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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.)

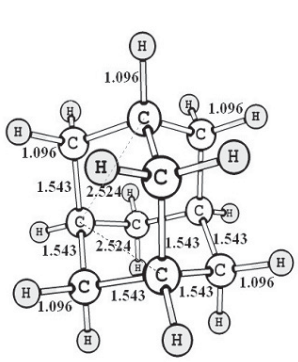
Atom	E / Ω
C	-37.4332
O	-75.9020
H	-0.6052
Total	-114.5456

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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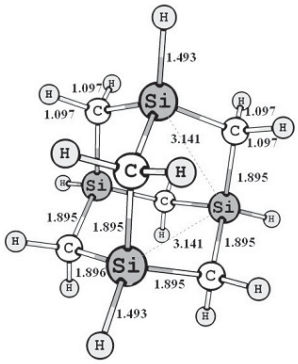

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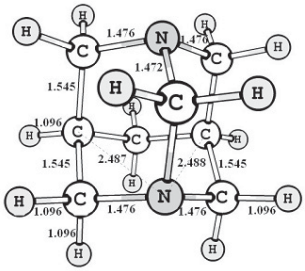

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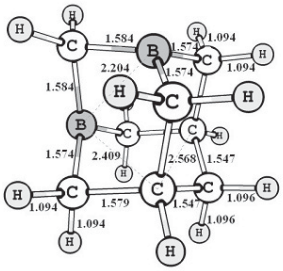

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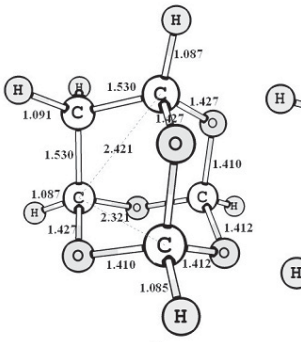

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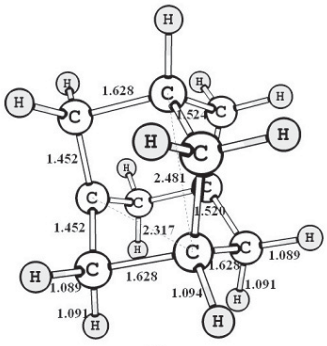

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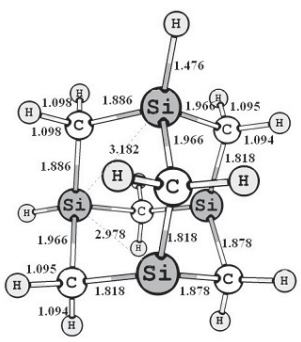

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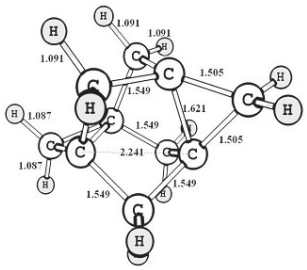

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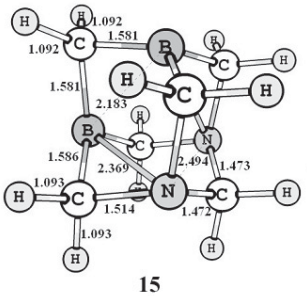

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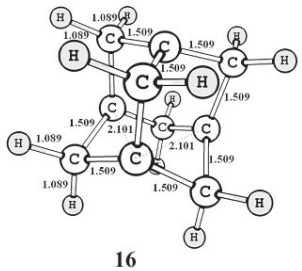

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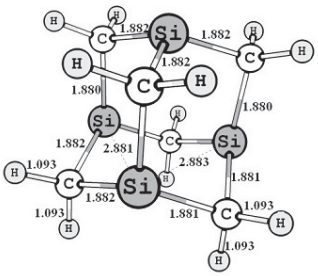

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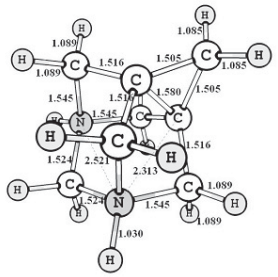

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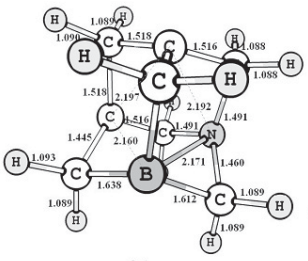

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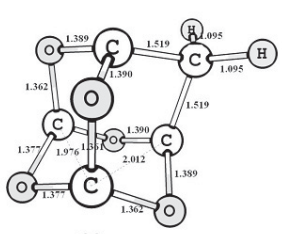

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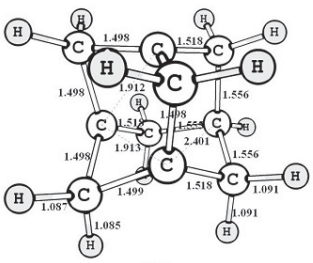

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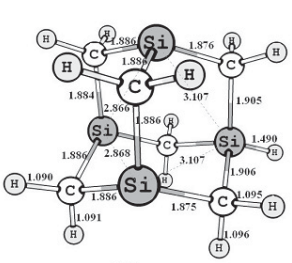

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Table S3. Computed energy values of the species **1** to **46**

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
H,0,-1.1276728184,2.1618743263,-2.7170058316
C,0,-0.6271775972,-1.2865592237,-2.284284324
H,0,0.374003746,-1.2544260003,-2.7290706337
H,0,-1.1278701617,-2.1609815422,-2.7175693656
C,0,-1.4146963501,0.0004520967,-2.6636467233
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
H,0,0.0230824187,-0.0324727264,1.0904333967
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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