.1415977946,-2.1049867758

Species 29

Charge = 0 Multiplicity = 1
C,0,0.0662530246,-0.1055426153,0.1044185463
H,0,-0.0011412372,-0.0536943287,1.1898745492
H,0,1.087089161,-0.3176842657,-0.21204353
C,0,-0.9427941659,-1.0340564433,-0.4874681424
C,0,-2.3120369894,-1.1490713227,0.0983865612
H,0,-2.3091659272,-1.0670394062,1.1840766667
H,0,-2.8455723582,-2.0433135041,-0.2225937785

C,0,-2.0863718458,1.5714978408,-0.1068966869
H,0,-2.4792570749,2.4680921559,-0.5859824442
H,0,-2.1316476835,1.6687487263,0.9776950489
C,0,-2.8371433471,0.0613937223,-2.2621444464
H,0,-3.3774203483,-0.8181212389,-2.6111582323
H,0,-3.1880936759,0.9593482065,-2.7679983255
C,0,-0.4588762747,1.1047590767,-2.2570140389
H,0,0.5552494317,0.9079827161,-2.6035701527
H,0,-0.8807539153,1.9721198972,-2.7622739357
C,0,-0.7701907566,-1.419176345,-1.9317716535
H,0,0.2689602339,-1.552838968,-2.2313343034
H,0,-1.3744945162,-2.2734721091,-2.2354962398
C,0,-1.3526607348,-0.0896884242,-2.32932039
B,0,-2.6691752268,0.2142286996,-0.6720927799
B,0,-0.6908706731,1.0824884032,-0.6678227655

Species 30

Charge = 0 Multiplicity = 1
C,0,0.0190448765,-0.0287820214,-0.0104922329
H,0,-0.0039207849,0.0015394757,1.0807728255
H,0,1.0448351678,-0.1632501986,-0.3565716025
C,0,-2.8799241249,-1.1512771764,-0.0681428146
H,0,-2.9190908837,-1.1247158668,1.0227468178
H,0,-3.5358778973,-1.9377236725,-0.4440710907
C,0,-2.2399451341,1.4987159909,-0.1319659595
H,0,-2.6034240565,2.4570383489,-0.5107065297
H,0,-2.2636707085,1.4972543498,0.960386596
C,0,-3.4008652976,0.3002058445,-2.2911461141
H,0,-4.0458133533,-0.5048728069,-2.6461313473
H,0,-3.7835351016,1.2628134126,-2.6363216164
C,0,-0.5003934643,1.4277889584,-2.2306242635
H,0,0.5305953612,1.2763567027,-2.5537902112
H,0,-0.8577677743,2.4004384994,-2.5747369119
C,0,-0.9697278814,-1.6497567367,-2.492926426
H,0,0.0525676066,-1.8088840107,-2.83640386
H,0,-1.6042249867,-2.4520806148,-2.869938
B,0,-2.9875855783,0.2524299153,-0.772533703
B,0,-0.8244916226,1.0917139384,-0.7262135562
Si,0,-1.0693918344,-1.4924842607,-0.5997747577
Si,0,-1.6269478715,0.0680992652,-2.9763202346

Species 31

Charge = 0 Multiplicity = 1
C,0,-0.1539752434,0.0001600263,-0.1059135719
H,0,-0.1945935366,-0.005339616,0.9840938345
H,0,0.8795794666,0.005573737,-0.4589929305
C,0,-2.5123598503,-1.2743502473,-0.2291147246
H,0,-2.6314571301,-1.2145888496,0.853555377
H,0,-3.1120753632,-2.0994493353,-0.6157918894
C,0,-2.5215154526,1.2584247368,-0.2162765798
H,0,-3.1272252633,2.0830394743,-0.5945866262
H,0,-2.6401680981,1.1868427043,0.8657278279
C,0,-3.2057968502,0.0001220382,-2.3052702825
H,0,-3.7696905619,-0.8910785199,-2.5841966614
H,0,-3.7762887229,0.8898795916,-2.5752070199
C,0,-0.9041712257,1.3797052571,-2.3540312535
H,0,0.1349012061,1.3737330737,-2.6905388307
H,0,-1.4279604349,2.2654640414,-2.7155491257
C,0,-0.8940157499,-1.3617804044,-2.3679718222
H,0,0.1451552394,-1.3448105174,-2.7038557439
H,0,-1.4109355602,-2.2479136091,-2.7383366589
N,0,-3.0231945599,-0.0067158935,-0.8255172793
B,0,-1.6436339358,0.0074806996,-2.6382021789
B,0,-1.040977762,1.1157944604,-0.7982319631
B,0,-1.0330024127,-1.1148372362,-0.8093130945

Species 32

Charge = 1 Multiplicity = 1
C,0,0.0100774119,-0.0000000011,0.0069447267
H,0,0.0002055283,-0.0000000011,1.1003366667
H,0,1.0624828612,-0.0000000027,-0.2929161119
C,0,-0.6778538122,1.2550921846,-0.5445257614
H,0,-0.2458800486,2.1686034617,-0.1314216926
C,0,-0.6778538177,-1.2550921844,-0.5445257612
H,0,-0.2458800544,-2.1686034618,-0.131421693
C,0,-2.2269897428,-1.2463673839,-0.0399524628
H,0,-2.2385608093,-1.2333706043,1.0488774826
H,0,-2.724876179,-2.1330802268,-0.4295598822
C,0,-2.2269897382,1.246367385,-0.0399524631
H,0,-2.7248761747,2.1330802281,-0.4295598814
H,0,-2.2385608045,1.2333706049,1.0488774823
C,0,-2.6560312219,0.0000000007,-0.6566596659
C,0,-2.9026546336,-0.0000000013,-2.0906863616
H,0,-3.3940538563,-0.898762383,-2.4603946608
H,0,-3.3940538604,0.8987623774,-2.4603946621
C,0,-0.6765573307,1.2674830853,-2.0782653584
H,0,0.3551573237,1.3051287666,-2.4410964369
H,0,-1.1719594792,2.1643790112,-2.4598179057
C,0,-0.6765573286,-1.2674830833,-2.0782653582
H,0,0.355157328,-1.3051287598,-2.4410964317
H,0,-1.1719594714,-2.1643790108,-2.4598179082
C,0,-1.3586950886,0.0000000003,-2.6088093102
H,0,-1.4207298302,0.0000000008,-3.6987380535

Species 33

Charge = 2 Multiplicity = 1
C,0,0.0291780879,-0.0599255781,0.0204731065
H,0,0.0165204572,-0.065059312,1.1104666167

H,0,1.0525047257,-0.0652211105,-0.3550200494
C,0,-0.7201102321,1.2583465242,-0.509850067
H,0,-0.1556380083,2.1039509428,-0.1105786528
C,0,-0.835858974,-1.0668801382,-0.5911985086
C,0,-2.1407240855,-1.3123214616,0.0202109714
H,0,-2.1297011897,-1.304289951,1.110117731
H,0,-2.6472917563,-2.201261309,-0.3558561602
C,0,-2.1801836914,1.2618086469,0.0045916687
H,0,-2.218517682,1.3280474327,1.0941839857
C,0,-2.9079735631,-0.0038184264,-0.5093129677
H,0,-3.922385331,-0.0700552655,-0.1099967427
C,0,-2.909704578,-0.0009417896,-2.0568165999
H,0,-3.4741768016,-0.8465462082,-2.4560880141
C,0,-0.721841247,1.261223161,-2.0573536992
H,0,0.2925705209,1.3274600004,-2.4566699243
C,0,-0.6938671984,-1.3127767334,-2.0248900696
H,0,0.3375230729,-1.3037925355,-2.3775411503
H,0,-1.2169471032,-2.2016398334,-2.3776539908
C,0,-1.4496311187,-0.0044039123,-2.5712583355
H,0,-1.4112971281,-0.0706426982,-3.6608506525
C,0,-1.4890907245,2.5697261965,-2.5868776377
H,0,-0.9825230539,3.4586660437,-2.2108105051
H,0,-1.5001136204,2.5616946868,-3.6767843972
C,0,-2.9359476122,2.5701814678,-0.541776597
H,0,-3.9673378835,2.5611972687,-0.1891255166
H,0,-2.4128677081,3.4590445681,-0.1890126751
C,0,-3.6589928976,1.3173303127,-2.5871397734
H,0,-4.6823195356,1.3226258452,-2.2116466183
H,0,-3.6463352658,1.3224640467,-3.6771332837
C,0,-2.7939558361,2.3242848728,-1.9754681579

Species 34

Charge = 2 Multiplicity = 1
C,0,-0.0019145871,0.003721575,0.0279424178
H,0,0.0384150157,-0.017882517,1.1233086836
H,0,1.0369886494,0.027471721,-0.3093768015
C,0,-0.7209980584,1.2628367676,-0.4587822594
H,0,-0.2340269317,2.1883993079,-0.1498771409
C,0,-0.7371146649,-1.2379800528,-0.4570390737
C,0,-2.180549358,-1.2536902068,0.0283220846
H,0,-2.1811879017,-1.2980015756,1.1237302292
H,0,-2.7201815047,-2.1419279815,-0.3081595738
C,0,-2.1969399783,1.2894085762,-0.2371482243
C,0,-2.9121481325,-0.0013906365,-0.459139353
H,0,-3.9573525319,0.0399445048,-0.1508312211
C,0,-2.9088167511,-0.0054320328,-2.1078844081
H,0,-3.3957878778,-0.9309945731,-2.4167895266
C,0,-0.717666677,1.2587953712,-2.1075273144
H,0,0.3275377224,1.21746023,-2.4158354466
C,0,-0.7268025403,-1.2559438371,-2.1717585494
H,0,0.3209990933,-1.2531490096,-2.4666122724
H,0,-1.2521495856,-2.1622330677,-2.4673775201
C,0,-1.4328748312,-0.0320038415,-2.3295184433
C,0,-1.4492654519,2.5110949414,-2.5949887517
H,0,-0.9096333055,3.3993327161,-2.2585070931
H,0,-1.4486269085,2.5554063104,-3.6903968963
C,0,-2.9030122696,2.5133485716,-0.3949081171
H,0,-3.9508139033,2.5105537429,-0.1000543947
H,0,-2.3776652251,3.4196378025,-0.0992891461
C,0,-3.6279002234,1.2536831598,-2.594609084
H,0,-4.6668034588,1.2299330133,-2.2572898612
H,0,-3.6682298292,1.2752872522,-3.6899753497
C,0,-2.8927001449,2.4953847874,-2.1096275931
H,0,-3.4256034815,3.4184751841,-2.3436972488
H,0,-0.2042113283,-2.1610704492,-0.2229694175

Species 35

Charge = 0 Multiplicity = 1
C,0,0.0094928021,0.0000284218,0.0066997953
H,0,0.0098255548,-0.0001173976,1.0988211108
H,0,1.0481713571,0.0000189894,-0.3307628488
C,0,-0.7215903045,1.2452584354,-0.5243615989
C,0,-0.7217210331,-1.2449885377,-0.5246882444
C,0,-2.1695418206,-1.2625715992,-0.0203250431
H,0,-2.1811440429,-1.2868351631,1.072903957
H,0,-2.6729783562,-2.1660585437,-0.3752529612
C,0,-2.1694109484,1.2628616237,-0.0199990098
H,0,-2.6727517963,2.1664913783,-0.374698929
H,0,-2.1810145665,1.286847985,1.0732359879
C,0,-2.8892494641,0.0002497923,-0.544876574
H,0,-3.9206479453,0.0002558388,-0.1796905591
C,0,-2.873495508,0.0004494465,-2.0850018593
H,0,-3.4005716811,-0.879905059,-2.4680823149
H,0,-3.4004831101,0.8809567722,-2.4678526291
C,0,-0.6900668078,1.26283832,-2.0566900818
H,0,0.3461483863,1.2853348141,-2.4055398036
H,0,-1.1822456928,2.1667475684,-2.4258074321
C,0,-0.6902045014,-1.262177576,-2.0570211579
H,0,0.3460056355,-1.2847035059,-2.4058825288
H,0,-1.1824907553,-2.1659351091,-2.4263674243
C,0,-1.4133770437,0.0004379677,-2.5778088585
H,0,-1.3857487989,0.0005808995,-3.6716161424
Cl,0,0.1517916303,-2.7409312934,0.1102012207
Cl,0,0.152071915,2.7409465553,0.1109186182

Species 36

Charge = 0 Multiplicity = 1
C,0,0.3136571698,-0.000002237,0.2286569813
H,0,0.321521768,-0.0001406112,1.3238876878

H,0,1.3590616474,-0.0000134335,-0.0977767508
C,0,-2.3336256066,-1.5384445726,0.1975679929
H,0,-2.3564596615,-1.5627455037,1.2928392852
H,0,-2.8489011168,-2.4416691228,-0.1478389224
C,0,-2.33346574,1.5387025961,0.1979803157
H,0,-2.8486582163,2.4420753618,-0.1471621614
H,0,-2.3562835488,1.5626942361,1.2932591197
C,0,-3.1949910196,0.0005050428,-2.3181492156
H,0,-3.7265748539,-0.8770641243,-2.7047684135
H,0,-3.7264627719,0.8782465813,-2.7045321145
C,0,-0.533534825,1.5387652939,-2.2808282498
H,0,0.500449658,1.5623999961,-2.6428472665
H,0,-1.021271828,2.4423529735,-2.6630882833
C,0,-0.5336542562,-1.538022485,-2.28122483
H,0,0.5003457687,-1.5615810011,-2.643207617
H,0,-1.0213979365,-2.4414882652,-2.6637611947
Cl,0,0.4424973385,-3.2554213515,0.320605938
Cl,0,0.4428298938,3.2553779184,0.3214409448
Si,0,-0.5541407379,-1.5480349608,-0.4038637213
Si,0,-0.553985483,1.5482789399,-0.4034625891
Si,0,-3.259148569,0.000259178,-0.4255208187
H,0,-4.6641065052,0.0002685193,0.0687565389
Si,0,-1.4147418746,0.0004934641,-2.9666419886
H,0,-1.3792765078,0.0006775542,-4.4555829187

Species 37

Charge = 0 Multiplicity = 1
C,0,0.3862133842,-0.0000072389,0.2814782182
H,0,0.3809357848,-0.0001472979,1.3777158346
H,0,1.4287662615,-0.0000112802,-0.0569446164
C,0,-2.3723333603,-1.293345292,0.1106681535
H,0,-2.4818048195,-1.2662304177,1.2018926868
H,0,-2.9355088908,-2.1679594311,-0.2396619245
C,0,-2.3722094956,1.2936242508,0.1110171803
H,0,-2.9353096027,2.1683848843,-0.2390679321
H,0,-2.4816717217,1.2662211721,1.2022356727
C,0,-2.8527210076,0.0004556101,-2.0700859771
H,0,-3.3866188315,-0.8776978798,-2.4574974599
H,0,-3.3865307493,0.8787671903,-2.4572603987
C,0,-0.6291395364,1.2935065069,-2.2909327635
H,0,0.3748117025,1.2648240601,-2.7323632579
H,0,-1.1347632809,2.1692283207,-2.7177170752
C,0,-0.629252569,-1.2927413908,-2.2912700441
H,0,0.3747039438,-1.2640226177,-2.7326865402
H,0,-1.1349449222,-2.1683068961,-2.7182938796
Cl,0,0.246362285,-3.3073617135,0.1770515087
Cl,0,0.2466774536,3.3073784066,0.1779256405
Si,0,-0.5691200749,1.4683021703,-0.4142324806
Si,0,-0.5692547715,-1.4680485926,-0.4146157414
C,0,-2.9726836162,0.0002528978,-0.5220859779
H,0,-4.0477427564,0.0002740684,-0.2944659874
C,0,-1.4180889973,0.0004656151,-2.6660807806
H,0,-1.5353275857,0.000613143,-3.7586167343

Species 38

Charge = 0 Multiplicity = 1
C,0,0.0775183824,0.0000158925,0.0558971289
H,0,0.0824976328,-0.0001266179,1.1477358506
H,0,1.1173562597,0.0000050978,-0.2772849888
C,0,-0.628512909,1.2925940005,-0.4564599984
C,0,-0.6286488028,-1.2923548865,-0.456797899
C,0,-2.121460605,-1.2662287625,-0.072270503
H,0,-2.2865923196,-1.1808279355,1.0024147422
H,0,-2.626044287,-2.1675973425,-0.427113895
C,0,-2.1213274155,1.2665264303,-0.0719399864
H,0,-2.6258155526,2.1680402831,-0.4265504559
H,0,-2.2864690923,1.1808623949,1.0027225307
C,0,-2.5054960695,0.0002673367,-0.8288036281
C,0,-3.0606675585,0.0004768136,-2.2227234124
H,0,-3.5410677378,-0.9090461339,-2.571832046
H,0,-3.5409740062,0.9101389209,-2.5715981823
C,0,-0.7254345294,1.2669727378,-1.9944932239
H,0,0.245232833,1.1823149737,-2.4847459782
H,0,-1.2198752032,2.1681406874,-2.3639438188
C,0,-0.725568698,-1.266323934,-1.994824801
H,0,0.2451069932,-1.1816398813,-2.4850567188
H,0,-1.2201053254,-2.1673435731,-2.3645088347
C,0,-1.5632199055,0.0003860863,-2.1263452488
Cl,0,0.2646928922,-2.7590737947,0.1924172993
Cl,0,0.2649816697,2.7590510957,0.1931362033

Species 39

Charge = 0 Multiplicity = 1
C,0,0.3111121489,0.0000040586,0.2291165935
H,0,0.3191139671,-0.0001466036,1.3246991736
H,0,1.360177755,0.0000013677,-0.0861768994
C,0,-2.3309215561,-1.5579107548,0.1649084764
H,0,-2.3932213005,-1.5694186939,1.2582093148
H,0,-2.8503792177,-2.4515912321,-0.1929565658
C,0,-2.3307856148,1.5581627128,0.1653287287
H,0,-2.8501662158,2.4519851918,-0.1922938011
H,0,-2.3930851288,1.5693813347,1.2586326816
C,0,-3.3026028092,0.0005201794,-2.3909922339
H,0,-3.8164019874,-0.884977214,-2.7649135939
H,0,-3.8163203455,0.8861702217,-2.7646644576
C,0,-0.563112698,1.5556394679,-2.2702682838
H,0,0.4572801017,1.5600528765,-2.6680518554
H,0,-1.0584106555,2.4521963994,-2.6538113857
C,0,-0.5632554769,-1.5548779071,-2.2706912248

H,0,0.4571353444,-1.5592774333,-2.66847977
H,0,-1.0586363645,-2.4512865319,-2.6544736474
Cl,0,0.5210545319,-3.2391865058,0.3742046556
Cl,0,0.5213343199,3.2391362903,0.3750892783
Si,0,-3.2107334259,0.0002531777,-0.4941112939
Si,0,-1.4703547002,0.0005077693,-2.8992460889
Si,0,-0.534327828,1.5619624647,-0.3906784344
Si,0,-0.5344651372,-1.5617134628,-0.3911044376

Species 40

Charge = 0 Multiplicity = 1
C,0,0.3984590515,-0.0000102827,0.290470756
H,0,0.4088290405,-0.0001568778,1.3851334432
H,0,1.4434049618,-0.0000129778,-0.0355222687
C,0,-2.3341572747,-1.2992372991,0.0189747737
H,0,-2.5855957396,-1.1624120918,1.0703429065
H,0,-2.9464268812,-2.1143239272,-0.3737267199
C,0,-2.3340373737,1.299533884,0.0193311494
H,0,-2.9462358523,2.1147835039,-0.3731427457
H,0,-2.5854822998,1.1624417266,1.0706630571
C,0,-3.0059945484,0.0004802133,-2.182482725
H,0,-3.4877141059,-0.908564493,-2.5320850167
H,0,-3.4876260889,0.9096678726,-2.5318340797
C,0,-0.7042752137,1.2992374565,-2.2253880053
H,0,0.2170576609,1.1613843553,-2.7906370905
H,0,-1.2673051384,2.1144800646,-2.6855393071
C,0,-0.7043910291,-1.2984783362,-2.2257380739
H,0,0.2169558636,-1.1605531202,-2.7909468161
H,0,-1.2674920742,-2.113546105,-2.6861116312
Cl,0,0.4118651117,-3.310563875,0.296567404
Cl,0,0.4121706954,3.3105372991,0.2974563273
Si,0,-0.4989109226,1.5330127143,-0.3626802707
Si,0,-0.4990494069,-1.5327771206,-0.3630925349
C,0,-2.4777937058,0.000263292,-0.7774761841
C,0,-1.506227027,0.0004012989,-2.1152614122

Species 41

Charge = 0 Multiplicity = 1
C,0,0.8842460776,-0.0004324396,0.7360282396
H,0,0.8868823753,-0.0049047613,1.8277282312
H,0,1.9233805298,0.0039399115,0.4013112383
C,0,-1.2851526528,-1.3450727195,0.7122960345
H,0,-1.2924770174,-1.3579632471,1.8049309462
H,0,-1.7473082944,-2.2651534547,0.3462390037
C,0,-1.2925639538,1.3316337032,0.723464445
H,0,-1.7605291533,2.2519918564,0.3655160082
H,0,-1.2999337991,1.3349217832,1.8161886896
C,0,-2.0594974948,0.0001095766,-1.4770074295
H,0,-2.4873782712,-0.8879271645,-1.9446587597
H,0,-2.4922536593,0.8896575749,-1.9372561792
C,0,0.1264315789,1.2230899236,-1.3249598438
H,0,1.1382970476,1.2103245191,-1.7366975526
H,0,-0.3921012581,2.0993101121,-1.7190269979
C,0,0.1337612566,-1.2113960413,-1.3348467105
H,0,1.1456296683,-1.1886588467,-1.7461941426
H,0,-0.3789726991,-2.0875931416,-1.7364873876
B,0,-1.8408827747,-0.0056382672,0.0753276013
N,0,-0.5724993413,0.0054863107,-1.7596643578
C,0,0.1655599899,1.2630046917,0.2140433605
C,0,0.1729174425,-1.2636236782,0.2036454319
Cl,0,1.1361133595,2.7446933212,0.7605224577
Cl,0,1.1517960716,-2.7442248553,0.7385033207

Species 42

Charge = 0 Multiplicity = 1
C,0,-0.000173422,-0.2846073746,-0.2317837915
C,0,0.0780744153,0.0499617458,1.8647184915
C,0,1.4328002912,-0.0064942134,2.5127958533
H,0,1.9119412292,-0.9768123365,2.5579870644
H,0,1.6003435137,0.6573360561,3.3520867087
C,0,1.3217489161,0.6312883802,1.1566039503
C,0,-0.401516565,1.8190927796,0.7903997375
O,0,-0.4008147344,-0.9223029987,0.9782410341
O,0,1.3983217855,-0.0813714888,-0.0460996525
O,0,-0.6543789988,0.9819197874,-0.3409610506
O,0,-0.7940028797,1.1391700198,1.9800522858
O,0,1.0049639115,1.980230497,0.9555609269
Cl,0,-1.227559794,3.3352621509,0.5836080282
Cl,0,-0.3545722879,-1.2415474726,-1.6398965916

Species 43

Charge = 0 Multiplicity = 1
C,0,0.1427435025,0.0000497078,0.1046850054
H,0,0.1237513792,-0.0073308158,1.1963414168
H,0,1.1782234031,0.0073508689,-0.2412637848
O,0,-2.4202239379,1.2921810919,-0.1045565078
O,0,-2.4075428018,-1.3158710239,-0.1225347099
O,0,-3.1580093972,0.0000677659,-2.3014709356
O,0,-0.8525932573,1.3150989901,-2.2569733865
O,0,-0.8393827389,-1.2913500976,-2.2744237785
Si,0,-0.8023623722,-1.523935776,-0.6026866117
Si,0,-0.8176936155,1.5237026546,-0.5818997403
Si,0,-1.6232456467,0.0124802889,-2.9366502423
Si,0,-3.2915969342,-0.0125306224,-0.6458307161
Cl,0,-5.2165489112,-0.0242444745,-0.0321791919
Cl,0,-1.6287657979,0.0243314805,-4.9571742075

Species 44

Charge = 0 Multiplicity = 1
C,0,0.0830926864,-0.002763124,0.0597958466
H,0,0.0929722788,0.0177335644,1.1532132049
H,0,1.1257177112,0.0181781589,-0.2698880007
C,0,-0.6276268138,1.2842633615,-0.4556298191
C,0,-0.6035138691,-1.3173390097,-0.4385694558
C,0,-2.1083932867,-1.2677672708,-0.0738096247
H,0,-2.3010070303,-1.1743287662,0.9975234064
H,0,-2.6260010967,-2.1643560745,-0.4277964401
C,0,-2.1212093708,1.2625721036,-0.0735895025
H,0,-2.6228031137,2.1676742104,-0.4248856284
H,0,-2.2892854906,1.1726167716,1.0004379528
C,0,-2.5001838657,-0.0024227776,-0.8382997485
C,0,-3.0691609069,0.0023337868,-2.2292670975
H,0,-3.5476718281,-0.9089457936,-2.5772430686
H,0,-3.5524650662,0.9102768873,-2.5803658071
C,0,-0.726888062,1.2631399213,-1.9935889247
H,0,0.2423720989,1.174366391,-2.4862806186
H,0,-1.2174043651,2.1677925667,-2.3613852773
C,0,-0.7232352466,-1.2678858103,-1.9817776701
H,0,0.2356817625,-1.1758927329,-2.4973782723
H,0,-1.2217232408,-2.1638471762,-2.3637446313
C,0,-1.5702534999,-0.002202479,-2.1182762503
Cl,0,0.2616810956,2.7635275992,0.1910461565
H,0,-0.064835831,-2.1880498145,-0.0472714446

Species 45

Charge = 0 Multiplicity = 1
C,0,0.3229300814,-0.006570662,0.2377035797
H,0,0.3331787932,0.0032593282,1.3340350144
H,0,1.3733568341,0.0039367755,-0.0756878077
C,0,-2.3197901035,-1.5614078437,0.1649470614
H,0,-2.3955523655,-1.5761345984,1.2588686786
H,0,-2.8423338784,-2.4544826694,-0.1937461174
C,0,-2.3260862039,1.5479617731,0.1673141857
H,0,-2.8432111824,2.4427730228,-0.1909859272
H,0,-2.3891832072,1.5596337818,1.2606728893
C,0,-3.3008162077,-0.0126682825,-2.3895141069
H,0,-3.8102411053,-0.9021104676,-2.7602522478
H,0,-3.8193640701,0.8685129701,-2.7665417053
C,0,-0.5597091202,1.5452346886,-2.2661863276
H,0,0.460598623,1.549671829,-2.6644882803
H,0,-1.0544842194,2.4429469872,-2.64758649
C,0,-0.5599134508,-1.5582839175,-2.2604665955
H,0,0.4569347317,-1.565683959,-2.6712046384
H,0,-1.0568548189,-2.4542691575,-2.6468133075
Cl,0,0.526595565,3.2266109048,0.3788532982
Si,0,-3.2107024951,-0.0111475919,-0.490689688
Si,0,-1.4672922397,-0.0107909722,-2.9003693564
Si,0,-0.5299463146,1.5443828116,-0.3872418597
Si,0,-0.5025580943,-1.5995472681,-0.3682793497
H,0,0.249089852,-2.7793973694,0.1765191311

Species 46

Charge = 0 Multiplicity = 1
C,0,0.4089191446,-0.0163454894,0.2982079959
H,0,0.4207903682,-0.0029388662,1.3935744768
H,0,1.4555193587,-0.0025734129,-0.0248461456
C,0,-2.3154608935,-1.3075665733,0.0147312439
H,0,-2.5885158443,-1.1655883547,1.0610771871
H,0,-2.9348080176,-2.1176291142,-0.3808212829
C,0,-2.3289249752,1.2912327716,0.0193880649
H,0,-2.935747448,2.1108334848,-0.3731249893
H,0,-2.588936606,1.1486619561,1.0678445523
C,0,-3.0137787164,-0.0050926803,-2.188018742
H,0,-3.4920240346,-0.9168735206,-2.535100015
H,0,-3.4975587556,0.9027813266,-2.5386527676
C,0,-0.7025831482,1.2910551357,-2.2208132835
H,0,0.2133377797,1.1478674445,-2.7933755957
H,0,-1.2639592893,2.110780297,-2.6756161446
C,0,-0.7027567715,-1.3067293124,-2.2072834531
H,0,0.2068057651,-1.1640216768,-2.7920394624
H,0,-1.2710371752,-2.1169171111,-2.6728756897
Cl,0,0.4248923904,3.2896649925,0.3068354844
Si,0,-0.4918354869,1.5110280335,-0.3576619729
Si,0,-0.4692741727,-1.5825909593,-0.3420229248
C,0,-2.4642724052,-0.0057441846,-0.7878286899
C,0,-1.5120315475,-0.0054485423,-2.0998170454
H,0,0.1778858793,-2.8454155282,0.1270992394

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