ELECTRONIC SUPPLEMENTARY INFORMATION

for a paper in *PCCP* entitled

Nonseparable Exchange–Correlation Functional for Molecules, Including Homogeneous Catalysis Involving Transition Metals

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Database 2015

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Based on our previous Common Database 2.0,[1] we developed this new database called Database 2015. It comprises of 427 molecular data plus 56 solid-state data for a total of 483 data. The total of 483 data has been divided into 29 subdatabases in this new database, which includes 417 molecular energetic (ME417) data such as energies of atomization, isomerization energies, reaction barrier heights, proton affinities, electron affinities, ionization potentials, and atomic energies, ten molecular structural (MS10) data such as diatomic bond distances, 39 solid-state energetic (SSE39) data, in particular solid-state cohesive energies and semiconductor band gaps, and 17 solid-state structural (SSS17) data, in particular solid-state lattice constants..

As compared to Common Database 2.0, we have added additional 3d and 4d transition metal data, noble-gas-dimer weak interactions data, and 2p and 4p isomerization energy data into

this present database, and we reorganized the data into restructured subdatabases containing both new data and data from Common Database 2.0. In the new database we divide bond energies into those for single-reference (SR) systems and those for multi-reference (MR) systems, and we also classify each of these categories into three subcategories consisting of molecules containing only main-group nonmetals (MGN), those containing one or more main-group metals (MGM), and those containing one or more transition metals (TM). We believe that dividing molecules into such groups help in recognizing systematic performance trends in tested methods.

In many places, the subdatabases are called databases, and the subsubdatabases are called subdatabases or databases – the usage depends on the context. Next we give details about each subdatabase in Database 2015.

1. Single-Reference Main-Group-Metal Bond Energies (SR-MGM-BE9): Nine main group molecules are included, in particular, $AlCl_3$, AlF_3, AlCl, LiCl, KOH, NaO, LiO, ZnSe, and ZnCl. This database contains three subdatabases, namely, SRM2, SRMGD5, and 3dBESR2.

-Single-reference main-group bond energy (SRM2): we selected two single-reference molecules, $AlCl_3$ and AlF_3 that contain main-group metals from the previous database (MGAE109/11)[1,2,3,38].

-Single-reference main-group diatomic molecules (SRMGD5): this subset includes bond dissociation energies of five main-group single-reference diatomic molecules, AlCl, LiCl, KOH, NaO, and LiO. Among these five molecules, AlCl and LiCl are selected from the previous database (SRMBE13),[1,4] whereas KOH, NaO, and LiO are selected from eight main-group single-reference molecules, first reported in our recent work[5]. We carried out representative-database analysis for these eight molecules; and we selected KOH, NaO, and LiO as best representing all eight molecules. For details of representative analysis, see references 6 and 7. The benchmark values of bond dissociation energies of KOH and NaO are from references 8 and 9, respectively. The benchmark value of the bond dissociation energy of LiO is obtained by $CCSDT(Q)_2$/aug-cc-pCVQZ.

-3d single-reference metal-ligand bond energies (3dSRBE2): This subset includes two zinc-ligand molecules, in particular ZnCl and ZnSe. They are selected from the 3d transition metal-ligand bond energies (3dBE70) database, which was first reported in our previous paper,[10] by careful representative analysis. Actually, the 3dBE70 database consists of 19 single-reference

(denoted as 3dSRBE19) and 51 multi-reference (denoted as 3dMRBE51) molecules, and we did representative analysis separately for the single-reference subset and the multi-reference subset. Six molecules are selected from each of the subset since the percentage errors in representation (PEIR, see definition in ref 7) resulted from them are only 15.0% and 11.3%, respectively. The six molecules selected from 3dMRBE51 are integrated as the 3dMRBE6 subset, which will be illustrated in detail below, while the ones selected from 3dSRBE19 are divided into two subsets, namely 3dSRBE2 (which includes ZnCl and ZnSe) and 3dSRBE4 (which includes $CrCl_2$, MnF_2, $FeCl_2$, and $CoCl_2$), and are ranged respectively to the single-reference main group metal bond energies (SR-MGM-BE9) and single-reference transition metal bond energies (SR-TM-BE17) databases, because the 3*d* orbitals of zinc are fully occupied. The best estimates of bond energies for all these representative subsets are from reference 10.

2. Single-Reference Main-Group Nonmetal Bond Energies (SR-MGN-BE107): This is a regrouped database that combines the previously reported alkyl bond dissociation energies (ABDE12) database[1,3,11,49,50] with 95 single-reference molecules selected from the previous so-called main-group atomization energies (MGAE109/11)[1,2,3,38] database. These 95 molecules were categorized as single-reference ones on the basis of their B_1 diagnostic values.[13] A molecule with B_1 value less than 10 kcal/mol per bond was considered to be a single-reference system. The ABDE12 database consists of the alkyl bond dissociation energies (ABDE4/05) and the larger set of alkyl bond dissociation energies (ABDEL8) subsets. The D_0 values for ABDE4/05 and ABDEL8 subsets are taken from a paper by Izgorodina *et al*.,[11] and we use the B3LYP/6-31G(d) zero-point vibrational energies scaled with a scale factor of 0.9806 to obtain our best estimate of the D_e values in the database. In this work, we denote the 95 single-reference molecules as the single-reference nonmetal atomization energies (SRNM95) subset. This subset is composed of all main group single-reference molecules in the MGAE109/11 database. For more information about the source of molecules in these three subsets, please see reference 1.

3. Single-Reference Transition Metal Bond Energies (SR-TM-BE17): SR-TM-BE17 is obtained by merging the 3dSRBE4 subset as mentioned above when we illustrated the 3dBESR2 subset, ten molecules selected from the previously reported single-reference metal bond energies

(SRMBE10) subset, two palladium complexes (PdBE2), and FeCl molecule (unpublished). Each of these subsets is described next.

-3d single-reference metal-ligand bond energies (3dSRBE4): 3dSRBE4 include four molecules, in particular $CrCl_2$, MnF_2, $FeCl_2$, and $CoCl_2$, and they are chosen from representative analysis of the 3dBE19 subset that is presented in a 2013 paper.[10]

-Single-reference metal bond energies (SRMBE10): This database is selected from the subset SRMBE13 of Database 2.0. More detailed information about the source of the 13 data has been explained in our earlier work.[1,4] We select ten molecules containing transition metals from the original SRMBE13 database to form the new database SRMBE10. Bond energies for all molecules in this database are equilibrium ones (D_e), obtained from the experimental bond energies in the ground vibrational state (D_0). Two molecules, CoH and FeH, were corrected for their bond energies compared to their original reference values in Database 2.0.

-Palladium complex bond energies (PdBE2): The two palladium complexes, namely $Pd(PH_3)_2C_6H_8$ and $Pd(PH_3)_2C_{10}H_{12}$, are selected from our previous study[12] on the binding energies of d^{10} transition metals to alkenes. They are set into this SR-TM-BE17 database because the B_1[13] diagnostic shows that both of them are single-reference systems. As it is stated in reference 12, there are two possible conformations for $Pd(PH_3)_2C_{10}H_{12}$ and here we chose the less planar conjugated conformation (denoted as 10b in reference 12) as it has an energy of about 2 kcal/mol lower than the other one (denoted as 10a in reference 12).

4. Multi-Reference Main-Group Metal Bond Energies (MR-MGM-BE4): This database includes four main-group multi-reference diatomic molecules, CaO, LiO^-, KO^-, and MgS. Representative analysis has been done for 7 multi-reference molecules,[5] where LiO^-, KO^-, and MgS have been found to be the best representative of all the seven molecules. Besides these three, we selected CaO from our recent paper[14]. The bond energies of CaO and MgS are from references15, 16, 17, and 18. The benchmark bond energy of LiO^- is obtained by $CCSDT(Q)_2$/aug-cc-pCVQZ and that of KO^- is obtained by CCSD(T)/aug-cc-pCVQZ.

5. Multi-Reference Main-Group Nonmetal Bond Energies (MR-MGN-BE17): This database is composed of subsets of MGAE109/11[1,2,3,38] and MRBE10.[1,4] Twelve multi-reference

nonmetal molecules were selected from the previous MGAE109/11 database, namely, NF_3, CO_2, SiO, SO_2, CO, SO, ClO, F_2, N_2, O_2, NO, and CN. Five non-metal molecules were selected from the previous MRBE10 database, namely, B_2, O_3, C_2, S_4, and Cl_2O. All seventeen molecules of this database were classified as multi-reference molecules based on their B_1 diagnostic values being greater than 10 kcal/mol per bond.

6. Multi-Reference Transition Metal Bond Energies (MR-TM-BE13): MR-TM-BE13 includes three subsets, namely 3d multi-reference metal-ligand bond energies (3dMRBE6), multi-reference bond energies (MRBE5), and 3d transition metal containing molecules such as CuH, VO, CuCl, and NiCl (*taken from a manuscript under preparation*).

-3d multi-reference metal-ligand bond energies (3dMRBE6): 3dMRBE6 is constructed as a representative of the 3dMRBE51 database.[10] This subset consists of six molecules, in particular TiCl, VF_5, CrCl, CrOF, $(FeBr_2)_2$, and $Co(CO)_4H$.

-Multi-reference bond energies (MRBE3): Three transition metal molecules are selected from a previous database MRBE10,[1] namely, $NiCH_2^+$, $Fe(CO)_5$, and VS.

7. Multi-Reference Transition Metal Dimer Bond Energies (MR-TMD-BE2): Cr_2 and V_2 are selected from a previous database MRBE10.[1,4] The bond energy for Cr_2 is corrected compared to its original reference value in Database 2.0.

8. Ionization Potential (IP23): Sc and Co are added to the previous database IP21.[1,3,19,20,2144,48,] Sc and Co are selected as representative data from 3d atoms of a recent paper "Density Functional Theory of Open-Shell Systems. The 3d-Series Transition Metal Atoms and Their Cations."[22]

9. Noncovalent Complexation Energies (NCCE30): This database is obtained by selecting 27 data from NCCE31/05 database[1,44,45] and then combining them with three new data, in particular the complexation energies of $CO_2\cdots Ar$, parallel-displaced $(CO_2)_2$ (denoted as $(CO_2)_2PD$), and pyridine dimer $(C_5H_5N)_2$. These three new data are selected from Voorhis' 2012 paper,[23] and the reference complexation energies for $CO_2\cdots Ar$, $(CO_2)_2PD$, and $(C_5H_5N)_2$ are from refs. 24, 25, and 26, respectively.

10. Noble Gas Dimer Weak Interactions (NGDWI21): This database is composed of seven noble gas dimers, four of which are taken from the previous NCCE31/05 database[1,44,45] and three of them are new dimers, He_2, Ar_2, and Kr_2. For each dimer, three data points are selected from the potential energy curve,[27] where one of them is the equilibrium point and the other two points are 0.3 Å away from the equilibrium point (on either side). This results in 21 data points.

11. 3d Transition Metal Atomic Excitation Energies (3dAEE7): The 3dAEE7 database is composed of the excitation energies of Ca^+ and six 3d transition metal atoms or cations, namely, Sc, V, Mn^+, Fe, Ni^+, and Zn. These six transition metal atoms or cations are chosen as a representative subset of the excitation energies of the ten 3d-series transition metal atoms and their cations.[15] The Ca^+ is included in this database because of its excitation from Ca^+(4s) state to Ca^+(3d) state.[14]

12. 4d Transition Metal Atomic Excitation Energies (4dAEE5): The 4dAEE5 database is composed of five multiplicity-changing excitation energies of 4d transition metal atoms or cations, namely, Mo^+, Ru^+, Rh^+, Pd, and Y^+. They are selected as a representative subset of a recent study on 4d transition metal atoms and their cations.[28]

13. p-block Excitation Energies (pEE5): The pEE5 database is chosen as a representative subset from the previously reported database[29] that contains nine multiplicity-changing valence (V9 database) and eight Rydberg (R8 database) excitation energies of p-block elements. The five p-block elements or cations included in this representative database are F, Ar, C^+, Al, and Si^+. The best-estimated excitation energies are experimental values with spin-orbit coupling excluded.

14. 4p Isomerization Energies (4pIsoE4): The 4pIsoE4 database was chosen from ref. 30.

15. 2p Isomerization Energies (2pIsoE4): The 2pIsoE4 database was chosen from ref. 30.

16. Diatomic Geometries of Light-Atom Molecules (DGL6): Diatomic geometries for molecules containing only light (DG6L) atoms. DG6L is selected from the previous databases MGNHBL11[31,51] and MGHBL9[31] which were also reported in reference 1.

17. Diatomic Geometries of Heavy-Atom Molecules (DGH4): Diatomic geometries for molecules with one or more heavy (DG4H) atoms. The reference geometries for DG4H molecules are taken from the NIST website[32] and reference 33.

18. Lattice Constants (LC17): The LC17 database is a subset of the previous lattice constant database, solid-state structure database 47 (SSS47).[1]

19. Other Databases: Besides the 18 new databases mentioned above, there are another 11 databases in Database 2015, namely

- IsoL6/11: six isomerization energies of large organic molecules
- EA13/03: 13 electron affinities
- PA8: eight proton affinities
- πTC13: 13 thermochemical data for π systems
- HTBH38/08: 38 hydrogen transfer barrier heights
- NHTBH38/08: 38 non-hydrogen transfer barrier heights
- AE17: 17 atomic energies
- HC7/11: seven hydrocarbon data
- DC9/12: nine difficult cases
- SBG31: semiconductor band gaps
- SSCE8: solid-state cohesive energies

that were part of Common Database 2.0 and are used with no changes. For more information about these 11 previous databases, please see reference 1.

DETAILS

Spin-orbit coupling

The reference data in Database 2015 are from experiments or from high-level quantum mechanical calculations, and they include spin-orbit coupling when it is nonzero.

When testing density functional methods, similar to what was done in the previous work,[34,35] we include spin-orbit effects post-SCF using the following equation for the electronic energy:

$$E = E(\mathrm{SCF}) - E(\mathrm{SO})$$

where E(SO) is a positive value, usually taken from experiment but in a few cases taken from theory. All E(SO) values needed for Database 2015 are in Table S3. There is one database that is an exception to the inclusion of spin-orbit effects, namely the AE17 database. For the AE17 database, we compare to experimental results that exclude relativistic effects;[36,37] therefore, we do not include the SO values given in Table S3 for the AE17 database.

Scalar relativistic effects

We use two protocols for the treatment of scalar relativistic effects. For the comparison of databases pEE5, 3dAEE7, and 4dAEE5 to the reference values, we include scalar relativistic effects in our calculations. For all other databases, we neglect scalar relativistic effects when we compare to the reference data. Because of this second protocol, when we took reference data from Karton et al.[38] for bond energies, we took the values that do not include scalar relativistic effects. For other reference data, taken from experiment, the neglect of scalar relativistic effects can only be justified by these effects being small relative to the typical error in the methods being tested.

Vibrational contributions

As already mentioned, the data in Database 2015 are from experiments or high-level quantum mechanical calculations. Throughout the database, as in previous work,[1] we only present vibration-exclusive energies (also sometimes called zero-point-exclusive energies). When the data is from high-level calculations, it corresponds to the electronic energy, including nuclear repulsion but not zero-point energy or thermal energy. When the data comes from experiments, vibrational and rotational contributions (both thermal energy and zero-point energy, where the latter is abbreviated ZPE) are removed theoretically. Thus, for example, bond energies are D_e and not D_0.

For the 3dSRBE2, 3dSRBE4, 3dMRBE6, SRMBE13, and MRBE5 subdatabases and for the FeCl, CuH, VO, CuCl, and NiCl molecules, vibration-exclusive data is obtained by

subtracting vibrational energies from experimental data to get the reference data. For the alky bond dissociation energies (ABDE12), which are included in the SR-MGN-BE107 database in Database 2015, a scalar factor of 0.9806 is used to estimate the vibrational contribution from B3LYP/6-31G(d) calculations, and this is added to D_0 values to get D_e.[1] For the SSCE8 database, Table S4 provides the calculated ZPEs.[1]

In summary, all the energetic data in the database are Born-Oppenheimer potential energy differences without ZPE or thermal vibrational, rotational, or translational contributions.

Geometries and basis sets for testing with Database 2015

In using the molecular energetics database ME417 for testing electronic structure methods, we perform single-point calculations; the sources of the geometries used for these single-point calculations are given in Table S1. For databases MS10, SSS17, and SSE39, we use geometries or lattice constants optimized self-consistently by the method being tested (in such cases we put "optimized" in the geometries column of Table S1). The basis sets used for these tests are given in Table S2.

Energetic data of Database 2015

In order to make our new database available for use by other groups, all the reference data are provided in Table S5. We also include the energetic data calculated by BLYP, PBE, N12, and GAM. We selected BLYP and PBE because of their wide availability in software packages; reproducing this data may be useful for checking. We included N12 and GAM because they are the only published NGAs, and again, this data may be useful for checking.

There is one thing worth emphasizing about Table S5. Since the reference data include the spin-orbit correction, the values in the third, fourth, fifth, and sixth columns have the spin-orbit values that are provided in Table S3 already subtracted (when they are nonzero).

Geometries of Database 2015

We provide the information about the geometries for single-point calculations on Database 2015 in Table S7. Some geometries are from Common Database 2 (CD2), which can be found at http://comp.chem.umn.edu/db/. All the geometries used in Database 2015, incldung

the ones that were part of CD2, are given in Table S7 (in Å units) along with charges and multiplicities.

Table S1. Geometries for testing electronic structure methods.

primary subset[b]	secondary	description	geometries	Ref.
ME417				
SR-MGM-BE9		single-reference main-group metal bond energies		
	SRM2	single-reference main-group bond energies	QCISD/MG3	39
	SRMGD5	single-reference main-group diatomic molecules	CCSDT(Q)2/aug-cc-pCVQZ	40
	3dSRBE2	3d single-reference metal-ligand bond energies	M05/def2-TZVP (metals), ma-TZVP (non-metals)	-*a*-
SR-MGN-BE107		single-reference main-group non-metal bond energies	QCISD/MG3	39
SR-TM-BE17		single-reference TM[c] bond energies		
	3dSRBE4	3d single-reference metal-ligand bond energies	M05/def2-TZVP (metals), ma-TZVP (non-metals)	-*a*-
	SRMBE10	single-reference metal bond energies	experiment	1
	PdBE2	palladium complex bond energies	M06/BS3	-*a*-
	FeCl	FeCl bond energy	experiment	41
MR-MGM-BE4		multi-reference main-group metal bond energies	M06-L/aug-cc-pCVQZ	14
MR-MGN-BE17		multi-reference main-group non-metal bond energies	QCISD/MG3	39
MR-TM-BE13		multi-reference TM bond energies		
	CuH and VO	CuH and VO bond energies	experiment	42
	CuCl	CuCl bond energy	experiment	43
	NiCl	NiCl bond energy	M06-L/ma-TZVP	-*a*-
	3dMRBE6	3d multi-reference metal-ligand bond energies	M05/def2-TZVP (metals), ma-TZVP (non-metals)	-*a*-
	MRBE3	Multi-reference bond energies	QCISD/MG3	39
MR-TMD-BE2		Multi-reference TM dimer bond energies (Cr_2 and V_2)	QCISD/MG3	39
IP23		ionization potentials		
NCCE30		noncovalent complexation energies		
	CO_2···Ar	complexation energy of CO_2···Ar	experiment	24
	$(CO_2)_2$PD	complexation energy of parallel-displaced $(CO_2)_2$	experiment	25
	$(C_5H_5N)_2$	complexation energy of pyridine dimer	experiment	26
	rest	noncovalent complexation energies of remaining 27 complexes	MC-QCISD/3	44,45
NGDWI21		noble gas dimer weak interaction		27
3dAEE7		3d TM atomic excitation energies		
4dAEE5		4d TM atomic excitation energies		
pEE5		p-block excitation energies		
4pIsoE4		4p isomerization energies	PBE0-D3/def2-TZVPP	-*a*-
2pIsoE4		2p isomerization energies	PBE0-D3/def2-TZVPP	-*a*-
IsoL6/11		isomerization energies of large molecules	B97-D/TZVP	46
EA13/03		electron affinities	QCISD/MG3	39

NHTBH38/08	non-hydrogen transfer barrier heights	QCISD/MG3	39
AE17	atomic energies		
HC7/11	hydrocarbon chemistry	MP2/6-311+G(d,p)	50
DC9/12	difficult cases	MP2/6-311+G(d,p)	51
MS10			
DGL6	diatomic geometries for light-atom molecules	optimized	
DGH4	diatomic geometries for heavy-atom molecules	optimized	
SSS17			
LC17	lattice constants	optimized	
SSE39			
SBG31	Semiconductor band gaps	optimized	
SSCE8	solid-state cohesive energies	optimized	

[a]Geometries were calculated in this work.

[b]In the name of a database or subdatabase, the number at the end of the name or before the solidus is the number of data. For example, ME417, SR-MGM-BE9, and IsoL6/11 contain respectively 417, 9, and 6 data.

[c]TM denotes transition metal.

Table S2. Basis sets for testing density functional theory.

primary subset	secondary	description	basis set
ME417			
SR-MGM-BE9		single-reference main-group metal bond energies	
	SRM2	single-reference main-group bond energies	MG3S
	SRMGD5	single-reference main-group diatomic molecules	aug-cc-pcVQZ; cc-pcVQZ
	3dSRBE2	3d single-reference metal-ligand bond energies	def2-TZVP(metal); ma-TZVP(non-metal)
SR-MGN-BE107		single-reference main-group non-metal bond energies	MG3S
SR-TM-BE17		single-reference TM^b bond energies	
	3dSRBE4	3d single-reference metal-ligand bond energies	def2-TZVP (metal); ma-TZVP (non-metal)
	SRMBE10	single-reference metal bond energies	def2-TZVP
	PdBE2	palladium complex bond energies	SDD-2fg (Pd); cc-pVTZ (non-metal)
	FeCl	FeCl bond energy	aug-pwCVTZ (Fe); aug-pVTZ (Cl)
MR-MGM-BE4		multi-reference main-group metal bond energies	cc-pCVQZ (metal); aug-cc-pCVQZ (non-metal)
MR-MGN-BE17		multi-reference main-group non-metal bond energies	MG3S
MR-TM-BE13		multi-reference TM bond energies	
	CuH, CuCl, NiCl, VO	CuH, CuCl, NiCl, and VO bond energies	aug-cc-pwCVTZ (metal); aug-cc-pVTZ (non-metal)
	3dMRBE6	3d multi-reference metal-ligand bond energies	def2-TZVP (metal); ma-TZVP (non-metal)
	MRBE3	Multi-reference bond energies	def2-TZVP
MR-TMD-BE2		Multi-reference TM dimer bond energies (Cr_2 and V_2)	def2-TZVP
IP23		ionization potentials	MG3S
NCCE30		noncovalent complexation energies	MG3S
NGDWI21		noble gas dimer weak interaction	aug-cc-pVQZ
3dAEE7		3d TM atomic excitation energies	cc-pCVQZ (Ca); cc-pVQZ-DK
4dAEE5		4d TM atomic excitation energies	cc-pVTZ-DK
pEE5		p-block excitation energies	cc-pVQZ-DK; d-aug-cc-pVQZ-DK (F, Ar)
4pIsoE4		4p isomerization energies	cc-pVQZ
2pIsoE4		2p isomerization energies	cc-pVQZ
IsoL6/11		isomerization energies of large molecules	MG3SXP
EA13/03		electron affinities	MG3S
PA8		proton affinities	MG3S
πTC13		thermochemistry of π systems	MG3S
HTBH38/08		hydrogen transfer barrier heights	MG3S
NHTBH38/08		non-hydrogen transfer barrier heights	MG3S
AE17		atomic energies	For H, He, atoms from B to Ne, and atoms from Al to Ar, the basis set is cc-pwCV5Z; for Li, Be, Na, and Mg, the basis set is cc-pCVQZ.
HC7/11		hydrocarbon chemistry	6-311+G(2df,2p)
DC9/12		difficult cases	MG3S

MS10			
DGL6		diatomic geometries for light-atom molecules	6-311+G(2df,2p)
DGH4		diatomic geometries for heavy-atom molecules	
	HBr, ZnS	diatomic geometries for HBr and ZnS	aug-cc-pVQZ (H, Zn, S), B2 for Zn,[52] cc-pwCVQZ
	NaBr	diatomic geometry for NaBr	-DK[a] for Br
	Ag_2	diatomic geometry for Ag_2	jun-cc-pVTZ-PP
SSS17			
LC17		lattice constants	m-6-311G*
SSE39			
SBG31		semiconductor band gaps	m-6-311G*
SSCE8		solid-state cohesive energies	m-6-311G*

[a]A scalar relativistic correction of 0.003 Å was added to the geometry.

[b]TM denotes transition metal.

Table S3. Spin-orbit coupling in kcal/mol.[a]

Chemical species	Spin-orbit coupling	Chemical species	Spin-orbit coupling
Al	0.21	NiCl	1.50
B	0.03	NO	0.18
Br	3.51	O	0.22
C	0.09	O^-	0.16
C^+	0.13	OH	0.20
$CH(^2\Pi)$	0.04	P^-	0.28
Cl	0.84	P^+	0.90
Cl^+	1.05	S	0.56
ClO	0.46	S^-	0.55
Co	2.27	Se	2.70
CoH	2.10	SH	0.54
F	0.38	Si	0.43
Fe	1.15	Si^+	0.58
$Fe[CO]_5$	1.52	Si_2 (triplet)	0.20
FeH	1.10	TiCl	0.50
FeCl	1.10	Ti	0.60
HS	0.54	V_2	1.83
Li	0.14	V	0.90
LiCl	0.84	VS	1.47
Ni	2.80	Zr_2	3.30
$NiCH_2^+$	1.72		

[a]In all cases the spin–orbit coupling lowers the energy.

Table S4. Zero point energy (in kcal/mol) of solids in the SSCE8 database.

Solid	ZPE
C	4.985
Si	1.431
SiC	2.754
Ge	0.827
NaCl	0.718
NaF	1.100
LiCl	0.943
LiF	1.636

Table S5. Energetic data (in kcal/mol) of ME417 computed using BLYP, PBE, N12, a GAM exchange-correlation functionals.

SR-MGM-BE9	Reference	BLYP	PBE	N12	GAM
$AlCl_3$	309.91	286.79	303.85	317.30	300.75
AlF_3	429.60	418.56	424.60	435.52	419.88
KOH	85.00	81.04	83.07	74.85	84.31
NaO	65.23	67.84	67.28	55.75	65.57
LiO (aug-cc-pCVQZ)	82.54	89.51	87.56	73.92	82.19
LiCl	113.90	107.13	108.43	105.23	110.50
AlCl	121.56	117.05	121.11	124.77	119.95
ZnSe	25.20	23.13	29.25	32.98	22.81
ZnCl	53.48	43.10	51.36	50.40	49.49

SR-MGN-BE107	Reference	BLYP	PBE	N12	GAM
C_2H_6	97.39	90.42	96.87	97.56	96.26
iPr-CH_3	95	80.83	86.95	87.48	84.27
C_2H_6O	89.79	82.66	89.61	90.17	88.89
iPr-OCH_3	91.51	77.36	83.89	84.37	80.88
Et-H	108.92	104.83	104.87	106.75	104.93
Et-CH_3	95.89	86.43	93.08	93.89	92.31
Et-OCH_3	95.26	80.14	86.38	87.11	83.42
Et-OH	100.29	93.53	99.77	99.95	96.09
tBu-H	103.86	97.35	97.32	98.98	97.54
tBu-CH_3	93.67	78.82	86.16	86.29	85.52
tBu-OCH_3	89.27	73.12	80.12	80.10	77.08
tBu-OH	115.02	90.50	97.19	96.81	93.34
$CH(^2\prod)$	84.18	85.40	84.51	80.99	81.42
$CH_2(^3B_1)$	190.66	179.65	178.62	176.18	195.06

$CH_2(^1A_1)$	181.37	189.93	194.44	191.44	182.06
$CH_3(^2A''_2)$	307.79	306.94	309.94	306.25	307.42
CH_4	420.34	416.89	420.10	417.98	417.89
NH	83.1	89.26	88.25	78.29	80.39
NH_2	182.59	189.11	188.24	174.57	176.41
NH_3	298.02	301.42	301.71	289.63	289.95
OH	107.19	109.37	109.55	103.94	103.58
H_2O	232.75	231.94	233.52	228.80	226.60
HF	141.25	140.26	141.21	142.49	139.80
$SiH_2(^1A_1)$	151.79	151.45	147.42	151.74	146.18
$SiH_2(^3B_1)$	131.05	130.04	131.24	132.63	134.03
SiH_3	227.58	223.90	221.98	226.76	221.80
SiH_4	324.52	317.27	312.98	321.34	311.40
PH_2	153.2	157.41	154.44	158.56	149.27
PH_3	242.27	242.35	239.12	246.92	233.62
H_2S	183.35	180.09	181.46	188.11	179.79
HCl	106.66	103.45	105.43	109.40	106.07
C_2H_2	405.35	404.85	414.68	402.31	407.93
CH_2CH_2	563.51	560.54	571.44	562.25	565.12
CH_3CH_3	712.8	704.26	716.76	710.12	711.16
HCN	313.34	320.00	326.04	302.03	309.67
HCO	279.11	286.54	294.70	279.70	282.47
H_2CO	374.35	377.36	385.59	373.13	374.34
CH_3OH	513.22	510.23	519.53	510.32	507.71
NH_2NH_2	438.6	446.84	452.61	425.34	426.44
HOOH	268.57	274.47	281.01	265.58	261.91
Si_2 (triplet)	75.72	73.67	79.25	82.53	78.92
P_2	117.59	121.42	121.47	129.41	110.57
S_2	103.13	105.70	113.56	119.78	109.53
Cl_2	58.07	55.64	63.19	67.61	59.24
SC	171.11	171.41	178.79	176.17	171.94
ClF	61.57	64.46	69.61	69.65	63.22
Si_2H_6	535.03	519.14	519.15	533.93	516.41
CH_3Cl	395.51	388.55	398.90	398.78	395.42
CH_3SH	473.84	467.02	477.54	479.83	472.41
HOCl	165.17	166.39	173.27	167.73	161.86
BCl_3	322.9	308.88	332.71	341.14	330.10
BF_3	469.79	466.79	479.89	482.08	468.32
C_2Cl_4	466.28	451.41	496.50	492.42	486.81
C_2F_4	589.36	594.16	628.83	615.24	604.92

C_3H_4 (propyne)	704.79	701.22	720.82	703.95	710.88
C_4H_4O	993.74	988.72	1030.93	1000.59	1003.85
C_4H_4S	962.73	951.06	995.57	977.60	977.89
C_4H_5N	1071.57	1067.91	1110.71	1074.00	1080.97
C_4H_6 (*trans*-1,3-butadiene)	1012.37	1005.67	1034.35	1013.33	1020.71
C_4H_6 (2-butyne)	1004.13	996.22	1025.60	1004.20	1012.53
C_5H_5N	1237.69	1235.63	1284.97	1240.67	1251.80
CCH	265.13	266.02	276.77	262.38	254.71
CCl_4	312.74	293.79	329.07	332.08	320.70
CF_3CN	639.85	646.33	679.13	647.45	646.80
CF_4	476.32	473.15	500.35	494.93	482.04
CH_2OH	409.76	411.59	421.12	409.88	408.70
CH_3CN	615.84	619.75	635.43	607.16	615.98
CH_3NH_2	582.22	581.82	590.75	574.11	574.71
CH_3NO_2	601.27	616.78	641.46	600.83	610.34
$CHCl_3$	343.18	329.33	355.85	358.23	349.63
CHF_3	457.5	456.81	476.75	472.22	462.22
ClF_3	125.33	143.00	159.31	154.07	141.60
H_2	109.49	109.49	104.71	106.52	105.91
CH_2CH	445.91	446.54	457.74	446.49	451.86
$HCOOCH_3$	785.26	786.49	810.81	786.50	785.61
HCOOH	500.98	505.35	521.63	502.00	501.48
PF_3	363.87	361.13	370.39	376.70	351.77
SH	86.98	87.66	87.92	90.76	85.91
$SiCl_4$	384.94	352.77	381.23	400.42	375.99
SiF_4	574.35	555.50	567.60	581.43	556.57
C_2H_5	603.75	599.45	611.88	603.29	606.16
C_4H_6 (bicylobutane)	987.2	970.69	1011.27	989.09	1007.13
C_4H_6 (cyclobutene)	1001.61	987.94	1023.83	1003.96	1010.29
HCOCOH	633.35	639.96	662.71	635.23	638.69
CH_3CHO	677.03	676.30	694.27	677.31	679.57
C_2H_4O	650.7	647.42	669.49	651.40	655.29
C_2H_5O	698.64	692.44	710.32	694.91	698.29
CH_3OCH_3	798.05	792.05	809.67	795.64	792.99
CH_3CH_2OH	810.36	802.12	820.99	807.14	805.72
C_3H_4 (allene)	703.2	704.15	723.86	707.10	713.24
C_3H_4 (cyclopropene)	682.74	676.44	701.38	684.07	696.22
CH_3COOH	803.04	801.52	827.56	803.57	803.88
CH_3COCH_3	977.96	972.06	999.98	978.37	981.84
C_3H_6 (cyclopropane)	853.41	841.68	867.94	853.98	862.39

CH_3CHCH_2	860.61	852.80	873.53	859.57	863.85
C_3H_8	1006.87	992.73	1014.92	1003.52	1005.99
$C_2H_5OCH_3$	1095.12	1083.83	1111.06	1092.36	1090.93
C_4H_{10} (isobutane)	1303.04	1281.53	1313.84	1297.40	1301.58
C_4H_{10} (antiperiplanar butane)	1301.32	1281.13	1313.05	1296.86	1300.78
C_4H_8 (cyclobutane)	1149.01	1130.27	1167.07	1149.95	1153.75
C_4H_8 (isobutene)	1158.61	1144.50	1175.33	1156.45	1162.33
C_5H_8 (spiropentane)	1284.28	1265.51	1315.19	1289.02	1306.62
C_6H_6	1367.56	1355.87	1409.19	1375.72	1386.66
CH_3CO	581.58	585.72	603.41	584.40	587.89
$(CH_3)_2CH$	900.75	892.06	914.25	900.86	905.15
$(CH_3)_3C$	1199.34	1184.20	1216.44	1198.28	1203.91
H_2CCO	532.32	539.73	557.87	537.84	543.21

SR-TM-BE17	Reference	BLYP	PBE	N12	GAM
$CrCl_2$	181.13	172.66	175.77	175.75	174.00
MnF_2	232.26	246.27	254.45	257.54	238.28
$FeCl_2$	190.29	183.66	196.13	199.82	187.54
$CoCl_2$	182.9	172.64	183.99	184.99	178.35
Ag_2	38.3	38.46	40.57	44.66	39.10
AgH	54	56.54	55.86	57.34	51.99
CoH	45.5	61.04	60.33	61.35	70.27
$CrCH_3^+$	28.8	42.24	43.74	39.71	41.86
Cu_2	47.2	45.71	47.98	51.09	40.27
CuAg	40.7	39.14	44.30	46.27	36.10
CuH_2O^+	38.8	41.52	43.06	42.60	38.23
FeH	36.9	52.15	51.58	55.45	52.19
VCO^+	28.2	34.69	38.34	30.87	39.89
Zr_2	70.8	78.99	92.93	103.08	70.85
$Pd(PH_3)_2C_6H_8$	16.2	2.38	13.32	9.05	6.40
$Pd(PH_3)_2C_{10}H_{12}$ (structure b)	17.3	-3.85	9.11	3.64	1.78
FeCl	78.5	75.98	84.87	81.32	79.43

MR-MGM-BE4	Reference	BLYP	PBE	N12	GAM
CaO	96.15	118.39	124.23	117.38	107.75
LiO^-	57.59	62.43	61.83	51.71	63.27
KO^-	33.14	35.50	37.69	27.50	40.40
MgS	55.68	50.14	55.31	59.35	49.17

MR-MGN-BE17	Reference	BLYP	PBE	N12	GAM
NF_3	204.53	225.18	242.56	217.54	214.80
CO_2	389.61	398.98	415.56	391.92	398.39
SiO (singlet)	192.4	194.66	195.65	190.28	183.14
SO_2	259.61	262.95	277.06	264.61	255.30
CO	259.42	261.25	268.30	253.14	255.74
SO (triplet)	125.69	133.23	139.56	133.92	128.27
ClO	64.84	73.41	79.92	72.01	69.03
F_2	38.27	47.14	51.24	44.69	41.45
N_2	228.48	239.62	242.97	206.41	218.77
O_2	120.37	134.46	142.81	123.85	131.19
NO	152.7	166.03	171.75	143.46	151.87
CN	181.27	190.72	197.02	170.36	181.80
$B_2 \rightarrow 2B$	67.4	67.02	76.97	70.77	77.18
$O_3 \rightarrow O_2 + O$	26.61	34.51	41.16	23.89	23.86
$C_2 \rightarrow 2C$	146.88	145.45	93.61	125.16	148.78
$S_4 \rightarrow 2S_2$	25.75	18.84	28.37	31.54	23.61
$Cl_2O \rightarrow Cl_2 + O$	41.71	48.21	53.04	41.99	41.33

MR-TM-BE13	Reference	BLYP	PBE	N12	GAM
TiCl	100.78	106.35	115.67	121.31	103.16
VF_5	564.15	609.78	629.82	622.37	584.58
CrCl	90.15	87.52	88.95	90.22	94.00
CrOF	247.58	255.56	254.80	241.31	229.25
$(FeBr_2)_2$	366.8	336.68	367.57	371.83	338.57
$Co(CO)_4H$	1230.13	1250.35	1310.05	1246.10	1225.99
$NiCH_2^+ \rightarrow Ni^+ + CH_2$	76.3	93.69	94.26	87.90	82.90
$Fe(CO)_5 \rightarrow Fe + 5CO$	147.4	161.10	194.57	198.47	149.54
$VS \rightarrow V + S$	106.9	64.48	129.75	133.08	116.34
CuH	62.6	65.68	64.51	65.28	57.84
CuCl	87.7	80.11	86.40	91.21	79.96
VO	151	171.71	182.07	173.27	154.03
NiCl	88	83.11	89.44	95.69	82.09

MR-TMD-BE2	Reference	BLYP	PBE	N12	GAM
$Cr_2 \rightarrow 2Cr$	36.0	44.36	21.46	38.70	23.00
$V_2 \rightarrow 2V$	64.2	-14.65	104.05	115.63	70.71

IsoL6/11	Reference	BLYP	PBE	N12	GAM
10-	6.82	1.81	5.26	4.76	5.36
13-	33.52	29.73	31.06	31.28	32.43
14-	5.3	3.85	6.23	6.02	5.50
20-	4.66	4.09	4.90	4.99	5.05
3-	9.77	3.28	7.18	9.44	4.45
9-	21.76	16.68	17.65	17.04	18.49

IP23	Reference	BLYP	PBE	N12	GAM
C	259.7	263.05	266.14	261.75	264.76
S	238.9	240.60	240.91	239.04	232.52
SH	238.9	238.46	239.82	238.94	233.95
Cl	299.1	297.26	298.84	299.44	293.21
Cl_2	265.3	255.07	256.88	256.52	254.46
OH	299.1	305.17	304.59	295.83	295.91
O	313.9	326.99	324.72	306.87	309.00
O_2	278.9	283.57	282.78	288.56	281.75
P	241.9	233.95	241.03	238.23	241.51
PH	234.1	230.02	236.20	232.83	235.28
PH_2	226.3	224.68	229.94	225.61	227.00
S_2	216	213.46	217.27	214.88	216.79
Si	187.9	182.99	188.89	185.16	186.03
Cr	156.009	167.19	170.50	158.24	165.25
Cu	178.173	194.47	193.05	183.51	188.80
FeC	173.71	185.31	186.16	175.96	171.52
Mo	163.71	168.09	172.08	160.20	164.40
Pd	192.24	203.75	204.21	206.52	202.45
Rh	172.11	180.21	180.85	173.76	171.35
Ru	169.86	177.18	178.98	167.96	171.74
Zn	216.629	223.84	221.22	219.05	216.67
Co	181.1	187.88	187.23	173.65	195.61
Sc	151.32	148.34	146.89	132.85	156.38

EA13/03	Reference	BLYP	PBE	N12	GAM
C	29.1	30.26	35.75	29.09	34.68
S	47.9	48.64	49.60	45.75	44.79
SH	53.3	50.76	52.70	49.61	50.05
Cl	83.4	81.23	83.12	81.03	80.41
Cl_2	55.6	62.46	59.76	53.44	58.32
OH	42.1	41.98	42.32	35.11	37.82
O	33.7	39.24	38.26	25.62	29.03
O2	10.8	11.16	8.63	3.70	-1.88
P	17.2	20.53	20.16	14.93	14.48
PH	23.2	23.21	24.02	19.50	19.71
PH_2	29.4	26.26	28.18	24.49	25.54
S_2	38.5	34.51	35.69	31.39	30.53
Si	31.9	26.98	33.26	28.95	32.90

PA8	Reference	BLYP	PBE	N12	GAM
NH_3	211.9	209.55	210.89	212.97	214.43
H_2O	171.8	168.96	170.39	172.03	172.70
C_2H_2	156.6	157.00	158.91	160.66	163.56
SiH_4	156.5	158.14	157.01	157.68	162.00
PH_3	193.1	191.29	190.24	192.98	195.47
H_2S	173.7	174.44	174.38	175.41	178.21
HCl	137.1	138.25	138.93	139.21	141.94
H_2	105.9	104.17	106.03	105.57	109.02

πTC13	Reference	BLYP	PBE	N12	GAM
E2-E1	-1.4	3.07	3.10	3.40	2.49
E4-E3	-8.8	0.06	0.16	0.51	-0.64
E6-E5	-14.3	-1.60	-1.42	-0.98	-2.35
P-2	167.81	166.27	167.91	170.06	172.61
P-4	193.45	197.47	196.42	199.75	200.44
P-6	209.68	215.55	214.26	217.78	218.28
P-8	219.67	227.12	225.72	229.39	229.78
P-10	225.95	235.42	233.96	237.75	238.05
SB-2	214.46	213.17	213.72	217.46	218.09
SB-4	226.15	227.96	228.25	232.69	232.63
SB-6	233.44	238.09	238.26	243.07	242.66
SB-8	238.16	245.25	245.34	250.39	249.76
SB-10	240.97	250.68	250.72	255.95	255.14

HTBH38/08	Reference	BLYP	PBE	N12	GAM
$H + HCl \rightarrow H_2 + Cl$	5.7	-2.67	0.34	2.04	3.12
	8.7	3.37	-0.38	-0.85	2.96
$OH + H_2 \rightarrow H_2O + H$	5.1	-2.91	-5.74	-2.44	-0.95
	21.2	10.18	13.53	15.90	16.15
$CH_3 + H_2 \rightarrow CH_4 + H$	12.1	7.35	4.02	6.13	7.83
	15.3	7.81	9.47	11.35	12.38
$OH + CH_4 \rightarrow H_2O + CH_3$	6.7	-2.14	-5.00	-1.87	-0.35
	19.6	10.49	8.82	11.26	12.20
$H + H_2 \rightarrow H_2 + H$	9.6	2.96	3.77	6.53	7.73
	9.6	2.96	3.77	6.53	7.73
$OH + NH_3 \rightarrow H_2O + NH_2$	3.2	-8.67	-11.35	-7.57	-5.57
	12.7	1.60	-0.85	2.23	3.91
$HCl + CH_3 \rightarrow CH_4 + Cl$	1.7	-3.28	-5.71	-3.89	-2.08
	7.9	3.22	-0.98	-1.56	2.31
$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	3.4	-5.57	-8.45	-5.17	-4.02
	19.9	12.19	10.65	12.86	13.99
$F + H_2 \rightarrow HF + H$	1.8	-10.74	-12.05	-9.36	-8.65
	33.4	20.03	24.46	26.61	25.24
$O + CH_4 \rightarrow OH + CH_3$	13.7	2.33	0.16	6.72	7.40
	8.1	1.75	-0.44	-1.07	0.51
$H + PH_3 \rightarrow H_2 + PH_2$	3.1	-2.50	-1.65	0.72	0.37
	23.2	22.05	18.38	18.88	21.93
$H + HO \rightarrow H_2 + O$	10.7	1.58	3.76	3.28	4.46
	13.1	1.69	-1.08	5.86	6.79
$H + H_2S \rightarrow H_2 + HS$	3.5	-2.12	-1.13	1.09	1.92
	17.3	14.94	10.04	10.25	13.95
$O + HCl \rightarrow OH + Cl$	9.8	-8.14	-9.88	-1.80	-1.20
	10.4	-2.22	-5.75	-7.27	-3.69
$CH_3 + NH_2 \rightarrow CH_4 + NH$	8	3.48	0.66	0.78	2.67
	22.4	13.57	10.83	16.23	17.11
$C_2H_5 + NH_2 \rightarrow C_2H_6 + NH$	7.5	5.87	2.86	2.87	5.11
	18.3	10.83	7.76	13.42	14.09
$NH_2 + C_2H_6 \rightarrow NH_3 + C_2H_5$	10.4	5.31	1.52	4.42	6.02
	17.4	12.80	10.12	12.65	14.54
$NH_2 + CH_4 \rightarrow NH_3 + CH_3$	14.5	8.08	4.51	7.18	9.08
	17.8	10.43	7.82	10.52	12.14
s-trans cis-$C_5H_8 \rightarrow$ *s-trans cis*-C_5H_8	38.4	36.04	31.43	33.25	36.56

	38.4	36.04	31.43	33.25	36.56

NHTBH38/08	Reference	BLYP	PBE	N12	GAM
$H + N_2O \rightarrow OH + N_2$	17.13	8.95	10.46	11.34	16.15
	82.47	62.18	53.04	59.00	57.69
$H + FH \rightarrow HF + H$	42.18	26.78	27.98	30.53	36.09
	42.18	26.78	27.98	30.53	36.09
$H + ClH \rightarrow HCl + H$	18	10.53	10.40	13.69	15.85
	18	10.53	10.40	13.69	15.85
$H + FCH_3 \rightarrow HF + CH_3$	30.38	16.33	18.73	20.71	23.07
	57.02	42.33	41.14	43.39	47.98
$H + F_2 \rightarrow HF + F$	2.27	-11.45	-9.59	-10.37	-6.85
	106.18	81.67	80.38	87.43	91.50
$CH_3 + FCl \rightarrow CH_3F + Cl$	6.73	-6.91	-6.41	-5.90	-5.64
	60	42.89	42.79	44.25	46.03
$F^- + CH_3F \rightarrow FCH_3 + F^-$	-0.34	-7.88	-8.33	-7.45	-6.28
	-0.34	-7.88	-8.33	-7.45	-6.28
$F^-\cdots CH_3F \rightarrow FCH_3\cdots F^-$	13.38	6.11	6.66	7.06	9.06
	13.38	6.11	6.66	7.06	9.06
$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	3.1	-3.87	-3.73	-1.07	0.16
	3.1	-3.87	-3.73	-1.07	0.16
$Cl^-\cdots CH_3Cl \rightarrow ClCH_3\cdots Cl^-$	13.41	5.56	6.94	8.39	11.12
	13.41	5.56	6.94	8.39	11.12
$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	-12.54	-19.31	-19.51	-17.89	-16.20
	20.11	12.88	12.09	14.10	14.49
$F^-\cdots CH_3Cl \rightarrow FCH_3\cdots Cl^-$	3.44	-1.96	-0.98	-0.20	1.76
	29.42	20.72	21.04	22.00	24.18
$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	-2.44	-9.78	-10.66	-9.62	-8.14
	17.66	9.59	9.63	11.92	12.47
$OH^-\cdots CH_3F \rightarrow HOCH_3\cdots F^-$	10.96	3.20	3.37	3.87	6.52
	47.2	39.80	42.72	44.31	43.34
$H + N_2 \rightarrow HN_2$	14.36	5.59	5.57	6.92	9.17
	10.61	8.58	9.24	12.58	11.54
$H + CO \rightarrow HCO$	3.17	-1.93	-1.69	-0.34	0.57
	22.68	23.36	24.72	26.22	27.30
$H + C_2H_4 \rightarrow CH_3CH_2$	1.72	-0.61	-0.04	1.28	1.52
	41.75	38.29	40.39	42.31	42.55
$CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$	6.85	4.75	1.57	3.14	3.11
	32.97	24.87	29.72	30.85	31.08

HCN → HNC	48.07	47.04	45.95	46.48	48.54
	32.82	32.10	30.97	33.81	32.82

NCCE30	Reference	BLYP	PBE	N12	GAM
$(NH_3)_2$	3.15	2.36	3.34	2.40	3.64
$(HF)_2$	4.57	4.37	5.00	4.84	5.06
$(H_2O)_2$	4.97	4.55	5.44	4.99	5.55
$NH_3\cdots H_2O$	6.41	6.01	7.15	6.43	7.09
$(HCONH_2)_2$	14.94	12.02	14.24	13.31	14.18
$(HCOOH)_2$	16.15	13.80	16.33	16.41	15.53
$C_2H_4\cdots F_2$	1.06	2.68	3.17	2.76	3.49
$NH_3\cdots F_2$	1.81	4.95	5.45	4.79	5.62
$C_2H_2\cdots ClF$	3.81	4.36	6.18	4.74	6.25
$HCN\cdots ClF$	4.86	4.75	5.93	4.80	6.04
$NH_3\cdots Cl_2$	4.88	6.46	7.95	6.37	7.50
$H_2O\cdots ClF$	5.36	6.08	7.41	6.27	7.30
$NH_3\cdots ClF$	10.62	14.62	17.09	15.67	15.28
$(H_2S)_2$	1.66	0.73	1.80	0.67	2.33
$(HCl)_2$	2.01	1.13	2.11	1.13	2.54
$HCl\cdots H_2S$	3.35	2.80	4.16	2.98	4.42
$CH_3Cl\cdots HCl$	3.55	1.90	3.39	2.07	3.90
$HCN\cdots CH_3SH$	3.59	2.16	3.52	2.29	3.87
$CH_3SH\cdots HCl$	4.16	3.63	5.61	4.10	5.80
$CH_4\cdots Ne$	0.22	-0.10	0.27	-0.05	0.26
$C_6H_6\cdots Ne$	0.47	-0.39	0.35	-0.26	0.43
$(CH_4)_2$	0.51	-0.82	0.01	-1.02	0.49
$CO_2\cdots Ar$	0.57	0.43	-0.26	0.65	-0.45
$(C_2H_2)_2$	1.34	0.10	1.00	-0.03	1.47
$(C_2H_4)_2$	1.42	-1.08	0.36	-1.19	1.27
sandwich $(C_6H_6)_2$	1.81	-3.69	-1.56	-2.60	0.73
T-shaped $(C_6H_6)_2$	2.74	-1.81	0.11	-0.20	1.88
parallel-displaced $(C_6H_6)_2$	2.78	-3.49	-0.97	-2.12	1.37
parallel-displaced $(CO_2)_2$	1.49	0.13	-0.71	0.29	-0.98
sandwich $(C_5H_5N)_2$	2.89	2.48	0.19	2.69	-1.31

NGDWI21	Reference	BLYP	PBE	N12	GAM
He_2	0.022	-0.08	0.06	-0.05	0.041
Ne_2	0.080	-0.14	0.12	-0.10	0.080
Ar_2	0.290	-0.38	0.11	-0.46	0.271
Kr_2	0.400	-0.52	0.09	-0.64	0.439
HeNe	0.040	-0.10	0.09	-0.07	0.058
HeAr	0.060	-0.14	0.09	-0.13	0.086
NeAr	0.130	-0.20	0.13	-0.20	0.139
HeHe_L_0.3A	0.007	-0.14	0.07	-0.10	0.031
HeHe_R_0.3A	0.017	-0.05	0.04	-0.02	0.029
ArAr_L_0.3A	0.141	-0.82	-0.18	-0.87	0.155
ArAr_R_0.3A	0.239	-0.22	0.14	-0.27	0.209
NeNe_L_0.3A	0.015	-0.30	0.04	-0.22	-0.002
NeNe_R_0.3A	0.067	-0.09	0.10	-0.06	0.067
KrKr_L_0.3A	0.236	-1.10	-0.29	-1.17	0.251
KrKr_R_0.3A	0.343	-0.29	0.16	-0.39	0.361
HeNe_L_0.3A	0.006	-0.19	0.08	-0.14	0.030
HeNe_R_0.3A	0.033	-0.07	0.06	-0.03	0.045
HeAr_L_0.3A	0.025	-0.26	0.06	-0.25	0.074
HeAr_R_0.3A	0.049	-0.09	0.07	-0.07	0.061
NeAr_L_0.3A	0.053	-0.41	0.02	-0.39	0.085
NeAr_R_0.3A	0.109	-0.12	0.11	-0.11	0.104

AE17	Reference	BLYP	PBE	N12	GAM
H	-0.50	-0.50	-0.50	-0.50	-0.50
He	-2.90	-2.91	-2.89	-2.92	-2.92
Li	-7.48	-7.46	-7.46	-7.53	-7.52
Be	-14.67	-14.63	-14.63	-14.71	-14.71
B	-24.65	-24.65	-24.61	-24.69	-24.70
C	-37.85	-37.84	-37.80	-37.87	-37.88
N	-54.59	-54.59	-54.54	-54.61	-54.62
O	-75.07	-75.08	-75.01	-75.07	-75.07
F	-99.73	-99.75	-99.68	-99.73	-99.73
Ne	-128.94	-128.95	-128.87	-128.95	-128.93
Na	-162.25	-162.27	-162.17	-162.29	-162.24
Mg	-200.05	-200.08	-199.95	-200.08	-200.06
Al	-242.35	-242.37	-242.24	-242.37	-242.35
Si	-289.36	-289.38	-289.23	-289.38	-289.36
P	-341.26	-341.27	-341.12	-341.27	-341.27
S	-398.11	-398.12	-397.95	-398.12	-398.11

Cl	-460.15	-460.15	-459.97	-460.17	-460.15

HC7/11	Reference	BLYP	PBE	N12	GAM
E22-E1	14.34	-11.53	13.78	17.05	15.57
E31-E1	25.02	-13.37	18.42	22.69	17.68
octane iso	1.90	-9.58	-5.18	-7.16	-5.84
DE (reaction a)	9.81	4.07	5.78	4.71	5.96
DE (reaction b)	14.84	6.01	8.59	6.96	8.86
DE (reaction c)	193.99	135.86	193.00	196.37	184.95
DE (reaction d)	127.22	83.93	124.90	126.79	118.74

3dAEE7	Reference	BLYP	PBE	N12	GAM
Sc	32.91	17.34	13.28	4.95	26.67
Mn^+	27.08	19.64	26.57	15.69	15.46
Fe	34.32	18.98	21.35	12.36	45.39
Ni^+	25.02	24.14	25.21	43.42	37.44
Zn	93.48	104.03	97.93	104.59	97.48
Ca^+	39.10	25.91	26.44	22.76	21.45
V	5.60	-3.31	-12.57	-16.77	-0.17

4dAEE5	Reference	BLYP	PBE	N12	GAM
Mo^+	43.96	26.07	33.40	32.07	39.93
Ru^+	25.15	26.50	22.98	34.74	30.35
Rh^+	18.62	10.83	11.74	9.59	14.12
Pd	21.96	21.11	21.90	29.79	27.24
Y^+	3.41	2.63	-0.42	-9.44	10.53

pEE5	Reference	BLYP	PBE	N12	GAM
F	292.88	296.52	293.55	285.45	293.88
Ar	268.12	260.68	262.05	262.85	268.53
C^+	122.92	124.88	114.12	87.95	115.91
Al	82.98	90.82	82.87	74.38	86.58
Si^+	126	130.64	121.83	107.96	123.09

DC9/12	Reference	BLYP	PBE	N12	GAM
$HCN\cdots BF_3 \rightarrow HCN + BF_3$	5.70	2.71	4.33	4.04	4.80
$C_6Cl_6 + 6HCl \rightarrow 6Cl_2 + C_6H_6$	148.30	114.96	135.99	141.13	160.55
$P_4 \rightarrow 4P$	289.90	283.42	308.07	325.38	304.77
$SF_6 \rightarrow S + 6F$	477.50	463.87	501.88	503.59	472.41
$PF_5 \rightarrow P + 5F$	556.40	540.64	562.00	571.23	535.61
$P_4O_{10} \rightarrow P_4 + 5O_2$	719.70	605.03	618.57	656.30	539.58
$C_6F_6 \rightarrow 6C + 6F$	1388.10	1398.03	1485.06	1443.03	1434.16
$Si(OCH_3)_4 \rightarrow Si + 4C + 4O + 12H$	2023.50	1996.50	2046.37	2012.09	1987.05
urotropin → 6C + 4N + 12H	2151.10	2122.01	2214.43	2121.45	2122.96

2pIsoE4	Reference	BLYP	PBE	N12	GAM
C	3.8	0.35	1.45	0.81	1.39
N	57.1	71.19	64.37	65.84	70.26
O	9.9	10.53	9.43	8.78	5.62
F	26.9	23.27	26.06	26.11	26.68

4pIsoE4	Reference	BLYP	PBE	N12	GAM
As	33.0	45.84	37.90	37.40	42.29
Br	-6.3	-6.44	-5.22	-5.88	-6.01
Ge	24.6	23.25	22.73	24.44	20.73
Se	20.8	22.47	22.67	22.73	19.96

Table S6. MUEs (in kcal/mol for energetics and Å for distances) for each primary subdatabase using GAM exchange–correlation functional.

Subset	MUE	Subset	MUE
MSR2	3.15	PA-CP5/06	8.52
MGDSR5	1.06	PA-SB5/06	9.02
3dSRBE2	3.19	HATBH12/08	9.06
ABDE12	7.95	NSBH16/08	4.15
ABDE4/05	5.85	UABH10/08	2.04
ABDEL8	8.99	DBH24/08	4.93
NMSR95	1.55	HB6/04	0.60
AE6/11	3.48	CT7/04	2.73
3dSRBE4	2.56	DI6/04	0.75
SRMBE12	8.34	EDCE19	1.43
MBE15	8.32	WI8	0.16

TMBE15	8.32	pSI7	1.47
3dMRBE6	4.11	SB1AE97	1.59
MRBE5	8.26	MGLC4	0.038
IP13/03	3.77	ILC5	0.096
IPM10	5.65	TMLC4	0.087
πIE3/06	8.00	SLC5	0.134

Table S7. Geometries (in Å), Charge, and Multiplicity for Single-Point Calculations.

SR-MGM-BE9			
KOH			
0, 1			
K	0.0000000	0.0000000	2.1800000
O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	-0.9700000
NaO			
0, 2			
Na	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	2.0500000
LiO			
0, 2			
Li	0.0000000	0.0000000	1.6800000
O	0.0000000	0.0000000	0.0000000
ZnSe			
0, 1			
Zn	0.0000000	0.0000000	-1.1906800
Se	0.0000000	0.0000000	1.0506000
ZnCl			
0, 2			
Zn	0.0000000	0.0000000	0.7864940
Cl	0.0000000	0.0000000	-1.3879310

$AlCl_3$
0, 1

Al	0.0000000	0.0000000	0.0000000
Cl	2.0713000	0.0000000	0.0000000
Cl	-1.0356500	-1.7938000	0.0000000
Cl	-1.0356500	1.7938000	0.0000000

AlF_3
0, 1

Al	0.0000000	0.0000000	0.0000000
F	1.6284800	0.0000000	0.0000000
F	-0.814240	-1.410310	0.0000000
F	-0.814240	1.4103100	0.0000000

LiCl
0, 1

Li	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.0206700

AlCl
0, 1

Cl	0.0000000	0.0000000	-1.0705300
Al	0.0000000	0.0000000	1.0705300

SR-MGN-BE107

C_2H_6
0, 1

C	-0.7652700	0.0000000	0.0000000
C	0.7652700	0.0000000	0.0000000
H	1.1643500	1.0209400	0.0000000
H	1.1643500	-0.5104700	0.8841600
H	1.1643500	-0.5104700	-0.8841600
H	-1.1643500	-1.0209400	0.0000000
H	-1.1643500	0.5104700	0.8841600
H	-1.1643500	0.5104700	-0.8841600

iPr-CH_3
0, 1

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.1005600
C	1.4620900	0.0000000	-0.4685500
C	-0.7310500	-1.2662100	-0.4685500
C	-0.7310500	1.2662100	-0.4685500
H	1.5211800	0.0000000	-1.5650500
H	-0.7605900	-1.3173800	-1.5650500
H	-0.7605900	1.3173800	-1.5650500

H	1.9975500	0.8862200	-0.1072300
H	1.9975500	-0.8862200	-0.1072300
H	-0.2312900	-2.1730400	-0.1072300
H	-1.7662600	-1.2868200	-0.1072300
H	-1.7662600	1.2868200	-0.1072300
H	-0.2312900	2.1730400	-0.1072300

C_2H_6O
0, 1

O	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.4098600
C	1.3043100	0.0000000	-0.5352500
H	-1.0441800	0.0000000	1.7341000
H	1.2078600	0.0000000	-1.6243400
H	0.5010100	0.8929500	1.8197700
H	1.8737300	0.8929500	-0.2273700
H	0.5010100	-0.8929500	1.8197700
H	1.8737300	-0.8929500	-0.2273700

iPr-OCH_3
0, 1

O	0.2581800	0.9378800	0.0407400
C	1.6365600	1.0423000	0.3233000
H	1.8990700	2.1004100	0.2355500
H	2.2623400	0.4702400	-0.3784700
C	-0.2958100	-0.3651000	0.2296100
H	0.0737300	-0.7702300	1.1884200
C	0.0999600	-1.3221900	-0.8997900
C	-1.8070700	-0.1766000	0.3188300
H	-2.3094100	-1.1343600	0.4933800
H	-2.0591700	0.5065000	1.1358100
H	-2.1901500	0.2507100	-0.6147500
H	-0.3461700	-2.3107400	-0.7410700
H	-0.2515800	-0.9340800	-1.8625300
H	1.1853100	-1.4555200	-0.9606300
H	1.8687800	0.7036000	1.3466100

Et-H
0, 1

C	-0.7652700	0.0000000	0.0000000
C	0.7652700	0.0000000	0.0000000
H	1.1643500	1.0209400	0.0000000
H	1.1643500	-0.5104700	0.8841600
H	1.1643500	-0.5104700	-0.8841600
H	-1.1643500	-1.0209400	0.0000000
H	-1.1643500	0.5104700	0.8841600
H	-1.1643500	0.5104700	-0.8841600

Et-CH_3
0, 1

C	0.0000000	0.0000000	0.5864600
H	0.8776200	0.0000000	1.2471600
H	-0.8776200	0.0000000	1.2471600
C	0.0000000	-1.2771800	-0.2598900
C	0.0000000	1.2771800	-0.2598900
H	0.0000000	-2.1759600	0.3676200
H	-0.8846200	-1.3221900	-0.9073900
H	0.8846200	-1.3221900	-0.9073900
H	0.0000000	2.1759600	0.3676200
H	0.8846200	1.3221900	-0.9073900
H	-0.8846200	1.3221900	-0.9073900

Et-OCH_3
0, 1

C	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.4096200
C	1.3060800	0.0000000	1.9578700
C	1.1922100	0.0000000	3.4735300
H	2.1866600	0.0000000	3.9333200
H	-1.0441000	0.0000000	-0.3247400
H	0.5007900	-0.8926700	-0.4105100
H	0.5007900	0.8926700	-0.4105100
H	1.8643500	-0.8872800	1.6105600
H	1.8643500	0.8872800	1.6105600
H	0.6498100	-0.8869000	3.8167300
H	0.6498100	0.8869000	3.8167300

Et-OH
0, 1

H	-1.8176300	-0.8062000	0.0000000
O	-0.8507800	-0.8715100	0.0000000
C	-0.3229800	0.4520600	0.0000000
C	1.1930800	0.3476000	0.0000000
H	1.6489800	1.3439400	0.0000000
H	-0.6606200	1.0125200	-0.8875300
H	-0.6606200	1.0125200	0.8875300
H	1.5377700	-0.1943400	-0.8868200
H	1.5377700	-0.1943400	0.8868200

tBu-H
0, 1

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.1005600
C	1.4620900	0.0000000	-0.4685500
C	-0.7310500	-1.2662100	-0.4685500
C	-0.7310500	1.2662100	-0.4685500

H	1.5211800	0.0000000	-1.5650500
H	-0.7605900	-1.3173800	-1.5650500
H	-0.7605900	1.3173800	-1.5650500
H	1.9975500	0.8862200	-0.1072300
H	1.9975500	-0.8862200	-0.1072300
H	-0.2312900	-2.1730400	-0.1072300
H	-1.7662600	-1.2868200	-0.1072300
H	-1.7662600	1.2868200	-0.1072300
H	-0.2312900	2.1730400	-0.1072300

tBu-CH_3
0, 1

C	0.0000000	0.0000000	0.0000000
C	1.5402500	-0.0000900	-0.0000400
C	-0.5133300	1.4521900	-0.0000500
C	-0.5134900	-0.7261100	-1.2575600
C	-0.5134200	-0.7259900	1.2576500
H	-1.6099900	1.4848900	-0.0000200
H	-1.6101500	-0.7423700	-1.2858000
H	-1.6100800	-0.7422500	1.2859600
H	-0.1631200	1.9963800	0.8859100
H	-0.1631600	1.9963000	-0.8860800
H	-0.1633300	-0.2309600	-2.1718600
H	-0.1633900	-1.7655100	-1.2858000
H	-0.1633200	-1.7653900	1.2859600
H	-0.1632000	-0.2307700	2.1718900
H	1.9365200	-1.0231600	-0.0000100
H	1.9365800	0.5113800	-0.8860700
H	1.9366300	0.5114600	0.8859200

tBu-OCH_3
0, 1

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.5330700
O	1.4034400	0.0000000	1.8630700
C	1.7631400	0.0000000	3.2288700
H	-1.0228900	0.0000000	-0.3917600
H	0.5199500	-0.8862500	-0.3781500
H	0.5199500	0.8862500	-0.3781500
H	2.8567700	0.0000000	3.2541300
H	1.4070800	-0.8921700	3.7647500
H	1.4070800	0.8921700	3.7647500
C	-0.6925200	-1.2669400	2.0622200
C	-0.6925200	1.2669400	2.0622200
H	-0.1536600	-2.1608800	1.7298200
H	-0.1536600	2.1608800	1.7298200
H	-1.7201100	-1.3251500	1.6864900

H	-1.7201100	1.3251500	1.6864900
H	-0.7436500	-1.2818800	3.1563800
H	-0.7436500	1.2818800	3.1563800

tBu-OH
0, 1

C	-1.5323300	0.0224700	0.0000000
C	-0.0019200	0.0142100	0.0000000
O	0.3723900	1.4035600	0.0000000
H	1.3424800	1.4403600	0.0000000
H	-1.9299100	-0.9981900	0.0000000
H	-1.9079700	0.5438200	-0.8865300
H	-1.9079700	0.5438200	0.8865300
C	0.5430300	-0.6646600	-1.2658000
C	0.5430300	-0.6646600	1.2658000
H	0.1783600	-0.1475200	-2.1594300
H	0.1783600	-0.1475200	2.1594300
H	0.2375200	-1.7160000	-1.3228000
H	0.2375200	-1.7160000	1.3228000
H	1.6408400	-0.6376700	-1.2803200
H	1.6408400	-0.6376700	1.2803200

$CH(^2\prod)$
0, 2

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.1191300

$CH_2(^3B_1)$
0, 3

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0767200
H	0.7766500	0.0000000	-0.7457500

$CH_2(^1A_1)$
0, 1

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.1077100
H	1.0837800	0.0000000	-0.2289900

$CH_3(^2A''_2)$
0, 2

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0773200
H	0.9329800	0.0000000	-0.5386600
H	-0.9329800	0.0000000	-0.5386600

CH_4
0, 1

C	0.0000000	0.0000000	0.0000000

H	0.0000000	0.0000000	1.0874400
H	1.0252500	0.0000000	-0.3624800
H	-0.5126300	0.8878900	-0.3624800
H	-0.5126300	-0.8878900	-0.3624800

NH
0, 3

N	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0367300

NH_2
0, 2

N	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0240500
H	0.9971600	0.0000000	-0.2331400

NH_3
0, 1

N	0.0000000	0.0000000	0.1128900
H	0.0000000	0.9380200	-0.2634100
H	0.8123500	-0.4690100	-0.2634100
H	-0.8123500	-0.4690100	-0.2634100

OH
0, 2

O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9689000

H_2O
0, 1

O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9569100
H	0.9263600	0.0000000	-0.2398700

HF
0, 1

F	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9153800

$SiH_2(^1A_1)$
0, 1

Si	0.0000000	0.0000000	0.1309600
H	0.0000000	1.0947500	-0.9167600
H	0.0000000	-1.0947500	-0.9167600

$SiH_2(^3B_1)$
0, 3

Si	0.0000000	0.0000000	0.0000000
H	1.2694600	0.0000000	0.7575200
H	-1.2694600	0.0000000	0.7575200

SiH_3
0, 2

Si	0.0000000	0.0000000	0.0791800
H	0.0000000	1.4079800	-0.3694900
H	1.2193500	-0.7039900	-0.3694900
H	-1.2193500	-0.7039900	-0.3694900

SiH_4
0, 1

Si	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.4767000
H	1.3922500	0.0000000	-0.4922300
H	-0.6961200	-1.2057200	-0.4922300
H	-0.6961200	1.2057200	-0.4922300

PH_2
0, 2

P	0.0000000	0.0000000	-0.1156600
H	1.0201300	0.0000000	0.8674300
H	-1.0201300	0.0000000	0.8674300

PH_3
0, 1

P	0.0000000	0.0000000	0.1264100
H	1.1913400	0.0000000	-0.6320600
H	-0.5956700	-1.0317300	-0.6320600
H	-0.5956700	1.0317300	-0.6320600

H_2S
0, 1

S	0.0000000	0.0000000	0.1025200
H	0.0000000	0.9662500	-0.8201500
H	0.0000000	-0.9662500	-0.8201500

HCl
0, 1

Cl	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.2744500

C_2H_2
0, 1

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.2031400
H	0.0000000	0.0000000	2.2657500
H	0.0000000	0.0000000	-1.0626100

CH_2CH_2
0, 1

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.3311900

H	0.9214900	0.0000000	-0.5660700
H	-0.9214900	0.0000000	-0.5660700
H	0.9214900	0.0000000	1.8972600
H	-0.9214900	0.0000000	1.8972600

CH_3CH_3
0, 1

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.5261800
H	1.0160700	0.0000000	1.9214000
H	0.5096000	-0.8790400	-0.3952200
H	-0.5080300	-0.8799400	1.9214000
H	-0.5080400	0.8799400	1.9214000
H	-1.0160700	-0.0018000	-0.3952200
H	0.5064700	0.8808400	-0.3952200

HCN
0, 1

C	0.0000000	0.0000000	-0.5003600
N	0.0000000	0.0000000	0.6526400
H	0.0000000	0.0000000	-1.5662900

HCO
0, 2

C	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.1766100
H	0.9129300	0.0000000	-0.6428700

H_2CO
0, 1

O	0.0000000	0.0000000	0.6746200
C	0.0000000	0.0000000	-0.5297100
H	0.0000000	0.9354900	-1.1093700
H	0.0000000	-0.9354900	-1.1093700

CH_3OH
0, 1

C	-0.0464200	0.6630700	0.0000000
O	-0.0464200	-0.7550600	0.0000000
H	-1.0869600	0.9759400	0.0000000
H	0.8605900	-1.0570400	0.0000000
H	0.4381500	1.0715900	0.8895400
H	0.4381500	1.0715900	-0.8895400

NH_2NH_2
0, 1

N	0.0000000	0.0000000	0.0000000
N	0.0000000	0.0000000	1.4338300
H	0.9401400	0.0000000	-0.3744700

H	-0.4512800	0.8508900	-0.3007000
H	0.8350000	0.4320200	1.8083100
H	-0.0098000	-0.9631000	1.7345400

HOOH
0, 1

O	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.4398400
H	0.9448300	0.0000000	-0.1771600
H	-0.3850500	0.8628100	1.6170000

Si_2
0, 3

Si	0.0000000	0.0000000	0.0000000
Si	0.0000000	0.0000000	2.1579200

P_2
0, 1

P	0.0000000	0.0000000	0.0000000
P	0.0000000	0.0000000	1.8903800

S_2
0, 3

S	0.0000000	0.0000000	0.0000000
S	0.0000000	0.0000000	1.8925900

Cl_2
0, 1

Cl	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.0078300

SC
0, 1

C	0.0000000	0.0000000	0.0000000
S	0.0000000	0.0000000	1.5363500

ClF
0, 1

F	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	1.6303300

Si_2H_6
0, 1

Si	0.0000000	0.0000000	0.0000000
Si	0.0000000	0.0000000	2.3406100
H	1.3881100	0.0000000	-0.5151800
H	-0.6940500	-1.2021400	-0.5151800
H	-0.6940500	1.2021400	-0.5151800
H	-1.3881100	0.0000000	2.8557900
H	0.6940500	-1.2021400	2.8557900

H	0.6940500	1.2021400	2.8557900

CH_3Cl
0, 1

C	0.0000000	0.0000000	-1.1258900
Cl	0.0000000	0.0000000	0.6568300
H	0.0000000	1.0279900	-1.4702600
H	0.8902700	-0.5140000	-1.4702600
H	-0.8902700	-0.5140000	-1.4702600

CH_3SH
0, 1

C	-0.0477500	1.1501100	0.0000000
S	-0.0477500	-0.6636400	0.0000000
H	1.2780600	-0.8296600	0.0000000
H	-1.0912000	1.4564300	0.0000000
H	0.4317800	1.5453800	0.8910000
H	0.4317800	1.5453800	-0.8910000

HOCl
0, 1

O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9621100
Cl	1.6421500	0.0000000	-0.3923200

BCl_3
0, 1

B	0.0000000	0.0000000	0.0000000
Cl	1.7406400	0.0000000	0.0000000
Cl	-0.8703200	-1.5074400	0.0000000
Cl	-0.8703200	1.5074400	0.0000000

BF_3
0, 1

B	0.0000000	0.0000000	0.0000000
F	0.0000000	0.0000000	1.3083600
F	1.1330800	0.0000000	-0.6541800
F	-1.1330800	0.0000000	-0.6541800

C_2Cl_4
0, 1

C	0.0000000	0.0000000	0.6692300
C	0.0000000	0.0000000	-0.6692300
Cl	0.0000000	1.4473800	1.5854300
Cl	0.0000000	-1.4473800	1.5854300
Cl	0.0000000	-1.4473800	-1.5854300
Cl	0.0000000	1.4473800	-1.5854300

C_2F_4
0, 1

C	0.0000000	0.0000000	0.6594900
C	0.0000000	0.0000000	-0.6594900
F	0.0000000	1.0941800	1.3815800
F	0.0000000	-1.0941800	1.3815800
F	0.0000000	1.0941800	-1.3815800
F	0.0000000	-1.0941800	-1.3815800

C_3H_4 (propyne)
0, 1

C	0.0000000	0.0000000	0.2195100
C	0.0000000	0.0000000	1.4239600
C	0.0000000	0.0000000	-1.2437600
H	0.0000000	0.0000000	2.4862600
H	0.0000000	1.0190100	-1.6281500
H	0.8824900	-0.5095000	-1.6281500
H	-0.8824900	-0.5095000	-1.6281500

C_4H_4O
0, 1

O	0.0000000	0.0000000	1.1581400
C	0.0000000	1.0901600	0.3453000
C	0.0000000	-1.0901600	0.3453000
C	0.0000000	0.7197300	-0.9560100
C	0.0000000	-0.7197300	-0.9560100
H	0.0000000	2.0445000	0.8383500
H	0.0000000	-2.0445000	0.8383500
H	0.0000000	1.3774800	-1.8066100
H	0.0000000	-1.3774800	-1.8066100

C_4H_4S
0, 1

S	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.7153500
C	1.7144200	0.0000000	-0.0563700
C	1.2669400	0.0000000	2.2200500
C	2.2604900	0.0000000	1.1933000
H	-0.9296100	0.0000000	2.2586800
H	2.2269100	0.0000000	-1.0033400
H	1.4872000	0.0000000	3.2762300
H	3.3233300	0.0000000	1.3787300

C_4H_5N
0, 1

H	0.0000000	0.0000000	2.1206400
N	0.0000000	0.0000000	1.1195600
C	0.0000000	1.1209700	0.3297700
C	0.0000000	-1.1209700	0.3297700
C	0.0000000	0.7133800	-0.9798900

C	0.0000000	-0.7133800	-0.9798900
H	0.0000000	2.1059300	0.7609900
H	0.0000000	-2.1059300	0.7609900
H	0.0000000	1.3609300	-1.8390300
H	0.0000000	-1.3609300	-1.8390300

C_4H_6 (*trans*-1,3-butadiene)
0, 1

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.3365900
C	1.2146700	0.0000000	2.1485300
C	1.2146700	0.0000000	3.4851100
H	-0.9202300	0.0000000	-0.5659600
H	0.9256700	0.0000000	-0.5614600
H	-0.9424700	0.0000000	1.8733100
H	2.1571400	0.0000000	1.6118000
H	0.2890000	0.0000000	4.0465700
H	2.1349000	0.0000000	4.0510700

C_4H_6 (2-butyne)
0, 1

C	0.0000000	0.0000000	2.0668000
C	0.0000000	0.0000000	0.6024600
C	0.0000000	0.0000000	-0.6024600
C	0.0000000	0.0000000	-2.0668000
H	0.0000000	1.0181800	2.4549300
H	-0.8817700	-0.5090900	2.4549300
H	0.8817700	-0.5090900	2.4549300
H	0.0000000	1.0181800	-2.4549300
H	0.8817700	-0.5090900	-2.4549300
H	-0.8817700	-0.5090900	-2.4549300

C_5H_5N
0, 1

N	0.0000000	0.0000000	1.4170400
C	0.0000000	0.0000000	-1.3813400
C	0.0000000	1.1387000	0.7191500
C	0.0000000	-1.1387000	0.7191500
C	0.0000000	-1.1941300	-0.6708000
C	0.0000000	1.1941300	-0.6708000
H	0.0000000	0.0000000	-2.4624000
H	0.0000000	2.0514200	1.3012600
H	0.0000000	-2.0514200	1.3012600
H	0.0000000	-2.1490300	-1.1757800
H	0.0000000	2.1490300	-1.1757800

CCH
0, 2

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.2073000
H	0.0000000	0.0000000	-1.0634000

CCl_4
0, 1

C	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	1.7673000
Cl	1.6662300	0.0000000	-0.5891000
Cl	-0.8331100	-1.4429900	-0.5891000
Cl	-0.8331100	1.4429900	-0.5891000

CF_3CN
0, 1

C	0.0000000	0.0000000	-0.3272500
C	0.0000000	0.0000000	1.1573200
F	0.0000000	1.2425200	-0.7832100
F	1.0760500	-0.6212600	-0.7832100
F	-1.0760500	-0.6212600	-0.7832100
N	0.0000000	0.0000000	2.3094600

CF_4
0, 1

C	0.0000000	0.0000000	0.0000000
F	0.0000000	0.0000000	1.3150700
F	1.2398600	0.0000000	-0.4383600
F	-0.6199300	-1.0737500	-0.4383600
F	-0.6199300	1.0737500	-0.4383600

CH_2OH
0, 2

C	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.3655800
H	0.9036400	0.0000000	1.6815100
H	0.8719400	-0.3709600	-0.5186200
H	-0.9828100	-0.0804900	-0.4321400

CH_3CN
0, 1

C	0.0000000	0.0000000	-1.1809800
C	0.0000000	0.0000000	0.2814900
N	0.0000000	0.0000000	1.4359800
H	0.0000000	1.0224300	-1.5516200
H	0.8854500	-0.5112100	-1.5516200
H	-0.8854500	-0.5112100	-1.5516200

CH_3NH_2
0, 1

C	0.0499200	0.7059500	0.0000000

N	0.0499200	-0.7576300	0.0000000
H	-0.9437300	1.1656200	0.0000000
H	-0.4400800	-1.111100	0.8099800
H	-0.4400800	-1.111100	-0.8099800
H	0.5874700	1.0621800	0.8774800
H	0.5874700	1.0621800	-0.8774800

CH_3NO_2
0, 1

C	-0.0768600	-1.3131100	0.0000000
N	0.0000000	0.1727500	0.0000000
H	0.9467500	-1.6772100	0.0000000
H	-0.5893500	-1.6219200	0.9026500
H	-0.5893500	-1.6219200	-0.9026500
O	0.0433200	0.7244000	-1.0826900
O	0.0433200	0.7244000	1.0826900

$CHCl_3$
0, 1

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0807800
Cl	1.6785000	0.0000000	-0.5432000
Cl	-0.8392500	-1.4536200	-0.5432000
Cl	-0.8392500	1.4536200	-0.5432000

CHF_3
0, 1

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0857600
F	1.2460100	0.0000000	-0.4651500
F	-0.6230100	-1.0790800	-0.4651500
F	-0.6230100	1.0790800	-0.4651500

ClF_3
0, 1

Cl	0.0000000	0.0000000	0.0000000
F	0.0000000	0.0000000	1.5930300
F	1.6936800	0.0000000	0.0795300
F	-1.6936800	0.0000000	0.0795300

H_2
0, 1

H	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.7418800

CH_2CH
0, 2

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.3101200

H	0.9288100	0.0000000	-0.5674600
H	-0.9189000	0.0000000	-0.5736300
H	0.7321600	0.0000000	2.1005700

$HCOOCH_3$
0, 1

C	-0.9275600	-0.0857100	0.0000000
O	-0.7114800	-1.2656400	0.0000000
O	0.0000000	0.8739100	0.0000000
H	-1.9224400	0.3673100	0.0000000
C	1.3533600	0.3993700	0.0000000
H	1.9750400	1.2876700	0.0000000
H	1.5422100	-0.2015300	0.8862300
H	1.5422100	-0.2015300	-0.8862300

HCOOH
0, 1

O	-1.0277800	-0.4408400	0.0000000
C	0.0000000	0.4208800	0.0000000
O	1.1564300	0.1106400	0.0000000
H	-0.6554300	-1.3309800	0.0000000
H	-0.3737200	1.4472900	0.0000000

PF_3
0, 1

P	0.0000000	0.0000000	0.4976300
F	0.0000000	1.3566900	-0.2764600
F	1.1749300	-0.6783400	-0.2764600
F	-1.1749300	-0.6783400	-0.2764600

SH
0, 2

S	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.3402000

$SiCl_4$
0, 1

Si	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.0232000
Cl	1.9074900	0.0000000	-0.6744000
Cl	-0.9537500	1.6519400	-0.6744000
Cl	-0.9537500	-1.6519400	-0.6744000

SiF_4
0, 1

Si	0.0000000	0.0000000	0.0000000
F	0.0000000	0.0000000	1.5546000
F	1.4656900	0.0000000	-0.5182000
F	-0.7328400	-1.2693300	-0.5182000

F	-0.7328400	1.2693300	-0.5182000

C_2H_5
0, 2

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.4901400
H	1.0137700	0.0000000	1.8911400
H	-0.8485500	0.3741300	-0.5528700
H	-0.5010600	-0.8876800	1.8958500
H	-0.5250100	0.8674800	1.8910500
H	0.7721800	-0.5127000	-0.5535700

C_4H_6 (bicylobutane)
0, 1

C	0.0000000	1.1302800	0.3160500
C	0.0000000	-1.1302800	0.3160500
C	0.7434800	0.0000000	-0.3229700
C	-0.7434800	0.0000000	-0.3229700
H	0.0000000	1.2135600	1.4001700
H	0.0000000	2.0775200	-0.2094500
H	0.0000000	-1.2135600	1.4001700
H	0.0000000	-2.0775200	-0.2094500
H	1.4300500	0.0000000	-1.1492100
H	-1.4300500	0.0000000	-1.1492100

C_4H_6 (cyclobutene)
0, 1

C	0.0000000	0.6699900	0.8138700
C	0.0000000	-0.6699900	0.8138700
C	0.0000000	0.7834000	-0.7000700
C	0.0000000	-0.7834000	-0.7000700
H	0.0000000	1.4137500	1.5983600
H	0.0000000	-1.4137500	1.5983600
H	0.8868400	1.2396000	-1.1406000
H	-0.8868400	1.2396000	-1.1406000
H	-0.8868400	-1.2396000	-1.1406000
H	0.8868400	-1.2396000	-1.1406000

HCOCOH
0, 1

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.5207100
O	1.0278300	0.0000000	-0.6264700
H	-0.9966700	0.0000000	-0.4673100
O	-1.0278300	0.0000000	2.1471800
H	0.9966700	0.0000000	1.9880200

CH_3CHO
0, 1

O	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.2063100
H	0.9556900	0.0000000	1.7610900
C	-1.2379700	0.0000000	2.0569500
H	-2.1301100	0.0000000	1.4366300
H	-1.2331800	-0.8777200	2.7058000
H	-1.2331800	0.8777200	2.7058000

C_2H_4O
0, 1

C	0.0000000	0.7314100	-0.3719900
O	0.0000000	0.0000000	0.8518000
C	0.0000000	-0.7314100	-0.3719900
H	0.9175100	1.2638800	-0.5876200
H	-0.9175100	1.2638800	-0.5876200
H	-0.9175100	-1.2638800	-0.5876200
H	0.9175100	-1.2638800	-0.5876200

C_2H_5O
0, 2

C	0.9987900	-0.5824500	0.0000000
C	0.0000000	0.5875900	0.0000000
O	-1.2553700	0.0196200	0.0000000
H	0.1587600	1.1938600	0.8972900
H	0.1587600	1.1938600	-0.8972900
H	2.0101900	-0.1790700	0.0000000
H	0.8612500	-1.1982200	0.8860000
H	0.8612500	-1.1982200	-0.8860000

CH_3OCH_3
0, 1

C	0.0000000	1.1633600	-0.1970300
O	0.0000000	0.0000000	0.5943900
C	0.0000000	-1.1633600	-0.1970300
H	0.0000000	2.0176100	0.4751400
H	0.8891600	1.2096900	-0.8352500
H	-0.8891600	1.2096900	-0.8352500
H	0.0000000	-2.0176100	0.4751400
H	-0.8891600	-1.2096900	-0.8352500
H	0.8891600	-1.2096900	-0.8352500

CH_3CH_2OH
0, 1

C	1.1696900	-0.4020600	0.0000000
C	0.0000000	0.5564400	0.0000000
O	-1.1919800	-0.2204100	0.0000000
H	-1.9440300	0.3707200	0.0000000
H	0.0381200	1.1990000	0.8847500

H	0.0381200	1.1990000	-0.8847500
H	2.1122800	0.1453700	0.0000000
H	1.1366100	-1.0385400	0.8832700
H	1.1366100	-1.0385400	-0.8832700

C_3H_4 (allene)
0, 1

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.3074000
C	0.0000000	0.0000000	-1.3074000
H	0.0000000	0.9267900	1.8643900
H	0.0000000	-0.9267900	1.8643900
H	0.9267900	0.0000000	-1.8643900
H	-0.9267900	0.0000000	-1.8643900

C_3H_4 (cyclopropene)
0, 1

C	0.0000000	0.0000000	0.8615500
C	0.0000000	0.6467600	-0.5000200
C	0.0000000	-0.6467600	-0.5000200
H	-0.9101700	0.0000000	1.4542000
H	0.9101700	0.0000000	1.4542000
H	0.0000000	1.5750900	-1.0387600
H	0.0000000	-1.5750900	-1.0387600

CH_3COOH
0, 1

C	0.0000000	0.1554800	0.0000000
O	0.1886000	1.3427200	0.0000000
O	-1.2395900	-0.3822500	0.0000000
H	-1.8599400	0.3553500	0.0000000
C	1.0581000	-0.9077600	0.0000000
H	2.0391000	-0.4460200	0.0000000
H	0.9400900	-1.5397000	0.8787500
H	0.9400900	-1.5397000	-0.8787500

CH_3COCH_3
0, 1

O	0.0000000	0.0000000	1.3963400
C	0.0000000	0.0000000	0.1859100
C	0.0000000	1.2837400	-0.6128900
C	0.0000000	-1.2837400	-0.6128900
H	0.0000000	2.1402400	0.0548200
H	0.0000000	-2.1402400	0.0548200
H	-0.8777300	1.3200100	-1.2602600
H	0.8777300	1.3200100	-1.2602600
H	0.8777300	-1.3200100	-1.2602600
H	-0.8777300	-1.3200100	-1.2602600

C_3H_6 (cyclopropane)
0, 1

C	0.0000000	0.8683500	0.0000000
C	0.7520100	-0.4341800	0.0000000
C	-0.7520100	-0.4341800	0.0000000
H	0.0000000	1.4538200	0.9074400
H	0.0000000	1.4538200	-0.9074400
H	1.2590400	-0.7269100	-0.9074400
H	1.2590400	-0.7269100	0.9074400
H	-1.2590400	-0.7269100	0.9074400
H	-1.2590400	-0.7269100	-0.9074400

CH_3CHCH_2
0, 1

C	1.2889400	0.1419900	0.0000000
C	0.0000000	0.4780000	0.0000000
H	1.6010900	-0.8950200	0.0000000
H	2.0682600	0.8910400	0.0000000
H	-0.2662900	1.5298300	0.0000000
C	-1.1369500	-0.4994900	0.0000000
H	-0.7725000	-1.5263000	0.0000000
H	-1.7712600	-0.3612800	0.8775000
H	-1.7712600	-0.3612800	-0.8775000

C_3H_8
0, 1

C	0.0000000	0.0000000	0.5902000
C	0.0000000	1.2666700	-0.2605000
C	0.0000000	-1.2666700	-0.2605000
H	-0.8741500	0.0000000	1.2454900
H	0.8741500	0.0000000	1.2454900
H	0.0000000	2.1658900	0.3560800
H	0.0000000	-2.1658900	0.3560800
H	0.8805900	1.3026700	-0.9045700
H	-0.8805900	1.3026700	-0.9045700
H	-0.8805900	-1.3026700	-0.9045700
H	0.8805900	-1.3026700	-0.9045700

$C_2H_5OCH_3$
0, 1

O	0.0089100	-0.7126500	0.0000000
C	0.0000000	0.6986900	0.0000000
C	1.3170600	-1.2306700	0.0000000
C	-1.4372800	1.1699900	0.0000000
H	0.5305800	1.0734800	0.8844300
H	0.5305800	1.0734800	-0.8844300
H	1.2407900	-2.3151300	0.0000000
H	1.8715200	-0.9111700	-0.8890900

H	1.8715200	-0.9111700	0.8890900
H	-1.9575100	0.8021600	-0.8833600
H	-1.9575100	0.8021600	0.8833600
H	-1.4799200	2.2593800	0.0000000

C_4H_{10} (isobutane)
0, 1

C	0.0000000	0.0000000	0.3798500
H	0.0000000	0.0000000	1.4745100
C	0.0000000	1.4511200	-0.0963600
H	0.0000000	1.4938600	-1.1884700
H	-0.8829100	1.9856900	0.2577200
H	0.8829100	1.9856900	0.2577200
C	1.2567100	-0.7255600	-0.0963600
H	1.2937200	-0.7469300	-1.1884700
H	2.1611100	-0.2282200	0.2577200
H	1.2782000	-1.7574700	0.2577200
C	-1.2567100	-0.7255600	-0.0963600
H	-1.2937200	-0.7469300	-1.1884700
H	-1.2782000	-1.7574700	0.2577200
H	-2.1611100	-0.2282200	0.2577200

C_4H_{10} (antiperiplanar butane)
0, 1

C	0.7032400	1.8211500	0.0000000
C	0.7032400	0.2956900	0.0000000
C	-0.7032400	-0.2956900	0.0000000
C	-0.7032400	-1.8211500	0.0000000
H	1.7167600	2.2231500	0.0000000
H	-1.7167600	-2.2231500	0.0000000
H	0.1897600	2.2111700	0.8807000
H	0.1897600	2.2111700	-0.8807000
H	-0.1897600	-2.2111700	0.8807000
H	-0.1897600	-2.2111700	-0.8807000
H	1.2472100	-0.0730500	-0.8746200
H	1.2472100	-0.0730500	0.8746200
H	-1.2472100	0.0730500	-0.8746200
H	-1.2472100	0.0730500	0.8746200

C_4H_8 (cyclobutane)
0, 1

C	0.0000000	1.0762900	0.1428600
C	0.0000000	-1.0762900	0.1428600
C	-1.0762900	0.0000000	-0.1428600
C	1.0762900	0.0000000	-0.1428600
H	0.0000000	1.9792000	-0.4651600
H	0.0000000	1.3592200	1.1958200
H	0.0000000	-1.9792000	-0.4651600

H	0.0000000	-1.3592200	1.1958200
H	-1.9792000	0.0000000	0.4651600
H	-1.3592200	0.0000000	-1.1958200
H	1.9792000	0.0000000	0.4651600
H	1.3592200	0.0000000	-1.1958200

C_4H_8 (isobutene)
0, 1

C	0.0000000	0.0000000	1.4566700
C	0.0000000	0.0000000	0.1226300
H	0.0000000	0.9233200	2.0208000
H	0.0000000	-0.9233200	2.0208000
C	0.0000000	1.2726600	-0.6780000
H	0.0000000	2.1519200	-0.0358900
H	0.8773800	1.3196300	-1.3274100
H	-0.8773800	1.3196300	-1.3274100
C	0.0000000	-1.2726600	-0.6780000
H	0.0000000	-2.1519200	-0.0358900
H	-0.8773800	-1.3196300	-1.3274100
H	0.8773800	-1.3196300	-1.3274100

C_5H_8 (spiropentane)
0, 1

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.7639500	1.2655500
C	0.0000000	-0.7639500	1.2655500
C	0.7639500	0.0000000	-1.2655500
C	-0.7639500	0.0000000	-1.2655500
H	-0.9112200	1.2621800	1.5665000
H	0.9112200	1.2621800	1.5665000
H	-0.9112200	-1.2621800	1.5665000
H	0.9112200	-1.2621800	1.5665000
H	1.2621800	-0.9112200	-1.5665000
H	1.2621800	0.9112200	-1.5665000
H	-1.2621800	-0.9112200	-1.5665000
H	-1.2621800	0.9112200	-1.5665000

C_6H_6
0, 1

C	0.0000000	0.0000000	1.3920000
C	1.2055100	0.0000000	0.6960000
C	1.2055100	0.0000000	-0.6960000
C	0.0000000	0.0000000	-1.3920000
C	-1.2055100	0.0000000	-0.6960000
C	-1.2055100	0.0000000	0.6960000
H	0.0000000	0.0000000	2.4730000
H	2.1416800	0.0000000	1.2365000
H	2.1416800	0.0000000	-1.2365000

H	0.0000000	0.0000000	-2.4730000
H	-2.1416800	0.0000000	-1.2365000
H	-2.1416800	0.0000000	1.2365000

CH_3CO
0, 2

C	-0.9672500	-0.6655400	0.0000000
C	0.0000000	0.4955700	0.0000000
H	-0.4314100	-1.6151600	0.0000000
H	-1.6038900	-0.5858900	0.8790800
H	-1.6038900	-0.5858900	-0.8790800
O	1.1803300	0.4758400	0.0000000

$(CH_3)_2CH$
0, 2

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.4913100
C	1.2901600	0.0000000	-0.7480000
H	-0.9066100	-0.2740800	-0.5223300
H	-0.9920000	0.1918900	1.8986700
H	1.1450200	0.1918900	-1.8105100
H	0.3376000	-0.9638500	1.8960300
H	0.6835400	0.7566300	1.8851500
H	1.9737200	0.7566300	-0.3541900
H	1.8096200	-0.9638500	-0.6589300

$(CH_3)_3C$
0, 2

C	0.0000000	0.0000000	0.1870700
C	0.0000000	1.4803200	-0.0194300
C	1.2819900	-0.7401600	-0.0194300
C	-1.2819900	-0.7401600	-0.0194300
H	0.0000000	1.7342100	-1.0900200
H	-0.8847600	1.9473100	0.4162300
H	0.8847600	1.9473100	0.4162300
H	1.5018700	-0.8671000	-1.0900200
H	2.1288000	-0.2074300	0.4162300
H	1.2440400	-1.7398800	0.4162300
H	-1.5018700	-0.8671000	-1.0900200
H	-1.2440400	-1.7398800	0.4162300
H	-2.1288000	-0.2074300	0.4162300

H_2CCO
0, 1

C	0.0000000	0.0000000	-1.2099700
C	0.0000000	0.0000000	0.1033300
H	0.0000000	0.9391200	-1.7354400
H	0.0000000	-0.9391200	-1.7354400

O	0.0000000	0.0000000	1.2638400

SR-TM-BE17

$CrCl_2$
0, 5

Cr	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.2187740
Cl	0.0000000	0.0000000	-2.2187740

MnF_2
0, 6

Mn	0.0000000	0.0000000	0.0193710
F	0.0000000	-1.8063110	-0.0269050
F	0.0000000	1.8063110	-0.0269050

$FeCl_2$
0, 5

Cl	0.0000000	0.0000000	2.1363190
Cl	0.0000000	0.0000000	-2.1363190
Fe	0.0000000	0.0000000	0.0000000

FeCl
0, 6

Fe	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.1790000

$CoCl_2$
0, 4

Co	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.0970190
Cl	0.0000000	0.0000000	-2.0970190

$Pd(PH_3)_2$-C_6H_8
0, 1

Pd	0.0000000	0.0000000	0.4610420
P	0.0000000	2.0283390	1.6528010
P	0.0000000	-2.0283390	1.6528010
C	-0.0156460	0.6959950	-1.6527290
C	0.0156460	-0.6959950	-1.6527290
C	-1.1645900	-1.5150630	-1.8460670
C	1.1645900	1.5150630	-1.8460670
C	-1.1532730	-2.8279860	-2.0672590
C	1.1532730	2.8279860	-2.0672590
H	0.2497020	3.2063260	0.9016430
H	-0.2497020	-3.2063260	0.9016430

H	-2.0651990	-3.3906710	-2.2076860
H	2.0651990	3.3906710	-2.2076860
H	-0.2202650	-3.3784220	-2.1224910
H	0.2202650	3.3784220	-2.1224910
H	-1.1308210	2.5271000	2.3447330
H	1.1308210	-2.5271000	2.3447330
H	0.9248650	2.3236040	2.6838690
H	-0.9248650	-2.3236040	2.6838690
H	-2.1167780	-0.9903400	-1.8017850
H	2.1167780	0.9903400	-1.8017850
H	0.9747710	-1.1906290	-1.7979420
H	-0.9747710	1.1906290	-1.7979420

$Pd(PH_3)_2$-$C_{10}H_{12}$ (structure b)
0, 1

Pd	0.0000000	0.0000000	0.7447810
P	0.0000000	2.0439550	1.9232440
P	0.0000000	-2.0439550	1.9232440
H	1.1951430	2.5845990	2.4580770
H	-1.1951430	-2.5845990	2.4580770
H	-0.3511360	3.1794590	1.1487350
H	0.3511360	-3.1794590	1.1487350
H	-0.8074810	2.3657750	3.0415330
H	0.8074810	-2.3657750	3.0415330
C	-2.3976420	-1.5445540	-0.9389140
C	2.3976420	1.5445540	-0.9389140
C	-0.0457350	-0.7116120	-1.3610510
C	0.0457350	0.7116120	-1.3610510
C	1.3190410	1.3955350	-1.6918520
C	-1.3190410	-1.3955350	-1.6918520
C	1.1475720	-1.5365100	-1.5546620
C	-1.1475720	1.5365100	-1.5546620
H	3.2739190	2.0591700	-1.3118030
H	-3.2739190	-2.0591700	-1.3118030
H	2.4451790	1.1467830	0.0702080
H	-2.4451790	-1.1467830	0.0702080
H	1.3263670	1.8346400	-2.6895280
H	-1.3263670	-1.8346400	-2.6895280
C	1.1561870	-2.8596560	-1.7155340
C	-1.1561870	2.8596560	-1.7155340
H	2.0936840	-1.0068370	-1.5584990
H	-2.0936840	1.0068370	-1.5584990
H	0.2478210	-3.4507230	-1.7084020
H	-0.2478210	3.4507230	-1.7084020
H	2.0849580	-3.3948690	-1.8568730

H	-2.0849580	3.3948690	-1.8568730

Fragments for Pd complexes

$Pd(PH_3)_2$

0, 1

Pd	0.0000000	0.0000000	0.0000000
P	0.0000000	0.0000000	2.2871160
P	0.0000000	0.0000000	-2.2871160
H	0.0000000	1.2143280	3.0122300
H	-1.0516390	-0.6071640	3.0122300
H	1.0516390	-0.6071640	3.0122300
H	0.0000000	1.2143280	-3.0122300
H	1.0516390	-0.6071640	-3.0122300
H	-1.0516390	-0.6071640	-3.0122300

C_6H_8

0, 1

C	0.0005840	0.6694290	0.0000000
C	-0.0005840	-0.6694290	0.0000000
C	-1.1920100	-1.4779660	0.0000000
C	1.1920100	1.4779660	0.0000000
C	-1.1920100	-2.8082660	0.0000000
C	1.1920100	2.8082660	0.0000000
H	-2.1087740	-3.3807360	0.0000000
H	2.1087740	3.3807360	0.0000000
H	-0.2630920	-3.3668520	0.0000000
H	0.2630920	3.3668520	0.0000000
H	-2.1373860	-0.9410450	0.0000000
H	2.1373860	0.9410450	0.0000000
H	0.9510550	-1.1978100	0.0000000
H	-0.9510550	1.1978100	0.0000000

$C_{10}H_{12}$

0, 1

C	-0.4356080	1.5045070	-2.6253710
C	0.0000000	0.0000000	-0.6825400
C	0.0000000	0.0000000	0.6825400
C	0.0737730	-1.2610230	1.4219420
C	-0.4356080	-1.5045070	2.6253710
C	0.0737730	1.2610230	-1.4219420
C	-0.0737730	-1.2610230	-1.4219420
C	-0.0737730	1.2610230	1.4219420
H	-0.3351350	-2.4797430	3.0819790
H	-0.9792650	-0.7544040	3.1850580
H	0.5871610	-2.0743360	0.9195970
H	0.5871610	2.0743360	-0.9195970

H	-0.3351350	2.4797430	-3.0819790
H	-0.9792650	0.7544040	-3.1850580
C	0.4356080	-1.5045070	-2.6253710
H	-0.5871610	-2.0743360	-0.9195970
H	0.9792650	-0.7544040	-3.1850580
H	0.3351350	-2.4797430	-3.0819790
C	0.4356080	1.5045070	2.6253710
H	-0.5871610	2.0743360	0.9195970
H	0.3351350	2.4797430	3.0819790
H	0.9792650	0.7544040	3.1850580

Ag_2
0, 1

Ag	0.0000000	0.0000000	0.0000000
Ag	0.0000000	0.0000000	2.5871100

AgH
0, 1

Ag	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.6180000

CoH
0, 3

Co	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.5310000

$CrCH_3^+$
1, 5

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.1000000
H	1.0370900	0.0000000	-0.3666700
H	-0.5185500	0.8981500	-0.3666700
Cr	-0.8956700	-1.5513400	-0.6333300

Cu_2
0, 1

Cu	0.0000000	0.0000000	0.0000000
Cu	0.0000000	0.0000000	2.2200000

CuAg
0, 1

Cu	0.0000000	0.0000000	0.0000000
Ag	0.0000000	0.0000000	2.2592900

CuH_2O^+
1, 1

Cu	0.0000000	0.0000000	-0.4938500
O	0.0000000	0.0000000	1.3361500
H	-0.8313800	0.0000000	1.8161500
H	0.8313800	0.0000000	1.8161500
FeH			
0, 4			
Fe	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.6100000
VCO^+			
1, 5			
V	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	2.1131400
O	0.0000000	0.0000000	3.2335100
Zr_2			
0, 3			
Zr	0.0000000	0.0000000	0.0000000
Zr	0.0000000	0.0000000	2.2400000

MR-MGM-BE4			
CaO			
0, 1			
Ca	0.0000000	0.0000000	1.8210000
O	0.0000000	0.0000000	0.0000000
LiO^-			
-1, 1			
Li	0.0000000	0.0000000	1.6300000
O	0.0000000	0.0000000	0.0000000
KO^-			
-1, 1			
K	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	2.1900000
MgS			
0, 1			
Mg	0.0000000	0.0000000	2.1400000
S	0.0000000	0.0000000	0.0000000

MR-MGN-BE17			
NF_3			
0, 1			
N	0.0000000	0.0000000	0.4761000
F	0.0000000	1.2217200	-0.1234300
F	1.0580400	-0.6108600	-0.1234300
F	-1.0580400	-0.6108600	-0.1234300
CO_2			
0, 1			
C	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.1594900
O	0.0000000	0.0000000	-1.1594900
SiO			
0, 1			
Si	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.5126700
SO_2			
0, 1			
S	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.4295000
O	1.2486200	0.0000000	-0.6960100
CO			
0, 1			
O	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.1296100
SO			
0, 3			
O	0.0000000	0.0000000	0.0000000
S	0.0000000	0.0000000	1.4789100
ClO			
0, 2			
Cl	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.5791800
F_2			
0, 1			
F	0.0000000	0.0000000	0.0000000
F	0.0000000	0.0000000	1.3952000
N_2			
0, 1			
N	0.0000000	0.0000000	0.0000000

N	0.0000000	0.0000000	1.0971100
O_2			
0, 3			
O	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.2013200
NO			
0, 2			
N	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.1520600
CN			
0, 2			
C	0.0000000	0.0000000	0.0000000
N	0.0000000	0.0000000	1.1672100
B_2			
0, 3			
B	0.0000000	0.0000000	0.8070500
B	0.0000000	0.0000000	-0.8070500
O_3			
0, 1			
O	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.2688100
O	1.1293300	0.0000000	-0.5783600
C_2			
0, 1			
C	0.0000000	0.0000000	-0.6200000
C	0.0000000	0.0000000	0.6200000
S_4			
0, 1			
S	0.0000000	0.0000000	0.0000000
S	0.0000000	0.0000000	1.9063400
S	2.0670400	0.0000000	2.4487200
S	3.0030300	0.0000000	0.7879800
Cl_2O			
0, 1			
O	0.0000000	0.0000000	0.6424200
Cl	1.4011700	0.0000000	-0.3212100
Cl	-1.4011700	0.0000000	-0.3212100

MR-TM-BE13			
CuH			
0, 1			
Cu	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.4630000
VO			
0, 4			
V	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.5890000
CuCl			
0, 1			
Cu	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.0500000
NiCl			
0, 2			
Ni	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.0730000
TiCl			
0, 4			
Ti	0.0000000	0.0000000	0.9818810
Cl	0.0000000	0.0000000	-1.2706690
VF_5			
0, 1			
V	0.0000010	0.0000450	0.0000010
F	0.0000140	-1.7058210	-0.0037130
F	1.7441660	-0.0009970	-0.0000090
F	-0.0000110	0.8570820	-1.4748060
F	-0.0000050	0.8506400	1.4785310
F	-1.7441660	-0.0010180	-0.0000040
CrCl			
0, 6			
Cr	0.0000000	0.0000000	0.9180970
Cl	0.0000000	0.0000000	-1.2961370
CrOF			
0, 4			
Cr	0.0000000	0.2573080	0.0000000
O	1.5735830	0.1639690	0.0000000
F	-1.3987410	-0.8319050	0.0000000

$(FeBr_2)_2$
0, 9

Fe	-0.0000020	-1.6229260	0.0000000
Br	-0.0000010	-3.9000320	0.0000000
Br	-1.8673960	0.0000090	0.0000000
Br	1.8673980	0.0000050	0.0000000
Fe	0.0000030	1.6229180	0.0000000
Br	-0.0000020	3.9000240	0.0000000

$Co(CO)_4H$
0, 1

Co	-0.0000800	-0.0000580	-0.1676540
H	-0.0001330	-0.0004420	-1.6561860
C	-0.0001160	0.0003720	1.6358970
C	0.8428780	1.5665600	-0.4703810
C	-1.7783250	-0.0535760	-0.4701430
C	0.9355020	-1.5133300	-0.4697490
O	1.5195610	-2.4577630	-0.7227620
O	-0.0001190	0.0006460	2.7733640
O	-2.8882110	-0.0870000	-0.7233710
O	1.3691010	2.5443470	-0.7235950

$NiCH_2^+$
1, 2

C	0.0000000	0.0000000	0.0000000
Ni	0.0000000	0.0000000	1.7813000
H	0.9328700	0.0000000	-0.5871800
H	-0.9328700	0.0000000	-0.5871800

$Fe(CO)_5$
0, 1

Fe	-0.2017300	-0.0720500	0.0000000
C	1.7282600	-0.0720500	0.0000000
O	2.8436700	-0.0720500	0.0000000
C	-0.2017000	-0.0720500	-1.9300000
O	-0.2017300	-0.0720500	-3.0454000
C	-0.2017000	-0.0720500	1.9300000
O	-0.2017300	-0.0720500	3.0454000
C	-1.1667500	-1.7434700	0.0000000
O	-1.7244300	-2.7094400	0.0000000
C	-1.1667500	1.5993800	0.0000000

O	-1.7244300	2.5653500	0.0000000
VS			
0, 4			
V	0.0000000	0.0000000	0.0000000
S	0.0000000	0.0000000	2.0480000

MR-TMD-BE2			
Cr_2			
0, 1			
Cr	0.0000000	0.0000000	0.0000000
Cr	0.0000000	0.0000000	1.6800000
V_2			
0, 3			
V	0.0000000	0.0000000	0.0000000
V	0.0000000	0.0000000	1.7700000

IsoL6/11			
10-educt			
0, 1			
C	-1.6793600	1.0830800	0.4844300
C	-2.9806200	1.5998300	0.4358800
C	-4.0358900	0.8127200	-0.0239200
C	-3.7924300	-0.4963800	-0.4472200
C	-2.4917100	-1.0064900	-0.3913700
C	-1.4111200	-0.2483400	0.0800200
O	-0.7084100	1.9397500	0.9476600
C	0.0100200	-0.8372900	0.2376100
C	1.0129000	0.1012600	-0.4883300
C	2.2481200	0.4648500	-0.0652400
C	0.4986800	0.5726200	-1.8464400
C	3.0950800	1.4584700	-0.8408100
C	2.9697300	-0.0732800	1.1614900
C	0.1533500	-2.2321300	-0.4141600
H	0.1712000	1.5743700	0.7285700
C	0.1970300	-1.0227100	1.7697200
H	-3.1399700	2.6265800	0.7574500
H	-5.0421900	1.2259700	-0.0570300
H	-4.6039400	-1.1186300	-0.8182100
H	-2.3188500	-2.0268800	-0.7218700
H	1.3059300	0.6508900	-2.5817000

H	-0.2470800	-0.1282700	-2.2354300
H	0.0007300	1.5503600	-1.7791500
H	2.5252500	2.0641200	-1.5503800
H	3.8951900	0.9391300	-1.3932700
H	3.5941300	2.1400100	-0.1371000
H	2.9276600	-1.1660500	1.2144300
H	4.0276200	0.2140200	1.1226300
H	2.5591800	0.3188400	2.1005300
H	1.1842300	-2.5801100	-0.2784700
H	-0.5197900	-2.9575700	0.0605000
H	-0.0667500	-2.2039400	-1.4875700
H	1.0795100	-1.6207100	2.0098000
H	0.2637000	-0.0632500	2.2925100
H	-0.6811200	-1.5548600	2.1544700

10-product
0, 1

C	-1.5103100	0.6260600	0.2649700
C	-2.6479900	0.7065000	1.0899500
C	-3.8460500	0.1109600	0.6998600
C	-3.9359900	-0.5786600	-0.5165800
C	-2.8059400	-0.6583100	-1.3331900
C	-1.5959400	-0.0633000	-0.9565200
O	-0.3981200	1.2421000	0.7697400
C	0.8929000	1.2400900	0.0720600
C	1.3965100	-0.1741400	-0.2887800
C	1.2212400	-1.2519700	0.5055600
C	0.5552900	-1.2431300	1.8652900
C	1.6565600	-2.6529300	0.1165200
C	2.1630800	-0.2369800	-1.5937000
C	0.7546700	2.1959600	-1.1324900
C	1.8563800	1.8776500	1.0858200
H	-2.5671000	1.2397600	2.0344200
H	-4.7146600	0.1848100	1.3520200
H	-4.8705700	-1.0450300	-0.8199700
H	-2.8557100	-1.1911800	-2.2813900
H	-0.7319800	-0.1586800	-1.6012100
H	-0.4606200	-1.6599200	1.7872600
H	0.4704600	-0.2540000	2.3136500
H	1.1175900	-1.8987800	2.5468200
H	1.7857000	-2.7979800	-0.9598800
H	2.6006600	-2.9222900	0.6165900
H	0.9025600	-3.3754600	0.4595800

H	2.6811900	-1.1875500	-1.7345900
H	2.9261100	0.5537800	-1.6245900
H	1.5088900	-0.0682800	-2.4628500
H	0.0973900	1.7959300	-1.9089100
H	1.7323800	2.4089400	-1.5766100
H	0.3275400	3.1356000	-0.7658800
H	1.9322800	1.2626900	1.9870800
H	1.5100100	2.8827000	1.3582700
H	2.8515900	1.9550400	0.6317000

13-educt
0, 1

C	-1.4762800	-1.1531600	-0.2928000
C	-2.8689200	-1.1588100	-0.2946900
C	-3.5922600	0.0018500	0.0382400
C	-2.8682400	1.1615900	0.3732800
C	-1.4756900	1.1545000	0.3734000
C	-0.7393100	0.0002300	0.0410600
C	1.4762800	1.1531600	-0.2928000
C	0.7393100	-0.0002300	0.0410600
C	1.4756900	-1.1545000	0.3734000
C	2.8682400	-1.1615900	0.3732800
C	3.5922600	-0.0018500	0.0382400
C	2.8689200	1.1588100	-0.2946900
N	4.9909600	0.0138500	0.0923700
N	-4.9909600	-0.0138500	0.0923700
H	-0.9455800	-2.0578500	-0.5825900
H	-3.4077600	-2.0666000	-0.5655400
H	-3.4066700	2.0680500	0.6490400
H	-0.9444300	2.0599200	0.6597400
H	0.9455800	2.0578500	-0.5825900
H	0.9444300	-2.0599200	0.6597400
H	3.4066700	-2.0680500	0.6490400
H	3.4077600	2.0666000	-0.5655400
H	5.4353400	-0.8878400	-0.0246400
H	5.4345400	0.7312700	-0.4668800
H	-5.4345400	-0.7312700	-0.4668800
H	-5.4353400	0.8878400	-0.0246400

13-product
0, 1

C	-4.1262200	-0.7529900	0.2299600
C	-4.3421600	0.3006800	-0.6664900

C	-3.2616300	1.1094400	-1.0359100
C	-1.9811300	0.8770400	-0.528900
C	-1.7679300	-0.1822300	0.3704800
C	-2.8543900	-0.9939100	0.7496100
N	-0.4884100	-0.4923700	0.8579100
N	0.4884100	0.4923700	0.8579100
C	1.7679300	0.1822300	0.3704800
C	2.8543900	0.9939100	0.7496100
C	4.1262200	0.7529900	0.2299600
C	4.3421600	-0.3006800	-0.6664900
C	3.2616300	-1.1094400	-1.0359100
C	1.9811300	-0.8770400	-0.5289000
H	-0.4691500	-1.1191800	1.6584400
H	0.4691500	1.1191800	1.6584400
H	-4.9548300	-1.3903500	0.5336400
H	-5.3356900	0.4891800	-1.0666100
H	-3.4123400	1.9327500	-1.7321500
H	-1.1415400	1.5016200	-0.8197700
H	-2.6940900	-1.8138900	1.4498000
H	2.6940900	1.8138900	1.4498000
H	4.9548300	1.3903500	0.5336400
H	5.3356900	-0.4891800	-1.0666100
H	3.4123400	-1.9327500	-1.7321500
H	1.1415400	-1.5016200	-0.8197700

14-educt
0, 1

C	-3.2493600	-0.2121800	0.1908800
C	-3.0180100	-0.0802600	1.5531100
C	-1.7187000	0.1430800	2.0465000
C	-0.6589000	0.2373800	1.1580500
C	-0.8503600	0.1108100	-0.2400800
C	-2.1808600	-0.1271900	-0.7220400
C	0.2573700	0.1928900	-1.2009100
O	-2.4617900	-0.2774000	-2.0266500
O	0.0637500	0.0215200	-2.4210600
C	1.6870000	0.5139100	-0.7364000
C	1.8296500	1.9616500	-0.2365800
C	2.2643100	-0.5377300	0.2414000
O	2.8380100	-0.2185100	1.2650300
C	2.0956200	-1.9843500	-0.1848100
H	-4.2473000	-0.3900700	-0.2016900
H	-3.8548500	-0.1517400	2.2455300

H	-1.5451900	0.2414400	3.1150000
H	0.3377000	0.4112900	1.5486000
H	-1.5891000	-0.2042600	-2.5089900
H	2.2866900	0.3979800	-1.6510100
H	1.2305300	2.1423500	0.6600400
H	1.5072800	2.6582500	-1.0195000
H	2.8780100	2.1597800	0.0111800
H	2.3814800	-2.1134300	-1.2371200
H	1.0319400	-2.2538900	-0.1095600
H	2.6851000	-2.6413300	0.4610700

14-product
0, 1

C	-1.3563800	2.1276300	-0.6540100
C	-2.6522200	1.7556300	-0.2927700
C	-2.9054900	0.4540500	0.1530600
C	-1.8607200	-0.4674800	0.2205000
C	-0.5396600	-0.1112600	-0.1120000
C	-0.3060700	1.2116900	-0.5480600
H	-1.1387100	3.1250000	-1.0287700
H	-3.4620700	2.4783900	-0.3672800
H	-3.9125000	0.1554500	0.4350800
H	-2.0661000	-1.4803800	0.5567600
C	0.5731100	-1.1202200	-0.0010100
O	0.9385000	1.6089000	-1.0131200
C	1.9281700	2.1110300	-0.1534000
O	2.9882900	2.3977500	-0.6350700
C	1.5342900	2.2745500	1.2971100
O	1.6896300	-0.797400	0.3747500
C	0.2394400	-2.5602300	-0.3912300
C	1.4619600	-3.4802100	-0.4296100
H	0.6192500	2.8726200	1.3887000
H	2.3579400	2.7588000	1.8262900
H	1.3409500	1.2863300	1.7279900
H	-0.2786800	-2.5355500	-1.3614000
H	-0.5058800	-2.9397200	0.3254400
H	2.1958300	-3.1167400	-1.1580500
H	1.1612500	-4.4977400	-0.7078100
H	1.9558600	-3.5108900	0.5479000

20-educt
0, 1

C	-0.3221800	2.3985500	0.0027900

C	-0.1277700	0.9875700	0.5860100
C	-1.2755100	0.0545200	0.2098100
C	-1.2507900	-0.7026400	-0.9688200
C	-2.3284500	-1.5264700	-1.3037700
C	-3.4432500	-1.6059500	-0.4621800
C	-3.4742800	-0.8546000	0.7167700
C	-2.3957100	-0.0296200	1.0483300
H	-0.3823000	-0.6524600	-1.6200300
H	-2.2957300	-2.1100300	-2.2219900
H	-4.2800500	-2.2515800	-0.7217900
H	-4.3360800	-0.9111500	1.3791700
H	-2.4227300	0.5612800	1.9622400
C	1.2532500	0.4161300	0.2925900
C	1.8853800	-0.3395900	1.2925500
C	3.1350500	-0.9223100	1.0721600
C	3.7775300	-0.7551100	-0.1596300
C	3.1587700	-0.0036400	-1.1622100
C	1.9041800	0.5757900	-0.9408500
H	1.3855000	-0.4737600	2.2510400
H	3.6077100	-1.5042300	1.8611600
H	4.7524600	-1.2057100	-0.3347000
H	3.6504400	0.1330400	-2.1235800
H	1.4344900	1.1499300	-1.7339800
H	-0.1815800	1.1501700	1.6709600
H	0.5510600	3.0438400	0.1719100
F	-0.5642300	2.3747200	-1.3571900
F	-1.4151900	3.0033200	0.5932400

20-product
0, 1

C	0.6193700	-0.4719800	-1.9508600
C	-0.6193700	0.4719800	-1.9508600
C	-1.4764000	0.3631100	-0.7195800
C	1.4764000	-0.3631100	-0.7195800
C	-1.1971400	1.1168700	0.4288400
C	-1.9664200	0.9458800	1.5817800
C	-3.0076300	0.0110000	1.6019700
C	-3.2848600	-0.7468900	0.4591400
C	-2.5249000	-0.5659800	-0.6999000
H	-0.3806000	1.8328800	0.4113500
H	-1.7479600	1.5379400	2.4683600
H	-3.6032300	-0.1232400	2.5029500
H	-4.0965700	-1.4716700	0.4670600

H	-2.7371100	-1.1532800	-1.5913500
C	1.1971400	-1.1168700	0.4288400
C	1.9664200	-0.9458800	1.5817800
C	3.0076300	-0.0110000	1.6019700
C	3.2848600	0.7468900	0.4591400
C	2.5249000	0.5659800	-0.6999000
H	0.3806000	-1.8328800	0.4113500
H	1.7479600	-1.5379400	2.4683600
H	3.6032300	0.1232400	2.5029500
H	4.0965700	1.4716700	0.4670600
H	2.7371100	1.1532800	-1.5913500
H	-1.2060300	0.2360500	-2.8489800
F	-0.1149900	1.7812300	-2.1107800
F	0.1149900	-1.7812300	-2.1107800
H	1.2060300	-0.2360500	-2.8489800

3-educt
0, 1

C	1.2327000	-0.3352000	1.2550400
C	-0.1570000	0.1589600	1.7053800
C	-1.2109500	-0.2386000	0.6753000
C	-0.7951300	0.2548000	-0.7101300
C	0.6195500	-0.2519600	-1.0505800
O	1.5378700	0.1955200	-0.0337700
O	-0.5423000	-0.4136600	2.9572600
O	-2.4976600	0.3243200	0.9626100
O	-1.7031900	-0.2076900	-1.7197500
C	1.1370600	0.2874000	-2.3926100
O	0.5160900	-0.3393100	-3.5096000
H	0.1846900	-0.2551400	3.5776500
H	-2.7502300	0.0142400	1.8438900
H	-0.4420500	-0.2643300	-3.3733500
H	-2.5929800	0.0469600	-1.4344000
O	2.2363900	0.0574600	2.1564300
H	2.3186800	1.0222600	2.0868800
H	1.2515400	-1.4369100	1.2393400
H	-0.1174200	1.2613400	1.7703000
H	-1.2747800	-1.3396600	0.6501900
H	-0.7694500	1.3573500	-0.6972000
H	0.6083100	-1.3544000	-1.0903300
H	1.0011600	1.3839800	-2.4076200
H	2.2091200	0.0722600	-2.4609200

3-product
0, 1

C	3.0719700	0.2664900	-1.0660100
O	4.0164900	-0.4802300	-1.1145500
C	2.1498200	0.4694700	0.1350800
O	2.6047200	-0.2762200	1.2483200
C	0.7072700	0.0550700	-0.2707700
H	0.4746200	0.4932400	-1.2519100
C	-0.3436100	0.5816200	0.7320300
O	-0.0051300	0.2319600	2.0897800
C	-1.7778800	0.0975400	0.4212800
H	-2.4668400	0.6255600	1.0916100
C	-2.2210400	0.3467100	-1.0242500
O	-3.6040500	0.0557000	-1.2037900
H	2.7653800	0.8916200	-1.9444900
H	2.1337700	1.5585500	0.3375100
H	1.9252200	-0.1331600	1.9358900
O	0.6359100	-1.3744500	-0.4243300
H	-0.3244600	1.6793400	0.6786400
H	-0.4828400	-0.5949100	2.2773000
O	-1.9209800	-1.2984400	0.7615900
H	-1.5981100	-0.2606900	-1.7040400
H	-2.0867600	1.4056300	-1.2827200
H	-3.7422700	-0.8361100	-0.8495200
H	1.3086900	-1.7495900	0.1708000
H	-1.2199000	-1.7546700	0.2565500

9-educt
0, 1

C	0.0000000	-1.2609500	-1.2883200
C	0.0000000	0.0000000	-2.1791800
C	0.0000000	1.2609500	-1.2883200
C	-1.2582200	1.2557400	-0.3954300
C	-1.2792000	0.0000000	0.5078700
C	-1.2582200	-1.2557400	-0.3954300
C	1.2582200	-1.2557400	-0.3954300
C	1.2582200	1.2557400	-0.3954300
C	1.2792000	0.0000000	0.5078700
C	0.0000000	0.0000000	1.3758600
C	-2.5252200	0.0000000	1.3959700
H	0.0000000	-2.1605500	-1.9193800
H	0.8883700	0.0000000	-2.8276000
H	-0.8883700	0.0000000	-2.8276000

H	0.0000000	2.1605500	-1.9193800
H	-1.2766200	2.1567100	0.2363400
H	-2.1644100	1.2684100	-1.0196100
H	-1.2766200	-2.1567100	0.2363400
H	-2.1644100	-1.2684100	-1.0196100
H	1.2766200	-2.1567100	0.2363400
H	2.1644100	-1.2684100	-1.0196100
H	1.2766200	2.1567100	0.2363400
H	2.1644100	1.2684100	-1.0196100
C	2.5252200	0.0000000	1.3959700
H	0.0000000	0.8877800	2.0270600
H	0.0000000	-0.8877800	2.0270600
H	-3.4382800	0.0000000	0.7836800
H	-2.5422300	-0.8908400	2.0398800
H	-2.5422300	0.8908400	2.0398800
H	3.4382800	0.0000000	0.7836800
H	2.5422300	0.8908400	2.0398800
H	2.5422300	-0.8908400	2.0398800

9-product
0, 1

C	-2.9560100	-0.5899700	-0.5483100
C	-1.8200800	0.3447100	-1.0324900
C	-0.4710600	-0.4076900	-0.9015600
C	-0.2546000	-0.4641700	0.6649400
C	-1.5028800	0.2736200	1.2124400
C	-2.7395800	-0.6351800	1.0062700
C	-1.7353300	1.3569400	0.1340800
C	0.6895700	0.2981500	-1.6146000
C	2.0514800	-0.3100000	-1.2344700
C	2.2583400	-0.4388900	0.3115500
C	1.0763700	0.1708400	1.0856100
C	3.5906400	0.1784800	0.7566300
H	-2.8871200	-1.5828000	-1.0105000
H	-3.9386100	-0.1695000	-0.7965900
H	-1.9858900	0.7676800	-2.0303100
H	-0.5615200	-1.4244400	-1.3088600
H	-0.2541500	-1.5086200	1.0070900
H	-1.3794400	0.6321400	2.2411400
H	-2.5603800	-1.6527100	1.3758700
H	-3.6115200	-0.2315200	1.5360900
H	-0.9009400	2.0614500	0.0395100
H	-2.6654700	1.9207900	0.2833700

H	0.5443600	0.2434400	-2.7022500
H	0.6805400	1.3644300	-1.3495700
H	2.8526800	0.3065400	-1.6663600
H	2.1394500	-1.3032200	-1.6967600
H	2.2800600	-1.5100800	0.5629700
H	1.2295100	0.0289700	2.1646800
H	1.0469400	1.2565000	0.9102500
H	3.5997900	1.2564500	0.5378900
H	4.4362600	-0.2804500	0.2260000
H	3.7485600	0.0481100	1.8362700

IP23

SH
0, 2

S	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.3402000

Cl_2
0, 1

Cl	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.0078300

OH
0, 2

O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9689000

O_2
0, 3

O	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.2013200

PH
0, 3

P	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.4220200

PH_2
0, 2

P	0.0000000	0.0000000	-0.1156600
H	1.0201300	0.0000000	0.8674300
H	-1.0201300	0.0000000	0.8674300

S_2
0, 3

S	0.0000000	0.0000000	0.0000000
S	0.0000000	0.0000000	1.8925900
FeC			
0, 3			
Fe	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.5960000
Co	0, 4	Co^+	1, 3
Sc	0, 2	Sc^+	1, 3

EA13/03			
SH			
0, 2			
S	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.3402000
Cl_2			
0, 1			
Cl	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	2.0078300
OH			
0, 2			
O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9689000
O_2			
0, 3			
O	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.2013200
PH			
0, 3			
P	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.4220200
PH_2			
0, 2			
P	0.0000000	0.0000000	-0.1156600
H	1.0201300	0.0000000	0.8674300
H	-1.0201300	0.0000000	0.8674300
S_2			

0, 3			
S	0.0000000	0.0000000	0.0000000
S	0.0000000	0.0000000	1.8925900

PA8

NH_3
0, 1

N	0.0000000	0.0000000	0.1164900
H	0.0000000	0.9397300	-0.2718100
H	0.8138300	-0.4698600	-0.2718100
H	-0.8138300	-0.4698600	-0.2718100

H_2O
0, 1

O	0.0000000	0.0000000	0.1192600
H	0.0000000	0.7632400	-0.4770500
H	0.0000000	-0.7632400	-0.4770500

C_2H_2
0, 1

C	0.0000000	0.0000000	0.6080800
C	0.0000000	0.0000000	-0.6080800
H	0.0000000	0.0000000	-1.6739900
H	0.0000000	0.0000000	1.6739900

SiH_4
0, 1

Si	0.0000000	0.0000000	0.0000000
H	0.8561300	0.8561300	0.8561300
H	-0.8561300	-0.8561300	0.8561300
H	-0.8561300	0.8561300	-0.8561300
H	0.8561300	-0.8561300	-0.8561300

PH_3
0, 1

P	0.0000000	0.0000000	0.1246200
H	0.0000000	1.2006500	-0.6230900
H	1.0397900	-0.6003200	-0.6230900
H	-1.0397900	-0.6003200	-0.6230900

H_2S
0, 1

S	0.0000000	0.0000000	0.1021400
H	0.0000000	0.9742700	-0.8170800
H	0.0000000	-0.9742700	-0.8170800

HCl			
0, 1			
Cl	0.0000000	0.0000000	0.0711100
H	0.0000000	0.0000000	-1.2088700
H_2			
0, 1			
H	0.0000000	0.0000000	0.3685800
H	0.0000000	0.0000000	-0.3685800

πTC13			
E2-E1			
π1			
0, 1			
C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.3154600
C	0.0000000	0.0000000	-1.3154600
H	0.0000000	0.9270900	1.8729500
H	0.0000000	-0.9270900	1.8729500
H	0.9270900	0.0000000	-1.8729500
H	-0.9270900	0.0000000	-1.8729500
π2			
0, 1			
C	0.0000000	0.0000000	0.2137600
C	0.0000000	0.0000000	1.4361600
C	0.0000000	0.0000000	-1.2496500
H	0.0000000	0.0000000	2.4997000
H	0.0000000	1.0192400	-1.6337700
H	0.8826900	-0.5096200	-1.6337700
H	-0.8826900	-0.5096200	-1.6337700
E4-E3			
π3			
0, 1			
C	-2.6092400	0.0002900	0.0001900
C	-1.2853700	-0.0000800	0.0000200
C	0.0000000	-0.0005700	-0.0001600
C	1.2853700	-0.0002300	-0.0008500
C	2.6092400	0.0003100	0.0004000
H	-3.1676500	-0.6809900	-0.6295600
H	-3.1671000	0.6818200	0.6301600
H	3.1678400	0.6303100	-0.6804800
H	3.1669000	-0.6294800	0.6822700

π4
0, 1

C	2.7552700	-0.0000200	0.0000000
C	1.5271600	0.0000100	0.0000000
C	0.1534700	0.0000400	0.0000000
C	-1.0756000	0.0000200	0.0000100
C	-2.5367900	-0.0000200	-0.0000100
H	3.8194600	-0.0000600	-0.0000100
H	-2.9201900	1.0193900	-0.0373100
H	-2.9201300	-0.5420500	-0.8642100
H	-2.9201500	-0.4774500	0.9014900

E6-E5

π5
0, 1

C	3.8996200	-0.0019000	-0.0004000
C	2.5720800	0.0030400	0.0009400
C	1.2896200	0.0418900	0.0083800
C	0.0001700	-0.0163500	-0.0016400
C	-1.2895800	0.0161300	0.0020000
C	-2.5723100	-0.0213200	-0.0041700
C	-3.8995500	-0.0055500	-0.0015100
H	4.4580500	-0.1791500	0.9108300
H	4.4575600	0.1595600	-0.9148500
H	-4.4453600	0.9146500	0.1699000
H	-4.4697300	-0.9109000	-0.1701200

π6
0, 1

C	-4.0619400	0.0000500	-0.0000300
C	-2.8316300	0.0000100	-0.0000100
C	-1.4656600	-0.0000300	0.0000200
C	-0.2274100	-0.0000600	0.0000500
C	1.1369900	-0.0000500	0.0000300
C	2.3687400	-0.0000400	0.0000300
C	3.8292000	0.0000600	-0.0000400
H	-5.1265100	0.0000900	-0.0000600
H	4.2122800	-0.8071700	-0.6241800
H	4.2121600	0.9442300	-0.3871000
H	4.2123100	-0.1367800	1.0111100

P-2
0, 1

C	0.0000000	0.6695200	-0.0000200
C	0.0000000	-0.6695200	-0.0000200
H	-0.9224900	1.2337800	0.0000400

H	0.9224900	1.2337800	0.0000800
H	0.9224900	-1.2337800	0.0000400
H	-0.9224900	-1.2337800	0.0000800

P-2H
1, 1

C	-0.6916100	0.0000000	-0.0627800
C	0.6916100	-0.0000100	-0.0628200
H	-1.2413800	0.9338700	-0.0717200
H	0.0003000	-0.0002800	1.0403400
H	-1.2419000	-0.9335500	-0.0715700
H	1.2415500	-0.9337800	-0.0719500
H	1.2414700	0.9338200	-0.0714700

P-4
0, 1

C	1.8497400	0.1106700	0.0000200
C	0.6057800	-0.4054000	-0.0000500
C	-0.6057500	0.4054100	-0.0000100
C	-1.8497600	-0.1106800	0.0000200
H	2.7242600	-0.5244100	0.0000800
H	2.0128900	1.1811800	0.0000100
H	0.4744200	-1.4836100	0.0000400
H	-0.4743900	1.4836200	0.0000100
H	-2.7242800	0.5244000	0.0000200
H	-2.0129300	-1.1811900	0.0000200

P-4H
1, 1

C	1.8467200	0.0819700	-0.0001900
C	0.4606700	-0.3731200	-0.0000700
C	-0.6643400	0.4580000	0.0001200
C	-1.9055700	-0.1304300	-0.0000400
H	2.3571400	-0.3606800	-0.8642400
H	2.3545000	-0.3557100	0.8681300
H	1.9532400	1.1616300	-0.0027100
H	0.2873800	-1.4478500	0.0001300
H	-0.5525500	1.5343000	0.0000400
H	-2.8136700	0.4591900	-0.0002300
H	-2.0109400	-1.2093500	-0.0000500

P-6
0, 1

C	-3.0752600	0.1707900	-0.0000300
C	-1.8654500	-0.4259200	0.0000500
C	-0.6084300	0.2994200	-0.0000200

C	0.6084300	-0.2994200	-0.0000500
C	1.8654500	0.4259200	0.0000700
C	3.0752600	-0.1707900	-0.0000400
H	-3.9886700	-0.4070100	0.0001700
H	-3.1688100	1.2496500	-0.0000700
H	-1.8079000	-1.5107600	0.0001600
H	-0.6621600	1.3858100	-0.0002200
H	0.6621600	-1.3858100	-0.0003800
H	1.8079000	1.5107600	0.0003100
H	3.9886700	0.4070100	-0.0001400
H	3.1688100	-1.2496500	0.0002600

P-6H
1, 1

C	-3.0690100	0.0960000	0.0000300
C	-1.6867800	-0.4118100	-0.0001400
C	-0.5536600	0.3737900	0.0003400
C	0.7051800	-0.2364900	-0.0001500
C	1.9369200	0.4630000	-0.0005000
C	3.1078800	-0.2361000	0.0002700
H	-3.5974200	-0.3012800	0.8717500
H	-3.5978400	-0.3014000	-0.8713600
H	-3.1196800	1.1810200	0.0000400
H	-1.5540900	-1.4918300	-0.0004700
H	-0.6346100	1.4545100	0.0005700
H	0.7446000	-1.3242300	-0.0001200
H	1.9374500	1.5458500	-0.0005700
H	4.0655700	0.2665200	0.0005500
H	3.1129200	-1.3195200	0.0004300

P-8
0, 1

C	-4.3079200	-0.2022100	0.0000200
C	-3.1093200	0.4185600	-0.0000100
C	-1.8394300	-0.2799200	-0.0000200
C	-0.6330600	0.3462800	-0.0000200
C	0.6330600	-0.3462800	-0.0000300
C	1.8394300	0.2799200	0.0000500
C	3.1093200	-0.4185600	0.0000500
C	4.3079200	0.2022000	-0.0000400
H	-5.2324500	0.3576900	0.0000600
H	-4.3801200	-1.2827600	0.0000300
H	-3.0741100	1.5045000	0.0000100
H	-1.8693000	-1.3673400	-0.0000600
H	-0.6066200	1.4339200	0.0000200
H	0.6066200	-1.4339200	-0.0000900

H	1.8693100	1.3673400	0.0001100
H	3.0741100	-1.5045000	0.0001200
H	5.2324500	-0.3576900	-0.0000500
H	4.3801200	1.2827500	-0.0001200

P-8H
1, 1

C	-4.2964900	0.0728400	0.0007400
C	-2.9082100	-0.4374000	0.0001800
C	-1.7832200	0.3463500	-0.0002800
C	-0.5041700	-0.2477200	-0.0010100
C	0.6980200	0.4625100	-0.0011000
C	1.9069000	-0.2154300	-0.0000700
C	3.1836800	0.4167900	0.0007100
C	4.3214700	-0.3275700	0.0004900
H	-4.8288300	-0.3125000	-0.8725500
H	-4.3379500	1.1590400	0.0003400
H	-4.8279400	-0.3117700	0.8749000
H	-2.7760000	-1.5172400	-0.0000300
H	-1.8707900	1.4272100	-0.0000600
H	-0.4527800	-1.3350200	-0.0012000
H	0.6841600	1.5468400	-0.0012400
H	1.8865900	-1.3036300	0.0000300
H	3.2347900	1.4990600	0.0010800
H	5.2982700	0.1357900	0.0006500
H	4.2826000	-1.4100300	0.0001700

P-10
0, 1

C	-5.5415400	-0.2215900	0.0068000
C	-4.3478400	0.4093900	0.0045400
C	-3.0725700	-0.2773200	0.0026200
C	-1.8711100	0.3601400	-0.0287400
C	-0.6010300	-0.3193400	-0.0305000
C	0.6009700	0.3195800	0.0308900
C	1.8710600	-0.3599500	0.0290600
C	3.0726100	0.2773600	-0.0027300
C	4.3478200	-0.4095100	-0.0046800
C	5.5416100	0.2213100	-0.0071900
H	-6.4707500	0.3305200	0.0057800
H	-5.6044500	-1.3027400	0.0082500
H	-4.3222200	1.4956500	0.0010000
H	-3.0920400	-1.3649500	0.0141600
H	-1.8554800	1.4481000	-0.0349500
H	-0.6153200	-1.4069000	-0.0598300
H	0.6152800	1.4071400	0.0601900

H	1.8553500	-1.4479000	0.0356200
H	3.0922200	1.3649800	-0.0146300
H	4.3220600	-1.4957700	-0.0009600
H	6.4707400	-0.3309300	-0.0061900
H	5.6046700	1.3024500	-0.0088400

P-10H
1, 1

C	-5.5244500	0.0285700	0.0040700
C	-4.1290800	-0.4732900	0.0039000
C	-3.0139700	0.3169200	0.0164800
C	-1.7179000	-0.2561900	0.0092800
C	-0.5371200	0.4729700	-0.0102500
C	0.6989400	-0.1754700	-0.0352700
C	1.9402400	0.4820600	-0.0233600
C	3.1188300	-0.2357900	0.0002300
C	4.4210100	0.3542900	0.0147600
C	5.5386200	-0.4159300	0.0165500
H	-6.0568700	-0.3517700	-0.8706000
H	-5.5682500	1.1151800	0.0059700
H	-6.0552200	-0.3542000	0.8789300
H	-3.9898100	-1.5520800	-0.0037700
H	-3.1137600	1.3972200	0.0226200
H	-1.6482000	-1.3424400	0.0058100
H	-0.5739000	1.5572400	-0.0032200
H	0.7025100	-1.2640100	-0.0453800
H	1.9689000	1.5666800	-0.0193100
H	3.0618300	-1.3225800	-0.0003600
H	4.5021800	1.4351800	0.0184900
H	6.5260100	0.0238500	0.0205800
H	5.4738800	-1.4970100	0.0118900

SB-2
0, 1

N	0.6767500	-0.1536300	0.0000100
C	-0.5943800	0.0276300	-0.0000300
H	1.1530200	0.7508400	-0.0000200
H	-1.2405900	-0.8433500	0.0000500
H	-1.0833900	1.0021000	0.0000800

SB-2H
1, 1

N	0.6034300	-0.0000100	-0.0000300
C	-0.6792500	0.0000100	0.0000100
H	1.1352400	0.8679800	0.0002000
H	1.1351900	-0.8680300	-0.0000700

H	-1.2095500	-0.9421600	0.0001200
H	-1.2094000	0.9422200	-0.0001300

SB-4
0, 1

N	1.7937000	-0.2281200	0.0000700
C	0.6419100	0.3556000	-0.0001300
C	-0.5891500	-0.4306900	-0.0000700
C	-1.8054000	0.1439000	0.0000600
H	2.5375500	0.4725900	0.0000500
H	0.5208500	1.4440400	0.0003200
H	-0.4714700	-1.5080100	-0.0001000
H	-2.7108200	-0.4460000	0.0003500
H	-1.9161700	1.2213600	-0.0002700

SB-4H
1, 1

N	-1.7424300	0.0805100	-0.0001100
C	-0.5256200	-0.3807300	0.0001200
C	0.6393800	0.4494300	0.0000700
C	1.8586800	-0.1364700	-0.0002000
H	-2.5425200	-0.5425700	-0.0000100
H	-1.9347800	1.0774600	-0.0002800
H	-0.4191700	-1.4605400	0.0006700
H	0.5262800	1.5263700	0.0004300
H	2.7625100	0.4559900	0.0003800
H	1.9700600	-1.2136500	-0.0003400

SB-6
0, 1

N	3.0094000	-0.2532800	0.0000700
C	1.8804700	0.3782200	0.0000200
C	0.6234300	-0.3527100	-0.0000800
C	-0.5790300	0.2713200	-0.0001300
C	-1.8538900	-0.4233400	-0.0000400
C	-3.0432700	0.2119700	0.0000900
H	3.7807600	0.4172200	0.0001400
H	1.8070700	1.4710700	0.0000500
H	0.6920200	-1.4357800	-0.0000800
H	-0.6093800	1.3589600	-0.0000600
H	-1.8257300	-1.5086500	0.0000900
H	-3.9749000	-0.3358800	0.0002800
H	-3.1019200	1.2933100	-0.0000100

SB-6H
1, 1

N	-2.9541800	0.0845700	0.0000300
C	-1.7360700	-0.4017400	0.0000900
C	-0.5641600	0.3847900	-0.0002000
C	0.6576800	-0.2370800	-0.0001300
C	1.9166700	0.4491600	0.0001100
C	3.0814000	-0.2418800	0.0000200
H	-3.7624100	-0.5242900	0.0003000
H	-3.1288200	1.0827300	-0.0002900
H	-1.6584600	-1.4840000	0.0004000
H	-0.6405900	1.4661000	0.0000300
H	0.6881100	-1.3248000	-0.0003500
H	1.9193600	1.5326600	0.0002700
H	4.0359400	0.2650300	0.0002300
H	3.0930000	-1.3248600	-0.0001900

SB-8
0, 1

N	-4.3373400	0.1686100	0.0020300
C	-3.2018600	-0.4527700	-0.0018500
C	-1.9524600	0.2875000	0.0023100
C	-0.7428400	-0.3290200	-0.0017700
C	0.5209300	0.3688800	0.0021500
C	1.7245900	-0.2614900	-0.0021200
C	2.9979800	0.4310100	0.0017400
C	4.1906100	-0.2005100	-0.0025000
H	-5.1022100	-0.5093400	-0.0018000
H	-3.1190800	-1.5450800	-0.0083300
H	-2.0285400	1.3701400	0.0089400
H	-0.7085300	-1.4167700	-0.0084300
H	0.4926400	1.4557300	0.0088500
H	1.7501900	-1.3490500	-0.0088300
H	2.9700600	1.5168100	0.0084300
H	5.1201700	0.3508800	0.0006200
H	4.2529400	-1.2816400	-0.0091500

SB-8H
1, 1

N	-4.1775300	0.0456300	-0.0000200
C	-2.9445500	-0.4218100	-0.0000500
C	-1.7894100	0.3733200	-0.0000600
C	-0.5498300	-0.2329800	0.0000300
C	0.6858500	0.4583900	0.0002100
C	1.8756100	-0.2243400	0.0000300
C	3.1680900	0.4016700	-0.0001300
C	4.3071400	-0.3303400	-0.0000100
H	-4.9736400	-0.5766700	-0.0000300

H	-4.3685700	1.0394600	0.0000300
H	-2.8529000	-1.5029100	-0.0000900
H	-1.8776300	1.4539300	0.0000100
H	-0.5104100	-1.3208000	0.0000500
H	0.6839900	1.5433200	0.0003500
H	1.8508000	-1.3123400	0.0000000
H	3.2158300	1.4847700	-0.0003600
H	5.2795200	0.1412900	-0.0001400
H	4.2784300	-1.4129100	0.0002200

SB-10
0, 1

N	-5.4710900	-0.2510500	0.0030100
C	-4.3452700	0.3884300	0.0027000
C	-3.0846700	-0.3309500	0.0049900
C	-1.8845200	0.3058900	-0.0196700
C	-0.6109900	-0.3684400	-0.0256300
C	0.5831000	0.2850900	0.0243500
C	1.8624200	-0.3773200	0.0247800
C	3.0525200	0.2808400	-0.0025000
C	4.3399600	-0.3830300	-0.0035700
C	5.5203400	0.2721300	-0.0074100
H	-6.2465300	0.4148500	0.0009400
H	-4.2801000	1.4820000	-0.0000800
H	-3.1424100	-1.4147600	0.0122600
H	-1.8694800	1.3942300	-0.0232800
H	-0.6181700	-1.4554500	-0.0508500
H	0.5838500	1.3729200	0.0492200
H	1.8631900	-1.4650500	0.0317200
H	3.0529600	1.3686600	-0.0139600
H	4.3350700	-1.4693800	0.0016100
H	6.4605800	-0.2609000	-0.0059800
H	5.5611900	1.3543200	-0.0109200

SB-10H
1, 1

N	5.4029600	-0.0149400	-0.0051400
C	4.1553100	-0.4578600	-0.0022000
C	3.0191200	0.3541800	-0.0007400
C	1.7613300	-0.2274800	-0.0035300
C	0.5465300	0.4833600	-0.0062400
C	-0.6648200	-0.1768000	0.0204400
C	-1.9298000	0.4659000	0.0201900
C	-3.0982100	-0.2505600	-0.0004700
C	-4.4089400	0.3410600	-0.0083900
C	-5.5332600	-0.4123500	-0.0108400

H	6.1847200	-0.6535500	-0.0039600
H	5.6142400	0.9738500	-0.0071900
H	4.0438700	-1.5370500	-0.0002100
H	3.1264800	1.4332500	-0.0029300
H	1.7019400	-1.3146000	0.0025100
H	0.5678700	1.5683100	-0.0187400
H	-0.6566900	-1.2653700	0.0314600
H	-1.9652100	1.5509500	0.0219300
H	-3.0423100	-1.3373000	-0.0053100
H	-4.4812000	1.4232400	-0.0082500
H	-6.5145400	0.0403900	-0.0126000
H	-5.4833700	-1.4941200	-0.0100600

HTBH38/08

Reaction 1: H + HCl → H_2 + Cl

HCl
0, 1

Cl	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.2744500

TS1
0, 2

H	0.0004800	-1.3406300	0.0000000
Cl	0.0000000	0.2032500	0.0000000
H	-0.0004800	-2.1146600	0.0000000

H_2
0, 1

H	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.7418800

Reaction 2: OH + H_2 → H_2O + H

OH
0, 2

O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9689000

TS2
0, 2

O	-0.3010600	-0.1080500	-0.0000100
H	-0.4279500	0.8515700	0.0000200
H	1.0154900	-0.1003700	0.0001200
H	1.8209700	0.1131900	-0.0000700

H_2O

0, 1			
O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9569100
H	0.9263600	0.0000000	-0.2398700

Reaction 3: $CH_3 + H_2 \rightarrow CH_4 + H$

CH_3			
0, 2			
C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0773200
H	0.9329800	0.0000000	-0.5386600
H	-0.9329800	0.0000000	-0.5386600
TS3			
0, 2			
C	0.0000000	0.2648100	0.0000000
H	1.0534300	0.5166700	0.0000000
H	-0.5266300	0.5170200	0.9122500
H	-0.5266300	0.5170200	-0.9122500
H	-0.0002600	-1.1177700	0.0000000
H	0.0000800	-2.0218300	0.0000000
CH_4			
0, 1			
C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0874400
H	1.0252500	0.0000000	-0.3624800
H	-0.5126300	0.8878900	-0.3624800
H	-0.5126300	-0.8878900	-0.3624800

Reaction 4: $OH + CH_4 \rightarrow H_2O + CH_3$

TS4			
0, 2			
C	-1.2114900	0.0079700	0.0004100
O	1.2939700	-0.1086900	0.0001300
H	0.0094800	-0.1180200	0.0028000
H	-1.5255300	-0.2332500	1.0100700
H	-1.4306700	1.0332300	-0.2780800
H	-1.5527100	-0.7101100	-0.7377000
H	1.4166400	0.8498900	-0.0005900

Reaction 5: $H + H_2 \rightarrow H_2 + H$

TS5			
0, 2			
H	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9294700

H	0.0000000	0.0000000	-0.9294700

Reaction 6: $OH + NH_3 \rightarrow H_2O + NH_2$

NH_3
0, 1

N	0.0000000	0.0000000	0.1128900
H	0.0000000	0.9380200	-0.2634100
H	0.8123500	-0.4690100	-0.2634100
H	-0.81235	-0.4690100	-0.2634100

TS6
0, 2

N	-1.1508200	-0.0439300	-0.1025600
O	1.1791900	-0.0927000	-0.0102900
H	-1.3031900	-0.5476400	0.7665700
H	-1.3389100	0.9358100	0.0918500
H	-0.0306900	-0.1538300	-0.3531800
H	1.2950100	0.8147500	0.2949900

NH_2
0, 2

N	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0240500
H	0.9971600	0.0000000	-0.2331400

Reaction 7: $HCl + CH_3 \rightarrow CH_4 + Cl$

TS7
0, 2

C	0.2441200	0.5999200	1.7024200
H	-0.6756000	0.2784800	2.1729400
H	0.3519100	1.6637900	1.5376700
H	1.1406900	0.0657900	1.9878200
H	0.0571600	0.1399700	0.3971100
Cl	-0.1375800	-0.3380900	-0.9594200

Reaction 8: $OH + C_2H_6 \rightarrow H_2O + C_2H_5$

C_2H_6
0, 1

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.5261800
H	1.0160700	0.0000000	1.9214000
H	0.5096000	-0.8790400	-0.3952200
H	-0.5080300	-0.8799400	1.9214000
H	-0.5080400	0.8799400	1.9214000
H	-1.0160700	-0.0018000	-0.3952200
H	0.5064700	0.8808400	-0.3952200

TS8
0, 2

C	1.4583300	-0.4463700	0.0254800
C	0.4694200	0.6974200	-0.0274900
O	-1.8530400	-0.3146600	-0.0530500
H	1.3017600	-1.0610800	0.9107400
H	1.3665800	-1.0861900	-0.8511200
H	2.4822400	-0.0668800	0.0571500
H	0.4710700	1.3254400	0.8610400
H	0.5335200	1.3035000	-0.9285600
H	-0.6302300	0.2078200	-0.0784600
H	-2.2672100	0.3883200	0.4657500

C_2H_5
0, 2

C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.4901400
H	1.0137700	0.0000000	1.8911400
H	-0.8485500	0.3741300	-0.5528700
H	-0.5010600	-0.8876800	1.8958500
H	-0.5250100	0.8674800	1.8910500
H	0.7721800	-0.5127000	-0.5535700

Reaction 9: $F + H_2 \rightarrow HF + H$

TS9
0, 2

H	0.1465700	-1.1283900	0.0000000
F	0.0000000	0.3304200	0.0000000
H	-0.1465700	-1.8454100	0.0000000

HF
0, 1

F	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9153800

Reaction 10: $O + CH_4 \rightarrow OH + CH_3$

TS10
0, 3

C	0.0002900	-1.1422900	0.0000000
H	-1.0559600	-1.3847400	0.0000000
H	0.5201700	-1.4073900	0.9124500
H	0.5201700	-1.4073900	-0.9124500
H	0.0115600	0.1601000	0.0000000
O	0.0002900	1.3616400	0.0000000

Reaction 11: $H + PH_3 \rightarrow H_2 + PH_2$			
PH_3			
0, 1			
P	0.0000000	0.0000000	0.1264100
H	1.1913400	0.0000000	-0.6320600
H	-0.5956700	-1.0317300	-0.6320600
H	-0.5956700	1.0317300	-0.6320600
TS11			
0, 2			
P	0.2174300	0.0000900	-0.1112500
H	0.2466100	1.0346700	0.8521600
H	0.2626600	-1.0250600	0.8616200
H	-1.2664200	-0.0109500	-0.1506300
H	-2.5042900	0.0000300	0.1055800
PH_2			
0, 2			
P	0.0000000	0.0000000	-0.1156600
H	1.0201300	0.0000000	0.8674300
H	-1.0201300	0.0000000	0.8674300

Reaction 12: $H + HO \rightarrow H_2 + O$			
TS12			
0, 3			
H	0.0000000	0.0000000	-0.8602900
O	0.0000000	0.0000000	0.3290200
H	0.0000000	0.0000000	-1.7719100

Reaction 13: $H + H_2S \rightarrow H_2 + HS$			
H_2S			
0, 1			
S	0.0000000	0.0000000	0.1025200
H	0.0000000	0.9662500	-0.8201500
H	0.0000000	-0.9662500	-0.8201500
TS13			
0, 2			
H	1.2621000	-0.2201000	0.0000000
S	0.0000000	0.2231500	0.0000000
H	-0.5005800	-1.1154500	0.0000000
H	-0.7615200	-2.2349100	0.0000000
HS			
0, 2			
S	0.0000000	0.0000000	0.0000000

H	0.0000000	0.0000000	1.3402000

Reaction 14: O + HCl → OH + Cl

TS14			
0, 3			
Cl	0.0188200	-0.8173000	0.0000000
H	-0.4704900	0.5694800	0.0000000
O	0.0188200	1.6655800	0.0000000

Reaction 15: $CH_3 + NH_2 \rightarrow CH_4 + NH$

TS15			
0, 3			
C	-1.1995800	-0.0111300	-0.0000300
N	1.4007100	0.1298600	0.0000200
H	-1.4266600	-0.5129300	0.9330600
H	-1.4199100	-0.5913800	-0.8881400
H	-1.5202400	1.0228100	-0.0457800
H	0.1889300	0.1269000	0.0010000
H	1.5703400	-0.8876700	-0.0000500
NH			
0, 3			
N	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0367300

Reaction 16: $C_2H_5 + NH_2 \rightarrow C_2H_6 + NH$

TS16			
0, 3			
C	-1.3949800	-0.4496600	0.0007000
C	-0.4357500	0.7140600	0.0020300
N	1.9275700	-0.3783500	0.0030400
H	-1.2000900	-1.1209500	-0.8356900
H	-1.3221000	-1.0278800	0.9217700
H	-2.4287100	-0.1053500	-0.0893300
H	-0.4176900	1.3084800	-0.9072000
H	-0.4411300	1.3290900	0.8974700
H	0.8285000	0.1805900	-0.0285600
H	2.4725900	0.4980700	0.0039100

Reaction 17: $NH_2 + C_2H_6 \rightarrow NH_3 + C_2H_5$

TS17			
0, 2			
C	-1.4857000	-0.4481600	-0.0000200
C	-0.5050400	0.7017400	0.0000300
N	1.8651600	-0.3401700	-0.0000600
H	-1.3541900	-1.0765100	-0.880500

H	-1.3541600	-1.0766100	0.8803800
H	-2.5170200	-0.0861700	0.0000300
H	-0.5222200	1.3161200	-0.8972200
H	-0.5222100	1.3160300	0.8973400
H	0.6650500	0.1479600	-0.0000300
H	2.2466400	0.1597200	-0.8048100
H	2.2464400	0.1591300	0.8051500

Reaction 18: $NH_2 + CH_4 \rightarrow NH_3 + CH_3$

TS18
0, 2

C	-1.2607500	-0.0000100	0.0122900
N	1.3132600	-0.0000100	-0.1367800
H	-1.5839900	0.9085400	-0.4847400
H	-1.4636700	-0.0045700	1.0773000
H	-1.5847500	-0.9038800	-0.4927000
H	0.0431100	-0.0000600	-0.1516900
H	1.4804600	0.8055800	0.4677500
H	1.4805600	-0.8055200	0.4678100

Reaction 19: *s-trans cis*-$C_5H_8 \rightarrow$ *s-trans cis*-C_5H_8

C_5H_8
0, 1

C	-2.0556400	-0.6122700	0.0000100
C	-1.2311000	0.6404500	0.0000500
C	0.1056300	0.7342700	0.0000300
C	1.0575600	-0.3744100	-0.0000400
C	2.3835800	-0.1989400	-0.0000400
H	-2.7050800	-0.6416000	0.8771300
H	-2.7051300	-0.6415100	-0.8770900
H	-1.4513300	-1.5160800	-0.0000600
H	-1.7936700	1.5675900	0.0001000
H	0.5457600	1.7256400	0.0000600
H	0.6652600	-1.3832400	-0.0001100
H	3.0646900	-1.0377200	-0.0000900
H	2.8192800	0.7922900	0.0000200

TS19
0, 1

C	-1.2996200	-0.9048500	-0.0201500
C	-1.2059500	0.5058200	-0.0134100
C	0.0000000	1.1833600	0.1533000
C	1.2059500	0.5058100	-0.0134200
C	1.2996300	-0.9048500	-0.0201500
H	2.1688000	-1.3275500	-0.5157000
H	1.0320400	-1.4543900	0.8731700

H	2.0371300	1.0855800	-0.3985000
H	0.0000000	2.2629100	0.0859000
H	-2.0371300	1.0855900	-0.3984800
H	-2.1688000	-1.3275400	-0.5157200
H	-0.0000100	-1.1819400	-0.5208100
H	-1.0320600	-1.4543900	0.8731600

NHTBH38/08

Reaction 1: $H + N_2O \rightarrow OH + N_2$

N_2O
0, 1

N	0.0000000	0.0000000	0.0000000
N	0.0000000	0.0000000	1.1205600
O	0.0000000	0.0000000	2.3076100

OH
0, 2

O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9689000

TS1
0, 2

H	-0.3032900	-1.9307100	0.0000000
O	-0.8610100	-0.6215300	0.0000000
N	0.0000000	0.2570300	0.0000000
N	1.0273300	0.7291000	0.0000000

N_2
0, 1

N	0.0000000	0.0000000	0.0000000
N	0.0000000	0.0000000	1.0971100

Reaction 2: $H + FH \rightarrow HF + H$

HF
0, 1

F	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9153800

TS2
0, 2

H	0.0000000	0.0000000	1.1372200
F	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	-1.1372200

Reaction 3: $H + ClH \rightarrow HCl + H$

HCl			
0, 1			
Cl	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.2744500
TS3			
0, 2			
H	0.0000000	0.0000000	1.4858000
Cl	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	-1.4858000

Reaction 4: $H + FCH_3 \rightarrow HF + CH_3$

CH_3F			
0, 1			
C	-0.6320700	0.0000000	0.0000000
F	0.7491200	0.0000000	0.0000000
H	-0.9831800	-0.3384900	0.9726200
H	-0.9832200	1.0115500	-0.1931700
H	-0.9832000	-0.6730800	-0.7794400
TS4			
0, 2			
H	-0.0397600	0.0000000	0.0441100
F	-0.0493200	0.0000000	1.2825500
C	-0.0615400	0.0000000	2.9511600
H	0.9905000	0.0000000	3.1942800
H	-0.5900700	0.9123600	3.1834800
H	-0.5900700	-0.9123600	3.1834800
CH_3			
0, 2			
C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0773000
H	0.9329800	0.0000000	-0.5386600
H	-0.9329800	0.0000000	-0.5386600

Reaction 5: $H + F_2 \rightarrow HF + F$

F_2			
0, 1			
F	0.0000000	0.0000000	0.0000000
F	0.0000000	0.0000000	1.3952000
TS5			
0, 2			
H	0.0000000	0.0000000	-2.2312700
F	0.0000000	0.0000000	-0.6162200

F	0.0000000	0.0000000	0.8641400

Reaction 6: $CH_3 + FCl \rightarrow CH_3F + Cl$			
FCl			
0, 1			
F	0.0000000	0.0000000	0.0000000
Cl	0.0000000	0.0000000	1.6303300
TS6			
0, 2			
Cl	1.4547500	-0.0012400	-0.0000400
F	-0.3235900	0.0046300	0.0001200
C	-2.3874200	-0.0021500	-0.0000700
H	-2.4950900	-0.8553600	-0.6494000
H	-2.4973100	-0.1386700	1.0631400
H	-2.5015400	0.9862700	-0.4137300

Reaction 7: $F^- + CH_3F \rightarrow FCH_3 + F^-$			
TS7			
-1, 1			
F	0.0031000	-0.0188900	-0.0154600
C	-0.0001500	-0.0001400	1.8078600
H	1.0694500	0.0017100	1.8097600
H	-0.5366100	0.9251300	1.7969300
H	-0.5326000	-0.9277800	1.8170600
F	-0.0031900	0.0199700	3.6318500

Reaction 8: $F^-\cdots CH_3F \rightarrow FCH_3\cdots F^-$			
FCH3F (complex)			
-1, 1			
F	0.0000000	0.0000000	-1.8476300
C	0.0000000	0.0000000	-0.4218700
H	0.0000000	1.0235800	-0.0738400
H	-0.8864500	-0.5117900	-0.0738400
H	0.8864500	-0.5117900	-0.0738400
F	0.0000000	0.0000000	2.1534900

Reaction 9: $Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$			
CH_3Cl			
0, 1			
C	0.0000000	0.0000000	-1.1258900
Cl	0.0000000	0.0000000	0.6568300
H	0.0000000	1.0279900	-1.4702600
H	0.8902700	-0.5140000	-1.4702600
H	-0.8902700	-0.5140000	-1.4702600

TS9
-1, 1

Cl	2.3225800	-0.0001300	0.0001400
C	-0.0000900	0.0004900	-0.0005100
H	0.0000800	-0.7442900	-0.7676000
H	-0.0003200	-0.2914400	1.0280200
H	0.0000800	1.0372200	-0.2619600
Cl	-2.3225400	-0.0001300	0.0001300

Reaction 10: $Cl^{-}\cdots CH_3Cl \rightarrow ClCH_3\cdots Cl^{-}$

$ClCH_3Cl$ (complex)
-1, 1

Cl	0.0000000	0.0000000	-2.3847400
C	0.0000000	0.0000000	-0.5663300
H	0.0000000	1.0250700	-0.2243800
H	-0.8877300	-0.5125300	-0.2243800
H	0.8877300	-0.5125300	-0.2243800
Cl	0.0000000	0.0000000	2.6242100

Reaction 11: $F^{-} + CH_3Cl \rightarrow FCH_3 + Cl^{-}$

TS11
-1, 1

F	0.0000000	0.0000000	-2.5379300
C	0.0000000	0.0000000	-0.4883700
H	0.0000000	1.0620900	-0.6149700
H	-0.9198000	-0.5310400	-0.6149700
H	0.9198000	-0.5310400	-0.6149700
Cl	0.0000000	0.0000000	1.6245000

Reaction 12: $F^{-}\cdots CH_3Cl \rightarrow FCH_3\cdots Cl^{-}$

FCH_3Cl (complex 1)
-1, 1

Cl	0.0000000	0.0000000	1.6231400
C	0.0000000	0.0000000	-0.2273600
H	0.0000000	1.0263200	-0.5551400
H	0.8888200	-0.5131600	-0.5551400
H	-0.8888200	-0.5131600	-0.5551400
F	0.0000000	0.0000000	-2.7293100

FCH_3Cl (complex 2)
-1, 1

F	0.0000000	0.0000000	-2.6485400
C	0.0000000	0.0000000	-1.2401700
H	0.0000000	1.0247200	-0.8864100
H	-0.8874300	-0.5123600	-0.8864100
H	0.8874300	-0.5123600	-0.8864100

Cl	0.0000000	0.0000000	1.9963000

Reaction 13: $OH^- + CH_3F \rightarrow HOCH_3 + F^-$

OH^-			
-1, 1			
O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9620400
TS13			
-1, 1			
F	0.0225400	-0.0074500	0.0055300
C	-0.0184200	0.0050400	1.7649300
H	1.0480500	0.0052400	1.8541500
H	-0.5478200	0.9347100	1.7922200
H	-0.5489500	-0.9234300	1.8057600
O	0.0012700	0.0192000	3.7506000
H	-0.9267600	0.0316100	3.9975800
CH_3OH			
0, 1			
C	-0.0464200	0.6630700	0.0000000
O	-0.0464200	-0.7550600	0.0000000
H	-1.0869600	0.9759400	0.0000000
H	0.8605900	-1.0570400	0.0000000
H	0.4381500	1.0715900	0.8895400
H	0.4381500	1.0715900	-0.8895400

Reaction 14: $OH^-\cdots CH_3F \rightarrow HOCH_3\cdots F^-$

$HOCH_3F$ (complex 1)			
-1, 1			
C	-1.2980000	-0.3895200	-0.0000300
O	-0.4772200	0.7280200	0.0000500
H	-2.3519200	-0.0802300	-0.0086400
H	-1.1408500	-1.0358200	-0.8781000
H	-1.1531800	-1.0275100	0.8863600
H	0.5105800	0.3711600	0.0002400
F	1.7490200	-0.1905200	-0.0000100
$HOCH_3F$ (complex 2)			
-1, 1			
F	0.0003700	-2.4683400	0.0213900
C	-0.2766400	-1.0744200	-0.0026900
H	0.6492900	-0.5165000	-0.0090200
H	-0.8419900	-0.8471200	-0.8970700
H	-0.8510300	-0.8265900	0.8814200
O	-0.3017100	1.5825200	-0.2065400

H	-0.6051100	2.4924300	-0.1643100

Reaction 15: H + N_2 → HN_2

TS15			
0, 2			
N	0.0000000	0.0000000	0.0000000
N	0.0000000	0.0000000	1.1228100
H	1.2684500	0.0000000	1.7843300
HN_2			
0, 2			
N	0.0000000	0.0000000	0.0000000
N	0.0000000	0.0000000	1.1782000
H	0.9366400	0.0000000	1.6449700

Reaction 16: H + CO → HCO

CO			
0, 1			
O	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.1296100
TS16			
0, 2			
H	-1.5208600	1.3888300	0.0000000
C	0.1086300	0.5493300	0.0000000
O	0.1086300	-0.5856000	0.0000000
HCO			
0, 2			
H	-0.0090600	0.0000000	-0.0070900
C	-0.0070300	0.0000000	1.1096800
O	0.9560400	0.0000000	1.7856600

Reaction 17: H + C_2H_4 → CH_3CH_2

C_2H_4			
0, 1			
C	0.0000000	0.0000000	0.6655900
C	0.0000000	0.0000000	-0.6655900
H	0.0000000	0.9214900	1.2316700
H	0.0000000	-0.9214900	1.2316700
H	0.0000000	0.9214900	-1.2316700
H	0.0000000	-0.9214900	-1.2316700
TS17			
0, 2			
C	-0.5678800	0.0000500	-0.2189600

C	0.7511400	-0.0000400	0.0419300
H	-1.4938800	-0.0004900	1.5317700
H	-1.1016900	0.9206500	-0.4086300
H	-1.1020200	-0.9202300	-0.4091100
H	1.2991300	-0.9223400	0.1737600
H	1.2989000	0.9223200	0.1743600

CH_3CH_2
0, 2

C	-0.2587200	-0.8168300	0.0000000
C	-0.2509900	0.6741900	0.0000000
H	0.7588300	-1.2259400	0.0000000
H	-0.7588300	-1.2138700	0.8834200
H	-0.7588300	-1.2138700	-0.8834200
H	-0.1700200	1.2259400	-0.9243200
H	-0.1700200	1.2259400	0.9243200

Reaction 18: $CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$

TS18
0, 2

C	-0.4721300	0.6459300	-0.0000400
C	-1.3826200	-0.3638900	0.0000000
H	-0.2320400	1.1645700	-0.9172600
H	-0.2323400	1.1647600	0.9171700
H	-1.7271300	-0.8098100	0.9225200
H	-1.7269400	-0.8101300	-0.9224400
C	1.6120100	-0.2421900	0.0000300
H	2.1951800	0.6686700	-0.0012700
H	1.5894200	-0.8096200	-0.9186300
H	1.5902400	-0.8076000	0.9199700

$CH_3CH_2CH_2$
0, 2

C	1.2084400	-0.2871900	0.0000600
C	-0.0653600	0.5761300	-0.0000600
C	-1.3147900	-0.2395200	-0.0000100
H	1.2413700	-0.9283900	0.8812300
H	1.2413900	-0.9285900	-0.8809800
H	2.1018700	0.3387300	0.0000000
H	-0.0482200	1.2268500	-0.8770900
H	-0.0482700	1.2270400	0.8768300
H	-1.7291500	-0.6157700	0.9244400
H	-1.7287600	-0.6164200	-0.9243700

Reaction 19: HCN → HNC

HCN

0, 1			
C	0.0000000	0.0000000	-0.5003600
N	0.0000000	0.0000000	0.6526400
H	0.0000000	0.0000000	-1.5662900
TS19			
0, 1			
C	0.0803200	0.6202600	0.0000000
N	0.0803200	-0.5681000	0.0000000
H	-1.0441500	0.2551200	0.0000000
HNC			
0, 1			
C	0.0000000	0.0000000	-0.7372500
N	0.0000000	0.0000000	0.4320900
H	0.0000000	0.0000000	1.4269600

NCCE30			
parallel-displaced $(CO_2)_2$			
0, 1			
C	0.5683590	1.6604200	0.0000000
C	-0.5683590	-1.6604200	0.0000000
O	1.7008450	1.9115690	0.0000000
O	-1.7008450	-1.9115690	0.0000000
O	-0.5683590	1.4145690	0.0000000
O	0.5683590	-1.4145690	0.0000000
CO_2			
0, 1			
C	0.0000000	0.0000000	0.0000000
O	0.0000000	0.0000000	1.1601000
O	0.0000000	0.0000000	-1.1601000
Ar-CO_2			
0, 1			
Ar	0.0000000	0.0000000	1.8832290
C	0.0000000	0.0000000	-1.5409710
O	0.0000000	1.1617000	-1.5407680
O	0.0000000	-1.1617000	-1.5407680
sandwich $(C_5H_5N)_2$			
0, 1			
N	1.3980380	0.0000000	0.0000000
C	0.6985370	1.1401300	0.0000000

C	-0.6941820	1.1953400	0.0000000
C	-1.4067470	0.0000000	0.0000000
C	-0.6941820	-1.1953400	0.0000000
C	0.6985370	-1.1401300	0.0000000
H	1.2816690	2.0568850	0.0000000
H	-1.1999250	2.1525480	0.0000000
H	-2.4885470	0.0000000	0.0000000
H	-1.1999250	-2.1525480	0.0000000
H	1.2816690	-2.0568850	0.0000000
N	-1.3980380	0.0000000	3.7000000
C	-0.6985370	1.1401300	3.7000000
C	0.6941820	1.1953400	3.7000000
C	1.4067470	0.0000000	3.7000000
C	0.6941820	-1.1953400	3.7000000
C	-0.6985370	-1.1401300	3.7000000
H	-1.2816690	2.0568850	3.7000000
H	1.1999250	2.1525480	3.7000000
H	2.4885470	0.0000000	3.7000000
H	1.1999250	-2.1525480	3.7000000
H	-1.2816690	-2.0568850	3.7000000

C_5H_5N
0, 1

N	0.0000000	0.0000000	1.4201100
C	0.0000000	1.1401300	0.7206090
C	0.0000000	1.1953400	-0.6721100
C	0.0000000	0.0000000	-1.3846750
C	0.0000000	-1.1953400	-0.6721100
C	0.0000000	-1.1401300	0.7206090
H	0.0000000	2.0568850	1.3037410
H	0.0000000	2.1525480	-1.1778530
H	0.0000000	0.0000000	-2.4664750
H	0.0000000	-2.1525480	-1.1778530
H	0.0000000	-2.0568850	1.3037410

$(NH_3)_2$
0, 1

N	1.5752300	0.0000900	-0.0426100
H	2.1311100	0.8139500	-0.2866100
H	1.4964500	-0.0029400	0.9702600
H	2.1317200	-0.8118900	-0.2914500
N	-1.6882400	0.0000800	0.1048500
H	-2.1264000	-0.8126800	-0.3173100
H	-2.1274400	0.8118400	-0.3181600
H	-0.7143000	0.0005400	-0.1924100

NH_3

0, 1

N	0.0000000	0.0000000	0.1150100
H	0.0000000	0.9397500	-0.2683600
H	0.8138500	-0.4698800	-0.2683600
H	-0.8138500	-0.4698800	-0.2683600

$(HF)_2$

0, 1

F	1.3237400	-0.0902300	-0.0000100
H	1.7404400	0.7333900	0.0000100
F	-1.4572000	0.0192600	-0.0000100
H	-0.5393100	-0.0946600	0.0001500

HF

0, 1

F	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9207400

$(H_2O)_2$

0, 1

O	1.5317500	0.0059200	-0.1208800
H	0.5759700	-0.0052500	0.0249700
H	1.9062500	-0.0375600	0.7632200
O	-1.3962300	-0.0049900	0.1067700
H	-1.7893700	-0.7422800	-0.3710100
H	-1.7770400	0.7776400	-0.3042600

H_2O

0, 1

O	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	0.9618300
H	0.9335800	0.0000000	-0.2314100

$NH_3\cdots H_2O$

0, 1

N	-1.3955900	-0.0215600	0.0000400
H	-1.6298100	0.9611000	-0.1062200
H	-1.8627700	-0.5125400	-0.7559700
H	-1.8335500	-0.3307700	0.8623100
O	1.5685000	0.1058900	0.0000100
H	0.6067400	-0.0339600	-0.0006300
H	1.9405200	-0.7800000	0.0002200

$(HCONH_2)_2$

0, 1

O	-1.1410900	1.4452100	0.0000000
C	-0.0617500	2.0309500	0.0000000
H	-0.0136900	3.1301700	0.0000000
N	1.1410900	1.4358800	0.0000000

H	1.2176900	0.4165300	0.0000000
H	1.9714500	2.0021000	0.0000000
O	1.1410900	-1.4452100	0.0000000
C	0.0617500	-2.0309500	0.0000000
H	0.0136900	-3.1301700	0.0000000
N	-1.1410900	-1.4358800	0.0000000
H	-1.2176900	-0.4165300	0.0000000
H	-1.9714500	-2.0021000	0.0000000

$HCONH_2$
0, 1

C	-0.1606800	0.3884000	-0.0005400
O	-1.1957100	-0.2463900	0.0001900
N	1.0833000	-0.1584200	-0.0002900
H	-0.1399200	1.4903500	0.0013900
H	1.1822600	-1.1604100	0.0011200
H	1.9043200	0.4197400	0.0012500

$(HCOOH)_2$
0, 1

C	-0.1202300	1.9140700	0.0000000
H	-0.1672900	3.0070200	0.0000000
O	-1.1218600	1.2209800	0.0000000
O	1.1218600	1.4804900	0.0000000
H	1.1275800	0.4890200	0.0000000
O	1.1218600	-1.2209800	0.0000000
C	0.1202300	-1.9140700	0.0000000
O	-1.1218600	-1.4804900	0.0000000
H	-1.1275800	-0.4890200	0.0000000
H	0.1672900	-3.0070200	0.0000000

HCOOH
0, 1

C	-0.1347000	0.4012500	-0.0002500
O	-1.1342600	-0.2645800	0.0000700
O	1.1186800	-0.0910800	0.0000600
H	-0.1076200	1.4954700	0.0005100
H	1.0404800	-1.0577100	-0.0000200

$C_2H_4\cdots F_2$
0, 1

C	0.0000000	-2.1928500	-0.6683900
C	0.0000000	-2.1928600	0.6683900
H	-0.9251900	-2.1923200	-1.2339800
H	0.9251900	-2.1923200	-1.2339800
H	-0.9251900	-2.1923200	1.2339800
H	0.9251900	-2.1923100	1.2339800
F	0.0000000	0.7856900	0.0000000

F	0.0000000	2.2056500	0.0000000

C_2H_4
0, 1

C	0.0000000	0.0000000	0.6680800
C	0.0000000	0.0000000	-0.6680800
H	0.0000000	0.9245300	1.2349200
H	0.0000000	-0.9245300	1.2349200
H	0.0000000	0.9245300	-1.2349200
H	0.0000000	-0.9245300	-1.2349200

F_2
0, 1

F	0.0000000	0.0000000	1.4142300
F	0.0000000	0.0000000	0.0000000

$NH_3\cdots F_2$
0, 1

N	0.0000000	0.0000000	-2.1499900
H	0.0000000	0.9396500	-2.5344000
H	0.8137600	-0.4698300	-2.5344000
H	-0.8137600	-0.4698300	-2.5344000
F	0.0000000	0.0000000	0.5457700
F	0.0000000	0.0000000	1.9712400

$C_2H_2\cdots ClF$
0, 1

H	0.0000000	1.6718900	-2.2125600
C	0.0000000	0.6052900	-2.1995600
C	0.0000000	-0.6052900	-2.1995600
H	0.0000000	-1.6718900	-2.2125600
Cl	0.0000000	0.0000000	0.6118800
F	0.0000000	0.0000000	2.2686500

C_2H_2
0, 1

C	0.0000000	-0.6042000	0.0000000
C	0.0000000	0.6042000	0.0000000
H	0.0067900	-1.6701300	0.0000000
H	-0.0068400	1.6701600	0.0000000

ClF
0, 1

F	0.0000000	0.0000000	-1.0740000
Cl	0.0000000	0.0000000	0.5685900

HCN-ClF
0, 1

F	0.0000000	0.0000000	2.4259200
Cl	0.0000000	0.0000000	0.7695700

N	0.0000000	0.0000000	-1.8395200
C	0.0000000	0.0000000	-2.9957300
H	0.0000000	0.0000000	-4.0650300

HCN
0, 1

C	0.0000000	0.0000000	-0.5010300
N	0.0000000	0.0000000	0.6570700
H	0.0000000	0.0000000	-1.5700500

$NH_3\cdots Cl_2$
0, 1

N	0.0000000	0.0000000	-2.8384500
H	0.0000000	0.9426900	-3.2153800
H	0.8163900	-0.4713400	-3.2153800
H	-0.8163900	-0.4713400	-3.2153800
Cl	0.0000000	0.0000000	-0.1500400
Cl	0.0000000	0.0000000	1.8862400

Cl_2
0, 1

Cl	0.0000000	0.0000000	1.0056600
Cl	0.0000000	0.0000000	-1.0056600

$H_2O\cdots ClF$
0, 1

O	2.2398200	0.0000300	-0.0882300
H	2.6008900	0.7619600	0.3770500
H	2.6010900	-0.7617300	0.3771900
Cl	-0.3158700	-0.0000700	-0.0169100
F	-1.9723100	0.0000700	0.0265700

$NH_3\cdots ClF$
0, 1

N	0.0000000	0.0000000	-2.0579000
H	0.0000000	0.9496100	-2.4144900
H	0.8223800	-0.4748000	-2.4144900
H	-0.8223800	-0.4748000	-2.4144900
Cl	0.0000000	0.0000000	0.2438500
F	0.0000000	0.0000000	1.9448000

$(H_2S)_2$
0, 1

S	-2.0310000	0.1032300	-0.0007800
H	-1.9340200	-0.8184600	0.9696800
H	-1.9404500	-0.8366200	-0.9543000
S	2.0798400	-0.0851100	0.0001800
H	2.3391500	1.2310200	-0.0022100
H	0.7538500	0.1341200	-0.0035400

H_2S
0, 1

S	0.0000000	0.0000000	0.1038900
H	0.0000000	0.9611600	-0.8311500
H	0.0000000	-0.9611600	-0.8311500

$(HCl)_2$
0, 1

Cl	1.8608200	-0.0654100	-0.0000700
H	1.7539400	1.2109800	0.0003400
Cl	-1.9252700	0.0055700	-0.0001000
H	-0.6584300	-0.1937000	0.0024800

HCl
0, 1

Cl	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.2790700

$HCl\cdots H_2S$
0, 1

S	1.8425300	0.0000100	-0.1015400
H	1.8227800	-0.9618100	0.8346500
H	1.8218800	0.9618600	0.8346200
Cl	-1.9116400	-0.0000100	0.0035000
H	-0.6273200	-0.0000600	-0.1040500

$CH_3Cl\cdots HCl$
0, 1

C	-1.4951300	1.1258000	0.0000000
Cl	-1.4024800	-0.6625400	0.0001400
H	-0.4810700	1.5183600	-0.0012200
H	-2.0271800	1.4351600	0.8953100
H	-2.0292400	1.4349200	-0.8941700
Cl	2.1396100	0.0373000	-0.0001400
H	0.9770000	-0.5140500	0.0000700

CH_3Cl
0, 1

C	0.0000000	0.0000000	-1.1262700
Cl	0.0000000	0.0000000	0.6582100
H	0.0000000	1.0309700	-1.4706000
H	0.8928500	-0.5154800	-1.4706000
H	-0.8928500	-0.5154800	-1.4706000

$HCN\cdots CH_3SH$
0, 1

C	1.9964400	0.0571800	-0.0064800
N	2.9802200	0.6583400	0.1094500
H	1.0723400	-0.4851900	-0.1064200

S	-1.5144000	-0.7999900	-0.1169800
C	-1.5701400	1.0129700	0.0116100
H	-1.5545800	-1.0526000	1.2004900
H	-1.5455600	1.3923800	-1.0102000
H	-0.7086600	1.4025500	0.5531000
H	-2.4931500	1.3399200	0.4866500

CH_3SH
0, 1

C	-0.0478800	1.1515100	0.0000000
S	-0.0478800	-0.6649600	0.0000000
H	1.2843400	-0.8210500	0.0000000
H	-1.0947100	1.4566200	0.0000000
H	0.4318900	1.5473700	0.8937100
H	0.4318900	1.5473700	-0.8937100

$CH_4\cdots Ne$
0, 1

Ne	0.0007100	-0.0350500	-1.7426000
C	-0.0007100	0.0350500	1.7425800
H	-0.0011600	0.0575200	2.8318600
H	-0.0212100	1.0543100	1.3583700
H	-0.8796100	-0.5037100	1.3901600
H	0.8991600	-0.4679200	1.3901600

CH_4
0, 1

C	0.0000000	0.0000000	0.0000000
H	0.0000000	0.0000000	1.0894700
H	1.0271600	0.0000000	-0.3631600
H	-0.5135800	0.8895500	-0.3631600
H	-0.5135800	-0.8895500	-0.3631600

$C_6H_6\cdots Ne$
0, 1

Ne	0.0000000	0.0000000	2.6001900
C	0.0000000	1.3956600	-0.6193500
C	-1.2086800	0.6978300	-0.6193500
C	-1.2086800	-0.6978300	-0.6193500
C	0.0000000	-1.3956600	-0.6193500
C	1.2086800	-0.6978300	-0.6193500
C	1.2086800	0.6978300	-0.6193500
H	0.0000000	2.4800400	-0.6175500
H	-2.1477800	1.2400200	-0.6175500
H	-2.1477800	-1.2400200	-0.6175500
H	0.0000000	-2.4800400	-0.6175500
H	2.1477800	-1.2400200	-0.6175500
H	2.1477800	1.2400200	-0.6175500

C_6H_6
0, 1

C	0.0000000	1.3956700	-0.6171600
C	-1.2086900	0.6978300	-0.6171600
C	-1.2086900	-0.6978300	-0.6171600
C	0.0000000	-1.3956700	-0.6171600
C	1.2086900	-0.6978300	-0.6171600
C	1.2086900	0.6978300	-0.6171600
H	0.0000000	2.4798800	-0.6170000
H	-2.1476400	1.2399400	-0.6170000
H	-2.1476400	-1.2399400	-0.6170000
H	0.0000000	-2.4798800	-0.6170000
H	2.1476400	-1.2399400	-0.6170000
H	2.1476400	1.2399400	-0.6170000

$(CH_4)_2$
0, 1

C	0.0000000	0.0000000	1.8072800
H	0.0000000	1.0266400	1.4424000
H	-0.8891000	-0.5133200	1.4424000
H	0.0000000	0.0000000	2.8968400
H	0.8891000	-0.5133200	1.4424000
C	0.0000000	0.0000000	-1.8072800
H	0.8891000	0.5133200	-1.4424000
H	0.0000000	0.0000000	-2.8968400
H	-0.8891000	0.5133200	-1.4424000
H	0.0000000	-1.0266400	-1.4424000

$(C_2H_2)_2$
0, 1

C	-0.4125500	1.6781700	0.0000000
C	0.4125500	2.5616300	0.0000000
H	-1.1320300	0.8908100	0.0000000
H	1.1346500	3.3457700	0.0000000
C	0.4125500	-1.6781700	0.0000000
C	-0.4125500	-2.5616300	0.0000000
H	1.1320300	-0.8908100	0.0000000
H	-1.1346500	-3.3457700	0.0000000

C_2H_2
0, 1

C	0.0000000	-0.6042000	0.0000000
C	0.0000000	0.6042000	0.0000000
H	0.0067900	-1.6701300	0.0000000
H	-0.0068400	1.6701600	0.0000000

$(C_2H_4)_2$
0, 1

C	1.8577700	0.4728000	0.4724200
C	1.8577700	-0.4728000	-0.4724200
H	0.9337700	0.8746900	0.8740600
H	2.7838200	0.8717100	0.8715600
H	2.7838200	-0.8717100	-0.8715600
H	0.9337700	-0.8746900	-0.8740600
C	-1.8577700	0.4728000	-0.4724200
C	-1.8577700	-0.4728000	0.4724200
H	-2.7838200	0.8717100	-0.8715600
H	-0.9337700	0.8746900	-0.8740600
H	-0.9337700	-0.8746900	0.8740600
H	-2.7838200	-0.8717100	0.8715600

sandwich $(C_6H_6)_2$
0, 1

C	0.0000000	1.9500000	1.3915000
H	0.0000000	1.9500000	2.4715000
C	1.2050700	1.9500000	0.6957500
H	2.1403800	1.9500000	1.2357500
C	1.2050700	1.9500000	-0.6957500
H	2.1403800	1.9500000	-1.2357500
C	0.0000000	1.9500000	-1.3915000
H	0.0000000	1.9500000	-2.4715000
C	-1.2050700	1.9500000	-0.6957500
H	-2.1403800	1.9500000	-1.2357500
C	-1.2050700	1.9500000	0.6957500
H	-2.1403800	1.9500000	1.2357500
C	-1.2050700	-1.9500000	-0.6957500
H	-2.1403800	-1.9500000	-1.2357500
C	0.0000000	-1.9500000	-1.3915000
H	0.0000000	-1.9500000	-2.4715000
C	1.2050700	-1.9500000	-0.6957500
H	2.1403800	-1.9500000	-1.2357500
C	1.2050700	-1.9500000	0.6957500
H	2.1403800	-1.9500000	1.2357500
C	0.0000000	-1.9500000	1.3915000
H	0.0000000	-1.9500000	2.4715000
C	-1.2050700	-1.9500000	0.6957500
H	-2.1403800	-1.9500000	1.2357500

T-shaped $(C_6H_6)_2$
0, 1

C	1.3915000	0.0000000	2.4957500
H	2.4715000	0.0000000	2.4957500
C	0.6957500	1.2050700	2.4957500
H	1.2357500	2.1403800	2.4957500
C	0.6957500	-1.2050700	2.4957500

H	1.2357500	-2.1403800	2.4957500
C	-0.6957500	1.2050700	2.4957500
H	-1.2357500	2.1403800	2.4957500
C	-0.6957500	-1.2050700	2.4957500
H	-1.2357500	-2.1403800	2.4957500
C	-1.3915000	0.0000000	2.4957500
H	-2.4715000	0.0000000	2.4957500
C	0.0000000	0.0000000	-1.1042500
C	0.0000000	-1.2050700	-1.8000000
H	0.0000000	-2.1403800	-1.2600000
H	0.0000000	0.0000000	-0.0242500
C	0.0000000	-1.2050700	-3.1915000
H	0.0000000	-2.1403800	-3.7315000
C	0.0000000	0.0000000	-3.8872500
H	0.0000000	0.0000000	-4.9672500
C	0.0000000	1.2050700	-3.1915000
H	0.0000000	2.1403800	-3.7315000
C	0.0000000	1.2050700	-1.8000000
H	0.0000000	2.1403800	-1.2600000

parallel-displaced $(C_6H_6)_2$
0, 1

C	-0.8000000	1.8000000	1.3915000
H	-0.8000000	1.8000000	2.4715000
C	0.4050700	1.8000000	0.6957500
H	1.3403800	1.8000000	1.2357500
C	-2.0050700	1.8000000	0.6957500
H	-2.9403800	1.8000000	1.2357500
C	0.4050700	1.8000000	-0.6957500
H	1.3403800	1.8000000	-1.2357500
C	-2.0050700	1.8000000	-0.6957500
H	-2.9403800	1.8000000	-1.2357500
C	-0.8000000	1.8000000	-1.3915000
H	-0.8000000	1.8000000	-2.4715000
C	0.8000000	-1.8000000	-1.3915000
C	2.0050700	-1.8000000	-0.6957500
H	2.9403800	-1.8000000	-1.2357500
H	0.8000000	-1.8000000	-2.4715000
C	2.0050700	-1.8000000	0.6957500
H	2.9403800	-1.8000000	1.2357500
C	0.8000000	-1.8000000	1.3915000
H	0.8000000	-1.8000000	2.4715000
C	-0.4050700	-1.8000000	0.6957500
H	-1.3403800	-1.8000000	1.2357500
C	-0.4050700	-1.8000000	-0.6957500
H	-1.3403800	-1.8000000	-1.2357500

NGDWI21

He_2
0, 1
He 0.0000000 0.0000000 0.0000000
He 0.0000000 0.0000000 2.9740000

Ne_2
0, 1
Ne 0.0000000 0.0000000 0.0000000
Ne 0.0000000 0.0000000 3.0910000

Ar_2
0, 1
Ar 0.0000000 0.0000000 0.0000000
Ar 0.0000000 0.0000000 3.7570000

Kr_2
0, 1
Kr 0.0000000 0.0000000 0.0000000
Kr 0.0000000 0.0000000 4.0110000

HeNe
0, 1
He 0.0000000 0.0000000 0.0000000
Ne 0.0000000 0.0000000 3.0310000

HeAr
0, 1
He 0.0000000 0.0000000 0.0000000
Ar 0.0000000 0.0000000 3.4800000

NeAr
0, 1
Ne 0.0000000 0.0000000 0.0000000
Ar 0.0000000 0.0000000 3.4890000

HeHe_L_0.3A
0, 1
He 0.0000000 0.0000000 0.0000000
He 0.0000000 0.0000000 2.6740000

HeHe_R_0.3A
0, 1
He 0.0000000 0.0000000 0.0000000
He 0.0000000 0.0000000 3.2740000

NeNe_L_0.3A
0, 1
Ne 0.0000000 0.0000000 0.0000000
Ne 0.0000000 0.0000000 2.7910000

NeNe_R_0.3A
0, 1
Ne 0.0000000 0.0000000 0.0000000
Ne 0.0000000 0.0000000 3.3910000

ArAr_L_0.3A
0, 1
Ar 0.0000000 0.0000000 0.0000000
Ar 0.0000000 0.0000000 3.4570000

ArAr_R_0.3A
0, 1
Ar 0.0000000 0.0000000 0.0000000
Ar 0.0000000 0.0000000 4.0570000

KrKr_L_0.3A
0, 1
Kr 0.0000000 0.0000000 0.0000000
Kr 0.0000000 0.0000000 3.7110000

KrKr_R_0.3A
0, 1
Kr 0.0000000 0.0000000 0.0000000
Kr 0.0000000 0.0000000 4.3110000

HeNe_L_0.3A
0, 1
He 0.0000000 0.0000000 0.0000000
Ne 0.0000000 0.0000000 2.7310000

HeNe_R_0.3A
0, 1
He 0.0000000 0.0000000 0.0000000
Ne 0.0000000 0.0000000 3.3310000

HeAr_L_0.3A
0, 1
He 0.0000000 0.0000000 0.0000000
Ar 0.0000000 0.0000000 3.1800000

HeAr_R_0.3A
0, 1
He 0.0000000 0.0000000 0.0000000
Ar 0.0000000 0.0000000 3.7800000

NeAr_L_0.3A
0, 1
Ne 0.0000000 0.0000000 0.0000000
Ar 0.0000000 0.0000000 3.1890000

NeAr_R_0.3A
0, 1
Ne 0.0000000 0.0000000 0.0000000
Ar 0.0000000 0.0000000 3.7890000

HC7/11
22
0, 1
C -0.2167300 1.3921000 0.4447800
C 0.3372000 -0.0023100 0.7598000
C -1.6101200 1.4687100 -0.1196700
C -2.5817900 0.5184600 -0.1900100
C -0.0932300 -1.0261000 -0.3235400
C -2.5160700 -0.9122500 0.1153100
C -1.3929400 -1.6663700 0.0314000
C 0.8693400 1.9551600 -0.4583100
C 1.8768700 0.0798000 0.5974700
H -1.9044500 2.4719300 -0.4354700
C 1.1348800 -1.8833700 -0.4918000
H -3.5554200 0.8673200 -0.5362100
H -3.4601900 -1.3991400 0.3545300
H -1.4333900 -2.7332600 0.2483400
H 0.7278700 2.8377000 -1.0784500
H 1.1349100 -2.8361700 -1.0161800
C 2.0172400 1.2561900 -0.3520400

C	2.2301600	-1.2618200	-0.0111600
H	2.9413500	1.4951300	-0.8727100
H	3.2464600	-1.6418600	-0.0781700
H	0.0386700	-0.3738800	1.7455700
H	-0.2259600	1.9914500	1.3727900
H	2.4090900	0.2657100	1.5410000
H	-0.2477600	-0.4540400	-1.2584700

1
0, 1

C	0.0000000	0.8784500	1.7965200
C	-0.7607600	-0.4392200	1.7965200
H	-1.3320600	-0.7690500	2.6584500
C	0.7607600	-0.4392200	1.7965200
C	-1.1998100	-0.6927100	0.3538900
H	0.0000100	1.5381200	2.6584500
C	1.1998100	-0.6927100	0.3538900
H	1.3320500	-0.7690700	2.6584500
H	0.0000000	2.4746500	0.2476400
C	-0.7607600	0.4392200	-1.7965200
H	-2.1431100	-1.2373300	0.2476400
C	1.1998100	0.6927100	-0.3538900
C	0.0000000	-1.3854200	-0.3538900
C	0.7607600	0.4392200	-1.7965200
H	2.1431100	-1.2373300	0.2476400
C	0.0000000	1.3854200	0.3538900
C	-1.1998100	0.6927100	-0.3538900
C	0.0000000	-0.8784500	-1.7965200
H	-2.1431100	1.2373300	-0.2476400
H	0.0000000	-2.4746500	-0.2476400
H	2.1431100	1.2373300	-0.2476400
H	-0.0000100	-1.5381200	-2.6584500
H	-1.3320500	0.7690700	-2.6584500
H	1.3320600	0.7690500	-2.6584500

31
0, 1

C	0.9946100	-0.0847100	0.0000000
C	1.0635400	-0.9851100	1.2024000
C	1.0635400	-0.9851100	-1.2024000
C	0.0925000	-1.8911100	-1.5216500
C	0.0925000	-1.8911100	1.5216500
C	-1.0108100	-2.2876000	-0.6884300
C	-1.0108100	-2.2876000	0.6884300
H	1.8699600	0.5747800	0.0000000
H	1.9155400	-0.8784500	1.8733200
H	1.9155400	-0.8784500	-1.8733200

H	0.1707800	-2.3893100	2.4877600
H	0.1707800	-2.3893100	-2.4877600
H	-1.8575700	-2.7614700	-1.1832100
H	-1.8575700	-2.7614700	1.1832100
C	-0.2510000	0.8397900	0.0000000
C	-0.2682000	3.0571100	0.7335000
C	-0.2682000	3.0571100	-0.7335000
C	-0.2586100	1.7706700	1.1781100
C	-0.2586100	1.7706700	-1.1781100
H	-0.2710700	3.9474100	1.3543600
H	-0.2710700	3.9474100	-1.3543600
H	-0.2567900	1.4391100	2.2108000
H	-0.2567900	1.4391100	-2.2108000
H	-1.1544700	0.2125100	0.0000000

octane-a
0, 1

C	0.0000000	0.0000000	0.7849100
C	0.0000000	0.0000000	-0.7849100
C	-0.8668700	1.1412000	1.3419100
C	1.4217500	0.1801300	1.3419100
C	-0.5548700	-1.3213300	1.3419100
C	0.8668700	1.1412000	-1.3419100
C	-1.4217500	0.1801300	-1.3419100
C	0.5548700	-1.3213300	-1.3419100
H	-0.5963400	2.1109100	0.9109100
H	-1.9314600	0.9668300	1.1578600
H	-0.7248400	1.2096000	2.4268700
H	1.8030300	1.1892800	1.1578600
H	1.4099700	0.0229300	2.4268700
H	2.1262700	-0.5390100	0.9109100
H	-1.5299300	-1.5719000	0.9109100
H	0.1284300	-2.1561000	1.1578600
H	-0.6851300	-1.2325300	2.4268700
H	0.5963400	2.1109100	-0.9109100
H	1.9314600	0.9668300	-1.1578600
H	0.7248400	1.2096000	-2.4268700
H	-1.8030300	1.1892800	-1.1578600
H	-1.4099700	0.0229300	-2.4268700
H	-2.1262700	-0.5390100	-0.9109100
H	1.5299300	-1.5719000	-0.9109100
H	-0.1284300	-2.1561000	-1.1578600
H	0.6851300	-1.2325300	-2.4268700

octane-b
0, 1

C	-0.1614600	4.4786700	0.0000000

C	-0.8406200	3.1086600	0.0000000
C	0.1614600	1.9538000	0.0000000
C	-0.5020900	0.5765400	0.0000000
C	0.5020900	-0.5765400	0.0000000
C	-0.1614600	-1.9538000	0.0000000
C	0.8406200	-3.1086600	0.0000000
C	0.1614600	-4.4786700	0.0000000
H	-0.8949200	5.2907700	0.0000000
H	0.4727800	4.5960200	0.8848800
H	0.4727800	4.5960200	-0.8848800
H	-1.4900900	3.0181000	-0.8799500
H	-1.4900900	3.0181000	0.8799500
H	0.8128500	2.0408900	-0.8807500
H	0.8128500	2.0408900	0.8807500
H	-1.1529600	0.4886800	-0.8809200
H	-1.1529600	0.4886800	0.8809200
H	1.1529600	-0.4886800	-0.8809200
H	1.1529600	-0.4886800	0.8809200
H	-0.8128500	-2.0408900	-0.8807500
H	-0.8128500	-2.0408900	0.8807500
H	1.4900900	-3.0181000	-0.8799500
H	1.4900900	-3.0181000	0.8799500
H	-0.4727800	-4.5960200	-0.8848800
H	0.8949200	-5.2907700	0.0000000
H	-0.4727800	-4.5960200	0.8848800

methane
0, 1

C	0.0000000	0.0000000	0.0000000
H	0.6294000	0.6294000	0.6294000
H	-0.6294000	-0.6294000	0.6294000
H	-0.6294000	0.6294000	-0.6294000
H	0.6294000	-0.6294000	-0.6294000

ethane
0, 1

C	0.0000000	0.0000000	0.7644500
C	0.0000000	0.0000000	-0.7644500
H	0.0000000	1.0197100	1.1590300
H	-0.8830900	-0.5098500	1.1590300
H	0.8830900	-0.5098500	1.1590300
H	0.0000000	-1.0197100	-1.1590300
H	-0.8830900	0.5098500	-1.1590300
H	0.8830900	0.5098500	-1.1590300

hexane
0, 1

C	1.4178600	2.8843800	0.0000000

C	-1.4178600	-2.8843800	0.0000000
C	0.0080600	0.7641400	0.0000000
C	-0.0080600	-0.7641400	0.0000000
C	-1.4178600	-1.3553700	0.0000000
C	1.4178600	1.3553700	0.0000000
H	-2.4357200	-3.2861500	0.0000000
H	2.4357200	3.2861500	0.0000000
H	0.9018100	3.2713400	0.8847500
H	0.9018100	3.2713400	-0.8847500
H	-0.9018100	-3.2713400	-0.8847500
H	-0.9018100	-3.2713400	0.8847500
H	1.9599000	0.9862400	-0.8798300
H	1.9599000	0.9862400	0.8798300
H	-1.9599000	-0.9862400	-0.8798300
H	-1.9599000	-0.9862400	0.8798300
H	-0.5370300	1.1311500	0.8806500
H	-0.5370300	1.1311500	-0.8806500
H	0.5370300	-1.1311500	-0.8806500
H	0.5370300	-1.1311500	0.8806500

ethylene
0, 1

C	0.0000000	0.0000000	-0.0093200
C	0.0000000	0.0000000	1.3297800
H	0.9263100	0.0000000	-0.5749100
H	-0.9263100	0.0000000	-0.5749100
H	0.9263100	0.0000000	1.8953700
H	-0.9263100	0.0000000	1.8953700

ethyne
0, 1

C	0.0000000	0.0000000	0.6081100
C	0.0000000	0.0000000	-0.6081100
H	0.0000000	0.0000000	-1.6731000
H	0.0000000	0.0000000	1.6731000

adamantane
0, 1

C	0.8883000	0.8883000	0.8883000
C	-0.8883000	-0.8883000	0.8883000
C	-0.8883000	0.8883000	-0.8883000
C	0.8883000	-0.8883000	-0.8883000
C	0.0000000	0.0000000	1.7730000
C	0.0000000	0.0000000	-1.7730000
C	0.0000000	1.7730000	0.0000000
C	0.0000000	-1.7730000	0.0000000
C	1.7730000	0.0000000	0.0000000
C	-1.7730000	0.0000000	0.0000000

H	1.5222000	1.5222000	1.5222000
H	-1.5222000	-1.5222000	1.5222000
H	-1.5222000	1.5222000	-1.5222000
H	1.5222000	-1.5222000	-1.5222000
H	2.4231000	-0.6263000	0.6263000
H	2.4231000	0.6263000	-0.6263000
H	-2.4231000	-0.6263000	-0.6263000
H	-2.4231000	0.6263000	0.6263000
H	-0.6263000	2.4231000	0.6263000
H	0.6263000	2.4231000	-0.6263000
H	0.6263000	-2.4231000	0.6263000
H	-0.6263000	-2.4231000	-0.6263000
H	-0.6263000	0.6263000	2.4231000
H	0.6263000	-0.6263000	2.4231000
H	0.6263000	0.6263000	-2.4231000
H	-0.6263000	-0.6263000	-2.4231000

bicycoct
0, 1

C	0.0000000	0.0000000	1.2955700
C	0.1332400	1.4353800	0.7641300
C	-0.1332400	1.4353800	-0.7641300
C	0.0000000	0.0000000	-1.2955700
C	1.1764600	-0.8330800	0.7641300
C	1.3097000	-0.6023000	-0.7641300
C	-1.3097000	-0.6023000	0.7641300
C	-1.1764600	-0.8330800	-0.7641300
H	0.0000000	0.0000000	2.3919200
H	-0.5697600	2.0999400	1.2795200
H	1.1431500	1.8070900	0.9786900
H	0.5697600	2.0999400	-1.2795200
H	-1.1431500	1.8070900	-0.9786900
H	0.0000000	0.0000000	-2.3919200
H	0.9934100	-1.8935400	0.9786900
H	2.1034800	-0.5565500	1.2795200
H	2.1365600	0.0864500	-0.9786900
H	1.5337300	-1.5434000	-1.2795200
H	-2.1365600	0.0864500	0.9786900
H	-1.5337300	-1.5434000	1.2795200
H	-0.9934100	-1.8935400	-0.9786900
H	-2.1034800	-0.5565500	-1.2795200

3dAEE7	Ground State	Excited State
Sc	0, 4	0, 2
Mn^+	1, 7	1, 5
Fe	0, 5	0, 3
Ni^+	1, 2	1, 4
Zn	0, 1	0, 3
Ca^+	1, 2 4s	1, 2 3d
V	0, 4	0, 6

4dAEE5	Ground State	Excited State
Mo^+	1, 6	1, 4
Ru^+	1, 4	1, 6
Rh^+	1, 3	1, 1
Pd	0, 1	0, 3
Y^+	1, 1	1, 3

pEE5	Ground State	Excited State
F	0, 2	0, 4
Ar	0, 1	0, 3
C^+	0, 2	0, 4
Al	0, 2	0, 4
Si^+	1, 2	1, 4

DC9/12			
$HCN\cdots BF_3 \rightarrow HCN + BF_3$			
$HCN\cdots BF_3$			
0, 1			
B	0.0000000	0.0000000	-0.8945200
F	0.0000000	1.3221800	-0.9740700
F	-1.1450400	-0.6610900	-0.9740700
F	1.1450400	-0.6610900	-0.9740700
N	0.0000000	0.0000000	1.5374400
C	0.0000000	0.0000000	2.7060100
H	0.0000000	0.0000000	3.7743100
HCN			
0, 1			
C	0.0000000	0.0000000	-0.5093900
N	0.0000000	0.0000000	0.6619500
H	0.0000000	0.0000000	-1.5773100
BF_3			
0, 1			
B	0.0000000	0.0000000	0.0000000

F	0.0000000	1.3183400	0.0000000
F	1.1417200	-0.6591700	0.0000000
F	-1.1417200	-0.6591700	0.0000000

$C_6Cl_6 + 6HCl \rightarrow 6Cl_2 + C_6H_6$

C_6Cl_6
0, 1

C	0.0000000	1.4068700	0.0000000
C	1.2183900	0.7034400	0.0000000
C	1.2183900	-0.7034400	0.0000000
C	0.0000000	-1.4068700	0.0000000
C	-1.2183900	-0.7034400	0.0000000
C	-1.2183900	0.7034400	0.0000000
Cl	2.7054600	1.5620000	0.0000000
Cl	2.7054600	-1.5620000	0.0000000
Cl	0.0000000	-3.1239900	0.0000000
Cl	-2.7054600	-1.5620000	0.0000000
Cl	-2.7054600	1.5620000	0.0000000
Cl	0.0000000	3.1239900	0.0000000

HCl
0, 1

Cl	0.0000000	0.0000000	0.0707200
H	0.0000000	0.0000000	-1.2023300

Cl_2
0, 1

Cl	0.0000000	0.0000000	1.0122600
Cl	0.0000000	0.0000000	-1.0122600

C_6H_6
0, 1

C	0.0000000	1.3987000	0.0000000
C	1.2113000	0.6994000	0.0000000
C	1.2113000	-0.6994000	0.0000000
C	0.0000000	-1.3987000	0.0000000
C	-1.2113000	-0.6994000	0.0000000
C	-1.2113000	0.6994000	0.0000000
H	0.0000000	2.4820000	0.0000000
H	2.1494000	1.2410000	0.0000000
H	2.1494000	-1.2410000	0.0000000
H	0.0000000	-2.4820000	0.0000000
H	-2.1494000	-1.2410000	0.0000000
H	-2.1494000	1.2410000	0.0000000

$P_4 \rightarrow 4P$

P_4			
0, 1			
P	-0.7805400	0.7805400	-0.7805400
P	0.7805400	-0.7805400	-0.7805400
P	0.7805400	0.7805400	0.7805400
P	-0.7805400	-0.7805400	0.7805400

$SF_6 \rightarrow S + 6F$			
SF_6			
0, 1			
S	0.0000000	0.0000000	0.0000000
F	0.0000000	0.0000000	1.5898900
F	0.0000000	1.5898900	0.0000000
F	0.0000000	0.0000000	-1.5898900
F	-1.5898900	0.0000000	0.0000000
F	1.5898900	0.0000000	0.0000000
F	0.0000000	-1.5898900	0.0000000

$PF_5 \rightarrow P + 5F$			
PF_5			
0, 1			
P	0.0000000	0.0000000	0.0000000
F	0.0000000	1.5608600	0.0000000
F	1.3517500	-0.7804300	0.0000000
F	-1.3517500	-0.7804300	0.0000000
F	0.0000000	0.0000000	1.5970500
F	0.0000000	0.0000000	-1.5970500

$P_4O_{10} \rightarrow P_4 + 5O_2$			
P_4O_{10}			
0, 1			
P	1.0197600	-1.0197600	1.0197600
O	0.0000000	0.0000000	1.7770100
P	-1.0197600	1.0197600	1.0197600
O	0.0000000	1.7770100	0.0000000
P	1.0197600	1.0197600	-1.0197600
O	1.7770100	0.0000000	0.0000000
O	-1.7770100	0.0000000	0.0000000
P	-1.0197600	-1.0197600	-1.0197600
O	0.0000000	0.0000000	-1.7770100
O	0.0000000	-1.7770100	0.0000000
O	-1.8564400	-1.8564400	-1.8564400
O	1.8564400	-1.8564400	1.8564400
O	-1.8564400	1.8564400	1.8564400
O	1.8564400	1.8564400	-1.8564400

O_2
0, 3

O	0.0000000	0.0000000	0.6118300
O	0.0000000	0.0000000	-0.6118300

$C_6F_6 \rightarrow 6C + 6F$

C_6F_6
0, 1

C	0.0000000	1.3949100	0.0000000
C	1.2080300	0.6974600	0.0000000
C	1.2080300	-0.6974600	0.0000000
C	0.0000000	-1.3949100	0.0000000
C	-1.2080300	-0.6974600	0.0000000
C	-1.2080300	0.6974600	0.0000000
F	2.3604400	1.3628000	0.0000000
F	2.3604400	-1.3628000	0.0000000
F	0.0000000	-2.7256000	0.0000000
F	-2.3604400	-1.3628000	0.0000000
F	-2.3604400	1.3628000	0.0000000
F	0.0000000	2.7256000	0.0000000

$Si(OCH_3)_4 \rightarrow Si + 4C + 4O + 12H$

$Si(OCH_3)_4$
0, 1

Si	0.0000000	0.0000000	0.0000000
O	0.0000000	1.3838100	0.8829800
O	-1.3838100	0.0000000	-0.8829800
O	0.0000000	-1.3838100	0.8829800
O	1.3838100	0.0000000	-0.8829800
C	-1.1313800	1.8377700	1.6222500
C	-1.8377700	-1.1313800	-1.6222500
C	1.1313800	-1.8377700	1.6222500
C	1.8377700	1.1313800	-1.6222500
H	-0.8746000	2.8067500	2.0528900
H	-2.0029400	1.9493300	0.9707200
H	-1.3749400	1.1420200	2.4323500
H	-2.8067500	-0.8746000	-2.0528900
H	-1.1420200	-1.3749400	-2.4323500
H	-1.9493300	-2.0029400	-0.9707200
H	0.8746000	-2.8067500	2.0528900
H	2.0029400	-1.9493300	0.9707200
H	1.3749400	-1.1420200	2.4323500
H	2.8067500	0.8746000	-2.0528900
H	1.1420200	1.3749400	-2.4323500
H	1.9493300	2.0029400	-0.9707200

urotropin → 6C + 4N + 12H			
urotropin			
0, 1			
N	-0.8672500	-0.8672500	-0.8672500
C	0.0000000	0.0000000	-1.6802700
N	0.8672500	0.8672500	-0.8672500
C	0.0000000	1.6802700	0.0000000
N	-0.8672500	0.8672500	0.8672500
C	-1.6802700	0.0000000	0.0000000
C	0.0000000	-1.6802700	0.0000000
C	1.6802700	0.0000000	0.0000000
C	0.0000000	0.0000000	1.6802700
N	0.8672500	-0.8672500	0.8672500
H	0.6305700	-0.6305700	-2.3170700
H	-0.6305700	0.6305700	-2.3170700
H	0.6305700	2.3170700	0.6305700
H	-0.6305700	2.3170700	-0.6305700
H	-2.3170700	0.6305700	-0.6305700
H	-2.3170700	-0.6305700	0.6305700
H	0.6305700	-2.3170700	-0.6305700
H	-0.6305700	-2.3170700	0.6305700
H	2.3170700	-0.6305700	-0.6305700
H	2.3170700	0.6305700	0.6305700
H	-0.6305700	-0.6305700	2.3170700
H	0.6305700	0.6305700	2.3170700

2pIsoE4			
C isomer 1			
0, 1			
C	0.8814440	0.8814440	0.8814440
H	0.2748330	1.5244710	1.5244710
H	1.5244710	0.2748330	1.5244710
H	1.5244710	1.5244710	0.2748330
C	-0.8814440	-0.8814440	0.8814440
H	-1.5244710	-0.2748330	1.5244710
H	-1.5244710	-1.5244710	0.2748330
H	-0.2748330	-1.5244710	1.5244710
C	0.8814440	-0.8814440	-0.8814440
H	0.2748330	-1.5244710	-1.5244710
H	1.5244710	-0.2748330	-1.5244710
H	1.5244710	-1.5244710	-0.2748330
C	-0.8814440	0.8814440	-0.8814440
H	-0.2748330	1.5244710	-1.5244710
H	-1.5244710	0.2748330	-1.5244710
H	-1.5244710	1.5244710	-0.2748330
C	0.0000000	0.0000000	0.0000000
C isomer 2			
0, 1			
C	-2.5347970	-0.3233130	-0.0000750
C	-1.2718400	0.5212990	0.0001220
H	-3.4346680	0.2949300	-0.0011990
H	-2.5746110	-0.9697140	-0.8806780
H	-2.5758640	-0.9683280	0.8814800
C	-0.0000610	-0.3113780	0.0000420
H	-1.2694200	1.1812980	-0.8743930
H	-1.2695020	1.1809150	0.8749290
C	1.2718570	0.5212550	-0.0001220
H	-0.0000730	-0.9728020	0.8751810
H	-0.0002640	-0.9728850	-0.8750320
H	1.2693680	1.1809840	-0.8748480
H	1.2693840	1.1813260	0.8743460
C	2.5348710	-0.3232740	0.0000320
H	2.5753550	-0.9693640	-0.8811750
H	3.4347120	0.2950700	-0.0001300
H	2.5754020	-0.9689680	0.8815230

N isomer 1
0, 1

C	1.1643200	-1.1946710	0.0034020
C	-0.2201670	-1.2001830	-0.0049420
C	-0.9344020	-0.0001110	-0.0086530
C	-0.2201200	1.2001960	-0.0049480
C	1.1641540	1.1947710	0.0034090
C	1.8704490	-0.0000260	0.0076640
H	1.6966260	-2.1388940	0.0074990
H	-0.7591750	-2.1417840	-0.0128110
H	-0.7594450	2.1416130	-0.0131950
H	1.6966690	2.1388760	0.0077400
H	2.9529460	0.0001660	0.0149150
H	-2.7673020	-0.8347840	0.2655590
H	-2.7671540	0.8347660	0.2659250
N	-2.3197960	0.0000270	-0.0730320

N isomer 2
0, 1

C	-1.1086170	0.7518350	0.6622030
C	0.2538470	0.1821170	1.0771000
C	0.2538470	0.1821170	-1.0771000
C	-1.1086170	0.7518350	-0.6622030
H	-1.8944760	1.0360010	1.3455810
H	-1.8944760	1.0360010	-1.3455810
C	0.2538470	-1.3055870	0.6635420
H	0.1775950	-2.1446220	1.3401070
C	0.2538470	-1.3055870	-0.6635420
H	0.1775950	-2.1446220	-1.3401070
H	0.5906060	0.4119760	2.0852970
H	0.5906060	0.4119760	-2.0852970
H	1.9796300	0.3343420	0.0000000
N	1.0691420	0.7883670	0.0000000

O isomer 1
0, 1

C	1.1228560	0.4660910	0.1556750
C	-1.1208000	0.4688070	0.1590000
C	-0.7723860	-1.0068490	-0.0523610
C	0.7689970	-1.0099100	-0.0479560
H	1.9928640	0.7958470	-0.4124690
H	1.3031980	0.6770990	1.2203450
H	-1.2947860	0.6762500	1.2255010
H	-1.9926390	0.8036420	-0.4033340
H	-1.1977310	-1.6390890	0.7276010
H	-1.1568330	-1.3595170	-1.0096840
H	1.1867110	-1.6378140	0.7396040
H	1.1578740	-1.3721080	-0.9998800
O	0.0011670	1.1933570	-0.2967290

O isomer 2
0, 1

C	1.5564450	0.0072220	-0.0149120
C	0.4495970	1.0769970	-0.1042910
C	-0.5391330	-0.0002920	0.3812740
C	0.4530940	-1.0686070	-0.0775670
H	2.3154780	-0.0012320	-0.7958720
H	2.0548970	0.0201420	0.9556360
H	0.2287160	1.3293700	-1.1433430
H	0.5543270	1.9929710	0.4788930
H	-0.6119940	0.0115690	1.4769130
H	0.2305030	-1.3447990	-1.1100680
H	0.5564250	-1.9719810	0.5233090
H	-2.3731770	0.5909260	0.1632250
O	-1.8093990	-0.0898610	-0.2069650

F isomer 1
0, 1

C	0.3713630	0.2464360	0.0000000
C	-1.1319490	0.2578520	0.0000000
H	-1.4404780	0.8247680	-0.8802270
H	-1.4404780	0.8247680	0.8802270
C	-1.7303620	-1.1371490	0.0000000
H	-1.4213700	-1.6968280	-0.8832920
H	-1.4213700	-1.6968280	0.8832920
H	-2.8188080	-1.0796950	0.0000000
F	0.8699330	-0.3779630	-1.0784030
F	0.8699330	1.4915900	0.0000000
F	0.8699330	-0.3779630	1.0784030

F isomer 2
0,1

C	-0.2741240	0.6174750	1.2486760
C	-0.0749060	-0.2024820	0.0000000
H	0.5366340	1.3434040	1.3596040
H	-1.2332120	1.1427920	1.2103110
C	-0.2741240	0.6174750	-1.2486760
H	-0.7709470	-1.0480990	0.0000000
H	-1.2332120	1.1427920	-1.2103110
H	0.5366340	1.3434040	-1.3596040
F	1.2041390	-0.7221480	0.0000000
F	-0.2741240	-0.2010980	-2.3535770
F	-0.2741240	-0.2010980	2.3535770

4pIsoE4

As isomer 1
0, 1

C	-2.2234030	1.1951000	0.0029320
C	-0.8365430	1.2104430	-0.0000780
C	-0.1179830	0.0174320	-0.0027290
C	-0.8128030	-1.1886830	-0.0099370
C	-2.2009650	-1.2044450	0.0023930
C	-2.9083740	-0.0122200	0.0076030
H	-2.7712220	2.1302660	0.0032780
H	-0.3122750	2.1589870	0.0018980
H	-0.2685690	-2.1269480	-0.0286920
H	-2.7289590	-2.1507930	0.0007860
H	-3.9917820	-0.0223720	0.0111520
As	1.8366410	-0.0551020	-0.0279900
H	2.0317630	0.3435680	1.4312930
H	2.0323330	1.3799120	-0.4971350

As isomer 2
0, 1

C	1.5777640	-0.4687930	0.6664430
C	0.3687710	0.2691700	1.2153390
C	0.3687710	0.2691700	-1.2153390
C	1.5777640	-0.4687930	-0.6664430
H	2.3337610	-0.9096860	1.3020780
H	2.3337610	-0.9096860	-1.3020780
C	0.3687710	1.6790510	0.6645770
H	0.4129830	2.5518670	1.3023110
C	0.3687710	1.6790510	-0.6645770
H	0.4129830	2.5518670	-1.3023110
H	0.2041640	0.1695680	2.2842240
H	0.2041640	0.1695680	-2.2842240
As	-0.9584790	-0.6604360	0.0000000
H	-2.0556700	0.4177480	0.0000000

Br isomer 1
0, 1

C	0.0388090	0.3025440	0.0000000
C	0.6039320	1.7125140	0.0000000
H	0.1878090	2.2107550	0.8792760
H	0.1878090	2.2107550	-0.8792760
C	2.1173570	1.8122710	0.0000000
H	2.5476410	1.3418800	0.8842040
H	2.5476410	1.3418800	-0.8842040
H	2.4069750	2.8639050	0.0000000
Br	0.6039320	-0.6744830	-1.5859990
Br	0.6039320	-0.6744830	1.5859990
Br	-1.9061060	0.4080200	0.0000000

Br isomer 2
0, 1

C	-0.5833050	1.0035800	1.2339360
C	-0.3112130	0.1693880	0.0000000
H	0.1575890	1.7908290	1.3568690
H	-1.5776660	1.4451230	1.1671690
C	-0.5833050	1.0035800	-1.2339360
H	-0.9295610	-0.7267740	0.0000000
H	-1.5776660	1.4451230	-1.1671690
H	0.1575890	1.7908290	-1.3568690
Br	-0.5833050	-0.0315530	2.8696410
Br	1.5276570	-0.4741640	0.0000000
Br	-0.5833050	-0.0315530	-2.8696410

Ge isomer 1
0, 1

C	1.1309840	1.1309840	1.1309840
H	0.5189590	1.7699440	1.7699440
H	1.7699440	0.5189590	1.7699440
H	1.7699440	1.7699440	0.5189590
C	-1.1309840	-1.1309840	1.1309840
H	-1.7699440	-0.5189590	1.7699440
H	-1.7699440	-1.7699440	0.5189590
H	-0.5189590	-1.7699440	1.7699440
C	1.1309840	-1.1309840	-1.1309840
H	0.5189590	-1.7699440	-1.7699440
H	1.7699440	-0.5189590	-1.7699440
H	1.7699440	-1.7699440	-0.5189590
C	-1.1309840	1.1309840	-1.1309840
H	-0.5189590	1.7699440	-1.7699440
H	-1.7699440	0.5189590	-1.7699440
H	-1.7699440	1.7699440	-0.5189590
Ge	0.0000000	0.0000000	0.0000000

Ge isomer 2
0, 1

C	-3.6771430	-0.4668290	0.0000370
C	-2.5075710	0.5028780	-0.0000310
H	-4.6348280	0.0571770	0.0000530
H	-3.6519360	-1.1130250	-0.8812030
H	-3.6518720	-1.1129680	0.8813170
C	-1.1563550	-0.1987100	-0.0000530
H	-2.5693700	1.1590410	-0.8750410
H	-2.5693050	1.1590890	0.8749510
C	0.0197400	0.7688280	0.0000280
H	-1.0975300	-0.8573630	0.8743670
H	-1.0974890	-0.8572540	-0.8745530
H	-0.0238530	1.4220730	-0.8764720
H	-0.0238820	1.4219570	0.8766140
Ge	1.7664250	-0.1190060	0.0000030
H	1.9071590	-1.0101980	-1.2481050
H	2.9081410	0.9129380	0.0000480
H	1.9071410	-1.0102910	1.2480460

Se isomer 1
0, 1

C	0.3831770	1.3825610	-0.1379460
C	0.3831800	-1.3824430	0.1374170
C	1.6754380	-0.7046920	-0.2865350
C	1.6751170	0.7048530	0.2867630
H	0.4294120	1.7254920	-1.1713840
H	0.1129800	2.2201670	0.5027500
H	0.4296070	-1.7263060	1.1706020
H	0.1134420	-2.2198770	-0.5037800
H	2.5426380	-1.2777480	0.0534710
H	1.7223390	-0.6538040	-1.3783930
H	1.7212430	0.6537410	1.3786980
H	2.5426850	1.2779830	-0.0522710
Se	-1.0092890	-0.0000390	0.0000620

Se isomer 2
0, 1

C	2.5483130	-0.0284000	-0.1110060
C	1.4719940	1.0755330	-0.1381750
C	0.5054690	0.0615380	0.4942920
C	1.4157480	-1.0706620	-0.0067920
H	3.2204540	-0.0990460	-0.9659410
H	3.1436280	0.0085870	0.8026200
H	1.1715570	1.3160530	-1.1589540
H	1.6573320	2.0013920	0.4067490
H	0.5204080	0.1187240	1.5823120
H	1.1123360	-1.4189560	-0.9968550
H	1.5507900	-1.9333940	0.6447740
Se	-1.3589340	-0.0388880	-0.0727750
H	-1.8218940	1.1007600	0.7297340

REFERENCES

[1] Peverati, R.; Truhlar, D. G. *Phil. Trans. R. Soc. A* **2014**, *372*, 20120476.

[2] Peverati, R.; Truhlar, D. G. *J. Chem. Phys.* **2011**, 135, 191102.

[3] Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Theory Comput.* **2005**, 2, 364-382.

[4] Peverati, R.; Truhlar, D. G. *J. Phys. Chem. Lett.* **2012**, 3, 117-124.

[5] Yu, H.; Truhlar, D. G. to be published.

[6] Lynch, B. J.; Truhlar, D. G. *J. Phys. Chem. A*. **2003**, *107*, 8996–8999. Erratum: **2003**, *108*, 1460.

[7] Zheng, J.; Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2007**, *3*, 569–582.

[8] Cotton, D. H.; Jenkins, D. R. *Trans. Faraday Soc.* **1969**, *65*, 1537–1543.

[9] https://www.webelements.com/sodium/bond_enthalpies.html, accessed on April 24, 2014.

[10] Zhang, W.; Truhlar, D. G.; Tang, M. *J. Chem. Theory Comput.* **2013**, *9*, 3965–3977.

[11] Izgorodina, E. I., Coote M. L., Radom, L. *J. Phys. Chem. A* **2005**, *109*, 7558–7566.

[12] Averkiev, B. B.; Zhao, Y.; Truhlar, D. G. *J. Mol. Cata A: Chem.* **2010**, 80–88.

[13] Schultz, N. E.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A*. **2005**, *109*, 11127–11143.

[14] Yu, H.; Truhlar, D. G. *J. Chem. Theory Comput*. **2014**, *10*, 2291–2305.

[15] Vasiliu, M.; Feller, D.; Gole, J. L.; Dixon, D. A. *J. Phys. Chem*. A **2010**, *114*, 9349–9358.

[16] Pedley, J. B.; Marshall, E. M. *J. Phys. Chem. Ref. Data*. **1983**, *12*, 967–1031.

[17] Lide, D. R. In *Handbook of Chemistry and Physics*, 87th edition; Lide, D. R., Ed.; CRC Press: Boca Raton, 2006; p. 9-89.

[18] Lide, D. R. In *Handbook of Chemistry and Physics*, 87th edition; Lide, D. R., Ed.; CRC Press: Boca Raton, 2006; p. 9-69.

[19] Peverati, R.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2012**, 14, 13171-13174.

[20] Li, R.; Peverati, R.; Isegawa, M.; Truhlar, D. G. *J. Phys. Chem. A* **2012**, 117, 169-173.

[21] Lynch, B. J.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2003**, 107, 1384-1388.

[22] Luo, S.; Averkiev, B. B.; Yang, K. R.; Xu, X.; Truhlar, D. G. *J. Chem. Theory Comput.* **2014**, *10*, 102–121.

[23] Vydrov, O. A.; Voorhis, T. V. *J. Chem. Theory Comput*. **2012**, *8*, 1929−1934.

[24] Lange, K. M.; Lane, J. R. *J. Chem. Phys*. **2011**, *134*, 034301.

[25] McMahon, J. D.; Lane, J. R. *J. Chem. Phys*. **2011**, *135*, 154309.

[26] Marshall, M. S.; Burns, L. A.; Sherrill, C. D. *J. Chem. Phys*. **2011**, *135*, 194102.

[27] Tang, K. T.; Toennies, J. P. *J. Chem. Phys*. **2003**, *118*, 4976–4983.

[28] Luo, S.; Truhlar, D. G. *J. Chem. Theory Comput*. **2012**, *8*, 4112−4126.

[29] Yang, K.; Peverati, R.; Truhlar, D. G.; Valero, R. *J. Chem. Phys*. **2011**, *135*, 044188.

[30] Schwabe, T. *Phys. Chem. Chem. Phys.* **2014**, *16*, 14559–14567.

[31] Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2008**, 128, 184109.

[32] http://cccbdb.nist.gov/expbondlengths1.asp, accessed on Oct. 29, 2014.

[33] Posada-Borbón, A.; Posada-Amarillas, A. *Chem. Phys. Lett*. **2015**, *618*, 66–71.

[34] Fast, P. L.; Corchado, J.; Sanchez, M. L.; Truhlar, D. G. *J. Phys. Chem. A* **1999**, *103*, 3139–3143.

[35] Lynch, B. J.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 1643–1649.

[36] Chakravorty, S.; Gwaltney, S.; Davidson, E. R.; Parpia, F.; Fischer, C. *Phys. Rev. A* **1993**, *47*, 3649–3670.

[37] Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215–241.

[38] Karton, A.; Tarnopolsky, A.; Lamere, J.-F.; Schatz, G. C.; Martin, J. M. L. *J. Phys. Chem. A* **2007**, *112*, 12868-12886.

[39] Pople, J. A.; Head-Gordon, M.; Raghavachari, K. *J. Chem. Phys.* **1987**, *87*, 5968–5975.

[40] http://cccbdb.nist.gov/ accessed on April 24, 2014.

[41] Bach, R. D.; Shobe, D. S.; Schlegel, H. B.; Nagel, C. J. *J. Phys. Chem.* **1996**, *100*, 8770–8776.

[42] Harrison, J. F. *Chem. Rev.* **2000**, *100*, 679−716.

[43] Jensen, K. P.; Roos, B. O.; Ryde, U. *J. Chem. Phys*. **2007**, *126*, 014103.

[44] Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 5656–5667.

[45] Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2005**, *1*, 415–432.

[46] Luo, S.; Zhao, Y.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2011**, *13*, 13683–13689.

[47] Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2006**, *110*, 10478–10486.

[48] Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Phys.* **2005**, *123*, 161103.

[49] Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101.

[50] Peverati, R.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. Lett.* **2011**, *2*, 1991–1997.

[51] Peverati, R.; Truhlar, D. G. *J. Chem. Theory Comput.* **2012**, *8*, 2310–2319.

[52] Amin, E. A.; Truhlar, D. G. *J. Chem. Theory Comput.* **2008**, *4*, 75–85.