

Theoretical Insight: Dual Roles of Electron-Pair Donors and Acceptors in Activating and Mediating Iodine Atom Transfer

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I. Original reaction mechanism.

The original reaction mechanism proposed by Daniele Leonori's group (J. Am. Chem. Soc. 2024, 146, 32, 22424-22430) highlights the Lewis base-mediated regulation of borane, wherein the boron radical acts as a halogen-atom transfer (XAT) agent to abstract halogen atoms from the substrate, thereby generating carbon-centered radicals. Subsequently, copper catalysis facilitates the formation of alkyl radicals and enables the construction of carbon-nitrogen bonds.

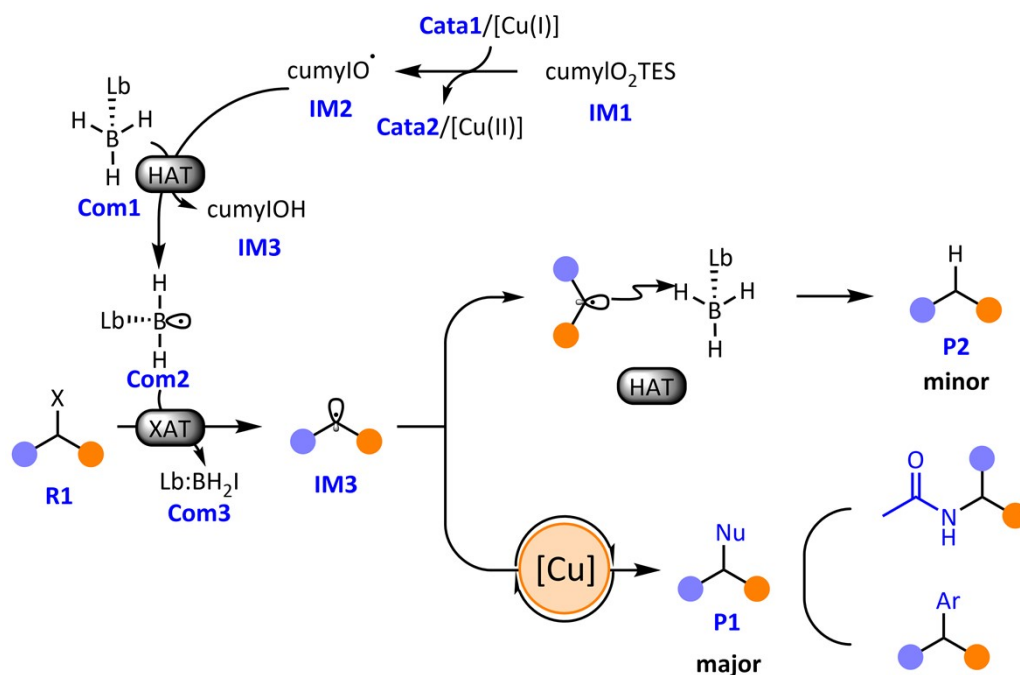


Figure S1. Original reaction mechanism.

The activation of carbon-iodine bonds by copper catalysts commonly proceeds through two primary mechanisms: oxidative addition and metal-halogen atom transfer. The corresponding activation barriers for these elementary steps are 30.8 and 33.8 kcal/mol, respectively, both of which are sufficiently high to render neither pathway dominant under ambient temperature conditions.

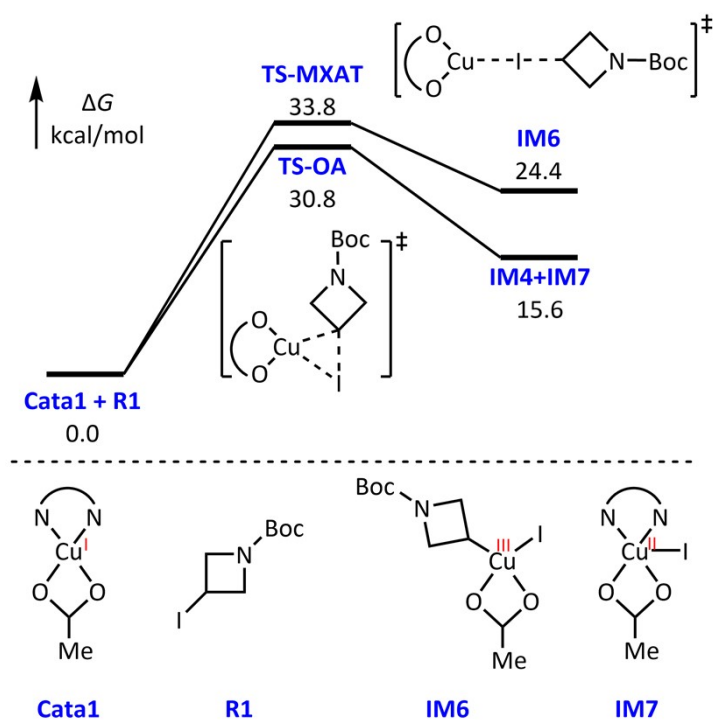


Figure S2. Copper-catalyzed C-I activation.

II. Linear correlation analysis between bond dissociation energy and atomic transfer.

Abscissa: Bond dissociation energy of Lb-BH₃ B-H bonds.

Ordinate: The activation energy of the alkyl radical R· and Lb-BH₃ is recorded as HAT2.

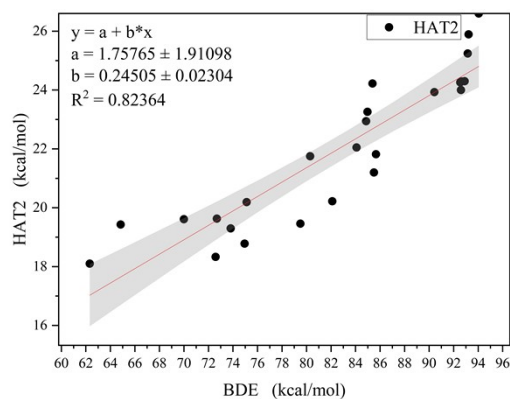


Figure S3. Linear correlation between the BDE of the B-H bond in Lb-BH₃ and the activation energy of the HAT2.

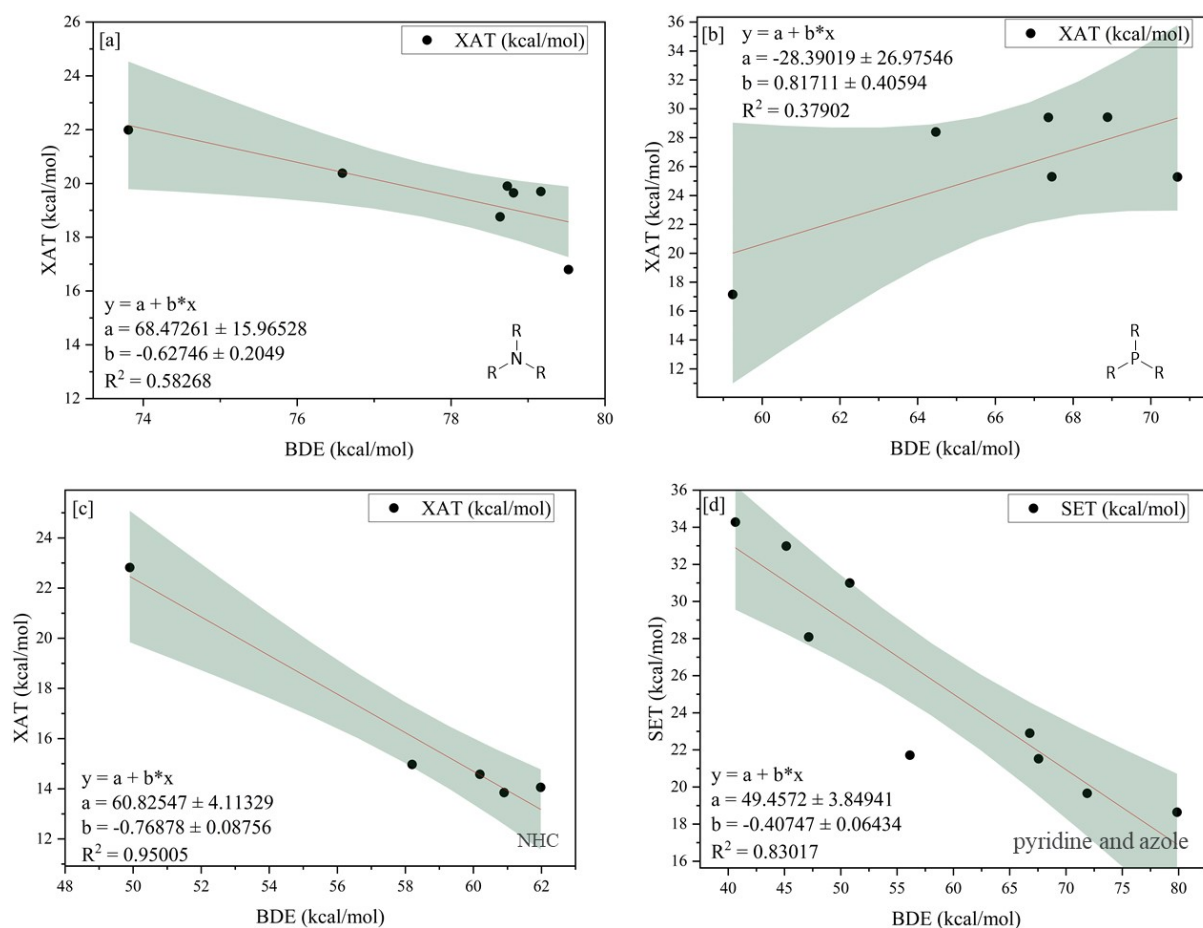


Figure S4. Linear correlation between the BDE of B-I in LbBH₂I and the energy barrier of SET. (a-d represent different structures of Lewis bases)

III. IBO analysis of the C-I bond heterolysis.

IBO analysis of the C-I bond heterolysis promoted by cooperative interaction between ComE3 and [Cu(II)].

To verify the mechanism of C-N bond formation between **ComE3** and [Cu(II)]-Nu complexes via a nucleophilic substitution pathway (Figure S5 and Table S1), we performed an IRC analysis on the **TS5** transition state. Six key points along the IRC path were analyzed, revealing gradual activation of the C-I bond, formation of a carbocation intermediate, and coupling between the N-containing nucleophilic fragments and the carbocation.

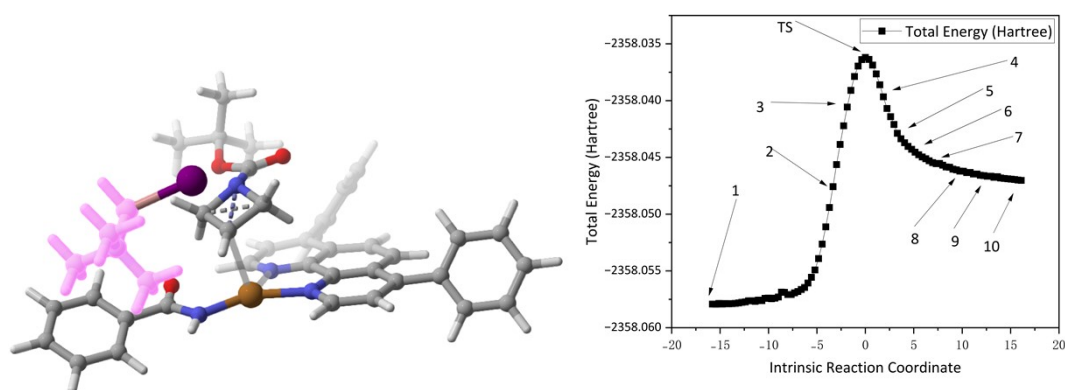
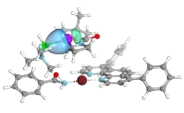
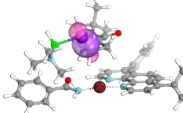
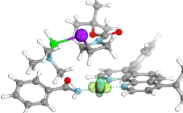
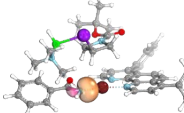
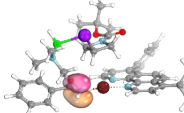
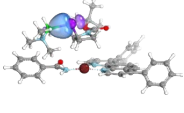
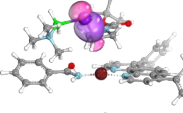
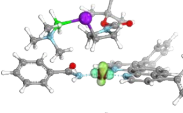
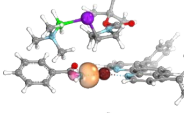
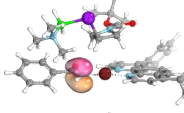
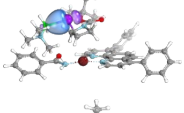
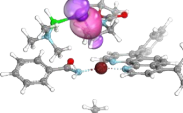
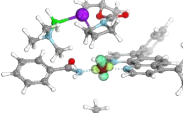
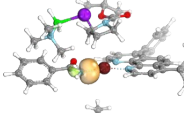
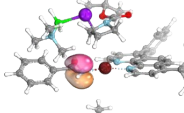
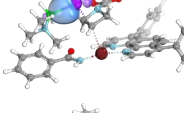
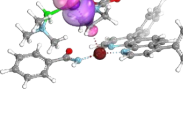
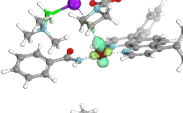
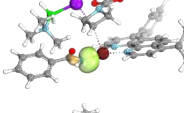
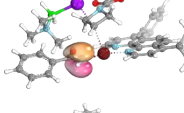
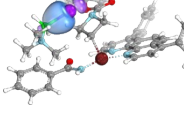
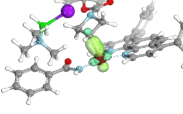
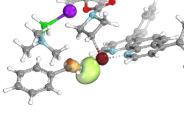
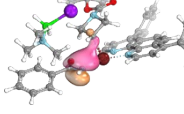
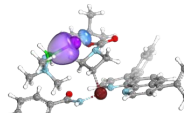
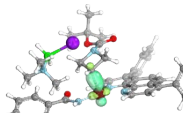
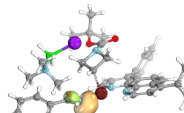
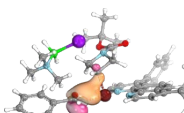
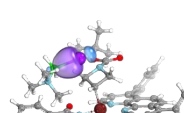
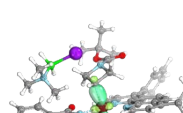
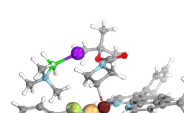
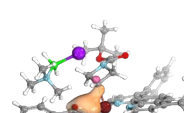
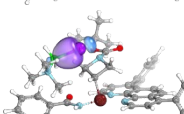
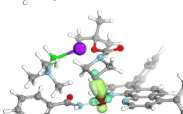
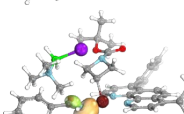
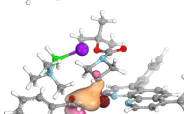
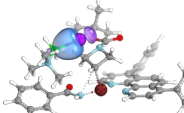
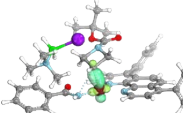
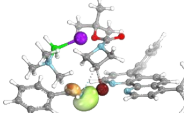
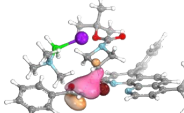
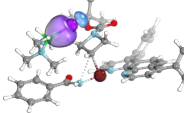
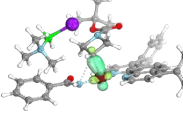
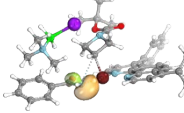
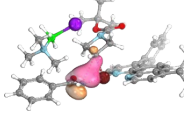
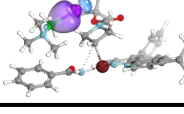
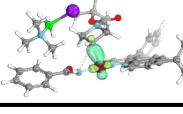
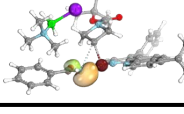
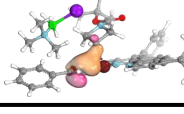


Figure S5. Structure of transition state TS5 and its IRC (key points along the reaction coordinate)

In Table 1, **Cata3** serves as the nucleophile, with its nitrogen-containing fragment attacking **ComE5**; intrinsic bond orbital (IBO) analysis along the reaction coordinate of **TS5** is used to characterize the electronic evolution during this nucleophilic substitution process.

Table S1. Intrinsic bond orbital analysis.

	I-B	I-C	Cu-C	N-C	N-Cu
1					
2					
3					
TS5					
4		/			
5		/			
6		/			
7		/			
8		/			
9		/			
10		/			

IV. Structural features of ComA and its potential reactivity

Theoretical calculations on the full model and complete reaction pathway reveal that the complexes and intermediates formed by Lbs and BH_3 play a dual role in the reaction: acting as Lewis bases (**ComB**) to mediate single-electron transfer, and simultaneously serving as Lewis acids (**ComD**) to activate the C–I bond. To ensure the reaction proceeds along the intended favorable pathway, computational analyses were performed to evaluate potential deactivation side reactions involving **ComA** and **ComB**, aiming to provide a theoretical foundation for the molecular design of Lewis base–borane complexes. Secondary reactions are primarily categorized into two types: $\text{Lbs} \rightarrow \text{BH}_3$ and $\text{Lbs} \rightarrow \text{BH}_2\cdot$. For $\text{Lbs} \rightarrow \text{BH}_3$, deactivation pathways include ligand exchange with other Lewis bases bearing lone electron pairs in the system, and hydrogen atom donation from BH_3 to form $[\text{Cu}]-\text{H}$ species, leading to catalyst Cata3 deactivation. For $\text{Lbs} \rightarrow \text{BH}_2\cdot$, deactivation occurs via reduction by proton-containing species to regenerate $\text{Lbs} \rightarrow \text{BH}_3$, or through transmetallation between the metal-like $\text{BH}_2\cdot$ radical and Cu-complexes. In the case of ligand exchange for $\text{Lbs} \rightarrow \text{BH}_3$, competing Lewis bases such as OAc^- , OTES^- , R_2 , and the solvent ethyl acetate can displace Lbs by coordinating to BH_3 . As shown in Figure *, the energy barriers for these ligand exchange processes are generally high under ambient conditions, indicating that the $\text{Lbs} \rightarrow \text{BH}_3$ structure exhibits good kinetic stability under the current reaction conditions. Moreover, the pathways involving BH_3 in **ComA** acting as a hydrogen donor to form $[\text{Cu}]-\text{H}$ species exhibit energy barriers exceeding $30.0 \text{ kcal}\cdot\text{mol}^{-1}$, rendering them kinetically inaccessible at room temperature—further supporting the robustness of this complex.

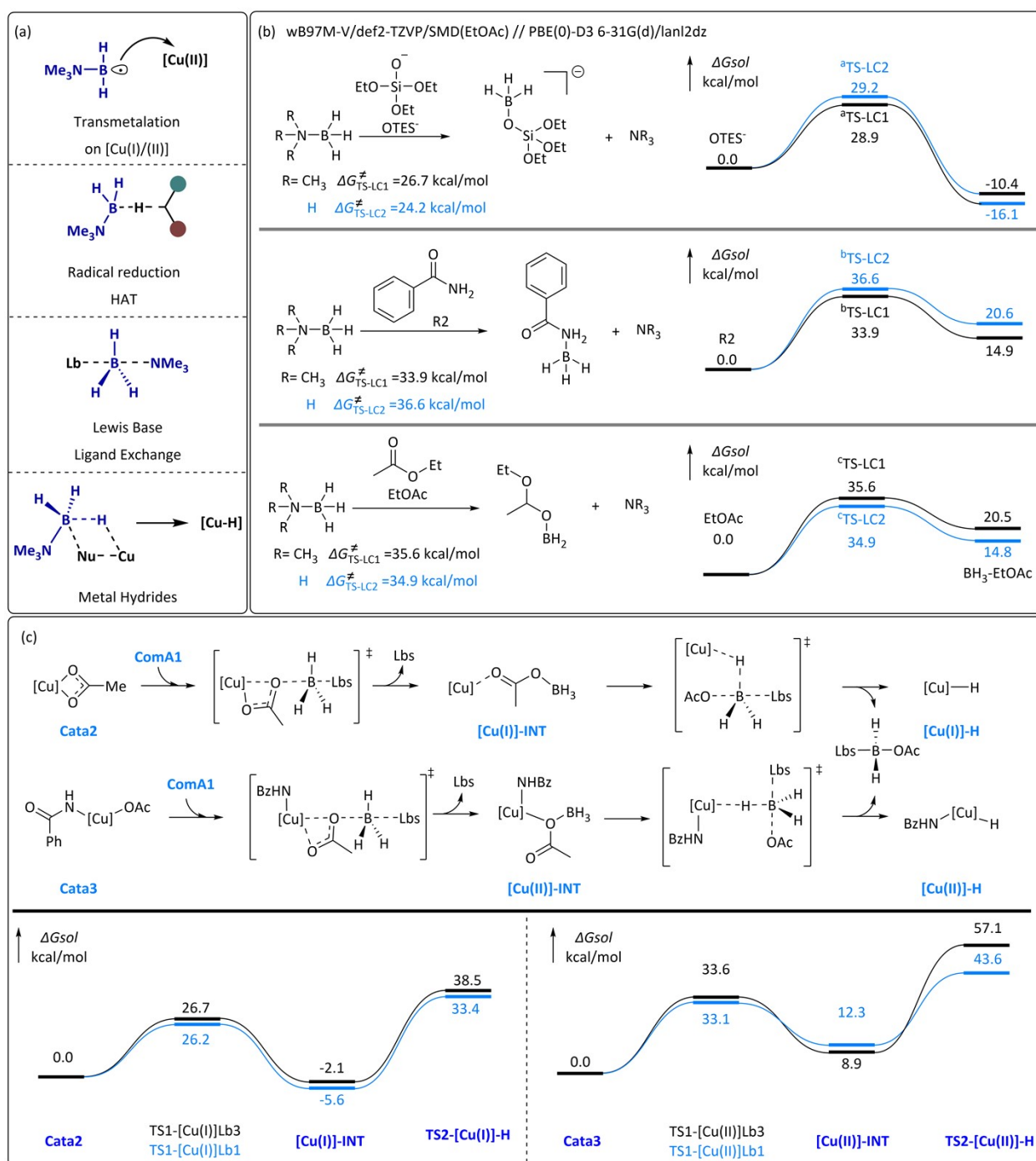


Figure S6. Inactivation mechanisms of the ComA complex. (a) Four prevalent pathways leading to ComA deactivation; (b) ligand exchange via competing Lewis bases; (c) formation of copper hydride species. (ω B97M-V/def2-TZVP/SMD(EtOAc)//PBE0-D3/6-31G(d)/LanL2DZ)

V. Estimation of energy barriers for SET using the Marcus–Hush theory

The Marcus-Hush equation decomposes the reorganization energy λ into two components, namely the inner-sphere nuclear reorganization energy λ_i and the outer-sphere solvent reorganization energy λ_o . The calculation of λ_i can be achieved through equations S1, S2, and S3:

$$\lambda_{i1} = \left| E^{D+}(Q_P) - E^{D+}(Q_R) \right| \quad \text{Equation S1}$$

$$\lambda_{i2} = \left| E^{A-}(Q_P) - E^{A-}(Q_R) \right| \quad \text{Equation S2}$$

$$\lambda_i = \lambda_{i1} + \lambda_{i2} \quad \text{Equation S3}$$

Where λ_{i1} represents the reorganization energy of the electron-donating substrates (D), λ_{i2} is the reorganization energy of the electron-accepting substrates (A). Q_R and Q_P are the equilibrium geometries of the reactants and products, respectively.

In addition, the outer-sphere solvent reorganization energy λ_o can be obtained according to the equation S4:

$$\lambda_o = \left(332 \text{ kcal mol}^{-1} \right) \left(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R} \right) \left(\frac{1}{\epsilon_{op}} - \frac{1}{\epsilon} \right) \quad \text{Equation S4}$$

where a_1 and a_2 are the radii of the electron-donating substrates (D) and the electron-accepting substrates (A), respectively, $R = a_1 + a_2$, ϵ_{op} and ϵ are the optical dielectric constant (2.1632994) and the static dielectric constant (2.20525) of DMSO solvent, respectively. The radius of a molecule can be obtained by calculating the molecular volume via a Monte-Carlo integration as implemented in the Gaussian 09 program. Therefore, the overall activation barrier of single-electron transfer (SET) process can be calculated from the equations S5 and S6:

$$\lambda = \lambda_i + \lambda_o \quad \text{Equation S5}$$

$$\Delta G_{SET}^\ddagger = (\lambda/4) \left(1 + \left(\frac{\Delta G_r}{\lambda} \right)^2 \right) \quad \text{Equation S6}$$

where ΔG_r is the reaction Gibbs Free Energy Change.

Table S2. Energy barriers for SET processes according to the Marcus-Hush theory. (unit: Hartree)

	ΔG_0	λ_i	λ_o	λ	$\Delta G_{SET}^\ddagger$
ComA1	-24.86801635	32.84975429	18.10380414	50.95355843	15.77261458
ComA2	-24.79789232	28.29501402	11.83973041	40.13474442	13.86412948
ComA3	-27.21973849	33.58329292	14.69130156	48.27459448	15.90562629
ComA4	-27.74352503	23.27882663	12.24841278	35.52723941	14.29809883
ComA5	-28.5843625	22.15129199	11.93271489	34.08400688	14.51403082
ComA6	-19.77097904	26.77369703	12.84357423	39.61727126	12.37099207
ComA7	-1.488167942	22.1033196	16.22183138	38.32515097	9.595734156
ComA8	-7.836025333	25.17266135	8.859375691	34.03203704	8.959079034
ComA9	-10.13186986	21.90192329	13.55457471	35.456498	9.587932493
ComA10	2.452188635	25.5862191	11.56935889	37.15557799	9.329354298
ComA11	-10.69967144	21.94377963	11.42036451	33.36414414	9.19886539
ComA12	24.29019008	26.33447733	15.32567103	41.66014835	13.95567099
ComA13	-7.982003464	28.07600549	11.83973041	39.91573589	10.37797697
ComA14	-13.34994887	19.87241874	11.70621443	31.57863316	9.305589647
ComA15	-8.943642083	20.09938578	10.01416061	30.11354639	8.192445995
ComA16	-12.92224242	20.10226677	7.751232752	27.85349953	8.462148393
ComA17	7.022751909	24.49488801	10.84021539	35.3351034	9.182713873
ComA18	-29.023162	19.75717266	12.59819421	32.35536687	14.59737503
ComA19	-22.24199378	20.06311145	12.65238873	32.71550019	11.95924127
ComA20	-7.97983615	21.91953253	11.99576503	33.91529757	8.948212761
ComA21	-28.37094746	20.59037201	9.725576528	30.31594854	14.21667042
ComA22	-3.821877863	21.72668941	10.46467178	32.19136119	8.161277178
ComA23	6.646897874	23.66462471	12.55644071	36.22106541	9.360208041
ComA24	-32.68327494	26.96392722	12.57429273	39.53821995	16.63875676
ComA25	-16.50812626	26.27867384	8.87110491	35.14977875	10.7257089
ComA26	7.052814126	22.38332191	10.10158455	32.48490645	8.504036605
ComA27	11.83709263	24.5081091	10.43203208	34.94014117	9.737583918
ComA28	-25.81936931	22.42343174	14.66544027	37.08887201	13.76574797

Note: SMD (ethyl ethanoate) ω B97X-D/def2-TZVP//SMD (ethyl ethanoate) PBE0(D3)/6-31G(d)/LANL2DZ.

VI. Linear correlation analysis between bond dissociation energy and pKa

As shown in Figure S7, we performed a correlation analysis between the pKa values of 28 Lewis bases (Lbs) and the reactivity of their corresponding radical intermediates, $\text{Lbs} \rightarrow \text{BH}_2\cdot$. The molecular structures were geometrically optimized and frequency analysis at the M06-2X/def2-TZVP level of theory, based on the pKa calculation protocol reported by the George C. Shields group, under both vacuum and solvated conditions (SMD model, solvent: ethyl acetate).

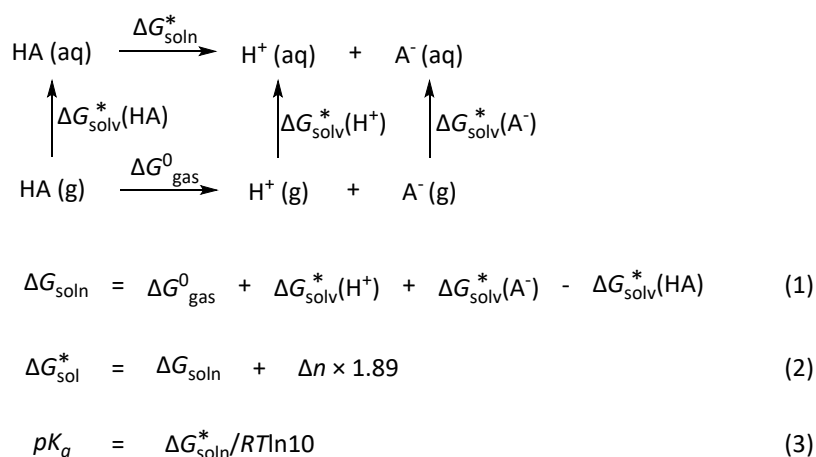


Figure S7. Thermodynamic Cycle for pKa Calculation^[1].

As illustrated in Figure S8, the pKa values of phosphines and their derivatives, carbenes, and nitrogen-containing heterocycles exhibit a strong linear correlation with the bond dissociation energy (BDE) of the B–H bond in Lb-BH_3 , whereas amines and their derivatives deviate significantly from this trend and display a weaker correlation. Thus, for these classes of Lewis bases showing clear correlation, pKa serves as an effective descriptor for predicting the reactivity of Lb-BH_3 complexes. We sincerely appreciate your feedback and will continue to investigate the relationship between the basicity and electron-donating ability of Lewis bases in our future work.

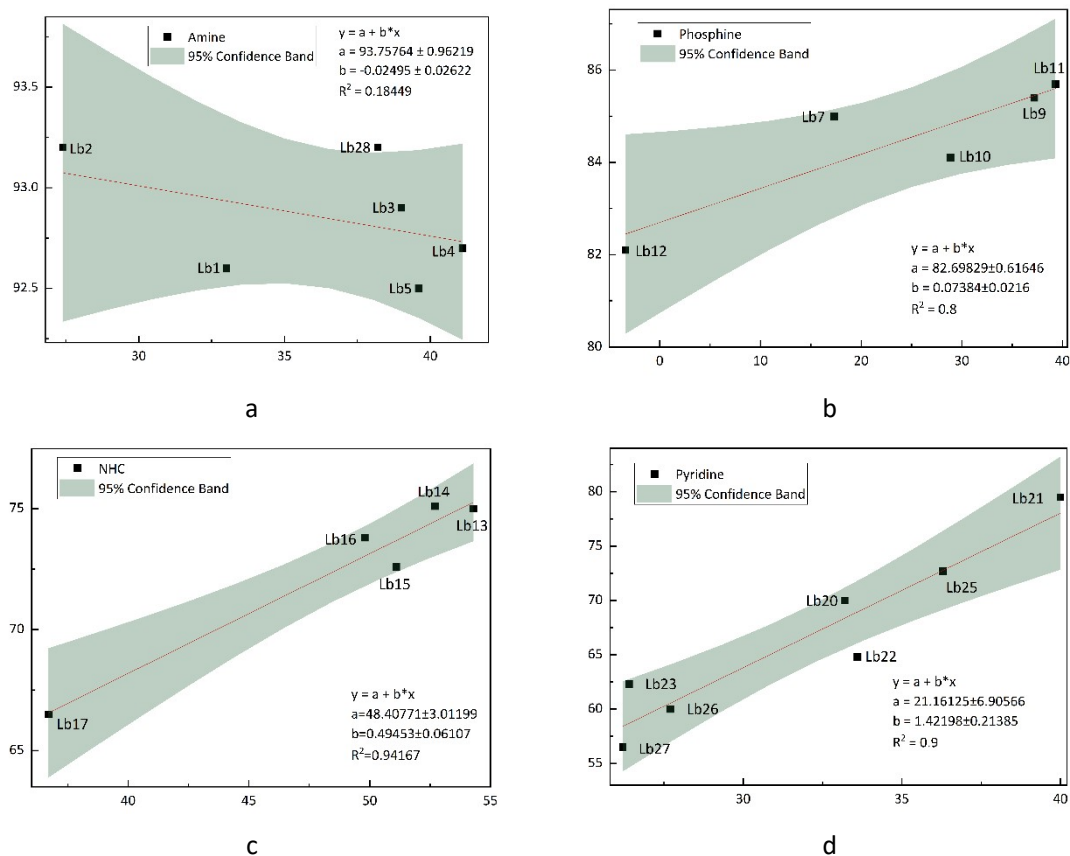


Figure S8. Linear correlation analysis between bond dissociation energy and pKa. (Figures S8 a–d present the correlation between B-H bond dissociation energy (BDE) and pKa for amines and their derivatives, phosphines and their derivatives, carbenes, and nitrogen-containing heterocycles, respectively. The x-axis displays the pKa values of the compounds, while the vertical axis denotes the bond dissociation energy (BDE).)

Reference

[1] Matthew D. Liptak, George C. Shields. Accurate pKa Calculations for Carboxylic Acids Using Complete Basis Set and Gaussian-n Models Combined with CPCM Continuum Solvation Methods. *J. Am. Chem. Soc.* **2001**, 123 (30), 7314-7319.

VII. Rate analysis of the primary competitive pathways for the transformation ComB3

Based on the transition state theory (TST) method reported by D. G. Truhlar et al.^[2], we have performed supplementary calculations of the reaction rates for multiple competing and reversible pathways involving the intermediate Lb3→BH₂· (ComB3). These results are presented in Section VII of the Supporting Information.

As shown in Reaction 1, the rate constant for the formation of ComB3 is $5.562 \times 10^3 \text{ s}^{-1}\text{M}^{-1}$, while that of the reverse reaction is $6.123 \times 10^0 \text{ s}^{-1}\text{M}^{-1}$. This kinetic profile enables effective maintenance of ComB3 concentration in the system, thereby facilitating the progression of subsequent reactions. In Reaction 2, ComB3 and R1 undergo an iodine atom transfer (XAT) to form Lb3→BH₂I (ComC3), with a rate constant of $3.180 \times 10^{-2} \text{ s}^{-1}\text{M}^{-1}$. As illustrated in Reaction 3, ComB3 reacts with the Lewis acid-activated substrate ComE3 via XAT to yield ComC3 and Lb3→BH₂I, with a significantly higher rate constant of $6.611 \times 10^1 \text{ s}^{-1}\text{M}^{-1}$. In Reaction 4, the substitution reaction between Cata3 and ComF3 proceeds with a rate constant of $2.599 \times 10^{-4} \text{ s}^{-1}\text{M}^{-1}$. Notably, both Reaction 3 and Reaction 4 exhibit substantially faster kinetics than Reaction 2, strongly suggesting that Lb3→BH₂·, acting as a Lewis acid, plays a crucial role in enhancing the efficiency of halogen atom transfer.

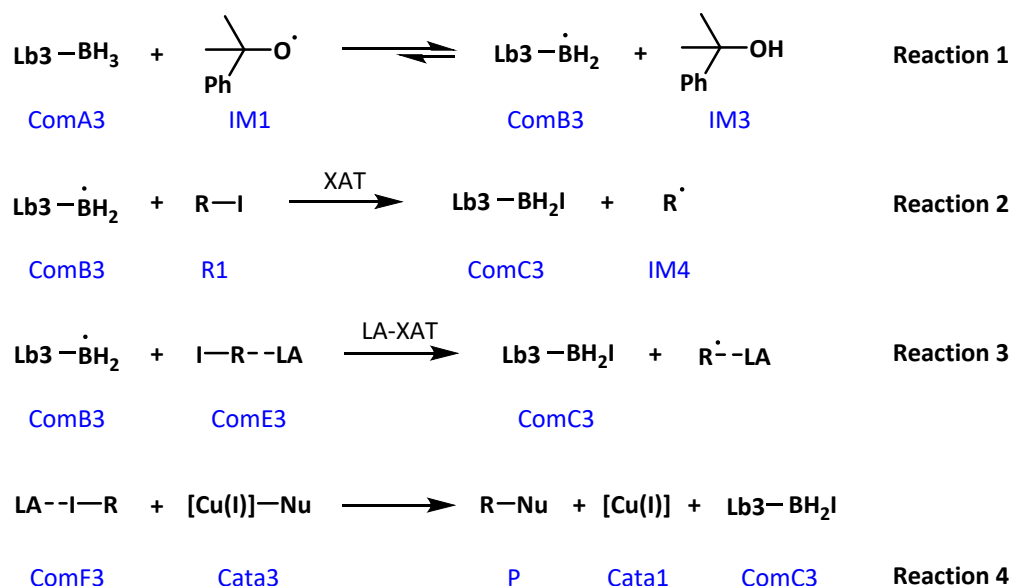


Figure S9. The reaction equations governing the formation and competitive pathways of ComB3

VIII. Intrinsic Reaction Coordinate for the Transition State ^{OS}TS-OS

We have performed supplementary intrinsic reaction coordinate (IRC) calculations for IM4 attacking the N-atom of Cata3 via an outer-sphere mechanism. Given the spin state change of the single electron during the transformation from reactant to transition state (TS-OS), the IRC pathway from reactant to TS was calculated in the triplet state, whereas the path from TS to product was computed in the singlet state. As shown in Figure S10, the IRC analysis confirms that direct C–N bond formation by the radical IM4 through an outer-sphere mechanism is feasible. Furthermore, the reaction is strongly exothermic from a thermodynamic standpoint, providing a substantial driving force for its spontaneous occurrence.

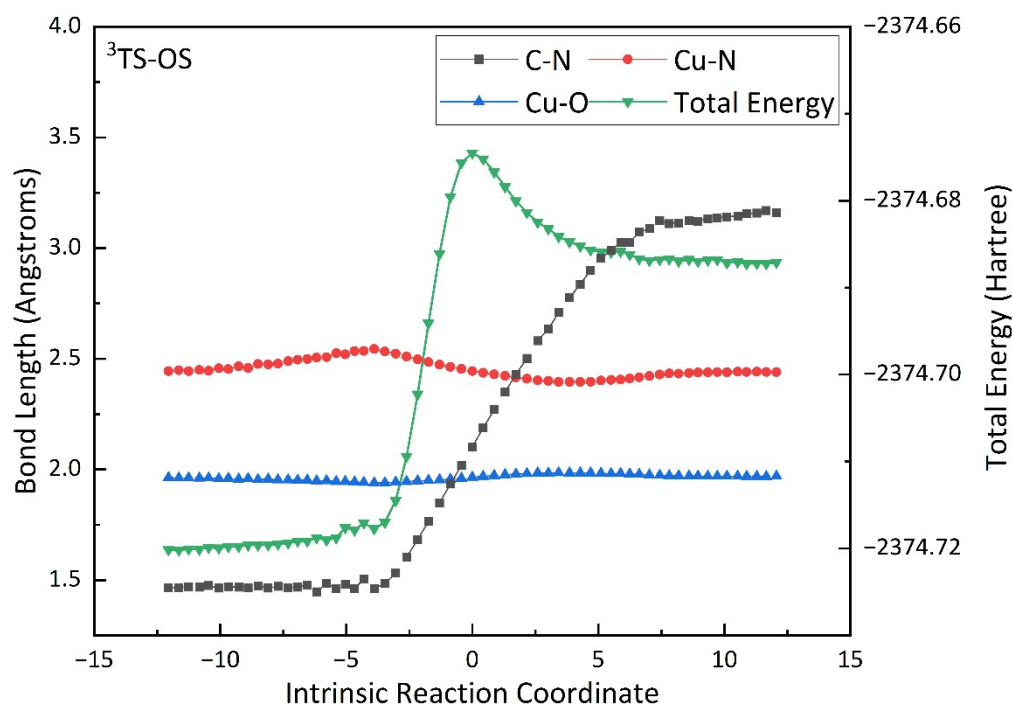


Figure S10. The intrinsic reaction coordinate of ^{OS}TS-OS and the evolution of key bond lengths

IX. Thermodynamic energies

Table S3. Energies were calculated at the PBE0(D3)/6-31G(d)/LANL2DZ level using the SMD(ethyl ethanoate) solvation model, followed by single-point energy corrections at the ω B97X-D/def2-TZVP level with the same solvent model. (Unit: hartree)

	$E_{ZPE-corr}$	E_{corr}	H_{corr}	G_{corr}	<i>sol-EE</i>
R2	0.125589	0.13317	0.134114	0.093741	-400.9793206
R1	0.21314	0.226835	0.227779	0.172604	-816.1747968
IM4	0.20805	0.220605	0.221549	0.170225	-518.4099763
IM0	0.391506	0.416699	0.147643	0.340306	-1252.966343
Cata1	0.378456	0.404474	0.405418	0.325545	-2902.77984
Cata2	0.381731	0.407114	0.408058	0.329495	-2902.624323
TS-NH	0.504288	0.538514	0.539458	0.442796	-3303.605497
Cata3	0.495396	0.530128	0.531072	0.433208	-3303.159692
TS-RC	0.705513	0.753534	0.754478	0.632256	-3821.584185
IM5	0.707724	0.755882	0.756826	0.633987	-3821.591562
TS-RE	0.707252	0.755042	0.755987	0.633754	-3821.573119
P	0.329581	0.349582	0.350526	0.283009	-918.868387
TS-OSM	0.706017	0.753495	0.754439	0.632173	-3821.552697
ComA3	0.15276	0.159528	0.160472	0.124923	-201.0935322
ComB3	0.141377	0.148263	0.149207	0.111782	-200.4278056
ComC3	0.145467	0.153663	0.154607	0.112082	-498.2388272
TS1	0.32425	0.341287	0.342231	0.281902	-625.8160695
TS2	0.35437	0.376296	0.37724	0.305012	-1016.591808
TS3	0.359874	0.380033	0.380977	0.313645	-719.4832214
ComD3	0.143113	0.150268	0.151213	0.113743	-200.3131132
ComF3	0.363725	0.38366	0.384604	0.317965	-1016.540504
TS4-ComD3	0.504635	0.532959	0.533903	0.450092	-1216.964524
ComE3	0.360297	0.381351	0.382295	0.313123	-1016.51616
TS5-ComE3	0.494323	0.529449	0.530394	0.432363	-3303.270057
ComA8	0.291747	0.30972	0.310664	0.248089	-1062.138189
ComF8	0.511088	0.542694	0.543639	0.453509	-1878.385797
TS4-ComD8	0.800006	0.851346	0.852291	0.722962	-2940.660153
ComE8	0.507794	0.540481	0.541426	0.448872	-1878.357772
TS5-ComE8	0.950328	1.013951	1.014896	0.862656	-4952.992513
ComA13	0.171593	0.181015	0.18196	0.138952	-331.890955
ComF13	0.391114	0.413789	0.414733	0.342041	-1148.1302
ComE13	0.387865	0.411734	0.412679	0.337379	-1148.10064
TS5-ComE13	0.831928	0.886556	0.8875	0.752535	-4222.72286
Cata4	0.443884	0.473534	0.474478	0.38691	-3074.636978
ComA18	0.094753	0.099922	0.100867	0.066663	-252.1326635
ComF18	0.312693	0.331783	0.332727	0.266536	-1068.356415
TS4-ComD18	0.404451	0.430356	0.4313	0.350831	-1320.593855
ComE18	0.310283	0.33032	0.331264	0.263093	-1068.322101

TS5-ComE18	0.753606	0.804453	0.805397	0.676592	-4142.947907
ComA24	0.15758	0.164479	0.165423	0.12737	-313.6484506
ComF24	0.375039	0.395924	0.396868	0.327523	-1129.873734
TS4-ComD24	0.528733	0.558755	0.559699	0.471225	-1443.621381
ComE24	0.372528	0.394457	0.395401	0.32381	-1129.84051
TS5-ComE24	0.816539	0.8692	0.870145	0.738182	-4204.470507
IM1	0.172967	0.182449	0.183393	0.138684	-424.7242247
IM3	0.1856668	0.1955405	0.19635	0.151923	-425.3965145
TS6-A3	0.446175	0.477882	0.478826	0.387496	-2985.956862
TS6-A1	0.530108	0.564982	0.565926	0.469176	-3103.849493
IM6	0.410386	0.43886	0.439804	0.354986	-2929.43744
TS7-A3	0.444359	0.47598	0.476924	0.386531	-2985.944435
TS7-A1	0.527467	0.562955	0.5639	0.465916	-3103.827537
TS8-A3	0.562404	0.602537	0.603481	0.495437	-3386.32611
TS8-A1	0.646826	0.690094	0.691038	0.577191	-3504.221996
IM7	0.527468	0.564049	0.564993	0.464078	-3329.795706
TS9-A3	0.562459	0.601391	0.602336	0.497167	-3386.289563
TS9-A1	0.643408	0.687107	0.688051	0.558901	-3504.184561
bTS-LC1	0.192608	0.205844	0.206788	0.153962	-484.142365
IM9	0.15843	0.167954	0.168898	0.124183	-427.6022916
bTS-LC3	0.277263	0.293378	0.294322	0.235442	-602.0312444
IM10	0.116108	0.122686	0.12363	0.085864	-307.7115218
IM11	0.147468	0.156287	0.157231	0.114585	-334.3343724
cTS-LC1	0.182334	0.195892	0.196837	0.143325	-390.869144
cTS-LC1	0.267157	0.28324	0.284184	0.225358	-508.7639364
IM12	0.225015	0.240574	0.241518	0.183844	-828.8614007
IM2	0.213218	0.228022	0.228967	0.172687	-828.3538401
aTS-LC1	0.291427	0.312986	0.31393	0.243857	-912.0211418
aTS-LC3	0.375805	0.400298	0.401242	0.325308	-1029.912219
IM8	0.213218	0.228022	0.228967	0.172687	-828.3538401
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X. Cartesian coordinates

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 C -3.07621600 -3.51732800 -0.98544000

C -3.38364500 -5.53789500 0.91073900
 H -1.51957300 -4.84444300 1.73318200
 C -4.18617500 -4.35467700 -1.03255300
 H -2.94701700 -2.74827500 -1.74224600
 C -4.34571100 -5.36181700 -0.08233100
 H -3.50324000 -6.32049200 1.65488200
 H -4.92567500 -4.22239800 -1.81753500
 H -5.21643800 -6.01083000 -0.11824700
 C -1.97047600 3.76324500 -0.02339400
 C -2.08127200 4.80020200 -0.95948500
 C -2.96107500 3.61941800 0.95797400
 C -3.17140300 5.66342600 -0.92575200
 H -1.32017400 4.91377900 -1.72727000
 C -4.04263200 4.49346900 0.99593100
 H -2.86824600 2.84132700 1.71092300
 C -4.15370800 5.51253300 0.05161200
 H -3.25330600 6.45562200 -1.66489100
 H -4.79746700 4.38076500 1.76932500
 H -5.00196600 6.19105300 0.08014400
 C 5.33317200 -0.07800200 0.04455900
 O 4.67951800 1.01591200 -0.00462300
 O 4.65677100 -1.15581500 0.09073100
 C 6.82009300 -0.08174000 0.05247300
 H 7.20870100 -1.10122600 0.05195000
 H 7.18906000 0.46155000 -0.82354200
 H 7.17524700 0.45028000 0.94170100
 Cu 3.00270300 -0.04860200 0.03946200

IM1:

C 1.50670600 -0.03994800 -0.06528000
 C 2.16500100 1.33831700 -0.11654500
 H 1.98423400 1.91134300 0.79906400
 H 3.24697100 1.20739600 -0.22341700
 H 1.80581500 1.91070500 -0.97709500
 C 2.04238000 -0.84858700 1.12294700
 H 1.59908400 -1.84769800 1.15170100
 H 3.12966900 -0.95664600 1.03566900
 H 1.82147600 -0.33859700 2.06666200
 C -0.03580900 0.01963400 -0.02929100
 C -0.75815700 -1.17861500 -0.10387000
 C -0.73244500 1.22668100 0.06274200
 C -2.14777900 -1.17061100 -0.05284800
 H -0.22631100 -2.11944600 -0.20837400

C -2.12452800 1.23113200 0.12511000
H -0.19783000 2.16975800 0.10714200
C -2.83616700 0.03551700 0.06627300
H -2.69415200 -2.10854200 -0.10973200
H -2.65265800 2.17674400 0.21776000
H -3.92225000 0.04359200 0.10878700
O 1.70384300 -0.71621600 -1.25295000

IM2:

O -0.46722800 0.38988200 -0.97439700
Si -1.61437000 0.09011100 0.03054600
O -3.12776600 -0.37180500 -0.56632100
O -2.07223600 1.38203100 1.03396700
O -1.29781400 -1.18445300 1.09093100
C -3.85041200 0.54422500 -1.34802100
H -4.01256900 1.48291100 -0.79337700
H -3.28921100 0.80974100 -2.25984800
C -5.18512800 -0.06297700 -1.73280300
H -5.77170200 0.62931800 -2.34924800
H -5.03466600 -0.98845800 -2.30074700
H -5.76756100 -0.30640200 -0.83645600
C -2.20270700 -1.47685300 2.12513100
H -2.38857000 -0.58291400 2.74182400
H -3.17777200 -1.78325800 1.71290500
C -1.64202000 -2.58842500 2.99083000
H -2.33151200 -2.83638000 3.80752700
H -1.47329400 -3.49298300 2.39473000
H -0.68271700 -2.28774000 3.42802000
C -1.13863400 2.39172900 1.32459100
H -1.43508900 2.85693100 2.27795500
H -0.12863100 1.97891900 1.47745900
C -1.08491600 3.44301500 0.23012300
H -2.07923600 3.87734700 0.06839300
H -0.39069100 4.25406000 0.48711500
H -0.75338700 2.96492900 -0.69700200

R2:

C 1.71711200 -0.13140300 -0.03354000
N 2.40524300 1.00942400 0.23417700
H 3.40756600 0.92509000 0.33484300
H 1.96813900 1.78378700 0.71213500
O 2.27943500 -1.18869900 -0.29676200

C 0.22206600 -0.02169700 -0.01606000
C -0.51061400 -1.20400200 0.11906800
C -0.45640600 1.19426700 -0.15006000
C -1.90008600 -1.17156400 0.14602500
H 0.02887400 -2.14260700 0.20521500
C -1.84797600 1.22516100 -0.13268700
H 0.09493800 2.11952000 -0.29809100
C -2.57150400 0.04422100 0.02182300
H -2.46107600 -2.09524900 0.26181600
H -2.36808300 2.17260200 -0.24695300
H -3.65809300 0.07058900 0.03847600

TS-NH:

C -2.88646700 -2.81930300 0.06430700
C -3.53606100 -1.60171300 0.21446300
C -2.76603300 -0.41342400 0.04090600
C -1.39046800 -0.56376600 -0.21708000
C -1.51470000 -2.86891000 -0.19800000
C -3.29637900 0.91499800 0.08873800
C -0.54966100 0.58398800 -0.38544800
C -1.09770600 1.88090400 -0.33769000
C -2.50091500 2.00712600 -0.08538700
C -0.20723700 2.97969000 -0.51854500
C 1.14180700 2.69437700 -0.67794000
C 1.59009900 1.37226400 -0.70830800
H -4.35791200 1.04871100 0.26244900
H -3.43373800 -3.74738700 0.18880100
H -0.97824500 -3.80615200 -0.29717100
H -2.93344600 2.99918100 -0.02465700
H 1.85758900 3.49716200 -0.81784400
H 2.64155400 1.14864800 -0.84987700
N 0.76817900 0.34137200 -0.58101200
N -0.78639300 -1.76936000 -0.31968000
C -4.97468500 -1.57712600 0.54467600
C -5.87253200 -2.34788000 -0.20505300
C -5.45294100 -0.83356200 1.63243200
C -7.22603100 -2.35822800 0.11486600
H -5.50825600 -2.92238100 -1.05268100
C -6.80535900 -0.85712100 1.95665100
H -4.75909800 -0.26182900 2.24270800
C -7.69487600 -1.61362700 1.19573400
H -7.91544400 -2.94873400 -0.48147800
H -7.16340500 -0.28729300 2.80910700

H -8.75145000 -1.62588800 1.44737400
 C -0.66440100 4.38300900 -0.53937500
 C -0.02269000 5.33331300 0.26523500
 C -1.69957700 4.79315600 -1.39078300
 C -0.42232200 6.66507600 0.23283900
 H 0.77554700 5.01988300 0.93285800
 C -2.08707100 6.12847300 -1.42938600
 H -2.18003100 4.07038100 -2.04472900
 C -1.45415300 7.06525900 -0.61430300
 H 0.07279200 7.39104600 0.87110500
 H -2.88204200 6.43786800 -2.10158400
 H -1.76256500 8.10637700 -0.64174500
 C 2.28050700 -4.34339300 -0.88270200
 O 3.47050400 -3.90094100 -0.87203300
 O 1.25277600 -3.60716700 -0.81543900
 C 2.07838000 -5.82615400 -0.95091200
 H 1.19599400 -6.05979700 -1.55022900
 H 2.96382400 -6.31852500 -1.35501800
 H 1.90368700 -6.19636500 0.06579400
 Cu 1.20411800 -1.65431800 -0.59342000
 C 3.48754500 -0.98411800 0.62259400
 N 3.19834900 -1.44428400 -0.65668300
 H 3.68319300 -0.96568800 -1.41188700
 H 3.42058700 -2.70485300 -0.76145200
 O 2.71266600 -1.28580200 1.53043300
 C 4.67967000 -0.13273900 0.85891000
 C 4.73325400 0.59307800 2.05531000
 C 5.73260100 -0.03313900 -0.05902300
 C 5.81681200 1.41920300 2.32325400
 H 3.91224000 0.49863200 2.75903000
 C 6.82086800 0.78789700 0.21646200
 H 5.72720700 -0.61603000 -0.97608500
 C 6.86110800 1.51800700 1.40330500
 H 5.85050600 1.98588900 3.24913100
 H 7.64021300 0.85403100 -0.49312900
 H 7.71043900 2.16181700 1.61383000

IM12:

O -0.50324400 0.44975100 -0.85857800
 Si -1.78769500 0.21252800 0.14581700
 O -3.14941300 -0.32685000 -0.59204800
 O -2.16710200 1.65430100 0.82537600
 O -1.32905900 -0.94631900 1.21424500

C -3.93740500 0.49965400 -1.44560000
 H -4.14175700 1.45820500 -0.95134300
 H -3.37918900 0.71332800 -2.36780800
 C -5.22840200 -0.21665000 -1.76629100
 H -5.85087900 0.39950700 -2.42504000
 H -5.02912400 -1.16902200 -2.26964400
 H -5.79237400 -0.42156200 -0.84970700
 C -2.23359700 -1.46191100 2.18990800
 H -2.52196000 -0.66012400 2.88394100
 H -3.14668200 -1.81980900 1.69663600
 C -1.55964000 -2.58724500 2.93907300
 H -2.23385500 -2.99244500 3.70204500
 H -1.28619500 -3.39754500 2.25447000
 H -0.65002300 -2.23105200 3.43464000
 C -1.19045600 2.53954300 1.36796600
 H -1.64472400 3.00972900 2.24818900
 H -0.30928000 1.98380600 1.71712100
 C -0.78809100 3.58768200 0.35358500
 H -1.66871200 4.13654900 0.00202200
 H -0.09023500 4.30506100 0.80136300
 H -0.30152600 3.12032300 -0.50862500
 H -0.02789600 -0.36256700 -1.08160400

Cata3:

C -2.35601100 -3.12631000 0.37575900
 C -3.23439800 -2.05433400 0.44930000
 C -2.70479200 -0.74621500 0.24760600
 C -1.31692900 -0.63759900 0.02801200
 C -0.99198100 -2.91371500 0.15212400
 C -3.48136500 0.45713300 0.23301500
 C -0.71070400 0.64730300 -0.18222000
 C -1.49938500 1.81491300 -0.19570400
 C -2.90635600 1.67580100 0.03069800
 C -0.82804000 3.05215600 -0.41916200
 C 0.55068200 3.02175700 -0.56988200
 C 1.24562300 1.80730800 -0.53443500
 H -4.55360700 0.39192900 0.38198100
 H -2.71682500 -4.13878900 0.52538000
 H -0.27902100 -3.73115900 0.10752400
 H -3.52590200 2.56569300 0.04455400
 H 1.10019900 3.94097300 -0.74562600
 H 2.32107200 1.75829300 -0.65498700
 N 0.62685800 0.65388500 -0.35780500

N -0.48610400 -1.70201900 -0.00559000
 C -4.66584000 -2.30382700 0.72396300
 C -5.36114800 -3.25460200 -0.03444700
 C -5.33309800 -1.64109400 1.76309700
 C -6.70031900 -3.52435900 0.22968500
 H -4.85061800 -3.76817500 -0.84524400
 C -6.66981400 -1.92052600 2.03059000
 H -4.79582200 -0.92499500 2.37918700
 C -7.35789700 -2.85807400 1.26229900
 H -7.23104300 -4.25595500 -0.37370800
 H -7.17291000 -1.40750400 2.84581700
 H -8.40299700 -3.07146900 1.47029500
 C -1.54204100 4.34584200 -0.48460300
 C -1.11001600 5.41609400 0.30935300
 C -2.61814600 4.53836700 -1.36160800
 C -1.75237400 6.64857100 0.24027200
 H -0.27886700 5.27127800 0.99484000
 C -3.25154000 5.77534900 -1.43520300
 H -2.94222000 3.72433300 -2.00491800
 C -2.82421400 6.83110000 -0.63169400
 H -1.41480200 7.46736000 0.87004900
 H -4.07789200 5.91531900 -2.12690400
 H -3.32352400 7.79473700 -0.68749600
 C 1.78507600 -3.22818500 -1.87956000
 O 1.44065500 -2.25642100 -2.57354200
 O 1.92971400 -3.15981600 -0.60165400
 C 2.04367100 -4.58234900 -2.49993700
 H 1.28444500 -5.29439100 -2.15580500
 H 2.01266200 -4.52385500 -3.59009800
 H 3.01648000 -4.96614200 -2.17590200
 Cu 1.48039600 -1.23119700 -0.31799800
 C 3.87232600 0.04015900 0.72312600
 N 3.33266800 -0.69280100 -0.25551600
 H 3.99344000 -1.22472800 -0.80939800
 O 3.21327300 0.73623700 1.51566400
 C 5.38068200 0.04669400 0.84867300
 C 5.98620800 1.16346700 1.43219900
 C 6.18528700 -1.02422700 0.44636600
 C 7.36782400 1.22595100 1.58210500
 H 5.34784600 1.97567300 1.76806600
 C 7.56785200 -0.97180700 0.60993000
 H 5.73171400 -1.91954900 0.02692200
 C 8.16356700 0.15652800 1.17062700
 H 7.82621000 2.10629900 2.02635200

H 8.18011500 -1.81658100 0.30379500
 H 9.24295400 0.19906000 1.29384300

TS-RC-triplet:

C -0.77639811 -0.14269970 0.47529232
 C 0.54183789 -0.56244670 0.36372732
 C 0.77874589 -1.90801170 -0.04066568
 C -0.34458311 -2.69320270 -0.35956868
 C -1.82658611 -1.00538370 0.14295332
 C 2.06876189 -2.52645170 -0.10598068
 C -0.18126911 -4.04046370 -0.82848868
 C 1.10480289 -4.60207170 -0.95198268
 C 2.22342589 -3.81123870 -0.53281768
 C 1.19151889 -5.93171570 -1.45771668
 C 0.00526389 -6.59010870 -1.75263268
 C -1.22561911 -5.94447170 -1.59538068
 H 2.93600089 -1.95958170 0.21431332
 H -1.00192211 0.87422330 0.77767932
 H -2.86783411 -0.69750570 0.17948332
 H 3.21200689 -4.25665970 -0.54457468
 H 0.02716589 -7.60080370 -2.14643468
 H -2.16952711 -6.42027670 -1.84213468
 N -1.31332411 -4.69921570 -1.15731768
 N -1.61265611 -2.24030970 -0.27666468
 C 1.64487089 0.37894730 0.63646832
 C 2.65716589 0.57376630 -0.31309768
 C 1.65767389 1.12994130 1.81761832
 C 3.66894189 1.49817630 -0.07566768
 H 2.60926189 0.04047030 -1.25842268
 C 2.67631089 2.04793130 2.05416632
 H 0.87603189 0.97855130 2.55765232
 C 3.68413889 2.23236430 1.10922332
 H 4.44084789 1.65373830 -0.82408668
 H 2.68336689 2.61850030 2.97854432
 H 4.47705689 2.95186830 1.29342532
 C 2.48267389 -6.61294570 -1.68433268
 C 2.68610389 -7.90442870 -1.18200268
 C 3.49591289 -6.00679170 -2.43940868
 C 3.88544889 -8.56928070 -1.41581068
 H 1.90675289 -8.37698970 -0.58992768
 C 4.69004989 -6.67884570 -2.68012668
 H 3.33512789 -5.01785370 -2.86037768
 C 4.88949589 -7.95840570 -2.16494568

H 4.03621589 -9.56590470 -1.01085568
 H 5.46372389 -6.20309970 -3.27594868
 H 5.82444089 -8.47979770 -2.34974668
 C -4.63521911 -5.53788670 -0.32030668
 O -4.31223211 -5.03616570 0.77056432
 O -4.13401511 -5.16800370 -1.44654268
 C -5.70291511 -6.60676770 -0.39947768
 H -6.64133211 -6.13241970 -0.71041068
 H -5.44884811 -7.35845470 -1.15135268
 H -5.85405711 -7.07788770 0.57381032
 Cu -3.02409711 -3.59972270 -0.96263168
 C -5.50864611 -2.35277470 -1.64928268
 N -4.53994911 -2.40975570 -0.71843568
 H -4.91136411 -2.49484770 0.22269332
 O -5.29346811 -2.30500970 -2.87079168
 C -6.93848411 -2.31660770 -1.16634868
 C -7.88708411 -1.62731570 -1.92615068
 C -7.35188811 -2.99751070 -0.01566268
 C -9.21923611 -1.58723270 -1.52817868
 H -7.55757611 -1.12883370 -2.83318568
 C -8.68988611 -2.97628570 0.37229932
 H -6.63277911 -3.57585470 0.56183732
 C -9.62407111 -2.26311070 -0.37660868
 H -9.94593111 -1.03486670 -2.11850768
 H -9.00337811 -3.52094270 1.25918732
 H -10.66633511 -2.24054870 -0.06904768
 C -2.24811511 -2.58706170 -3.47903368
 C -0.80354011 -2.20694170 -3.68487468
 C -2.62720411 -1.15322670 -3.24279168
 H -2.83322511 -3.41363870 -3.85959368
 H -0.43198811 -2.31278770 -4.71607168
 H -0.05457911 -2.64418170 -3.01042568
 H -3.23646611 -0.69341170 -4.03330668
 H -3.08609311 -0.92301170 -2.27554768
 N -1.19590111 -0.84601270 -3.34505568
 C -0.44540211 0.24158630 -3.10176968
 O 0.77329289 0.27018930 -3.22379868
 O -1.23839711 1.25817830 -2.70662268
 C -0.76393911 2.63375230 -2.73542368
 C -2.00483811 3.42154530 -2.33833268
 H -1.78156711 4.49302030 -2.32614968
 H -2.81920711 3.24057830 -3.04727968
 H -2.34223811 3.12422130 -1.33970368
 C 0.35416589 2.85102330 -1.72508368

H 1.24534789 2.28739730 -2.00048368
 H 0.60280289 3.91704130 -1.68026768
 H 0.03797689 2.53283930 -0.72665168
 C -0.32497011 2.99256530 -4.15012668
 H -1.13521811 2.79301830 -4.85974568
 H -0.07645311 4.05779830 -4.20128068
 H 0.55459489 2.41389130 -4.44210168

TS-RC-OSS:

C 0.66709024 -0.26048284 0.00000000
 C -0.32015576 0.70651116 -0.12628100
 C 0.05583124 2.07031516 0.05079400
 C 1.40287124 2.33189316 0.37538700
 C 1.97846224 0.10329216 0.32525800
 C -0.82855776 3.18685416 -0.09787500
 C 1.85583624 3.68240016 0.57627100
 C 0.96333724 4.76210616 0.41577700
 C -0.39721276 4.46683116 0.08040800
 C 1.47856324 6.07461616 0.62262800
 C 2.80346624 6.19482516 1.01603800
 C 3.60791124 5.05906016 1.15518300
 H -1.86425276 3.00617716 -0.36376900
 H 0.42038424 -1.31029484 -0.12174300
 H 2.76751324 -0.63117184 0.45778100
 H -1.10030976 5.28603316 -0.02409200
 H 3.23721424 7.17508816 1.18559500
 H 4.65222124 5.13189416 1.44108300
 N 3.15089524 3.83949616 0.92618400
 N 2.33049224 1.36253416 0.51329900
 C -1.70640476 0.29387416 -0.43658600
 C -1.95060876 -0.55588184 -1.52315800
 C -2.78094476 0.69853116 0.36688000
 C -3.24505576 -0.97782184 -1.81056100
 H -1.12189176 -0.86954884 -2.15298500
 C -4.07278776 0.26614316 0.08261900
 H -2.59841676 1.33214116 1.23094100
 C -4.30893976 -0.56807584 -1.00880100
 H -3.42261476 -1.62720884 -2.66364600
 H -4.89610376 0.57832916 0.71955700
 H -5.31932576 -0.90012784 -1.23209200
 C 0.66105024 7.29226316 0.43299000
 C 0.60495324 8.25657716 1.44727600

C -0.02461176 7.52376516 -0.76725400
 C -0.13228476 9.42326516 1.26952000
 H 1.13051124 8.07986016 2.38230800
 C -0.75216776 8.69656616 -0.94534900
 H 0.03530524 6.79437316 -1.57086200
 C -0.81218376 9.64606316 0.07342800
 H -0.17576176 10.15938116 2.06782900
 H -1.27035276 8.87021416 -1.88471300
 H -1.38436776 10.55933716 -0.06648500
 C 4.63203424 0.19703716 2.72766400
 O 4.09532124 1.13378616 3.34497900
 O 4.84691324 0.22414816 1.46006900
 C 5.09239324 -1.05202184 3.44452500
 H 6.18642324 -1.10674084 3.40058200
 H 4.77453124 -1.04644284 4.48940500
 H 4.70327924 -1.94402784 2.94226300
 Cu 4.20992024 2.06951216 1.04482400
 C 6.27336724 3.38821416 0.06303300
 N 5.75952924 2.77640016 -0.98852900
 H 6.03357624 3.21825216 -1.86354700
 O 5.93921324 2.98873216 1.24800300
 C 7.20537524 4.54850216 -0.01168600
 C 7.54510124 5.21944316 1.17303300
 C 7.73170924 5.02869216 -1.22081000
 C 8.36115324 6.34578916 1.14803000
 H 7.15721124 4.83686916 2.11171800
 C 8.55259124 6.15112816 -1.24524200
 H 7.50553724 4.52555516 -2.15763200
 C 8.86502024 6.82166316 -0.06165500
 H 8.60876924 6.85129316 2.07822800
 H 8.94832024 6.50600316 -2.19365000
 H 9.50466124 7.70018816 -0.08307200
 C 6.74406724 0.85169616 -1.42791200
 C 7.37951524 0.40551716 -0.13775400
 C 8.09918324 1.20249316 -1.99348000
 H 5.91988224 0.37932116 -1.94849500
 H 7.29791824 -0.66425284 0.09829300
 H 7.10496124 0.97916116 0.75422300
 H 8.44445324 0.59594416 -2.84406400
 H 8.28087524 2.26009916 -2.22903700
 N 8.68081124 0.78662916 -0.70977300
 C 9.67454824 1.38833616 -0.00742700
 O 9.81747824 1.26564716 1.19883000
 O 10.46930824 2.08489516 -0.84175600

C 11.62211524 2.81330116 -0.33332100
 C 12.18779024 3.46137116 -1.58953200
 H 13.07830724 4.04958616 -1.34423600
 H 12.46644724 2.69982516 -2.32617700
 H 11.44604924 4.12800916 -2.04341900
 C 11.17570524 3.87945716 0.65819400
 H 10.75131924 3.42896316 1.55724000
 H 12.03306924 4.50036416 0.94272500
 H 10.42159224 4.52662916 0.20018600
 C 12.62732724 1.84274216 0.27280500
 H 12.89047624 1.06405816 -0.45224300
 H 13.54253024 2.37997016 0.54600400
 H 12.21798924 1.36789216 1.16685900

IM5:

C 1.58805500 2.48606700 1.53199200
 C 2.71897600 1.71496900 1.31799200
 C 2.54056000 0.41510100 0.76609700
 C 1.21771800 -0.01344400 0.52439900
 C 0.32228300 1.97667900 1.21915100
 C 3.61865800 -0.46840900 0.43832900
 C 0.98333700 -1.34461800 0.01551100
 C 2.06548600 -2.18897300 -0.30961500
 C 3.39334200 -1.70847800 -0.07336300
 C 1.76670300 -3.48429800 -0.82067300
 C 0.43379800 -3.85667800 -0.91921300
 C -0.57372800 -2.95402300 -0.57017800
 H 4.63705600 -0.13296500 0.60009700
 H 1.67766200 3.47778400 1.96320700
 H -0.56907100 2.57852700 1.37871800
 H 4.23226100 -2.35806800 -0.29630100
 H 0.16445800 -4.83401900 -1.30540700
 H -1.62923400 -3.19820900 -0.65931400
 N -0.29552800 -1.73685800 -0.13510300
 N 0.13711600 0.76118500 0.73953900
 C 4.04959900 2.25784600 1.66796200
 C 4.44586100 3.50560700 1.17131800
 C 4.90757400 1.56359000 2.53093700
 C 5.68206200 4.04165100 1.51901900
 H 3.78695100 4.04435700 0.49499600
 C 6.13927600 2.10612300 2.88372300
 H 4.59553000 0.60765800 2.94320100
 C 6.53125400 3.34351200 2.37560800

H 5.98291600 5.00547300 1.11791700
H 6.79176900 1.56261300 3.56126100
H 7.49518200 3.76368000 2.64880300
C 2.81857200 -4.42984100 -1.25223300
C 2.82476600 -5.74024400 -0.75890400
C 3.78472700 -4.05084400 -2.19371900
C 3.78771500 -6.64882000 -1.18723400
H 2.08195400 -6.03736300 -0.02325500
C 4.74029600 -4.96451500 -2.62718500
H 3.77001300 -3.04434700 -2.60354800
C 4.74686900 -6.26348600 -2.12195300
H 3.78911000 -7.65931500 -0.78846400
H 5.47802300 -4.66160300 -3.36482600
H 5.49635700 -6.97457800 -2.45791000
C -0.90956300 -1.56165500 3.05404100
O 0.29677000 -1.56399500 2.80373400
O -1.86631300 -1.16242900 2.28478100
C -1.41597600 -2.07019700 4.39945500
H -2.01735200 -1.29787300 4.89014800
H -2.06871200 -2.93584600 4.24406900
H -0.58221500 -2.35372000 5.04570900
Cu -1.75156700 -0.51382500 0.44533400
C -4.42763300 -0.91049700 0.14537800
N -3.56217400 0.02829200 0.52244600
H -3.90644000 0.91746700 0.86053600
O -4.06357500 -1.98148800 -0.38054800
C -5.89413000 -0.63898400 0.34026600
C -6.79854300 -1.26340800 -0.52287500
C -6.38066000 0.18935600 1.35614500
C -8.16532100 -1.04066300 -0.39348700
H -6.40775600 -1.92401900 -1.29086600
C -7.74980000 0.40238600 1.49491100
H -5.69209000 0.64641700 2.06259100
C -8.64420700 -0.20562200 0.61582100
H -8.85968400 -1.52256500 -1.07673700
H -8.11871200 1.03863900 2.29492000
H -9.71236400 -0.03613400 0.72235600
C -1.96803100 0.10408100 -1.43218000
C -0.71192100 0.30154900 -2.28509300
C -2.23642100 1.60047100 -1.53630000
H -2.71662300 -0.60624000 -1.77839900
H -0.76239700 -0.22834500 -3.24450000
H 0.27048000 0.12723800 -1.84265800
H -3.17298400 1.86576300 -2.03984700

H -2.16086500 2.17124000 -0.60490700
N -1.03974800 1.72173100 -2.37676600
C -0.09495200 2.70175500 -2.32912100
O 1.07218700 2.52031100 -2.63666500
O -0.65226400 3.85522200 -1.92849300
C 0.10170000 5.10330500 -1.97027100
C -0.92695200 6.13029300 -1.51840800
H -0.47477600 7.12659600 -1.49221900
H -1.77834500 6.15087200 -2.20628200
H -1.29520400 5.88855100 -0.51588400
C 1.26882800 5.04710900 -0.99328800
H 1.97740000 4.26797200 -1.28122700
H 1.78318800 6.01400100 -0.98155000
H 0.90403100 4.84068800 0.01769000
C 0.55816300 5.38943800 -3.39541200
H -0.29786100 5.36251600 -4.07815000
H 1.00280500 6.38906200 -3.44138600
H 1.29886900 4.65844600 -3.72462900

TS-RE:

C -1.97666800 -2.23377700 1.30784600
C -2.95714100 -1.25870900 1.22525800
C -2.58684300 0.01414100 0.70693200
C -1.23332300 0.21193500 0.35499000
C -0.66989300 -1.94828100 0.90334500
C -3.50886800 1.09080200 0.50759600
C -0.79856100 1.49736500 -0.14290400
C -1.73885200 2.53163400 -0.34358400
C -3.10550300 2.28982500 0.00689600
C -1.25700000 3.76906100 -0.85901800
C 0.10492100 3.89054300 -1.08659100
C 0.95775000 2.80581600 -0.84778900
H -4.55319800 0.93789800 0.75627600
H -2.21496300 -3.21603900 1.70178800
H 0.10617600 -2.70683600 0.95817800
H -3.82861900 3.08783700 -0.12071700
H 0.51153900 4.81575300 -1.48240800
H 2.02631500 2.86401600 -1.04068000
N 0.51619400 1.64371300 -0.39989400
N -0.30441400 -0.76408800 0.44653900
C -4.33270000 -1.57667200 1.66578700
C -4.97508200 -2.71337300 1.15947900
C -4.99066900 -0.79017300 2.62033000

C -6.25584900 -3.04862100 1.58762700
 H -4.47079000 -3.32317600 0.41388000
 C -6.26807100 -1.13288100 3.05309100
 H -4.48766900 0.07711000 3.03964900
 C -6.90509300 -2.25925700 2.53507400
 H -6.74786300 -3.92690600 1.17913400
 H -6.76417300 -0.52076000 3.80102600
 H -7.90409200 -2.52246100 2.87134900
 C -2.15234600 4.90708900 -1.16333600
 C -1.87124400 6.17607400 -0.64260900
 C -3.25614500 4.74957200 -2.01197600
 C -2.68534000 7.26150300 -0.95220300
 H -1.02019300 6.30324300 0.02134700
 C -4.06394400 5.83804600 -2.32635900
 H -3.46646300 3.77448300 -2.44358200
 C -3.78315100 7.09531400 -1.79435500
 H -2.46208600 8.23853500 -0.53281700
 H -4.91147800 5.70391900 -2.99270200
 H -4.41694100 7.94360000 -2.03743800
 C 1.36303200 0.50035900 3.01175800
 O 0.36755800 1.19241500 2.77060300
 O 2.08842200 -0.11448600 2.14630100
 C 1.84322300 0.32909500 4.45045100
 H 1.94765800 -0.73467400 4.68984500
 H 2.83508200 0.78248100 4.56120800
 H 1.15303500 0.79829300 5.15556500
 Cu 1.67163500 -0.09308800 0.15429800
 C 4.32153800 0.66869900 -0.45455100
 N 3.49740000 -0.37656300 -0.23677800
 H 3.82347900 -1.12804800 0.36200600
 O 4.06970800 1.58185500 -1.24705600
 C 5.59712100 0.64434200 0.33204400
 C 6.76835300 1.11890600 -0.26276100
 C 5.61260200 0.21299100 1.66297000
 C 7.95909100 1.12460200 0.45542300
 H 6.73001600 1.47810700 -1.28709200
 C 6.80435600 0.23667600 2.38349100
 H 4.68139500 -0.09467500 2.13677600
 C 7.97858800 0.68153700 1.77866500
 H 8.87286000 1.48022500 -0.01298500
 H 6.81390200 -0.08495100 3.42142400
 H 8.90841200 0.69417000 2.34104800
 C 2.25037800 -0.74312500 -1.77063300
 C 0.83738700 -0.76961500 -2.43976700

C 2.27003700 -2.26647400 -1.85779600
 H 2.97066800 -0.16303800 -2.33526500
 H 0.88333600 -0.29590200 -3.42874800
 H -0.04910900 -0.41526300 -1.91736600
 H 3.05877500 -2.68554400 -2.49196900
 H 2.26847800 -2.79497300 -0.89763700
 N 0.94750700 -2.22119900 -2.48501100
 C -0.10166100 -3.06529800 -2.28280300
 O -1.26403900 -2.74215400 -2.46435000
 O 0.35056400 -4.26569000 -1.88750600
 C -0.55221800 -5.40792300 -1.78197800
 C 0.38810400 -6.54257400 -1.40130000
 H -0.17809500 -7.47072400 -1.27592200
 H 1.14219600 -6.69567900 -2.17999900
 H 0.90010300 -6.31704800 -0.45998300
 C -1.57843300 -5.16824200 -0.68228700
 H -2.21527800 -4.31519000 -0.92451800
 H -2.20326400 -6.05995600 -0.56520700
 H -1.07339000 -4.97973700 0.27107900
 C -1.20757200 -5.67910200 -3.13032300
 H -0.44272200 -5.78260400 -3.90741500
 H -1.77370800 -6.61492700 -3.07882100
 H -1.88715600 -4.87052000 -3.40564900

TS-OSM:

C -3.30207200 -3.28631900 -0.27565500
 C -4.30892300 -2.34774200 -0.45480500
 C -3.98110800 -0.97435200 -0.25907500
 C -2.66516000 -0.67604400 0.14550000
 C -2.02215800 -2.88835700 0.12602900
 C -4.88250500 0.11964900 -0.46458700
 C -2.26300800 0.68371100 0.37340000
 C -3.16824900 1.74153600 0.15826200
 C -4.49735600 1.41087700 -0.26069000
 C -2.69407400 3.06457900 0.39674600
 C -1.39563500 3.21235600 0.86392800
 C -0.57438100 2.09471600 1.05114700
 H -5.89305400 -0.09037100 -0.79664600
 H -3.51239700 -4.34210400 -0.41069600
 H -1.21971900 -3.59775600 0.30402400
 H -5.21255000 2.21178700 -0.41154100
 H -0.99545800 4.20258200 1.05477100
 H 0.45224400 2.17860200 1.39446800

N -0.99602600 0.86768500 0.79940400
 N -1.71929400 -1.61952900 0.33936700
 C -5.66579600 -2.79497500 -0.83357600
 C -5.83514400 -3.66082100 -1.92117700
 C -6.78829600 -2.40523100 -0.09068500
 C -7.10377700 -4.11313900 -2.26986400
 H -4.96894900 -3.96251500 -2.50435200
 C -8.05428400 -2.86730000 -0.43610300
 H -6.66339800 -1.76079300 0.77538800
 C -8.21570800 -3.71742000 -1.52868900
 H -7.22360800 -4.77497300 -3.12287900
 H -8.91538900 -2.56664000 0.15388800
 H -9.20559400 -4.07357300 -1.79964000
 C -3.52760300 4.26282200 0.16384500
 C -3.65390000 5.22924300 1.16958400
 C -4.15809400 4.47551800 -1.06943500
 C -4.40886500 6.37734100 0.95181200
 H -3.17234100 5.06687400 2.13030900
 C -4.90462900 5.62915400 -1.28713400
 H -4.03910200 3.74725400 -1.86728700
 C -5.03594700 6.57968500 -0.27621400
 H -4.50832700 7.11409700 1.74384300
 H -5.37994300 5.78794700 -2.25092500
 H -5.62307700 7.47770300 -0.44642000
 C 0.50509900 -2.74501100 2.65372500
 O -0.07052800 -1.83517000 3.27380800
 O 0.74833300 -2.68431700 1.39003600
 C 0.97554100 -4.00274000 3.34812200
 H 2.06580500 -4.07081100 3.26960400
 H 0.68467000 -4.00079200 4.39988100
 H 0.55915100 -4.88350700 2.84865700
 Cu 0.09444400 -0.87853800 0.94986400
 C 2.09961800 0.42770700 0.03243800
 N 1.52393500 -0.27330400 -0.93889400
 H 1.71481000 0.09628300 -1.86607000
 O 1.74286000 0.14330100 1.25964600
 C 3.07718900 1.51323000 -0.16139100
 C 3.52390900 2.23343100 0.96089200
 C 3.53201300 1.91748900 -1.42938600
 C 4.37408300 3.32411200 0.81805600
 H 3.18488500 1.91848200 1.94223000
 C 4.38305400 3.00621400 -1.56952800
 H 3.21675000 1.38447500 -2.32264400
 C 4.80522600 3.72239800 -0.44703400

H 4.70560100 3.86528000 1.70065200
 H 4.71826100 3.29986800 -2.56100400
 H 5.47029800 4.57421000 -0.55890300
 C 2.45383900 -2.12273100 -1.30987000
 C 3.23858900 -2.49022700 -0.07343700
 C 3.74516400 -1.86193500 -2.05869600
 H 1.60151600 -2.66934400 -1.69632400
 H 3.16626600 -3.53419000 0.25406500
 H 3.08802300 -1.84022200 0.79611800
 H 3.97494200 -2.54964500 -2.88553600
 H 3.92289400 -0.83632500 -2.40821400
 N 4.46777200 -2.18590500 -0.82234100
 C 5.54300400 -1.55580400 -0.28716100
 O 5.83489400 -1.61353800 0.89790800
 O 6.22676600 -0.90672600 -1.24770500
 C 7.45561100 -0.19440600 -0.93257800
 C 7.81591600 0.44786800 -2.26574800
 H 8.75160300 1.00835000 -2.17301900
 H 7.94049200 -0.31558100 -3.04082500
 H 7.02460100 1.13766100 -2.57824600
 C 7.20712200 0.88023600 0.11905200
 H 6.98686000 0.43809000 1.09129100
 H 8.09826900 1.51191900 0.20651400
 H 6.36551500 1.51223400 -0.17908500
 C 8.52531300 -1.18928400 -0.49963400
 H 8.66629800 -1.95563500 -1.26979200
 H 9.47788200 -0.66867500 -0.35330200
 H 8.24136700 -1.67388800 0.43697600

P:

C -2.75024700 0.88517400 -0.37060500
 N -1.61742100 0.13266800 -0.35310400
 H -1.65226000 -0.79815200 0.04005500
 O -2.75359500 2.07278400 -0.68151400
 C -4.01167000 0.17548000 0.01706700
 C -5.07981400 0.96194000 0.45785000
 C -4.17206200 -1.21149700 -0.07063100
 C -6.28156600 0.37145500 0.83088600
 H -4.94805000 2.03888600 0.50142200
 C -5.37866300 -1.80133700 0.29513300
 H -3.37113500 -1.83926200 -0.45377000
 C -6.43243500 -1.01253100 0.75214600
 H -7.10322000 0.99067700 1.18109200

H -5.49807700 -2.87853700 0.21524500
 H -7.37290600 -1.47546500 1.03957100
 C -0.33161800 0.65635400 -0.70071200
 C 0.57006600 -0.27324300 -1.55349600
 C 0.76434400 0.61436200 0.39857100
 H -0.48665800 1.64630900 -1.12771000
 H 0.95379100 0.16436500 -2.48154300
 H 0.13789700 -1.25758500 -1.76975900
 H 1.25826800 1.56971900 0.60465400
 H 0.44816600 0.15632500 1.34296100
 N 1.53551500 -0.27777800 -0.46274700
 C 2.87720300 -0.41706500 -0.59263700
 O 3.40762900 -0.89922800 -1.58092600
 O 3.48918800 0.03043500 0.51773700
 C 4.94055500 -0.02293000 0.64422700
 C 5.17942500 0.57911700 2.02115100
 H 6.25117200 0.59271700 2.24427900
 H 4.80289100 1.60680700 2.06460500
 H 4.67148300 -0.00847800 2.79342200
 C 5.41728800 -1.46850200 0.60057700
 H 5.24343000 -1.90963800 -0.38288100
 H 6.48997300 -1.50769000 0.81963200
 H 4.89271500 -2.06518100 1.35522500
 C 5.59322500 0.83164200 -0.43426600
 H 5.18440500 1.84813600 -0.41293000
 H 6.67135400 0.89345500 -0.25030400
 H 5.43014800 0.40592000 -1.42624600

ComA3:

B -1.63369200 -0.00797100 0.01295000
 H -1.99433200 0.05628000 -1.15029600
 H -1.98375700 0.96741600 0.65580000
 H -1.97539900 -1.05234200 0.54167800
 N -0.01407600 -0.00009300 -0.00005000
 C 0.49958600 -0.07879100 1.38491900
 H 0.12730300 0.77762300 1.95035300
 H 0.13645400 -0.99921100 1.84614800
 H 1.59518300 -0.07299300 1.38171200
 C 0.48728000 -1.16033300 -0.76852100
 H 0.12063700 -2.07781600 -0.30411400
 H 0.10890600 -1.09958100 -1.79076100
 H 1.58289700 -1.16241100 -0.77808900
 C 0.47619400 1.24627900 -0.62795200

H 0.09490100 1.30268800 -1.64933700
 H 0.10413900 2.09998800 -0.05815200
 H 1.57170300 1.25793000 -0.64001700

TS1:

B 1.83802600 -0.68038700 -0.97008600
 H 0.96074300 0.06473800 -0.27326300
 H 1.49442900 -1.83999800 -0.90503500
 H 1.97089000 -0.20313200 -2.07551100
 N 3.18212900 -0.46914300 -0.13073300
 C 4.27689400 -1.24769900 -0.75324200
 H 4.00572500 -2.30538700 -0.75265800
 H 4.41301000 -0.90904600 -1.78237100
 H 5.20486300 -1.10239500 -0.18954100
 C 3.54104800 0.96971900 -0.11703700
 H 3.71181300 1.30041600 -1.14350400
 H 2.70406300 1.52555500 0.30989400
 H 4.44768600 1.12104900 0.47790000
 C 2.97976500 -0.93140800 1.26358100
 H 2.16093900 -0.36035800 1.70463400
 H 2.71869400 -1.99134300 1.24883900
 H 3.89913000 -0.78344200 1.83963200
 C -0.81757000 1.35085000 0.16696900
 C -0.60333800 2.04945500 -1.18078300
 H -1.51442800 2.53154400 -1.55045000
 H 0.16804600 2.81855900 -1.06480800
 H -0.26210600 1.33120800 -1.93341400
 C -1.34985300 2.36156900 1.19772900
 H -1.46707000 1.87980400 2.17382600
 H -0.64702900 3.19579100 1.30011400
 H -2.32349900 2.75515100 0.88527100
 C -1.82242400 0.20088700 0.04550800
 C -1.54235600 -1.04158800 0.61780500
 C -3.05229500 0.37088900 -0.60163400
 C -2.45612700 -2.09072800 0.53631900
 H -0.59276600 -1.17626800 1.12533700
 C -3.96841300 -0.67450900 -0.68428000
 H -3.30412200 1.33049200 -1.04686700
 C -3.67311700 -1.91315800 -0.11693600
 H -2.21377700 -3.05153600 0.98502700
 H -4.91600400 -0.52081500 -1.19552700
 H -4.38674900 -2.73076700 -0.18346700
 O 0.40365000 0.92255300 0.69593800

ComB3:

B -1.89609900 -0.46244800 -0.06795400
H -2.14425700 0.65981000 0.30978600
H -1.95252000 -1.39608300 0.69941700
N -0.53615700 -0.49539500 -0.90308300
C 0.61822200 -0.22036600 -0.01166100
H 0.48511300 0.76300200 0.44332200
H 0.64694600 -0.97985100 0.77180600
H 1.55487200 -0.24022600 -0.58265300
C -0.35987300 -1.82897800 -1.52283500
H -0.32756000 -2.58416700 -0.73521800
H -1.21177400 -2.02820600 -2.17592200
H 0.57067400 -1.85581500 -2.10073000
C -0.57531800 0.53051300 -1.97049400
H -1.42792600 0.32733200 -2.62153900
H -0.69886200 1.51364400 -1.51250200
H 0.35430300 0.50625500 -2.54988800

R1:

C 0.26224400 -0.70628300 0.53426700
C 1.43629400 0.23263300 0.86426700
C 0.62351600 1.40122700 0.27764000
H 0.46739900 -1.53003400 -0.15459400
H -0.25094100 -1.09202900 1.42312600
H 1.70398600 0.31429300 1.91544000
H 1.06186100 1.92748900 -0.57456000
H 0.29715400 2.13015700 1.02931000
N -0.41064200 0.43693200 -0.08338900
I 3.30988600 -0.21373200 -0.15296000
C -1.74073000 0.71502000 -0.12619800
O -2.18074600 1.84655200 -0.24594100
O -2.44393000 -0.42476900 -0.04000100
C -3.90276900 -0.40635200 -0.05936700
C -4.25809100 -1.88077900 0.06392600
H -5.34570200 -2.00645300 0.06192300
H -3.84077300 -2.45029900 -0.77340200
H -3.86250000 -2.29696400 0.99680600
C -4.40433000 0.15996100 -1.38127200
H -5.49336600 0.05295000 -1.43532200
H -4.14987900 1.21729400 -1.47781600
H -3.96530300 -0.38833100 -2.22234600

C -4.42864900 0.37354200 1.13845100
H -4.17154500 1.43224600 1.06343500
H -5.51891800 0.27916900 1.18829800
H -4.00846400 -0.02826400 2.06755400

TS2:

C 1.21139200 -1.02234200 -0.91942200
C -0.19403700 -0.45202900 -1.09162400
C 0.27261500 0.83940300 -0.42620800
H 1.29728400 -1.97825900 -0.39022100
H 1.79130200 -1.07108700 -1.85136800
H -0.67335500 -0.42873100 -2.06641200
H -0.29996600 1.18756300 0.44062200
H 0.40985500 1.67830600 -1.12293000
N 1.52399900 0.15424500 -0.10596400
I -1.78622900 -1.57459900 0.21007600
C 2.72059400 0.75687600 0.10378800
O 2.83660400 1.93018300 0.42190200
O 3.71198000 -0.13537600 -0.06768200
C 5.10487000 0.25023300 0.10964900
C 5.85029900 -1.04435500 -0.18162400
H 6.92981500 -0.88771600 -0.08686400
H 5.55007900 -1.82926800 0.52089100
H 5.63762100 -1.39117100 -1.19867000
C 5.35052300 0.69823700 1.54469400
H 6.42247100 0.86460900 1.69954400
H 4.81635100 1.62465100 1.76481400
H 5.02029600 -0.07565000 2.24679400
C 5.48282200 1.32495200 -0.90160600
H 4.94560500 2.25505800 -0.70517900
H 6.55940900 1.52132000 -0.84687800
H 5.24857500 0.98923000 -1.91831900
B -3.14527600 0.97629900 -1.05359200
H -2.25245900 1.77684100 -1.10556700
H -3.57633000 0.40241600 -2.01531200
N -4.25671900 1.36387200 -0.00608300
C -5.01897300 2.52491900 -0.54121800
H -5.46811300 2.24265800 -1.49531000
H -5.80441500 2.81203700 0.16844800
H -4.33240000 3.35994800 -0.69341500
C -3.64392800 1.74715500 1.29079200
H -4.42780800 2.03625900 1.99826400
H -3.08193900 0.89620100 1.67925900

H -2.96610700 2.58674100 1.12549700
C -5.19464600 0.23345600 0.20766300
H -5.64295800 -0.03838300 -0.74975700
H -4.63954900 -0.61855800 0.60354400
H -5.97555300 0.53291600 0.913699000

IM4:

C -2.15900100 1.28731600 -0.08166700
C -3.45959400 0.63681700 0.28660000
C -2.89124800 -0.72945400 0.03788200
H -2.16691100 1.95050800 -0.95870700
H -1.61901500 1.79853800 0.72950800
H -4.47631500 1.00765400 0.30677600
H -3.35734700 -1.32059200 -0.76359900
H -2.76832500 -1.38096500 0.91662500
N -1.64565400 -0.06390800 -0.36358700
C -0.40109600 -0.55795300 -0.13159000
O -0.17303300 -1.74301000 0.04900300
O 0.49676900 0.44150800 -0.16743200
C 1.91757100 0.17971100 0.02788700
C 2.53329400 1.56677100 -0.08496800
H 3.61780700 1.50764100 0.05240800
H 2.33175200 2.00132600 -1.06985100
H 2.12318600 2.23602100 0.67906500
C 2.44037200 -0.72980000 -1.07580000
H 3.52887500 -0.82062700 -0.99147400
H 1.99833500 -1.72559300 -1.00698700
H 2.20819900 -0.30649400 -2.05947400
C 2.15830600 -0.39949200 1.41581500
H 1.72309000 -1.39629900 1.50964400
H 3.23550500 -0.46685700 1.60347300
H 1.71923100 0.25161300 2.18018200

ComC3:

B -0.60324600 1.05858000 -0.00062100
H -0.64721100 1.68740100 1.02274500
H -0.64721500 1.68627100 -1.02468100
N -1.80462400 0.00197000 -0.00001600
C -3.04665600 0.82288800 -0.00003900
H -3.06030000 1.45223400 0.89188600
H -3.06089100 1.45131500 -0.89259900
H -3.91745400 0.16011800 0.00059700

C -1.80685800 -0.85544500 -1.21113800
H -1.80348700 -0.21700300 -2.09662500
H -0.91231200 -1.47983400 -1.21046700
H -2.70042600 -1.48699100 -1.20840100
C -1.80629500 -0.85454400 1.21174300
H -0.91155100 -1.47865700 1.21128600
H -1.80288300 -0.21544200 2.09675000
H -2.69966800 -1.48636900 1.20971200
I 1.46737500 -0.00107800 -0.00000700

TS3:

B 2.37591700 -0.80651100 -0.70057900
H 1.88555600 0.53945400 -0.56729900
H 1.58953400 -1.54225700 -0.13957800
H 2.57926000 -1.03559900 -1.87521400
N 3.77254100 -0.83766600 0.08721500
C 4.33642600 -2.20800500 0.04860000
H 3.63050900 -2.89335500 0.52126300
H 4.48186300 -2.50063400 -0.99297400
H 5.29442200 -2.23627900 0.58076700
C 4.73019900 0.09794600 -0.54527200
H 4.88609000 -0.20236100 -1.58307600
H 4.31053600 1.10543900 -0.52024300
H 5.68333200 0.08005800 -0.00596900
C 3.56687300 -0.43997400 1.49924900
H 3.17846100 0.57946700 1.52779800
H 2.84235200 -1.11712900 1.95524800
H 4.51590300 -0.48978500 2.04366000
C -0.12060300 1.60460200 -1.14970700
C 1.20107300 1.77899100 -0.40909800
C 0.44464100 1.73556500 0.91554200
H -0.46701100 2.45410100 -1.75273400
H -0.21457000 0.68579800 -1.74591000
H 1.87612700 2.60047800 -0.64864900
H 0.42938600 2.66210000 1.50516800
H 0.68570300 0.89669500 1.58446700
N -0.78848000 1.51435100 0.15647000
C -1.77984300 0.67194200 0.53687900
O -1.96474700 0.32269600 1.69313600
O -2.51840800 0.32247300 -0.53403100
C -3.61459900 -0.62548600 -0.40754500
C -4.12032100 -0.74580500 -1.83796100
H -4.96218600 -1.44445800 -1.88279600

H -4.45665500 0.22758400 -2.21094900
H -3.32759200 -1.11394300 -2.49804700
C -4.70235500 -0.05988900 0.49681700
H -5.57225300 -0.72604400 0.48771700
H -4.34493200 0.04048000 1.52339600
H -5.02261500 0.92403700 0.13586900
C -3.09172500 -1.96758300 0.08871000
H -2.72829700 -1.89187700 1.11550000
H -3.89388500 -2.71307700 0.05236400
H -2.27183300 -2.31429900 -0.55038100

P2:

C -3.52581700 0.61041300 0.13372400
C -2.84126900 -0.77324000 0.03751000
C -2.13087400 1.25280600 -0.04268900
H -4.21402800 0.81964200 -0.68791300
H -3.19716400 -1.43967000 -0.75523600
H -2.79247800 -1.33269100 0.97949800
H -2.01087700 1.93709300 -0.88904800
H -1.72278100 1.72446800 0.85902200
N -1.59446400 -0.08653500 -0.27935400
C -0.34368400 -0.57126800 -0.09572800
O -0.09489300 -1.75922100 0.04058500
O 0.54119100 0.44289700 -0.11298400
C 1.96979600 0.19199500 0.01881900
C 2.56591300 1.58973500 -0.06635500
H 3.65599500 1.53936800 0.02151100
H 2.31644200 2.05931600 -1.02384100
H 2.18196000 2.22373800 0.74012200
C 2.27112200 -0.43402500 1.37431900
H 1.84394800 -1.43577600 1.44977000
H 3.35545500 -0.50174000 1.51538200
H 1.86129800 0.18691900 2.17891100
C 2.46138500 -0.67070800 -1.13612300
H 2.18159700 -0.21849700 -2.09421500
H 3.55382200 -0.74567900 -1.10012300
H 2.03821000 -1.67572200 -1.08382400
H -4.01997000 0.82132000 1.08378600

Cata4:

C 1.79858400 -3.49592800 -0.10084600
C 2.81453900 -2.55285800 -0.07424800

C 2.43990500 -1.17906400 -0.08347900
C 1.06080800 -0.87184400 -0.06526900
C 0.46053900 -3.09121600 -0.09805300
C 3.37626100 -0.09830000 -0.16463100
C 0.63148500 0.50648600 -0.05239500
C 1.58437900 1.54849400 -0.06021500
C 2.96958100 1.20077300 -0.15431900
C 1.09237800 2.88587100 -0.02925200
C -0.28205400 3.06921900 -0.04017300
C -1.14565400 1.96515500 -0.04863200
H 4.43136100 -0.32897200 -0.26310400
H 2.03475600 -4.55500400 -0.09102400
H -0.33908400 -3.82518000 -0.10440200
H 3.70424300 1.99380600 -0.24372800
H -0.69630800 4.07218400 -0.01170100
H -2.22975100 2.06097900 -0.04665600
N -0.69845800 0.72083100 -0.04343100
N 0.09000700 -1.81799800 -0.06849200
C 4.22410300 -2.99654900 -0.03337000
C 5.10539200 -2.51462600 0.94396400
C 4.68243100 -3.95124700 -0.94994700
C 6.41738500 -2.97443700 0.99725500
H 4.75189000 -1.79564000 1.67818400
C 5.99752900 -4.40264600 -0.90001200
H 4.00686800 -4.32435500 -1.71530200
C 6.86801800 -3.91559800 0.07330500
H 7.08725900 -2.59992700 1.76611700
H 6.34308700 -5.13472500 -1.62446100
H 7.89406300 -4.27030000 0.11333100
C 1.98863400 4.06166100 0.01416600
C 1.80276400 5.11284300 -0.89256800
C 2.99783600 4.16944500 0.98055500
C 2.61655400 6.24026500 -0.84330300
H 1.02685100 5.03360700 -1.64958700
C 3.80540500 5.30142700 1.03279100
H 3.13216300 3.37262200 1.70740900
C 3.61991000 6.33736700 0.11899600
H 2.46741500 7.04351300 -1.55941700
H 4.57750400 5.37618100 1.79346000
H 4.25365500 7.21889400 0.15890100
Cu -1.82221600 -1.11855800 -0.03729200
C -4.52691600 -0.21491600 0.00280100
N -3.71040900 -1.27312800 -0.00190200
H -4.20986700 -2.15381800 -0.02548600

O -4.14749000 0.97197700 -0.05382500
 C -6.01758400 -0.46980600 0.06965500
 C -6.87695100 0.49147300 -0.47064000
 C -6.57272100 -1.60264500 0.67414800
 C -8.25603700 0.31174300 -0.44110800
 H -6.43610800 1.38069000 -0.91117300
 C -7.95389600 -1.77867300 0.72056500
 H -5.92535800 -2.34287800 1.13870000
 C -8.79946800 -0.82599300 0.15537400
 H -8.91019700 1.06188000 -0.87848100
 H -8.37010100 -2.65887600 1.20395100
 H -9.87695800 -0.96551300 0.18660400

ComD3:

B -1.71223600 -0.42606300 0.04398300
 H -2.19291400 0.64487500 0.21520100
 H -2.02081900 -1.43542100 0.58603700
 N -0.52976500 -0.49665700 -0.90784200
 C 0.61872200 -0.21335500 0.01924800
 H 0.49917100 0.78305100 0.45103400
 H 0.65482400 -0.97276800 0.80358900
 H 1.53890000 -0.24979900 -0.57035400
 C -0.36797400 -1.84713000 -1.51998600
 H -0.28996200 -2.59190000 -0.72724300
 H -1.23934700 -2.05665000 -2.14281300
 H 0.53758400 -1.84871400 -2.13096700
 C -0.58873300 0.54689900 -1.97295400
 H -1.46151900 0.35778300 -2.60060500
 H -0.66931000 1.52877500 -1.50513600
 H 0.32316200 0.48609300 -2.57134000

ComF3:

C 0.36632800 0.04032600 0.88963000
 C 1.61038900 0.37590100 0.07040900
 C 0.73403000 0.42342700 -1.17934400
 H 0.24006100 -1.02453900 1.08684900
 H 0.16734400 0.61365000 1.79367100
 H 0.73643900 -0.49544700 -1.76597700
 H 0.81954800 1.28334300 -1.84030500
 N -0.49530600 0.45292100 -0.29328900
 C -1.50553400 -0.55618100 -0.70020600
 O -1.63549800 -0.85435000 -1.85529200

O -2.12915900 -0.97047400 0.36619300
 C -3.25926300 -1.93732300 0.27179300
 C -3.66787900 -2.09409800 1.72473700
 H -4.50996600 -2.78958100 1.79130400
 H -2.84129000 -2.49288900 2.32192400
 H -3.97736600 -1.13280700 2.14754100
 C -2.74591400 -3.24333400 -0.30761400
 H -3.54508000 -3.99007100 -0.25628200
 H -2.44635600 -3.13328800 -1.35223200
 H -1.89535100 -3.61488700 0.27394900
 C -4.36936100 -1.31208600 -0.55462700
 H -4.07445200 -1.18267000 -1.59857500
 H -5.24431300 -1.96942300 -0.52456700
 H -4.65699200 -0.34007400 -0.13987200
 B -1.40204800 1.80924200 -0.21321900
 H -1.87731300 1.90954900 -1.31519400
 H -2.18876300 1.60093900 0.67162100
 C 0.28759800 3.68670400 -0.87413800
 C -0.11311900 3.29887100 1.48172800
 C -1.86284500 4.17192800 0.08146900
 H 1.20463300 3.10665500 -0.77857300
 H -0.12833200 3.57540800 -1.87704800
 H -0.83531300 2.92938400 2.21187900
 H 0.79861600 2.70240100 1.51878900
 H -2.60961400 3.86422100 0.81479400
 H -2.30006800 4.16185600 -0.91786800
 N -0.71070900 3.22086000 0.12321700
 H 0.52050900 4.73879100 -0.68615300
 H -1.50005200 5.17532100 0.31918800
 H 0.14027800 4.33915700 1.70543100
 H 2.07610900 1.32581800 0.32708500
 I 3.21981300 -1.06508900 0.09084900

TS4-ComD3:

C 0.98399700 -0.00782400 -1.24300500
 C -0.45083300 0.24375600 -0.81266200
 C 0.02927000 0.43890100 0.61691000
 H 1.22913300 -1.06844000 -1.34233500
 H 1.39874900 0.54248600 -2.08694200
 H -0.09316100 -0.43918900 1.25394400
 H -0.27143200 1.32411100 1.17315200
 N 1.45820500 0.50955000 0.10562100
 C 2.36768500 -0.40047000 0.83908400

O 2.19078000 -0.63549400 2.00321000
 O 3.28922700 -0.82231100 0.01657900
 C 4.38049600 -1.71834800 0.48174100
 C 5.19303900 -1.91881800 -0.78438200
 H 6.04767800 -2.56774400 -0.56949800
 H 4.58772000 -2.38995300 -1.56588300
 H 5.57005500 -0.96184800 -1.15963300
 C 3.77729600 -3.02474300 0.96882500
 H 4.58748000 -3.72708400 1.19027800
 H 3.18841900 -2.88320600 1.87776000
 H 3.14265900 -3.46924400 0.19463600
 C 5.18588600 -0.99983100 1.55052400
 H 4.60335800 -0.84967600 2.46234700
 H 6.06350800 -1.60538700 1.79958700
 H 5.53320100 -0.02834400 1.18295700
 B 2.25619000 1.92513700 0.19424900
 H 2.41259200 2.10671400 1.37552600
 H 3.26657000 1.75842700 -0.43849000
 C 0.30870200 3.66708400 0.27388400
 C 1.37223500 3.25327000 -1.85922800
 C 2.59538700 4.31392700 -0.08276600
 H -0.50071400 3.00542700 -0.03555800
 H 0.44017600 3.62130100 1.35633000
 H 2.29255100 2.92530900 -2.34580100
 H 0.55280000 2.58082600 -2.11129500
 H 3.53373200 4.05841900 -0.57765300
 H 2.75002700 4.36276400 0.99601300
 N 1.57729900 3.26450000 -0.38752400
 H 0.05740900 4.68937400 -0.02424900
 H 2.23186800 5.27712500 -0.45117200
 H 1.11500200 4.26249300 -2.19457400
 H -0.97919000 1.07095700 -1.28083200
 I -1.90651100 -1.50487500 -1.09537900
 N -4.62647400 0.25805600 1.06585600
 C -4.82988500 -1.14721300 1.50188500
 H -4.35686300 -1.81531400 0.78004800
 H -4.36899000 -1.28319500 2.48201400
 H -5.90195000 -1.36001400 1.56229000
 C -5.24636400 0.45101600 -0.26917700
 H -5.10311800 1.48817000 -0.57847200
 H -4.75855100 -0.21371300 -0.98400800
 H -6.31563100 0.22374000 -0.21456200
 C -5.29036500 1.16460600 2.04226700
 H -4.83464600 1.02208700 3.02396700

H -5.14893500 2.19794300 1.71920800
 H -6.36109300 0.93353200 2.09201400
 B -3.09346100 0.60443400 1.02349400
 H -2.84402900 1.60787000 0.41013000
 H -2.49749800 0.25958900 2.00572100

ComE3:

C 0.26079300 0.04706700 0.82857900
 C -0.40718000 1.11855600 -0.04516400
 C -1.09496500 -0.67054400 0.91096800
 H 0.75239300 0.34707300 1.75103100
 H 0.04863600 1.35837100 -1.00921200
 H -0.58036700 2.04776500 0.51298100
 H -1.14159000 -1.72843400 0.63963300
 H -1.56632200 -0.52985000 1.89182100
 N -1.57881900 0.25331800 -0.11261700
 C -2.85688100 0.71185100 -0.28226500
 O -3.10516100 1.78668200 -0.79735600
 O -3.71910300 -0.19913600 0.17578100
 C -5.16435500 0.00718500 0.06608300
 C -5.72795400 -1.26492000 0.68210900
 H -6.82153900 -1.23357100 0.66428300
 H -5.39509600 -2.14424000 0.12124900
 H -5.39938700 -1.36794300 1.72142100
 C -5.57451500 1.22961300 0.87626500
 H -5.16295800 2.14366200 0.44435800
 H -6.66662500 1.30667700 0.88913700
 H -5.22601300 1.13306900 1.91019300
 C -5.56223900 0.12129700 -1.39937900
 H -5.19791400 -0.74650100 -1.95935200
 H -6.65410500 0.14525700 -1.47699200
 H -5.15830400 1.03082200 -1.84795700
 I 1.76521300 -1.14115900 -0.24626100
 B 3.20125800 0.63985600 -0.91142300
 H 3.59212900 0.22976700 -1.96360300
 H 2.44332100 1.56609400 -0.88158100
 N 4.38714900 0.82960900 0.10908500
 C 5.14917800 1.98630800 -0.46096400
 H 4.50346200 2.86538400 -0.48211300
 H 6.02053400 2.17991800 0.16941900
 H 5.47158000 1.73867200 -1.47334800
 C 5.29174200 -0.35149400 0.17254400
 H 6.15011700 -0.11586100 0.80619600

H 4.75132500 -1.19884100 0.59774100
H 5.62745700 -0.59593200 -0.83592200
C 3.93567700 1.18936700 1.48063400
H 3.24296300 2.03019600 1.41932100
H 3.44126700 0.32925100 1.93507000
H 4.80244200 1.46478200 2.08601900

TS5-ComE3:

C -3.76932000 -2.04601800 1.53725800
C -4.50697700 -0.94585100 1.12764900
C -3.81338600 0.28646000 0.94729900
C -2.41467600 0.28341800 1.13509600
C -2.38546100 -1.94347100 1.70587300
C -4.45475300 1.52864400 0.64117500
C -1.65978800 1.49679200 0.93292400
C -2.31384300 2.68913800 0.55797000
C -3.74129000 2.67441500 0.45940100
C -1.50541300 3.84607900 0.34978500
C -0.14128100 3.73358900 0.57852400
C 0.41454700 2.50723100 0.95776000
H -5.53710700 1.55540400 0.58018100
H -4.25454400 -3.00499700 1.68450200
H -1.79692100 -2.80826900 1.99828200
H -4.26159100 3.60401100 0.25716200
H 0.50891600 4.58866600 0.42589400
H 1.48140500 2.37732600 1.12132400
N -0.32378100 1.41957100 1.11462800
N -1.71739800 -0.81956700 1.49684200
C -5.95629600 -1.08677000 0.88312700
C -6.52345200 -0.66785000 -0.32822000
C -6.77216300 -1.69564500 1.84513300
C -7.88162300 -0.85076700 -0.56701300
H -5.89160900 -0.22482800 -1.09336700
C -8.13185900 -1.86681600 1.60700200
H -6.33990400 -2.01527500 2.78978100
C -8.68909500 -1.44544600 0.40096500
H -8.30850900 -0.53298400 -1.51389100
H -8.75728800 -2.32875100 2.36547900
H -9.75037600 -1.58288700 0.21448200
C -2.06687800 5.13608700 -0.10048600
C -1.73448500 6.31494000 0.57937200
C -2.89117900 5.20996100 -1.23167700
C -2.23010100 7.54039500 0.14638900

H -1.10253100 6.26356800 1.46214600
C -3.37648400 6.43852500 -1.66798500
H -3.12911100 4.30541700 -1.78509600
C -3.05166700 7.60488600 -0.97760100
H -1.97595300 8.44612400 0.68948000
H -4.00567200 6.48465100 -2.55220100
H -3.43604500 8.56263100 -1.31672900
Cu 0.36842600 -0.44548500 1.65653500
C 3.06670200 -0.49050400 2.21299900
N 1.96124200 -1.23005600 2.31275400
H 2.08487900 -2.14594100 2.72819400
O 3.04061900 0.67032900 1.73598500
C 4.38260200 -1.06036400 2.65094400
C 5.36663100 -0.18413300 3.11983900
C 4.67110800 -2.42582400 2.56105200
C 6.61076700 -0.66609200 3.51207800
H 5.13675500 0.87585700 3.17267400
C 5.92180400 -2.90698600 2.93874200
H 3.92917700 -3.11537800 2.16544200
C 6.89139600 -2.02930400 3.42019700
H 7.36424200 0.02105000 3.88731100
H 6.14102600 -3.96756400 2.85239700
H 7.86557300 -2.40637700 3.71910800
C 1.33519100 -0.77002500 -0.47946100
C 0.13458300 -0.56294100 -1.36731100
C 1.18866400 -2.26507800 -0.63410600
H 2.04736200 -0.10448400 0.00393000
H 0.27316000 0.09752200 -2.22726300
H -0.77540300 -0.25081300 -0.84147000
H 2.06631200 -2.81827400 -0.97747900
H 0.79764100 -2.76124200 0.26276800
N 0.15203200 -1.99993400 -1.64449600
C -1.01755400 -2.70632400 -1.78849900
O -2.05593200 -2.18297100 -2.14873600
O -0.80564000 -3.99058800 -1.49788600
C -1.85846700 -4.99132000 -1.69141800
C -1.16072600 -6.28566500 -1.30123800
H -1.85481800 -7.12596400 -1.39789400
H -0.29842400 -6.46883700 -1.94998400
H -0.81431100 -6.23842900 -0.26358200
C -3.02575300 -4.70358300 -0.75750700
H -3.50590900 -3.75492700 -1.00471800
H -3.76499400 -5.50673100 -0.84278900
H -2.67863200 -4.67016600 0.28092000

C -2.27969200 -5.02147400 -3.15426800
 H -1.40532600 -5.16977300 -3.79668900
 H -2.96843500 -5.85718500 -3.31460100
 H -2.77991000 -4.09459600 -3.44088600
 I 3.33296900 -0.40362700 -2.52347700
 B 3.73979900 1.78350300 -1.80572900
 H 3.58466100 2.46236700 -2.78184700
 H 2.96895900 1.92703500 -0.89761500
 N 5.23212500 1.94327600 -1.27844900
 C 5.28233400 3.32864700 -0.72899600
 H 4.60109700 3.39636800 0.12049500
 H 6.30279500 3.55022200 -0.40430200
 H 4.97960200 4.03442900 -1.50480000
 C 6.22618400 1.82828700 -2.37610300
 H 7.22867100 2.01394300 -1.98092900
 H 6.17919000 0.82210900 -2.79601000
 H 5.98781600 2.55805300 -3.15145000
 C 5.57686800 0.99487800 -0.18373900
 H 4.78525000 1.01876300 0.57004300
 H 5.65394700 -0.01234600 -0.59557100
 H 6.53793900 1.28333600 0.25119200

ComA8:

B -0.08743200 0.30088500 2.68218000
 H -1.13030600 0.12562700 3.22395800
 H 0.87857800 0.74243400 3.21606900
 P 0.00087700 -0.00225100 0.77856500
 C 1.66512400 -0.38639300 0.21181900
 C 2.51139800 -1.12959700 1.04282300
 C 2.08762200 0.01674900 -1.06039000
 C 3.78225000 -1.47259600 0.59420500
 H 2.18436500 -1.43795100 2.03334600
 C 3.36087000 -0.33240500 -1.49786500
 H 1.43206800 0.60118000 -1.70026000
 C 4.20451500 -1.07507000 -0.67316700
 H 4.44406500 -2.04617400 1.23646000
 H 3.69515700 -0.02080000 -2.48319800
 H 5.19930200 -1.34223200 -1.01880400
 C -1.15871700 -1.26878100 0.22651900
 C -0.80492200 -2.13408500 -0.81439100
 C -2.41983900 -1.36087000 0.83102900
 C -1.71870900 -3.08787500 -1.25126000
 H 0.17470100 -2.06817500 -1.27882300

C -3.32509700 -2.31589600 0.38247400
 H -2.69542800 -0.69234900 1.64194000
 C -2.97468300 -3.17831000 -0.65547200
 H -1.44568600 -3.76244800 -2.05745600
 H -4.30327900 -2.38988300 0.84859600
 H -3.68368200 -3.92638600 -0.99907800
 C -0.49291700 1.62735800 0.15855600
 C -1.68260700 1.80419300 -0.55543600
 C 0.33606500 2.72058800 0.45247600
 C -2.03340200 3.07963600 -0.98587600
 H -2.32326400 0.95703200 -0.78189400
 C -0.02982900 3.98969200 0.01948700
 H 1.26517500 2.57792900 0.99868800
 C -1.21240000 4.16838300 -0.69681600
 H -2.95094700 3.22210100 -1.54936600
 H 0.60942600 4.83906600 0.24167700
 H -1.49457200 5.16204000 -1.03351400

ComF8:

C 2.38920300 0.37902900 -1.35461500
 C 2.84120700 -0.92543700 -0.70451300
 C 1.90261200 -0.62684400 0.46076600
 H 3.03823900 1.23261000 -1.15129400
 H 2.09072800 0.35793000 -2.40199800
 H 2.56834100 -1.81105100 -1.27487000
 H 2.37316400 -0.12279400 1.30521400
 H 1.24835600 -1.42548800 0.80794900
 N 1.19607100 0.40083700 -0.40048400
 I 4.94100800 -1.13476700 -0.25578400
 C 0.98909700 1.70857000 0.25455900
 O 1.02222900 1.80852000 1.45137400
 O 0.81355500 2.60268800 -0.67409200
 C 0.62557700 4.04326200 -0.34149100
 C 0.46689500 4.66530700 -1.71722300
 H 0.33045800 5.74553800 -1.61383900
 H 1.35542500 4.48351200 -2.32945600
 H -0.40660800 4.25091500 -2.22986200
 C 1.87354600 4.54739800 0.36353200
 H 1.78414700 5.62853200 0.50833400
 H 1.99753600 4.07913500 1.34248600
 H 2.76364300 4.35707100 -0.24495400
 C -0.63299700 4.19769900 0.49332600
 H -0.51466200 3.76409300 1.48758300

H -0.85299800 5.26409600 0.60377500
 H -1.48568400 3.72099700 -0.00018700
 B -0.09078100 -0.13611400 -1.19770800
 P -1.68896700 -0.58128000 -0.15088500
 C -1.47708400 -2.04412900 0.90546900
 C -0.69551400 -3.10469500 0.42347800
 C -2.14083200 -2.17549200 2.13093900
 C -0.56034400 -4.26797900 1.17337700
 H -0.20120400 -3.03034300 -0.54100500
 C -1.99984600 -3.34353900 2.87576400
 H -2.76846300 -1.37342000 2.50588700
 C -1.20730900 -4.38626400 2.40246300
 H 0.04933200 -5.08297600 0.79510900
 H -2.51432400 -3.43631500 3.82748200
 H -1.09829600 -5.29444100 2.98794200
 C -2.38238300 0.74484300 0.88090400
 C -1.80444600 1.03462900 2.12439800
 C -3.47583900 1.49461100 0.43142200
 C -2.32415000 2.05718200 2.91051900
 H -0.95375400 0.46551500 2.48505200
 C -3.98213600 2.52449200 1.21976700
 H -3.93971300 1.27153500 -0.52450100
 C -3.41069200 2.80418900 2.45892600
 H -1.87541000 2.27115100 3.87587800
 H -4.83154200 3.10132000 0.86633500
 H -3.81302200 3.60329000 3.07467500
 C -2.94836500 -1.02620700 -1.38200000
 C -3.82034700 -2.09256800 -1.13140800
 C -3.07147500 -0.28869400 -2.56732400
 C -4.80578300 -2.41522800 -2.05908900
 H -3.72965200 -2.67375900 -0.21872600
 C -4.06173500 -0.61767700 -3.48817100
 H -2.40152400 0.53897900 -2.77492300
 C -4.92730600 -1.67999300 -3.23632900
 H -5.47778500 -3.24488800 -1.86082900
 H -4.15289100 -0.04355400 -4.40539900
 H -5.69638000 -1.93608800 -3.95928900
 H -0.41215700 0.71638400 -1.97968900
 H 0.22562100 -1.16937200 -1.73407300

TS4-ComD8:

C -0.31601300 -0.45073200 1.22506900
 C 0.03070400 -1.61950400 0.33151000

C -1.36991500 -1.58644900 -0.23533300
 H -0.55081400 -0.71784200 2.25842600
 H 0.32313800 0.43126300 1.20471000
 H -2.05096200 -2.33764600 0.17156200
 H -1.48857600 -1.52325100 -1.31903500
 N -1.62039000 -0.25152600 0.45372800
 C -1.61178300 0.88968100 -0.48377700
 O -2.18205200 0.81106600 -1.54105300
 O -0.96707400 1.88746400 0.04788600
 C -0.70229500 3.14415800 -0.70740100
 C 0.12446200 3.93462300 0.29106100
 H 0.40326200 4.89745100 -0.14723500
 H -0.44620200 4.11919200 1.20641200
 H 1.03894200 3.39049800 0.54527000
 C -2.02083200 3.82970600 -1.01300900
 H -1.81444300 4.79211200 -1.49181900
 H -2.63994400 3.23167000 -1.68448500
 H -2.57734900 4.01753100 -0.09072200
 C 0.09868100 2.80959100 -1.95437700
 H 1.00025200 2.24635300 -1.69635600
 H -0.49335500 2.23275800 -2.66814800
 H 0.40410400 3.74491000 -2.43403600
 C 4.47905800 1.14409500 -0.37170200
 C 4.00163200 2.32937600 0.20275300
 C 4.67143700 1.06962700 -1.75404300
 C 3.73895500 3.43373200 -0.60074300
 H 3.84906800 2.39390000 1.27743200
 C 4.39697400 2.17742300 -2.55442300
 H 5.03909600 0.15265000 -2.20483700
 C 3.93391600 3.35797400 -1.98051200
 H 3.38406900 4.35604000 -0.14992900
 H 4.54929000 2.11501000 -3.62803600
 H 3.72550800 4.22146700 -2.60593600
 C 5.69885000 -1.50912500 -0.25820600
 C 5.09764800 -2.65168600 -0.79643800
 C 7.06195000 -1.27005800 -0.47597100
 C 5.85608400 -3.54569600 -1.54848400
 H 4.04180500 -2.83919800 -0.62936600
 C 7.81238500 -2.16530000 -1.22968700
 H 7.53919900 -0.39158400 -0.05027800
 C 7.20994000 -3.30308900 -1.76678200
 H 5.38592200 -4.43276000 -1.96302000
 H 8.86943300 -1.97761500 -1.39442800
 H 7.79916800 -4.00227500 -2.35346300

C 5.73931200 0.23551300 2.07646600
 C 6.64055100 1.29922000 1.95192100
 C 5.64248700 -0.45689400 3.28831100
 C 7.44229200 1.65859800 3.03203400
 H 6.70962500 1.85322800 1.01965100
 C 6.44785200 -0.09453900 4.36365300
 H 4.93263400 -1.27521400 3.38725800
 C 7.34747100 0.96260700 4.23588500
 H 8.13943800 2.48577300 2.93310000
 H 6.36930800 -0.63432800 5.30296100
 H 7.97254900 1.24780500 5.07741800
 P 4.70117800 -0.32220900 0.68289100
 B 3.02011300 -1.01684800 1.21789400
 H 2.36053400 -0.22146100 1.82561000
 H 2.92404600 -2.19862100 1.38333300
 I 1.58422800 -1.00551100 -1.32985200
 H 0.44468500 -2.53074800 0.75181000
 C -4.77600500 -1.76096400 -0.59854500
 C -5.37169700 -2.95676400 -0.18218100
 C -4.23237200 -1.66586300 -1.88834800
 C -5.41583500 -4.04861600 -1.04544500
 H -5.80597300 -3.03862600 0.80946100
 C -4.28696800 -2.76016400 -2.74501700
 H -3.76158000 -0.74493200 -2.21795100
 C -4.87493500 -3.95254900 -2.32491800
 H -5.88032900 -4.97324800 -0.71577300
 H -3.86724000 -2.67931700 -3.74341700
 H -4.91368900 -4.80519500 -2.99671900
 C -5.21376700 1.13410800 -0.30740400
 C -4.96910500 2.37303300 0.29751600
 C -5.97442600 1.07057400 -1.47979600
 C -5.47528000 3.53650300 -0.27208600
 H -4.38913800 2.43013500 1.21440100
 C -6.46604200 2.24107700 -2.05114500
 H -6.18722800 0.11433000 -1.94703300
 C -6.21760500 3.47276000 -1.44969000
 H -5.28421300 4.49478300 0.20198500
 H -7.04963500 2.18694700 -2.96535000
 H -6.60632600 4.38338300 -1.89621700
 C -5.84067700 -0.63638100 1.88865700
 C -7.11017000 -0.04991700 1.81471200
 C -5.51982500 -1.46100700 2.97532400
 C -8.04509000 -0.28550000 2.81771300
 H -7.36895300 0.59280000 0.97879000

C -6.46194400 -1.69334700 3.97307700
 H -4.54162800 -1.92448400 3.04615800
 C -7.72266500 -1.10532700 3.89703100
 H -9.02655800 0.17503400 2.75472500
 H -6.20649500 -2.33281500 4.81283700
 H -8.45379500 -1.28569000 4.67984700
 P -4.63920300 -0.35677100 0.55041100
 B -2.88800000 -0.17831700 1.42459400
 H -2.80794100 -1.13498400 2.15258600
 H -2.87566200 0.87281900 2.01387400

ComE8:

C -2.05215600 0.52675700 -1.28901700
 C -1.62634200 1.95540000 -1.64809900
 C -2.73663400 2.47769900 -0.72337900
 H -2.58571500 0.04505600 -2.11757500
 H -1.29817500 -0.16115300 -0.89892800
 H -3.58545600 2.88127300 -1.28936100
 H -2.46310500 3.18520700 0.06382600
 N -2.93560500 1.10300000 -0.27637200
 C -4.14874700 0.61934300 0.13111100
 O -5.01863600 1.33783800 0.58944100
 O -4.18684200 -0.70445000 -0.04263300
 C -5.38897400 -1.47047200 0.28764800
 C -4.98964000 -2.89169200 -0.08125100
 H -5.81895200 -3.57597100 0.12145000
 H -4.73617300 -2.95553400 -1.14436500
 H -4.12092200 -3.21332900 0.50154200
 C -6.55365700 -0.99815300 -0.57299500
 H -7.41538800 -1.65320500 -0.40868400
 H -6.83821000 0.02543000 -0.32260100
 H -6.28427400 -1.04601900 -1.63359300
 C -5.69041800 -1.35630600 1.77610900
 H -5.97371000 -0.33633400 2.04170000
 H -6.51430000 -2.03040700 2.03186100
 H -4.81551000 -1.64711100 2.36684000
 C 0.64812900 -1.08403000 0.68548700
 C 0.20852100 -2.38205600 0.40086900
 C -0.07569300 -0.27892300 1.57739500
 C -0.94578000 -2.86892400 1.00707100
 H 0.76703400 -3.01394400 -0.28329000
 C -1.22915800 -0.77393500 2.17592500
 H 0.26266000 0.72519100 1.81462900

C -1.66214600 -2.06749800 1.89276000
 H -1.28119100 -3.87857800 0.78968300
 H -1.78852500 -0.14733400 2.86356900
 H -2.55658800 -2.45466500 2.37072900
 C 3.04597200 0.56983900 0.98047700
 C 3.81872800 1.63753500 0.50479900
 C 3.06773400 0.24107800 2.34209300
 C 4.59826700 2.37548100 1.38974800
 H 3.82335100 1.88710500 -0.55268700
 C 3.85288900 0.98324000 3.21881700
 H 2.47043300 -0.58442900 2.71853000
 C 4.61397400 2.05020200 2.74474300
 H 5.19352700 3.20441200 1.01920100
 H 3.86669500 0.72813100 4.27408500
 H 5.22172400 2.62958700 3.43351800
 C 3.09263900 -1.77849000 -0.78870100
 C 4.12946600 -2.28290400 0.00420100
 C 2.82040200 -2.34745000 -2.03969200
 C 4.88379100 -3.35867100 -0.45214200
 H 4.35278000 -1.83504400 0.96807400
 C 3.57999700 -3.42471200 -2.48615300
 H 2.02225900 -1.95541800 -2.66376900
 C 4.60919600 -3.92945700 -1.69386300
 H 5.68961700 -3.74867400 0.16229900
 H 3.36972800 -3.86541700 -3.45595100
 H 5.20234600 -4.76783000 -2.04724100
 P 2.07788700 -0.40255300 -0.19569600
 B 1.54537300 0.64878900 -1.74305200
 H 0.71581000 0.08042100 -2.39736400
 H 2.48403500 1.10995300 -2.32467100
 I 0.38364500 2.51435900 -0.94644600
 H -1.62327100 2.25643400 -2.69273000

TS5-ComE8:

C 2.33919900 1.26385100 -2.72878800
 C 2.20758500 2.53345900 -2.18431500
 C 0.92975400 2.90705200 -1.67600000
 C -0.10017900 1.93981000 -1.70999000
 C 1.25765400 0.37805900 -2.71684800
 C 0.62454700 4.20878200 -1.16393800
 C -1.40905800 2.26371300 -1.19426600
 C -1.65244500 3.52979600 -0.62261800
 C -0.60369500 4.50297800 -0.65330500

C -2.95632700 3.77529500 -0.10004300
 C -3.91359600 2.78634100 -0.26176800
 C -3.57440300 1.56144700 -0.84929500
 H 1.38731000 4.97834600 -1.20687000
 H 3.29812500 0.92785500 -3.10956400
 H 1.36519100 -0.62839500 -3.10847200
 H -0.80892000 5.50394100 -0.28977900
 H -4.91878900 2.93592000 0.11725600
 H -4.28719900 0.74654100 -0.94831200
 N -2.35212300 1.30162100 -1.28419100
 N 0.07347300 0.69248300 -2.20963700
 C 3.39215600 3.41255100 -2.10728900
 C 3.77574800 3.99518200 -0.89173200
 C 4.19907500 3.59828700 -3.23616800
 C 4.94287700 4.74833800 -0.81007100
 H 3.17771700 3.82950100 0.00050900
 C 5.35997600 4.35979000 -3.15436000
 H 3.90597700 3.15114100 -4.18216600
 C 5.73570600 4.93513200 -1.94123800
 H 5.23560100 5.18494400 0.14044000
 H 5.97230600 4.50469600 -4.03967200
 H 6.64441500 5.52673500 -1.87733600
 C -3.29830700 5.02079000 0.61587900
 C -4.44628000 5.74347800 0.26854800
 C -2.51166500 5.46195600 1.68871700
 C -4.79051600 6.89471900 0.96970200
 H -5.05733400 5.40926600 -0.56584000
 C -2.86447200 6.60774700 2.39405100
 H -1.63849600 4.88715300 1.98673400
 C -4.00110500 7.32911900 2.03310200
 H -5.67667800 7.45411400 0.68378400
 H -2.25391400 6.93409600 3.23109300
 H -4.27342100 8.22624700 2.58179400
 Cu -1.61507300 -0.50778600 -2.13628000
 C -3.76816700 -2.31204200 -2.23948300
 N -2.53185800 -2.06541100 -2.67761500
 H -2.15195400 -2.77463500 -3.29394300
 O -4.36177900 -1.53186400 -1.45672400
 C -4.46861800 -3.56968700 -2.66866600
 C -5.86609600 -3.59087700 -2.62640000
 C -3.78409700 -4.72078000 -3.07346800
 C -6.56799900 -4.72854900 -3.00920500
 H -6.38633300 -2.70001700 -2.28848800
 C -4.48502400 -5.86531400 -3.44324100

H -2.69686200 -4.74342700 -3.07535700
 C -5.87837400 -5.86923300 -3.41928800
 H -7.65433000 -4.72873300 -2.98375100
 H -3.94194700 -6.75655700 -3.74541700
 H -6.42512200 -6.76123300 -3.71276800
 C -2.28188100 -2.20007500 0.62500200
 C -1.01198300 -1.93085500 -0.09416100
 C -0.74075700 -0.76242300 0.81120400
 H -3.15909300 -1.86479300 0.02472700
 H -2.47313700 -3.21662600 0.97949400
 H -0.90734100 0.21958100 0.35435400
 H 0.22819600 -0.74330500 1.30897300
 N -1.86648000 -1.20684300 1.62954300
 C -2.69045400 -0.31032200 2.26431700
 O -2.32316700 0.80748000 2.58078200
 O -3.87662000 -0.87533700 2.48609000
 C -4.92067400 -0.17617200 3.23562000
 C -6.05255500 -1.19252600 3.25176700
 H -6.91379400 -0.78198300 3.78768900
 H -6.36024600 -1.43853800 2.23030300
 H -5.73602700 -2.11306900 3.75239600
 C -5.33665400 1.08450900 2.49115900
 H -6.19691700 1.53797900 2.99446400
 H -4.52153900 1.80995800 2.46178500
 H -5.63163000 0.83316300 1.46665400
 C -4.43084100 0.11882100 4.64679500
 H -3.61120200 0.84001400 4.63486100
 H -5.25495100 0.53159000 5.23762800
 H -4.09025900 -0.80320500 5.12980200
 C 4.66960500 -2.42567300 1.76011400
 C 4.77963100 -3.81755400 1.68513800
 C 5.43301100 -1.71005200 2.69173900
 C 5.64786500 -4.48976800 2.54153700
 H 4.19142800 -4.37585100 0.96289800
 C 6.29747200 -2.38794000 3.54297500
 H 5.34513400 -0.62895500 2.75992100
 C 6.40457700 -3.77698900 3.46810100
 H 5.72883600 -5.57111600 2.48495000
 H 6.88653700 -1.83295200 4.26701300
 H 7.07948300 -4.30371600 4.13660100
 C 2.67980300 -0.31005200 1.58386200
 C 2.27409300 -0.62053900 2.88896700
 C 2.24922900 0.88384300 0.99035300
 C 1.44064100 0.25299900 3.58339900

H 2.59744200 -1.54507700 3.35769300
 C 1.42578000 1.75655100 1.69562800
 H 2.54749800 1.12283600 -0.02457900
 C 1.01201600 1.43746700 2.98774900
 H 1.11763600 -0.00017600 4.58845300
 H 1.08815500 2.67713600 1.22726700
 H 0.34314100 2.10320000 3.52337000
 C 4.60136800 -0.66925100 -0.60128400
 C 5.19507500 0.56372000 -0.30123500
 C 4.81619000 -1.25793900 -1.85351800
 C 5.97741200 1.20735700 -1.25396200
 H 5.03044500 1.03656100 0.66290100
 C 5.61200100 -0.61396200 -2.79756800
 H 4.36293800 -2.21428300 -2.09528600
 C 6.18600900 0.62054500 -2.50106600
 H 6.40745500 2.17852000 -1.02951800
 H 5.77506600 -1.07520300 -3.76718200
 H 6.79155900 1.13209500 -3.24337400
 P 3.57689200 -1.55136900 0.61200700
 B 2.36795600 -2.72474100 -0.36228500
 H 2.96876000 -3.60301000 -0.91688100
 H 1.70874300 -2.01228800 -1.07520200
 I 0.87904700 -3.72684500 1.07489700
 H -0.53072900 -2.36780200 -0.95507800

ComA13:

C 0.00000300 0.64583600 -0.00008800
 C 0.75620000 -1.51708400 0.11035100
 H 1.03422900 -1.82109300 1.12688700
 C -0.75621600 -1.51706400 -0.11043700
 H -1.30092900 -2.13318200 0.60817900
 N 1.09289300 -0.10266600 -0.07610600
 N -1.09288500 -0.10265000 0.07611100
 C 2.46279700 0.34982500 0.00772700
 H 2.53710300 1.38955000 -0.31696100
 H 2.83572900 0.26208500 1.03484900
 H 3.07877000 -0.27055300 -0.64815600
 C -2.46280500 0.34983800 -0.00754500
 H -3.07872600 -0.27056800 0.64836300
 H -2.53710400 1.38954900 0.31719400
 H -2.83581800 0.26213400 -1.03464000
 H 1.30093200 -2.13318800 -0.60826300
 H -1.03428500 -1.82103700 -1.12697300

B 0.00003000 2.22381200 -0.00007400
H 0.70003500 2.79817000 -0.77116700
H -0.70001500 2.79817600 0.77097800

ComF13:

C 1.03463500 -0.49030700 -0.60218800
C 2.19766600 -0.94960600 0.26971300
C 1.45753900 -0.39832900 1.48418500
H 1.18662200 0.48942100 -1.05619700
H 0.62868600 -1.19264100 -1.32627300
H 2.33743300 -2.02813000 0.29271800
H 1.74609500 0.61297900 1.77366900
H 1.36677500 -1.04314600 2.35703100
N 0.18981100 -0.34869500 0.65234000
I 4.14214900 -0.10978000 -0.16127600
C -0.57014700 0.89663600 0.77910400
O -0.64430800 1.47160200 1.83191400
O -1.09555700 1.17884200 -0.38561100
C -1.83410300 2.44926100 -0.62396300
C -2.17457700 2.34516900 -2.09926000
H -2.73037400 3.23492600 -2.41003800
H -1.26559300 2.27496200 -2.70541800
H -2.79516800 1.46398500 -2.29463200
C -0.89882600 3.61431200 -0.34980500
H -1.39009100 4.54204800 -0.66007800
H -0.65346300 3.69600800 0.71163500
H 0.02681300 3.51033300 -0.92639600
C -3.08376700 2.47936100 0.23658800
H -2.83913600 2.50224700 1.30057600
H -3.65460800 3.38196900 -0.00461000
H -3.71646900 1.61123700 0.02750500
C -2.19435300 -1.55471100 0.30722500
C -4.47688600 -1.26416900 0.06304300
H -5.06331000 -0.34667300 -0.03277800
C -3.88654600 -1.74890300 -1.25879500
H -3.89587300 -0.97440500 -2.03653700
N -3.28007700 -1.02303900 0.86963200
N -2.50285400 -2.04533000 -0.89015700
C -3.44453500 -0.55378800 2.22623300
H -2.48327400 -0.29314500 2.66453900
H -4.07914100 0.33702700 2.21565800
H -3.92690400 -1.32418200 2.84049000
C -1.60857500 -2.59610400 -1.87732100

H -1.37057900 -1.85058500 -2.64629200
H -0.69156600 -2.93796200 -1.39695500
H -2.09345600 -3.45094700 -2.35841300
H -5.09461600 -2.02555400 0.55516300
H -4.37714300 -2.64343500 -1.65063200
B -0.74708700 -1.63479200 1.02312200
H -0.87595500 -1.60652500 2.21994900
H -0.12854900 -2.60455600 0.65664100

ComE13:

C -0.50016100 -0.94577500 -1.10650400
C 0.42184600 -2.11242300 -0.72126000
C -0.51436200 -2.42649000 0.45507600
H -0.05561800 0.05246800 -1.15180900
H -1.06323400 -1.13843500 -2.02773600
H 0.59122600 -2.89414700 -1.45942200
H -0.07944700 -2.42444300 1.45833800
H -1.08679600 -3.34995600 0.30446800
N -1.25218200 -1.21659800 0.11496600
I 2.44835200 -1.53191100 -0.15402800
C -2.56821200 -0.99321700 0.38362800
O -3.17908700 -1.59895500 1.24562000
O -3.02813800 -0.01532100 -0.41092500
C -4.39571900 0.48479400 -0.26717500
C -4.46581000 1.57808700 -1.32238700
H -5.46639200 2.02176500 -1.33341400
H -3.73989900 2.37150400 -1.11173100
H -4.25707500 1.16980500 -2.31711100
C -4.59220300 1.06655300 1.12591600
H -5.56678500 1.56362400 1.17988000
H -4.55457500 0.28733300 1.89001200
H -3.81843600 1.81273300 1.34118300
C -5.38929500 -0.62633800 -0.57558800
H -5.34020700 -1.41748400 0.17527200
H -6.40469300 -0.21578000 -0.58692300
H -5.18519500 -1.05815300 -1.56183700
C 1.79301000 1.54049000 0.61896800
C 2.37862500 3.33145600 -0.71907700
H 2.46811400 3.09179500 -1.78627200
C 0.92663500 3.48801700 -0.27131300
H 0.22844200 3.62822200 -1.10042500
N 2.82291200 2.18530700 0.07276700
N 0.66570100 2.21485400 0.40255000

C 4.18212900 1.71776400 -0.04015600
 H 4.40278000 1.00441000 0.75525200
 H 4.35436400 1.24415800 -1.01508900
 H 4.85798100 2.57186800 0.06025800
 C -0.64180400 1.98304900 0.96966800
 H -1.38891900 1.97155900 0.17068600
 H -0.66678400 1.02709000 1.48867600
 H -0.88540300 2.78723200 1.67446000
 H 2.99514600 4.20741500 -0.50294800
 H 0.79106200 4.30691200 0.44570700
 B 1.90845900 0.16833800 1.43184800
 H 2.87077700 0.10743100 2.14506900
 H 0.88929800 -0.26587900 1.88137300

TS5-ComE13:

C 2.99831600 -3.41240900 -1.48863300
 C 4.04953700 -2.58020100 -1.13131500
 C 3.80484700 -1.17706200 -1.11476300
 C 2.48647300 -0.72852200 -1.35133000
 C 1.73792200 -2.87638500 -1.74843600
 C 4.83446400 -0.19964500 -0.93194600
 C 2.18428500 0.68098700 -1.28804500
 C 3.21218700 1.61196700 -1.01837900
 C 4.55433000 1.13141100 -0.89744300
 C 2.84598200 2.98537500 -0.91369900
 C 1.52047100 3.31732700 -1.15121700
 C 0.58151900 2.32026500 -1.44327400
 H 5.86154900 -0.53653400 -0.84870400
 H 3.13700400 -4.48729800 -1.52946500
 H 0.90762700 -3.51989600 -2.02174500
 H 5.36033900 1.84833900 -0.78704700
 H 1.19587900 4.35010400 -1.07479200
 H -0.47040900 2.54209700 -1.59914100
 N 0.90151400 1.03726900 -1.49852700
 N 1.47005000 -1.57775200 -1.64975700
 C 5.35764700 -3.16109700 -0.77429100
 C 6.00118100 -2.79343600 0.41590100
 C 5.94227500 -4.13302700 -1.59634100
 C 7.20865100 -3.38502300 0.77119500
 H 5.53674900 -2.06453300 1.07505700
 C 7.15625700 -4.71252900 -1.24361800
 H 5.45275700 -4.41631200 -2.52437000
 C 7.79100100 -4.34086100 -0.05961500

H 7.69243700 -3.10229600 1.70162000
 H 7.60774700 -5.45519500 -1.89497900
 H 8.73670800 -4.79800500 0.21707400
 C 3.81216700 4.04076000 -0.54464400
 C 3.88750700 5.21334400 -1.30697100
 C 4.61944500 3.91515400 0.59463500
 C 4.76299700 6.23243600 -0.94669300
 H 3.26972500 5.31402900 -2.19551800
 C 5.48615400 4.94085400 0.95804700
 H 4.54801000 3.02315700 1.21165200
 C 5.56363100 6.09885100 0.18624100
 H 4.82130000 7.13166500 -1.55321300
 H 6.09895000 4.83636900 1.84882900
 H 6.24487800 6.89642200 0.46859300
 Cu -0.30500900 -0.78336800 -2.02097200
 C -2.78060900 0.57518900 -2.20604900
 N -2.03595800 -0.42607800 -2.68813400
 H -2.51307500 -1.02421300 -3.35357300
 O -2.34270000 1.41109400 -1.38709100
 C -4.21269900 0.68758600 -2.64293200
 C -4.78682700 1.96011400 -2.72823300
 C -5.00796600 -0.43749000 -2.88283900
 C -6.12868800 2.10752500 -3.06188000
 H -4.16419100 2.82692200 -2.52730800
 C -6.35724400 -0.29161000 -3.19722600
 H -4.58580300 -1.43464900 -2.78518400
 C -6.91834500 0.98052200 -3.29128900
 H -6.56265400 3.10080500 -3.13696400
 H -6.97161000 -1.17243700 -3.36086400
 H -7.97011400 1.09368700 -3.53891900
 C -1.24595600 -0.45169600 0.70978200
 C -1.62002500 -1.66014200 -0.09330600
 C -0.72350500 -2.51842400 0.75196600
 H -0.63936600 0.29230700 0.17336300
 H -2.06824800 0.08957200 1.18290500
 H 0.17598900 -2.89426500 0.25031400
 H -1.21599800 -3.35695000 1.25261500
 N -0.47895800 -1.34387300 1.58859400
 C 0.73303900 -1.07953500 2.16641900
 O 1.52051800 -1.95424100 2.47402600
 O 0.86745300 0.24048400 2.33929800
 C 1.97118700 0.79030400 3.13022100
 C 1.74831100 2.28991600 2.99980800
 H 2.52520900 2.83414200 3.54506600

H 1.78394400 2.59223900 1.94762300
 H 0.77345300 2.57294000 3.41061600
 C 3.31459300 0.39213300 2.53391200
 H 4.11107700 0.94545400 3.04305200
 H 3.49924600 -0.67738100 2.64396700
 H 3.34718100 0.64644200 1.47159000
 C 1.82308900 0.32937600 4.57269900
 H 1.93820700 -0.75468800 4.64761500
 H 2.59109200 0.80505400 5.19107200
 H 0.84085300 0.61298900 4.96568900
 H -2.30890900 -1.85274800 -0.89834200
 C -4.41758800 0.64687800 2.27235200
 C -4.32800300 2.50787000 0.90447300
 H -4.98262500 3.38041800 0.83912400
 C -3.25520800 2.63025500 1.98483300
 H -3.47752100 3.40549600 2.72906500
 N -5.08276400 1.33485400 1.35082100
 N -3.30992400 1.31483200 2.62398100
 C -6.20135500 0.86159000 0.56952600
 H -6.72823500 0.08085200 1.11723400
 H -6.88150400 1.69743100 0.38438400
 H -5.85922300 0.46266900 -0.39206600
 C -2.40709000 1.01770700 3.71233400
 H -2.57470300 1.70944700 4.54665900
 H -2.55981900 -0.00453800 4.05363600
 H -1.37427100 1.12251300 3.36401100
 H -3.88459400 2.29535400 -0.07622900
 H -2.25838100 2.81339900 1.57314500
 B -4.85710300 -0.77883500 2.84163200
 H -6.04895800 -0.92074300 2.89178500
 H -4.25239600 -1.15075100 3.80538200
 I -4.24103000 -2.32075700 1.13900700

ComA18:

C 0.04431100 -1.07244300 0.00008700
 H -0.30415400 -2.09432100 0.00009500
 C 0.07601000 1.14230500 0.00005600
 H -0.33827600 2.13878800 0.00013500
 C 1.35760300 0.70891300 -0.00006400
 H 2.29733100 1.23887500 -0.00011200
 N 1.29806400 -0.67286500 -0.00005400
 H 2.10106800 -1.29500700 -0.00012100
 N -0.74614700 0.01955400 0.00007000

B -2.20185400 -0.00899500 0.00012600
 H -2.71554500 -1.08051900 -0.00063100
 H -2.76212300 1.03768700 -0.00057800

LA18-R1-1:

C 0.11495800 -0.12041900 0.83649700
 C 1.37711400 -0.30687400 -0.00175000
 C 0.55206000 0.00907600 -1.24773800
 H -0.40301400 -1.04978000 1.07581100
 H 0.16977800 0.52022200 1.71617300
 H 0.18851800 -0.86701500 -1.78572500
 H 0.94595600 0.74471300 -1.94875400
 N -0.54080500 0.54911900 -0.35527400
 C -1.88952700 0.08151700 -0.70959800
 O -2.17500400 -0.14605800 -1.85380100
 O -2.59864500 0.00300800 0.38269800
 C -4.03271000 -0.39394500 0.34547100
 C -4.41975600 -0.33324200 1.81172000
 H -5.47196300 -0.61266800 1.92194200
 H -3.81380400 -1.02672300 2.40412700
 H -4.28630800 0.67848700 2.20824900
 C -4.14143700 -1.80715100 -0.20076400
 H -5.17841700 -2.14475500 -0.10403800
 H -3.86240800 -1.85661800 -1.25569900
 H -3.50669100 -2.49176500 0.37211100
 C -4.80307700 0.62481800 -0.47579200
 H -4.52324700 0.59044900 -1.53117600
 H -5.87306100 0.40597000 -0.39706300
 H -4.63208900 1.63618700 -0.09192200
 H 2.16376000 0.41532800 0.21006900
 I 2.33430900 -2.24224300 0.08418000
 B -0.64932700 2.18263100 -0.28338800
 H -1.02653900 2.52860200 -1.37334700
 H -1.38839400 2.42681000 0.63328600
 N 0.74557200 2.78583800 -0.00270000
 C 2.53273700 3.58570200 1.04279600
 C 1.32384000 2.99128600 1.23485400
 H 0.81614600 2.71810100 2.14702300
 H 3.28921300 3.91768200 1.73682200
 C 1.58090000 3.26385800 -0.92382600
 N 2.66466400 3.74085800 -0.31515400
 H 3.45237500 4.17249700 -0.78513200
 H 1.40103400 3.26591700 -1.98787700

TS4-ComD18:

C 1.21807400 0.16082300 -1.08989800
C -0.17213100 0.36523000 -0.51900300
C 0.41475300 0.31685500 0.88198300
H 1.43510800 -0.87227800 -1.37513800
H 1.58041400 0.84203100 -1.86092900
H 0.32283900 -0.64869000 1.38451900
H 0.16956700 1.11662100 1.58083500
N 1.79788800 0.45581700 0.28214400
C 2.78667000 -0.49743400 0.79862200
O 2.71145000 -0.91821700 1.92189700
O 3.66289700 -0.73174200 -0.14233600
C 4.82317800 -1.62857500 0.09037200
C 5.53989000 -1.57723100 -1.24681900
H 6.43982400 -2.19824000 -1.20498900
H 4.89622900 -1.95363200 -2.04876500
H 5.83739500 -0.55131200 -1.48735900
C 4.31571200 -3.02723400 0.39593000
H 5.16765200 -3.71431400 0.43148600
H 3.79908800 -3.06918600 1.35744100
H 3.63497100 -3.36966300 -0.39101200
C 5.68055000 -1.04970100 1.20243800
H 5.16643300 -1.08011200 2.16566700
H 6.60022800 -1.63852700 1.28335900
H 5.95563700 -0.01421800 0.97538300
H -0.69930400 1.27214600 -0.80428600
I -1.72673400 -1.29834600 -0.95639000
B -2.95050700 0.46115400 1.25515600
H -2.28608300 -0.07552900 2.09244100
H -2.71844500 1.54167900 0.79336900
N -4.28028400 -0.09362100 0.99334500
C -6.30268900 -0.39843500 0.10368800
C -5.25628700 0.46474200 0.17275100
H -5.11247800 1.43183100 -0.28328000
H -7.24588100 -0.33361000 -0.41661700
C -4.73731700 -1.30055700 1.38585900
N -5.96465000 -1.48446800 0.86956200
H -6.53679600 -2.30523100 1.01665100
H -4.21626100 -1.98355800 2.03638500
B 2.47408900 1.93269800 0.45291000
H 2.75021700 2.03242500 1.62238700
H 3.40372900 1.97462900 -0.30999300
N 1.44331700 3.02311900 0.07455400

C 0.25742600 4.51000300 -1.06966200
C 1.20991700 3.54450700 -1.18238800
H 1.75334700 3.19581300 -2.04697500
H -0.20117200 5.15668700 -1.80154800
C 0.65952800 3.67243000 0.93291500
N -0.06737600 4.56460500 0.26350600
H -0.74158400 5.19430600 0.68249100
H 0.62365100 3.50197000 1.99783000

ComE18:

C -0.97315800 -0.05844500 1.31398900
C 0.42282300 0.20464700 0.72726400
C -0.22906200 1.06191900 -0.36905700
H -1.35991100 -1.07457800 1.18985700
H -1.09136000 0.25352600 2.35615400
H -0.22891900 0.63544200 -1.37727400
H 0.12972600 2.09569700 -0.41092500
N -1.49786000 0.89036600 0.33023000
C -2.71140100 0.86492000 -0.29552800
O -2.89375600 1.35099800 -1.39770300
O -3.60927100 0.26685700 0.49528100
C -5.00527200 0.13039400 0.07964500
C -5.64099400 -0.57009600 1.27084500
H -6.70549400 -0.73946400 1.07991100
H -5.16382300 -1.53945600 1.45109000
H -5.54340600 0.03850600 2.17620300
C -5.08945700 -0.73996400 -1.16644700
H -6.14000600 -0.94468400 -1.39950800
H -4.63089300 -0.24527400 -2.02531000
H -4.58481700 -1.69791600 -0.99659500
C -5.62502800 1.50496400 -0.13102800
H -5.17455800 2.01550700 -0.98451000
H -6.69948100 1.39585200 -0.31447600
H -5.49250900 2.12392800 0.76323300
H 1.13306800 0.70909400 1.37993400
I 1.50585300 -1.55032100 0.01817900
B 3.02264000 -0.28439300 -1.48008000
H 3.63732100 -1.19941800 -1.94056900
H 2.19859800 0.29512200 -2.12104600
N 3.83889400 0.61884600 -0.58859100
C 4.49295200 2.35092600 0.62732800
C 3.47157700 1.87056200 -0.13001200
H 2.52102700 2.30953300 -0.39318000

H 4.61891500 3.28218500 1.15754400
C 5.05933100 0.35033800 -0.12084400
N 5.46723500 1.38007400 0.61124400
H 6.36854600 1.43989200 1.07215200
H 5.61703200 -0.55336100 -0.31352100

TS5-ComE18:

C 2.26683600 -3.09003600 -1.11981300
C 3.48307400 -2.48434600 -0.84821200
C 3.53605700 -1.05957900 -0.87899100
C 2.32890700 -0.36904600 -1.11288300
C 1.11957200 -2.31503100 -1.32906100
C 4.73937800 -0.29933200 -0.74108600
C 2.31426700 1.07405400 -1.14082400
C 3.50784000 1.79626400 -0.92037400
C 4.72596500 1.06213900 -0.76143800
C 3.43334900 3.22015500 -0.91593400
C 2.20499900 3.80188500 -1.19628000
C 1.08144200 3.00253000 -1.41772500
H 5.68164400 -0.82748400 -0.64320400
H 2.18554300 -4.17190700 -1.10890100
H 0.13940700 -2.75838000 -1.48474800
H 5.65758700 1.61112200 -0.68225400
H 2.09971400 4.88164000 -1.19996000
H 0.11195900 3.45173200 -1.61258600
N 1.12198300 1.67727100 -1.37410600
N 1.14734000 -0.99245600 -1.30667000
C 4.65975700 -3.31143400 -0.51439500
C 5.38549200 -3.07057800 0.66014100
C 5.02696000 -4.38271100 -1.33753200
C 6.46220700 -3.88352500 0.99814400
H 5.08273000 -2.26316400 1.32191300
C 6.11120700 -5.18658300 -1.00165900
H 4.47101400 -4.56966200 -2.25264900
C 6.83046100 -4.93883400 0.16594800
H 7.01058800 -3.69623100 1.91686400
H 6.39560300 -6.00720800 -1.65398700
H 7.67457800 -5.56996200 0.42873600
C 4.59673800 4.07573300 -0.60983200
C 4.91566800 5.15270200 -1.44661600
C 5.36092300 3.85853500 0.54513000
C 5.98845500 5.98419400 -1.14361800
H 4.33315600 5.32113100 -2.34863500
C 6.42499300 4.69968900 0.85124400

H 5.10114700 3.04536300 1.21764100
C 6.74430200 5.76009800 0.00544200
H 6.23520200 6.80788200 -1.80715300
H 7.00250100 4.52966600 1.75523500
H 7.57918500 6.41299300 0.24301600
Cu -0.45385300 0.40187800 -1.60454400
C -2.69336400 -1.26206900 -2.01267800
N -2.19731700 -0.03182400 -2.20193400
H -2.83842600 0.62695300 -2.62946200
O -2.04249000 -2.15194400 -1.42479400
C -4.10171800 -1.56700600 -2.44337300
C -4.76147800 -2.61941900 -1.79991300
C -4.77668400 -0.84654400 -3.43472200
C -6.07895600 -2.93055700 -2.12196300
H -4.21809200 -3.18394200 -1.04864700
C -6.09126900 -1.16305200 -3.76555100
H -4.27210500 -0.05159400 -3.97839000
C -6.74803700 -2.20044000 -3.10520500
H -6.58173700 -3.74878500 -1.61353200
H -6.60037500 -0.60491900 -4.54613800
H -7.77324700 -2.44840200 -3.36619900
C -1.28899700 0.87134000 0.59176800
C -0.05438600 0.69088000 1.43364600
C -1.79226800 -0.45975800 1.03792200
H -1.69927200 1.68295100 0.00779900
H 0.18249400 1.50194500 2.12679600
H 0.85435100 0.43835300 0.87612100
H -2.80720800 -0.50674000 1.44222500
H -1.70008100 -1.24042300 0.25096200
N -0.69032400 -0.49084300 2.01498000
C 0.05740700 -1.61504500 2.29850600
O 1.25583100 -1.56961100 2.50056600
O -0.74375300 -2.67770600 2.33623400
C -0.23601200 -3.99787400 2.71337700
C -1.48679600 -4.86138800 2.64573700
H -1.24051700 -5.89611500 2.90289600
H -2.24317200 -4.49792400 3.34850300
H -1.90979900 -4.84251400 1.63595600
C 0.79736600 -4.46425200 1.69840200
H 1.68919000 -3.83507100 1.72294800
H 1.08717100 -5.49635200 1.92132200
H 0.36773000 -4.43824200 0.69166800
C 0.32168000 -3.94965900 4.12914100
H -0.43072400 -3.55498700 4.81997400

H 0.58426600 -4.96289400 4.45037300
H 1.21470900 -3.32358700 4.17940000
C -6.42700200 2.26809100 0.77077800
H -6.84518900 3.08338400 1.34039800
C -5.03243300 1.00008100 -0.33925000
H -4.09264900 0.71761300 -0.78715400
C -6.22920000 0.35333600 -0.32067200
H -6.53626100 -0.58726100 -0.75334000
N -7.08337900 1.17057100 0.38277600
H -8.05858300 0.98423100 0.57159500
N -5.17257500 2.18960900 0.34181400
B -4.07209800 3.23868700 0.55669600
H -4.52625200 4.30280400 0.86240000
H -3.28161300 3.20488200 -0.35073400
I -2.81058400 2.54919500 2.42816600

ComA24:

B -2.32539100 -0.00000100 -0.45850600
H -2.78570800 1.06927700 -0.67744100
H -2.78568700 -1.06928100 -0.67748000
C 1.00293400 1.19927700 -0.32307500
C -0.29081900 1.25122000 0.46099100
C -0.29081800 -1.25121900 0.46099300
C 1.00293400 -1.19927700 -0.32307300
H -0.14590900 1.21654800 1.54304300
H -0.95160300 2.07100800 0.18059300
H 0.77481600 1.27183200 -1.39392000
H 1.58541800 2.08566900 -0.05033000
H -0.14590800 -1.21654500 1.54304600
H -0.95160100 -2.07100800 0.18059700
H 1.58541900 -2.08566800 -0.05032600
H 0.77481700 -1.27183400 -1.39391700
O -1.06341100 0.00000000 0.14811100
N 1.78251400 0.00000100 -0.08718200
H 2.15720300 0.00000100 0.85903100

ComF24:

I -3.61040600 0.11730500 0.10155400
C -0.55028200 0.30297800 0.89448700
C -1.54648100 -0.51832300 0.08079400
C -0.73204900 -0.20163700 -1.17017200
H -0.86154400 1.33327700 1.07442500

H -0.14187700 -0.13483500 1.80544400
H -1.09858000 0.64669900 -1.74843300
H -0.47649500 -1.02709100 -1.83289500
N 0.40793900 0.25013200 -0.28319900
C 1.01679000 1.53385100 -0.68229300
O 0.95987600 1.91350200 -1.81956100
O 1.57463700 2.05649200 0.37337200
C 2.31698600 3.34769900 0.29483300
C 2.78261400 3.53538900 1.72635600
H 3.34578200 4.47026000 1.80521200
H 1.92907500 3.58669500 2.41035800
H 3.43336100 2.71107300 2.03546900
C 1.35315000 4.44244700 -0.12758100
H 1.86664800 5.40735200 -0.06459600
H 1.00839500 4.30505900 -1.15498500
H 0.48701500 4.47420600 0.54222700
C 3.48720800 3.18173700 -0.65803300
H 3.15428900 3.05110000 -1.69029300
H 4.11095900 4.08020000 -0.60978800
H 4.10219200 2.32349500 -0.36736500
H -1.56598400 -1.57499500 0.34074200
B 1.64853800 -0.78204200 -0.13420000
H 2.31076800 -0.68942800 -1.13176500
H 2.19836400 -0.54663200 0.90377800
C 1.26519600 -3.10898900 -1.20481600
C 2.59133300 -3.81661800 -1.01406700
C 2.38404600 -3.62574000 1.36864900
C 1.05432500 -2.91617000 1.21269700
H 2.72574600 -4.52713700 -1.83631100
H 0.41541400 -3.79836700 -1.19624300
H 1.23545800 -2.49079100 -2.10205600
H 2.36399300 -4.19539000 2.30368900
H 3.18031600 -2.87505900 1.45495800
H 0.21273400 -3.61360500 1.16474900
H 0.87330300 -2.16586800 1.98177900
H 3.40078900 -3.07786500 -1.07920300
O 1.03624000 -2.19276900 -0.07160700
N 2.69687600 -4.51144700 0.25883700
H 2.06195100 -5.30766700 0.26752800

TS4-ComD24:

I -1.71169000 -1.77120100 0.16029300
B -3.03597800 1.14946000 -0.30120500

H -2.75729500 1.75934600 0.69117500
 H -2.71572900 1.43433000 -1.41914100
 C -6.43714300 -0.18866100 -1.35746500
 C -4.92828500 -0.19136700 -1.36762900
 C -4.96807700 0.17679200 1.05091200
 C -6.47563600 0.16965400 0.99088000
 H -4.51496600 -1.19482800 -1.23618400
 H -4.51821900 0.27862300 -2.26130200
 H -6.79454300 0.83552400 -1.56723300
 H -6.77333000 -0.83879100 -2.17226600
 H -4.55507300 -0.81809300 1.23720700
 H -4.58460500 0.89328400 1.77718800
 H -6.84265800 -0.20876400 1.95083200
 H -6.83312800 1.20851200 0.87343800
 N -6.90460300 -0.70800900 -0.08412300
 H -7.91799000 -0.77646100 -0.09044600
 O -4.45041300 0.62732500 -0.24673600
 C 1.16248900 -0.52559200 -0.80905000
 C -0.02905300 -0.21294300 0.07738500
 C 0.91026200 -0.16732700 1.26918900
 H 1.30565800 -1.59483900 -0.98769500
 H 1.29989700 0.03142400 -1.73601800
 H 0.97734900 -1.10891400 1.81891100
 H 0.83496600 0.66517000 1.96780600
 N 2.08388800 -0.07039400 0.31384000
 C 3.21671800 -0.95166200 0.63706700
 O 3.42182400 -1.30192500 1.76747300
 O 3.86206500 -1.20620500 -0.46923700
 C 5.10304600 -2.02732100 -0.46419200
 C 5.49392000 -2.02961000 -1.93054700
 H 6.40920400 -2.61498900 -2.06073000
 H 4.70536500 -2.47797300 -2.54372900
 H 5.68024700 -1.01077000 -2.28546500
 C 4.77056100 -3.42601600 0.02546200
 H 5.65394900 -4.06120200 -0.09599000
 H 4.48780000 -3.42874900 1.08054600
 H 3.95691000 -3.85892600 -0.56633300
 C 6.14955800 -1.33141000 0.38872200
 H 5.87721600 -1.33380300 1.44676300
 H 7.10290200 -1.85825100 0.27808400
 H 6.29093200 -0.29755500 0.05595000
 H -0.59135200 0.69368200 -0.14584000
 B 2.71353500 1.40735000 0.13138300
 H 3.37631100 1.63894400 1.10621800

H 3.27660100 1.44343000 -0.92670200
 C 1.30585200 3.28654500 1.24106800
 C 2.09983900 4.56026700 1.03534400
 C 1.94868600 4.30392300 -1.34481500
 C 1.15089600 3.02661900 -1.17396800
 H 1.88697800 5.23907100 1.86780500
 H 0.22598000 3.46135900 1.26869300
 H 1.61744800 2.73273100 2.12630700
 H 1.62471900 4.79494000 -2.26847900
 H 3.00984200 4.04737000 -1.46032400
 H 0.07479400 3.21118800 -1.10040000
 H 1.34883000 2.29126200 -1.95302600
 H 3.17036200 4.31918700 1.06878500
 O 1.52808300 2.38748300 0.09704500
 N 1.81173700 5.22279000 -0.22637100
 H 0.86499100 5.59763400 -0.20679700

ComE24:

I 1.59465700 -1.82553400 0.44967300
 C -0.79190100 -0.17528600 -0.88164500
 C -0.02742600 -1.50516400 -0.96920600
 C -1.33899900 -2.24502200 -0.66354400
 H -0.62751600 0.39679100 0.03813000
 H -0.68917500 0.48117900 -1.75062000
 H -1.43207600 -2.63539200 0.35613400
 H -1.60940800 -3.02428700 -1.38142400
 N -2.02077200 -0.96763600 -0.84950800
 C -3.20908500 -0.63753800 -0.26030000
 O -4.00209400 -1.47065900 0.13803400
 O -3.33343300 0.69420400 -0.22965600
 C -4.54702200 1.32621400 0.28915800
 C -4.25468000 2.80753200 0.10489500
 H -5.09925900 3.40301400 0.46568800
 H -3.36031700 3.09900000 0.66652200
 H -4.09276300 3.04158300 -0.95283200
 C -4.71788400 0.98896300 1.76358000
 H -5.55154000 1.56778000 2.17557600
 H -4.92717600 -0.07356100 1.90478600
 H -3.81216800 1.25098500 2.32251500
 C -5.74986100 0.90628400 -0.54374000
 H -5.96669500 -0.15660400 -0.41878000
 H -6.62771100 1.48205800 -0.23129600
 H -5.56884500 1.10971400 -1.60509600

H 0.42892400 -1.72908800 -1.93232800
 B 3.36529200 -0.72572700 -0.86353100
 H 4.32364600 -1.30265800 -0.45549700
 H 2.91860800 -0.87311900 -1.95909700
 C 3.95208000 1.08851800 0.83472900
 C 4.41828000 2.52644500 0.73657200
 C 2.79771600 3.00292500 -0.95317700
 C 2.27952600 1.58000700 -0.90926400
 H 4.79175000 2.82485600 1.72160400
 H 3.15717400 0.94821200 1.57515600
 H 4.76646600 0.38558600 1.01180100
 H 1.96121000 3.65420400 -1.22729300
 H 3.55399300 3.08278600 -1.74375200
 H 1.47079200 1.44817700 -0.18224200
 H 1.98185100 1.20275400 -1.88822700
 H 5.25747400 2.58138800 0.03237600
 O 3.37798700 0.69606900 -0.47074400
 N 3.38403900 3.44627800 0.29826400
 H 2.66247000 3.52589100 1.01249100

TS5-ComE24:

C -0.91778400 3.89883900 -0.12077500
 C -2.29635900 3.85477900 -0.27566300
 C -2.96109400 2.62818400 0.02297200
 C -2.17537400 1.56400600 0.51309700
 C -0.22054000 2.77922300 0.34617300
 C -4.35591200 2.39519500 -0.19533500
 C -2.78979000 0.30562300 0.86285800
 C -4.18107300 0.13380600 0.69868300
 C -4.93584400 1.20508100 0.12364000
 C -4.74091500 -1.12403300 1.06794500
 C -3.87398600 -2.10573100 1.52265300
 C -2.50597300 -1.84449700 1.62911700
 H -4.95098800 3.17823600 -0.65216100
 H -0.37633200 4.81526100 -0.33148700
 H 0.85763700 2.78100700 0.48895500
 H -5.98857100 1.04743900 -0.08308000
 H -4.25798500 -3.07552600 1.81987600
 H -1.82132400 -2.61019000 1.98361700
 N -1.97139300 -0.67254900 1.32093100
 N -0.83604500 1.65021100 0.66269200
 C -3.02305600 5.05817600 -0.72819700
 C -4.12424300 5.54408500 -0.01014500

C -2.58281100 5.75857600 -1.85822300
 C -4.77268200 6.70440400 -0.41901100
 H -4.45287600 5.02522700 0.88652600
 C -3.24115100 6.91198500 -2.27116200
 H -1.73490800 5.38201900 -2.42449000
 C -4.33629400 7.38744100 -1.55253700
 H -5.61725200 7.07869800 0.15225700
 H -2.89903100 7.43946300 -3.15687400
 H -4.84723600 8.29049300 -1.87386700
 C -6.18601500 -1.41204700 0.97934900
 C -6.62245900 -2.57161400 0.32608100
 C -7.12966600 -0.56877400 1.58088700
 C -7.97862200 -2.87272500 0.26232800
 H -5.89497200 -3.22222200 -0.15300400
 C -8.48402600 -0.88019400 1.52570700
 H -6.79637300 0.31649200 2.11616500
 C -8.91119700 -2.02895700 0.86255700
 H -8.30802500 -3.76673900 -0.25915300
 H -9.20657600 -0.22680900 2.00604700
 H -9.96981500 -2.26762800 0.81585600
 Cu 0.03839800 -0.05293500 1.46082000
 C 2.69768600 0.41298000 2.07215000
 N 1.69169700 -0.43050100 2.30085200
 H 1.87132400 -1.12680300 3.01502900
 O 2.61577600 1.34280400 1.23212300
 C 3.98317300 0.23863300 2.82201000
 C 4.69005000 1.38168000 3.20697800
 C 4.51448200 -1.02405300 3.10121900
 C 5.89851400 1.26478100 3.88573500
 H 4.27637700 2.35674500 2.96621500
 C 5.73715200 -1.14053800 3.75711900
 H 3.98835900 -1.91789100 2.77481000
 C 6.42694300 0.00242800 4.15706600
 H 6.43421600 2.15747400 4.19666500
 H 6.15248000 -2.12469000 3.95538600
 H 7.37632600 -0.08949400 4.67717100
 C 1.05932000 -0.59416400 -0.56338000
 C -0.13727300 -0.67661300 -1.47763400
 C 1.08723000 -2.09988200 -0.46985700
 H 1.70266700 0.21119600 -0.20608700
 H -0.03184000 -0.18708100 -2.44990900
 H -1.08566400 -0.35081900 -1.03551100
 H 2.02356300 -2.59099900 -0.75016400
 H 0.77789000 -2.48738500 0.50910100

N 0.01886500 -2.12974900 -1.47601400
 C -1.06502000 -2.97152800 -1.47597900
 O -2.14991400 -2.64226900 -1.91632500
 O -0.71784900 -4.14827300 -0.94635200
 C -1.61319500 -5.30392400 -1.03550700
 C -0.78426200 -6.41573100 -0.41040900
 H -1.35422900 -7.34978400 -0.40795200
 H 0.13947000 -6.57228400 -0.97605900
 H -0.52215700 -6.16641900 0.62319000
 C -2.87724200 -5.04966900 -0.22550500
 H -3.44651300 -4.21753500 -0.64458300
 H -3.50163500 -5.94908400 -0.23304600
 H -2.62088900 -4.82391600 0.81539300
 C -1.91777500 -5.60624200 -2.49631700
 H -0.98691600 -5.72298600 -3.06092800
 H -2.47877100 -6.54398700 -2.56304700
 H -2.51150500 -4.80979200 -2.94920700
 B 4.54304200 -1.15453900 -0.87634000
 H 4.94234700 -2.21973200 -1.24103100
 H 3.84977600 -1.07179900 0.09225500
 C 8.06645000 0.23448200 -0.97979500
 C 6.83906900 -0.34348700 -1.66233300
 C 5.45079300 1.19451000 -0.36763000
 C 6.70432400 1.72578000 0.29592500
 H 6.57420000 0.18690200 -2.58452500
 H 6.92601100 -1.41203800 -1.85983600
 H 8.30998300 -0.38969500 -0.11070200
 H 8.91056800 0.17358900 -1.67466900
 H 5.20965900 1.72490500 -1.29636100
 H 4.57347000 1.18117700 0.28363500
 H 6.53820900 2.77660200 0.55490900
 H 6.86628000 1.18284200 1.23464300
 O 5.70182900 -0.20640000 -0.74913400
 N 7.89726500 1.60221300 -0.52563800
 H 7.84364300 2.23257100 -1.32253500
 I 3.13219700 -0.36873800 -2.61798000

IM3:

C 1.45323800 0.03622000 -0.00000500
 C 1.99108600 -0.64644500 1.26002400
 H 1.68665400 -1.69659400 1.31542100
 H 3.08851800 -0.61598000 1.26478700
 H 1.62508600 -0.13027000 2.15339800

C 1.99139100 -0.64606400 -1.26011600
 H 1.62541800 -0.12976200 -2.15342500
 H 3.08881700 -0.61535000 -1.26471300
 H 1.68722200 -1.69626900 -1.31581500
 C -0.06901500 0.02443800 -0.00010200
 C -0.80475100 1.21133300 -0.00002000
 C -0.76327100 -1.19121200 -0.00007900
 C -2.19881000 1.18439100 0.00000300
 H -0.27811800 2.15936600 0.00000000
 C -2.15441800 -1.21962700 -0.00003400
 H -0.21389700 -2.12985900 -0.00004300
 C -2.88016800 -0.02931100 -0.00001200
 H -2.75287500 2.12017800 0.00004100
 H -2.67301200 -2.17533900 -0.00000800
 H -3.96713300 -0.04985200 0.00002300
 O 1.85815300 1.40199700 0.00024600
 H 2.82641600 1.40142100 0.00041600

TS6-ComA1:

C -0.23640500 -3.49171200 0.26420300
 C -1.42340800 -2.79654400 0.09072100
 C -1.35265500 -1.37639600 0.02112600
 C -0.07314200 -0.77655600 0.07980300
 C 0.97942500 -2.80300200 0.32356700
 C -2.50101800 -0.52737000 -0.07789700
 C 0.05247500 0.66051800 -0.00506900
 C -1.10508900 1.46951600 -0.08124000
 C -2.38363100 0.82730500 -0.12715800
 C -0.92487300 2.88110800 -0.13272200
 C 0.37490300 3.36476300 -0.15600700
 C 1.45490600 2.47888600 -0.09004300
 H -3.48585600 -0.98059500 -0.10498500
 H -0.24133500 -4.57548700 0.32229900
 H 1.91606900 -3.34021200 0.44336600
 H -3.27471900 1.43924800 -0.21339600
 H 0.55925100 4.43370300 -0.19363000
 H 2.47939100 2.84295900 -0.08635700
 N 1.30596600 1.16628000 -0.00439200
 N 1.06984400 -1.48583700 0.22039800
 C -2.69785600 -3.54035100 -0.01419900
 C -3.03412300 -4.48632000 0.96207100
 C -3.55844100 -3.35303300 -1.10412700
 C -4.21335500 -5.21775600 0.85933200

H -2.37326100 -4.63347200 1.81236800
 C -4.73311800 -4.09152500 -1.20874800
 H -3.29147400 -2.64287100 -1.88230100
 C -5.06574700 -5.02193700 -0.22562100
 H -4.46713800 -5.94107000 1.62919100
 H -5.38668100 -3.94326200 -2.06379500
 H -5.98507900 -5.59506900 -0.30693700
 C -2.05860700 3.83104200 -0.15291600
 C -2.11672500 4.83082700 -1.13178800
 C -3.05768400 3.78227500 0.82859700
 C -3.16016500 5.75158700 -1.13833200
 H -1.34806600 4.87125500 -1.89917800
 C -4.09578900 4.70858000 0.82431000
 H -3.00585900 3.02881600 1.61012800
 C -4.15218400 5.69243100 -0.16129500
 H -3.19879600 6.51540400 -1.90991600
 H -4.85898200 4.66466400 1.59620800
 H -4.96528200 6.41289800 -0.16611700
 C 5.36765900 -0.69291400 -1.02985400
 O 5.80525500 -0.31823000 0.08438700
 O 4.14586000 -0.77119200 -1.36917200
 C 6.37619100 -1.10319500 -2.09040100
 H 7.40090700 -0.96773500 -1.73828100
 H 6.21888100 -2.15354400 -2.35889300
 H 6.21766200 -0.51151700 -2.99820300
 Cu 2.82943900 -0.31103300 0.09064000
 H 3.39212500 2.07414700 3.32620600
 H 3.03785100 0.54122600 3.78560100
 H 2.22918400 1.22876800 2.53670800
 B 4.52373300 0.39795000 1.51041400
 H 3.89975600 -0.67221400 1.55410400
 H 4.21877300 1.33084400 0.79833600
 H 5.44077400 0.49109700 2.27982300
 N 3.14152200 1.15187400 2.97933900

TS6-ComA3:

C -0.68086300 -3.47511300 -0.09003900
 C -1.85316400 -2.73389200 -0.09152600
 C -1.73851500 -1.31522900 -0.13411500
 C -0.43986500 -0.76173900 -0.22805700
 C 0.55724000 -2.83142200 -0.17616200
 C -2.85610500 -0.42357600 -0.06344800
 C -0.26846300 0.67263000 -0.28962300

C -1.39545000 1.52311700 -0.19967600
 C -2.69293100 0.92696800 -0.09783600
 C -1.16944200 2.92866100 -0.24007100
 C 0.13504100 3.36635400 -0.41489500
 C 1.18052300 2.44177800 -0.50440000
 H -3.85419100 -0.83824200 0.02721100
 H -0.71874800 -4.55965200 -0.05734300
 H 1.48074800 -3.40414300 -0.19437000
 H -3.56443300 1.57119900 -0.05602500
 H 0.35650900 4.42862600 -0.44925400
 H 2.20935300 2.77354000 -0.62041100
 N 0.99396700 1.13380100 -0.42832100
 N 0.68205700 -1.51589700 -0.26049100
 C -3.15626400 -3.43464100 -0.05176900
 C -3.39230200 -4.40725400 0.92853600
 C -4.14579300 -3.18492600 -1.01239000
 C -4.59673200 -5.10376400 0.95694500
 H -2.63133800 -4.60399000 1.67958900
 C -5.34581600 -3.88944800 -0.98682300
 H -3.96324900 -2.45311500 -1.79506800
 C -5.57623200 -4.84735100 -0.00069900
 H -4.76951000 -5.84835800 1.72950600
 H -6.10012700 -3.69324200 -1.74413600
 H -6.51530000 -5.39393900 0.01944200
 C -2.25749600 3.92241000 -0.09920700
 C -2.38806600 4.94990000 -1.04265400
 C -3.13619300 3.88856100 0.99240400
 C -3.38356600 5.91267600 -0.90547300
 H -1.71343600 4.98111800 -1.89465800
 C -4.12562600 4.85737600 1.13131900
 H -3.02915600 3.11283800 1.74637300
 C -4.25520900 5.86885000 0.18109700
 H -3.47900100 6.69774200 -1.65097000
 H -4.79426400 4.82358500 1.98741900
 H -5.03115100 6.62216900 0.28858600
 C 4.73662400 -0.50208000 -2.18601600
 O 5.36593200 -0.31083200 -1.11841700
 O 3.47672900 -0.58862200 -2.30920000
 C 5.54005300 -0.66252800 -3.46484500
 H 6.60110300 -0.46222400 -3.29782000
 H 5.42414300 -1.68568200 -3.84194500
 H 5.15369100 0.01141700 -4.23701600
 Cu 2.45722100 -0.40094600 -0.57925500
 B 4.45032900 -0.16247800 0.71941400

H 3.75615500 -1.16768400 0.52898000
H 4.04467300 0.95809300 0.48946100
H 5.53772800 -0.34283300 1.20051100
N 3.65245600 -0.05516200 2.69874100
C 4.42329400 0.95941600 3.39986000
H 5.48392800 0.69093600 3.38114800
H 4.30383200 1.92172600 2.89182700
H 4.10409400 1.07080100 4.44964600
C 2.24230300 0.29579700 2.66969500
H 2.11795400 1.27039200 2.18917300
H 1.69512400 -0.44695300 2.08009200
H 1.80601000 0.34029400 3.68212500
C 3.84551400 -1.36504800 3.29960600
H 3.27629200 -2.11116200 2.73554600
H 4.90545800 -1.63448600 3.25484400
H 3.51644400 -1.39140300 4.35186000

IM6:

C 0.43678400 3.39899100 -0.24055100
C -0.84885200 2.90690400 -0.07449600
C -1.01672500 1.49283500 -0.04277700
C 0.14496700 0.69071300 -0.12959400
C 1.51952600 2.51894700 -0.33495100
C -2.28920300 0.84268900 0.04225400
C 0.03310200 -0.75004600 -0.08099200
C -1.24205100 -1.35760300 -0.01076400
C -2.39633000 -0.51383500 0.05846500
C -1.29718500 -2.78076000 0.00899900
C -0.09528600 -3.47223000 0.01015000
C 1.11583800 -2.77563800 -0.05395300
H -3.18727800 1.44945300 0.08373600
H 0.61461400 4.46952200 -0.26871000
H 2.53162500 2.89558500 -0.45705400
H -3.37719500 -0.97039800 0.13464600
H -0.08757300 -4.55774300 0.02423300
H 2.06354300 -3.30768600 -0.07846000
N 1.18468200 -1.45582300 -0.11317800
N 1.38687000 1.20414000 -0.26852200
C -1.97704600 3.85523900 0.06089700
C -2.13465700 4.88366600 -0.87741300
C -2.86583600 3.78074700 1.14204000
C -3.16680600 5.80765600 -0.74612000
H -1.45156300 4.94607200 -1.72090900

C -3.89223000 4.71128700 1.27517500
H -2.73747400 3.00494800 1.89243200
C -4.04841100 5.72378100 0.32999400
H -3.28259800 6.59391200 -1.48740300
H -4.56869500 4.64732500 2.12330700
H -4.85271100 6.44727000 0.43361000
C -2.57061200 -3.53518300 0.02245900
C -2.77985500 -4.52895900 0.98725900
C -3.55668300 -3.31283900 -0.94838200
C -3.95504800 -5.27436700 0.98976600
H -2.02153800 -4.70435500 1.74618400
C -4.72680700 -4.06636200 -0.94906300
H -3.39405800 -2.56340300 -1.71866300
C -4.93112900 -5.04566800 0.02164000
H -4.10770500 -6.03540700 1.75042200
H -5.47821200 -3.89107700 -1.71438100
H -5.84729100 -5.63020100 0.02156300
C 5.60126400 -0.20143800 0.66476200
O 5.90455700 -0.57386900 -0.53804500
O 4.44492500 -0.03400600 1.07990600
C 6.77416200 0.05214500 1.56849700
H 7.71165200 -0.27164100 1.11285000
H 6.83029500 1.12513100 1.78524000
H 6.62257000 -0.46487400 2.52077100
Cu 2.91973500 -0.26467900 -0.37591600
B 4.80041800 -0.87363000 -1.52868700
H 4.10308300 0.15982400 -1.72797800
H 4.12175400 -1.83261500 -1.14001000
H 5.31429700 -1.14503900 -2.59323500

TS7-ComA1:

C -2.05348600 2.23840500 -0.19335400
C -0.72069300 2.59092200 -0.05874400
C 0.23961500 1.53991200 -0.05702100
C -0.23511600 0.20843800 -0.13113100
C -2.42418500 0.89292000 -0.28959500
C 1.65283400 1.76385500 -0.01817000
C 0.70677200 -0.88901800 -0.10123100
C 2.09827200 -0.62765000 -0.08459900
C 2.53942800 0.73244800 -0.03470500
C 2.98199500 -1.74429600 -0.08725900
C 2.42104200 -3.01163200 -0.05696600
C 1.02962600 -3.16045100 -0.05638100

H 2.01877700 2.78429000 0.00990500
 H -2.82328400 3.00361500 -0.20315900
 H -3.46702800 0.61377800 -0.40964700
 H 3.60351700 0.93853500 0.00070200
 H 3.05707400 -3.89120800 -0.06142400
 H 0.57777400 -4.14925500 -0.04390200
 N 0.19171600 -2.13737000 -0.08625600
 N -1.54846800 -0.10234600 -0.24416400
 C -0.35097900 4.01753000 0.07078800
 C -0.83828700 4.94895000 -0.85473300
 C 0.43822300 4.46959500 1.13694500
 C -0.53170600 6.30004000 -0.72526900
 H -1.44596200 4.60493400 -1.68765300
 C 0.73770100 5.82210600 1.26836300
 H 0.79804400 3.75953400 1.87697900
 C 0.25706600 6.73996100 0.33600400
 H -0.90843000 7.00991700 -1.45633700
 H 1.34312300 6.15992400 2.10484300
 H 0.49448600 7.79519500 0.43803300
 C 4.45404600 -1.59732200 -0.12164000
 C 5.24341200 -2.25805400 0.82765500
 C 5.08274100 -0.84424500 -1.12221900
 C 6.63059600 -2.15458800 0.78766400
 H 4.76223200 -2.84114800 1.60865200
 C 6.47025400 -0.74872900 -1.16492700
 H 4.48062800 -0.35203500 -1.88136000
 C 7.24722100 -1.39923500 -0.20797700
 H 7.23038800 -2.66392100 1.53676900
 H 6.94506700 -0.16895500 -1.95146500
 H 8.33028100 -1.32045100 -0.24029700
 C -5.40755000 -1.33161400 -0.49961600
 O -4.98184200 -1.15699700 0.78761300
 O -5.32975900 -0.38997100 -1.24967200
 C -5.96811200 -2.66798600 -0.87087600
 H -5.12316400 -3.36075200 -0.96704400
 H -6.65270400 -3.05149100 -0.11012300
 H -6.47456000 -2.58168200 -1.83258500
 Cu -2.06840100 -2.15150800 -0.34249300
 B -4.62099400 -2.14247300 1.67663900
 H -4.49973000 -1.76419200 2.80617000
 H -2.82630600 -3.24708400 -1.18766000
 H -4.63615200 -3.29838300 1.37881600
 N -2.05610700 -2.18062200 2.07294800
 H -2.06129300 -1.27284600 2.53100000

H -1.07851500 -2.40131900 1.88675200
 H -2.37723700 -2.86238700 2.75585700

TS7-ComA3:

C -1.47412100 2.73388200 -0.31716600
 C -0.11629700 2.88412200 -0.08863200
 C 0.69515100 1.71468600 -0.14638000
 C 0.05106900 0.47683800 -0.37050200
 C -2.01772300 1.46430200 -0.54376200
 C 2.12087500 1.73078400 -0.01972300
 C 0.83033900 -0.73926400 -0.42330600
 C 2.23899900 -0.68345600 -0.31219400
 C 2.85702800 0.58892000 -0.09734800
 C 2.95686000 -1.91095100 -0.39941000
 C 2.22300600 -3.07881900 -0.53556400
 C 0.82674400 -3.02415900 -0.62081100
 H 2.62134800 2.68110800 0.12954000
 H -2.13193900 3.59663700 -0.28884000
 H -3.08209100 1.33389500 -0.71197600
 H 3.93484900 0.63730900 0.01198500
 H 2.72860600 -4.03636500 -0.60970500
 H 0.24204000 -3.93255900 -0.74108800
 N 0.14575600 -1.89201100 -0.57775100
 N -1.28550200 0.35953800 -0.54825700
 C 0.43294000 4.22678300 0.19939100
 C 0.12893400 5.29934600 -0.64823700
 C 1.21325900 4.46139800 1.33947300
 C 0.60767400 6.57587200 -0.37027200
 H -0.47118400 5.12338600 -1.53722000
 C 1.68398700 5.74048900 1.61947000
 H 1.42977200 3.64218700 2.02002800
 C 1.38629600 6.79956400 0.76361500
 H 0.37302600 7.39676200 -1.04203700
 H 2.27992300 5.91049800 2.51176500
 H 1.75793000 7.79688600 0.98151900
 C 4.43407500 -1.97722100 -0.35731100
 C 5.06875000 -2.84962400 0.53533400
 C 5.21592900 -1.21763000 -1.23791000
 C 6.45658000 -2.94855600 0.55813700
 H 4.46816400 -3.43869100 1.22361600
 C 6.60305400 -1.32459800 -1.21875400
 H 4.73164900 -0.56057600 -1.95544500
 C 7.22677700 -2.18621400 -0.31817100

H 6.93677900 -3.62184700 1.26264500
H 7.19705600 -0.73758400 -1.91354400
H 8.31010500 -2.26596900 -0.30182200
C -5.34562900 -0.45787700 -1.61010500
O -4.90999100 0.02290300 -0.40453600
O -5.06849600 0.17719300 -2.59509300
C -6.14216700 -1.72396300 -1.60533700
H -5.45832200 -2.54907200 -1.37415300
H -6.92950700 -1.70599600 -0.84717100
H -6.57135200 -1.87202100 -2.59665600
Cu -2.03032700 -1.57357000 -0.79541300
B -4.75709500 -0.68893400 0.76262700
H -4.32533500 -0.03597600 1.66564400
H -3.16401200 -2.58052400 -1.17592000
H -5.17388100 -1.79972300 0.88851600
N -2.54000700 -2.06515600 2.41640600
C -1.96420200 -3.36550100 2.14032300
H -2.75585500 -4.06816400 1.86124200
H -1.27254400 -3.28858500 1.29633700
H -1.41665600 -3.78281500 3.00885900
C -3.50941900 -2.15149100 3.48795500
H -3.96103500 -1.16956100 3.66249100
H -4.30744800 -2.84830600 3.21008200
H -3.06126100 -2.49904500 4.43964200
C -1.51415400 -1.09024800 2.72280600
H -0.80269600 -1.03617200 1.89381300
H -1.96927400 -0.10105700 2.84458800
H -0.95341200 -1.33169600 3.64768500

ComG1:

N 0.00000000 0.00000000 0.12209900
H 0.00000000 0.93352300 -0.28489700
H 0.80845500 -0.46676100 -0.28489700
H -0.80845500 -0.46676100 -0.28489700

ComG3:

N 0.00011400 0.00001500 -0.38265100
C 1.27034600 0.53401500 0.06207700
H 2.08984800 -0.08306200 -0.32380600
H 1.40194100 1.55204200 -0.32201700
H 1.36299200 0.57191800 1.16623100
C -1.09766500 0.83309700 0.06205200

H -0.97255200 1.85161000 -0.32267300
H -2.04494600 0.43870300 -0.32309400
H -1.17759000 0.89360200 1.16616200
C -0.17270900 -1.36717500 0.06205900
H -1.11748500 -1.76757900 -0.32274600
H 0.64229200 -1.99063600 -0.32278000
H -0.18512600 -1.46632300 1.16615200

TS8-ComA1:

C -2.59909400 -3.25397600 0.24209000
C -3.55552100 -2.24876200 0.25145400
C -3.10856100 -0.90449900 0.08975400
C -1.72021600 -0.69402700 -0.02428700
C -1.24034400 -2.94171900 0.12807600
C -3.96757400 0.23893000 0.01741700
C -1.19687500 0.63301000 -0.19116100
C -2.06518900 1.73984000 -0.27175500
C -3.47080300 1.49705600 -0.14718200
C -1.47084800 3.02389200 -0.44969400
C -0.08573100 3.09336300 -0.49755600
C 0.69047500 1.93328000 -0.40115200
H -5.03994100 0.09508100 0.08993600
H -2.89536100 -4.29088400 0.36308300
H -0.46864000 -3.70469900 0.14971400
H -4.15458100 2.33801200 -0.17936300
H 0.40820500 4.04936900 -0.63864000
H 1.77331700 1.95846000 -0.45411100
N 0.14608300 0.73814700 -0.26156800
N -0.81292900 -1.69528100 0.01183900
C -4.98146200 -2.59795700 0.42769600
C -5.56385100 -3.58013400 -0.38357400
C -5.75284600 -1.99432900 1.43024900
C -6.89682900 -3.93836400 -0.20710300
H -4.97219800 -4.04836100 -1.16620700
C -7.08228000 -2.36345000 1.61074800
H -5.30108500 -1.25325500 2.08446700
C -7.65864900 -3.33122500 0.78972700
H -7.34106200 -4.69280800 -0.85079900
H -7.66729700 -1.89626300 2.39833100
H -8.69873900 -3.61393000 0.92871400
C -2.26488800 4.26488700 -0.57870000
C -1.94575900 5.37445000 0.21515800
C -3.29789600 4.37532000 -1.51974300

C -2.65589400 6.56346600 0.08255200
 H -1.14911000 5.29420600 0.95045800
 C -3.99970800 5.56926000 -1.65588300
 H -3.53274000 3.53289400 -2.16520900
 C -3.68415300 6.66403300 -0.85297800
 H -2.40501500 7.41291700 0.71218100
 H -4.79086400 5.64547000 -2.39699600
 H -4.23568700 7.59438600 -0.95891400
 C 2.65003400 -3.27010500 -0.69530200
 O 2.94457600 -2.56516100 -1.68661600
 O 1.73960600 -2.94279200 0.14001500
 C 3.39036700 -4.55113000 -0.41267500
 H 2.77459000 -5.24125400 0.16893000
 H 3.72224000 -5.01918500 -1.34231000
 H 4.28335500 -4.30837900 0.17637100
 Cu 1.14047900 -1.06617400 -0.02839100
 C 3.26853500 0.44748600 1.14559500
 N 2.89249000 -0.27965500 0.09265400
 H 3.62962700 -0.65597200 -0.49153900
 O 2.49179900 0.80319500 2.05082900
 C 4.71770800 0.88205400 1.21960600
 C 5.20198100 1.33802300 2.44876300
 C 5.57856400 0.87553200 0.11573100
 C 6.52329100 1.75302100 2.58457800
 H 4.51639400 1.35812800 3.29085000
 C 6.89897000 1.29962800 0.24672900
 H 5.22148800 0.54943400 -0.85748100
 C 7.37727200 1.73415500 1.48209700
 H 6.88779500 2.09514800 3.55026900
 H 7.55461400 1.29600100 -0.62142800
 H 8.40917300 2.06127500 1.58371800
 N 7.10422300 -1.72562300 -2.62404800
 H 7.74102500 -2.47409700 -2.36186700
 H 7.32935000 -0.93090100 -2.03043300
 H 7.33703500 -1.45956200 -3.57792400
 B 4.85893800 -2.27889700 -2.18548700
 H 4.56822000 -1.25375200 -2.75230100
 H 5.00600100 -3.29300300 -2.82169500
 H 5.21101200 -2.24204200 -1.03062300

TS8-ComA3:

C 2.55128000 -3.07128500 -0.78360400
 C 3.44242600 -2.01609300 -0.65120400

C 2.90646300 -0.69602200 -0.60225100
 C 1.51043100 -0.56016300 -0.74093700
 C 1.17765900 -2.83249800 -0.89492200
 C 3.67723100 0.49077200 -0.38227300
 C 0.89583700 0.73684300 -0.70566500
 C 1.67805200 1.88674500 -0.47990400
 C 3.09183800 1.71999200 -0.32546300
 C 1.00073800 3.13991400 -0.44051800
 C -0.36264400 3.14451100 -0.69216200
 C -1.05454400 1.94655700 -0.90852000
 H 4.74980200 0.40319600 -0.24728300
 H 2.91654600 -4.09227300 -0.82494700
 H 0.45735200 -3.63797400 -0.99386700
 H 3.70803400 2.59815300 -0.16537800
 H -0.91562700 4.07835000 -0.68638500
 H -2.11961200 1.92089200 -1.11918100
 N -0.44369800 0.77244000 -0.88448000
 N 0.67483600 -1.61016800 -0.88725000
 C 4.89206300 -2.29206600 -0.56216300
 C 5.36515500 -3.23348900 0.36097900
 C 5.80180800 -1.66200300 -1.42195800
 C 6.72335600 -3.52710000 0.43293200
 H 4.66510100 -3.72040700 1.03524800
 C 7.15801600 -1.96630700 -1.35427200
 H 5.43995500 -0.95239000 -2.16146900
 C 7.62238300 -2.89514300 -0.42437500
 H 7.07974900 -4.25083300 1.16097100
 H 7.85260000 -1.47994900 -2.03393600
 H 8.68245800 -3.12826100 -0.37041300
 C 1.69961900 4.40932700 -0.14626800
 C 1.56807100 5.49717500 -1.01821300
 C 2.46182700 4.55589800 1.02055300
 C 2.20184600 6.70375200 -0.73678900
 H 0.98157900 5.38626000 -1.92675700
 C 3.08396500 5.76781500 1.30443700
 H 2.54558600 3.72470600 1.71629100
 C 2.96009400 6.84186800 0.42451800
 H 2.10293900 7.53730400 -1.42697600
 H 3.66302100 5.87429600 2.21782100
 H 3.45194200 7.78558500 0.64500800
 C -2.43963800 -3.59754900 0.02170300
 O -2.61434000 -3.17094300 1.18168900
 O -1.79084800 -3.01316200 -0.91249800
 C -3.05812200 -4.92313600 -0.36216100

H -3.88630900 -4.74313500 -1.05763400
 H -2.32480000 -5.54646500 -0.88383200
 H -3.43646800 -5.44744600 0.51770800
 Cu -1.32300300 -1.10658400 -0.78049200
 C -3.96792200 0.19660200 -1.17158600
 N -3.15219500 -0.56992500 -0.45354600
 H -3.59382800 -1.11340500 0.27933900
 O -3.61950400 0.83344600 -2.18619700
 C -5.40325600 0.32165900 -0.70560400
 C -6.35816600 0.75114300 -1.63189900
 C -5.80658000 0.06417300 0.60948300
 C -7.69243500 0.89380100 -1.26424000
 H -6.02838400 0.97120400 -2.64306200
 C -7.13954700 0.21861400 0.98338700
 H -5.07732900 -0.23706900 1.35832500
 C -8.08726700 0.62756300 0.04668400
 H -8.42571400 1.21778500 -1.99897000
 H -7.43680300 0.02302600 2.01078800
 H -9.12821000 0.74361400 0.33849500
 B -1.52629400 -1.84317900 2.21182400
 H -1.15296300 -2.71183400 2.96123400
 H -2.49479200 -1.17537700 2.47448500
 H -0.80425400 -1.53269800 1.29065500
 N -0.30387000 -0.37426000 3.40142000
 C -0.60418800 0.94677400 2.88337300
 H -0.37375400 0.98024200 1.81453500
 H -1.67210900 1.15484400 3.00392300
 H -0.03008000 1.74233900 3.39179600
 C -0.68937900 -0.49755400 4.79414400
 H -1.76166200 -0.29989400 4.89438000
 H -0.49561900 -1.51874300 5.13796900
 H -0.14016800 0.20329200 5.44811500
 C 1.09225200 -0.71339700 3.20543100
 H 1.27017500 -1.73995700 3.54252100
 H 1.33625000 -0.65808400 2.13936600
 H 1.77363800 -0.03958000 3.75526200

IM7:

C -2.45101200 -3.16032300 0.28487700
 C -3.36000400 -2.11366200 0.35212300
 C -2.86249300 -0.78979900 0.16839700
 C -1.47383500 -0.64020600 -0.01545500
 C -1.08877700 -2.90919700 0.09642400

C -3.67271500 0.39077100 0.13839700
 C -0.90127700 0.66275000 -0.20073600
 C -1.72234500 1.80646900 -0.24152200
 C -3.12978600 1.62605400 -0.05151300
 C -1.08217500 3.06240500 -0.45499100
 C 0.30156700 3.07341800 -0.56033500
 C 1.03097000 1.88141700 -0.49500700
 H -4.74570800 0.29387300 0.26184200
 H -2.78558300 -4.18401000 0.41745700
 H -0.35732700 -3.71017200 0.06844000
 H -3.77577400 2.49696400 -0.05344500
 H 0.82865900 4.00711200 -0.72761000
 H 2.11058000 1.86073300 -0.59567100
 N 0.44073800 0.71089700 -0.33190800
 N -0.61143900 -1.68169300 -0.03526400
 C -4.78675200 -2.40430200 0.60649400
 C -5.44337500 -3.37979200 -0.15509600
 C -5.48551000 -1.75725300 1.63503900
 C -6.77689500 -3.68802000 0.09466400
 H -4.90810100 -3.88237300 -0.95675900
 C -6.81594400 -2.07602300 1.88856800
 H -4.97690600 -1.02366300 2.25487100
 C -7.46618800 -3.03698600 1.11638500
 H -7.27836200 -4.43815000 -0.51088300
 H -7.34349800 -1.57543100 2.69595500
 H -8.50672400 -3.28092700 1.31317800
 C -1.83201900 4.33167200 -0.56720300
 C -1.44709300 5.43470700 0.20588200
 C -2.89174400 4.47059400 -1.47422600
 C -2.12020200 6.64662600 0.08736300
 H -0.62868700 5.33177800 0.91392800
 C -3.55535600 5.68742700 -1.59739000
 H -3.17744800 3.63172500 -2.10376400
 C -3.17537300 6.77589400 -0.81406100
 H -1.81959000 7.49134000 0.70131100
 H -4.36757500 5.78611400 -2.31252200
 H -3.69798200 7.72394300 -0.90917300
 C 2.66872000 -3.46965700 -1.12181200
 O 2.99577900 -2.69736500 -2.08571700
 O 1.87949600 -3.06804800 -0.22928400
 C 3.22023600 -4.85567700 -1.03422200
 H 2.76585200 -5.39542300 -0.20270700
 H 3.05499700 -5.38815800 -1.97620800
 H 4.30538400 -4.79768000 -0.89033600

Cu 1.34733500 -1.12928700 -0.18570500
 C 3.56185000 0.20512200 0.95503600
 N 3.14372600 -0.46398500 -0.12400900
 H 3.85799100 -0.84368500 -0.73283500
 O 2.80128000 0.55492000 1.87503600
 C 5.02677100 0.56571600 1.04332000
 C 5.54465900 0.88948400 2.30077000
 C 5.87401900 0.60889300 -0.06955300
 C 6.88543300 1.22860500 2.45094700
 H 4.87137000 0.86884300 3.15263300
 C 7.21433800 0.95867400 0.07683500
 H 5.48870000 0.38737000 -1.06204400
 C 7.72473800 1.26388700 1.33750000
 H 7.27693200 1.46851900 3.43656100
 H 7.86028000 0.99481000 -0.79676200
 H 8.77212400 1.53242000 1.45086800
 B 4.01015300 -3.05020500 -3.19927100
 H 4.08378800 -2.04543200 -3.88828300
 H 3.58339100 -4.00180800 -3.84198400
 H 5.08750900 -3.31898900 -2.68167300

TS9-ComA1:

C -0.31594200 3.54591000 -1.00606900
 C 0.93763900 2.96715600 -0.88004300
 C 1.02451200 1.54737000 -0.95766500
 C -0.18561100 0.82432800 -1.06189500
 C -1.44703900 2.73510600 -1.16709300
 C 2.25885500 0.82303800 -0.94661500
 C -0.16083600 -0.61921200 -1.01319200
 C 1.07405900 -1.30317500 -1.02724100
 C 2.28195200 -0.53542800 -0.99892600
 C 1.04595400 -2.72701000 -0.98644800
 C -0.18769900 -3.34792600 -0.89691300
 C -1.35325800 -2.57824500 -0.82386300
 H 3.19118600 1.37487900 -0.90400300
 H -0.42911200 4.62380400 -0.94678700
 H -2.43612600 3.17594500 -1.27013900
 H 3.23231200 -1.05651500 -0.97968900
 H -0.25645400 -4.43012400 -0.86027800
 H -2.32513800 -3.04661400 -0.69960800
 N -1.34646800 -1.25818900 -0.88772700
 N -1.39400700 1.41482700 -1.17319200
 C 2.12092100 3.82049800 -0.63999000

C 2.36665500 4.93279100 -1.45406000
 C 2.97762000 3.56263300 0.43923200
 C 3.45590900 5.76197700 -1.20395400
 H 1.70869100 5.13519900 -2.29533000
 C 4.06054700 4.39864400 0.69165400
 H 2.77705300 2.71829300 1.09426500
 C 4.30513400 5.49706400 -0.13100500
 H 3.64213800 6.61589400 -1.84928600
 H 4.71142500 4.19353800 1.53715100
 H 5.15361400 6.14663800 0.06518400
 C 2.27915900 -3.54330000 -0.98894300
 C 2.48117400 -4.48868100 0.02443500
 C 3.24052500 -3.41206100 -1.99926800
 C 3.62890100 -5.27556400 0.03577400
 H 1.74050400 -4.59192900 0.81335700
 C 4.38230400 -4.20735800 -1.99126700
 H 3.08093200 -2.69744600 -2.80254300
 C 4.58163300 -5.13680200 -0.97166200
 H 3.77884600 -5.99708000 0.83396200
 H 5.11627400 -4.10267900 -2.78536800
 H 5.47650000 -5.75277400 -0.96387700
 C -5.70475300 0.05464200 0.67924000
 O -5.96108300 0.00594200 -0.56834400
 O -4.57039300 0.19211600 1.19854000
 C -6.89049400 -0.04535300 1.60437400
 H -7.78731400 -0.35058900 1.06339200
 H -6.66993900 -0.75056300 2.41003000
 H -7.06374200 0.93496100 2.06162800
 Cu -2.91893600 -0.25550300 0.16770700
 C -0.87587200 -0.72931500 2.07605500
 N -1.64106000 0.25055100 1.59388000
 H -1.17866400 1.15221900 1.56001700
 O -1.22971100 -1.92583000 2.09111000
 C 0.52438600 -0.38745600 2.53711900
 C 1.49240700 -1.39298000 2.46408700
 C 0.90943200 0.88498100 2.97100600
 C 2.82165400 -1.12988600 2.77742900
 H 1.17569100 -2.37926600 2.13940300
 C 2.23556200 1.14714100 3.31030900
 H 0.16961700 1.67642400 3.06630400
 C 3.19833100 0.14418100 3.20129700
 H 3.56443000 -1.91889900 2.68907400
 H 2.51645800 2.13672200 3.66287600
 H 4.23471400 0.35364500 3.45309900

B -4.88177700 0.43835500 -1.76549000
H -5.72948600 0.38083200 -2.63724600
H -3.96784600 -0.74296100 -0.98315000
H -4.52431200 1.53608600 -1.39221900
N -3.52893500 0.12602700 -2.89453500
H -2.65271600 0.40618500 -2.43910100
H -3.66072600 0.68654700 -3.73756800
H -3.45033000 -0.84916800 -3.17441100

TS9-ComA3:

C 2.16682000 -3.14299700 -1.08719500
C 3.18234200 -2.20303400 -1.00949100
C 2.83172400 -0.87562900 -0.63050300
C 1.46221500 -0.59743200 -0.40740000
C 0.84044100 -2.76281400 -0.84769600
C 3.78423200 0.17576300 -0.44190700
C 1.05296100 0.73287300 -0.01124400
C 2.02343500 1.74648600 0.16758700
C 3.39808300 1.42653800 -0.07038100
C 1.56807800 3.03880200 0.55660800
C 0.20129200 3.23328700 0.67849800
C -0.68352400 2.16623400 0.48276800
H 4.83665400 -0.03643800 -0.59522000
H 2.39117500 -4.16707500 -1.36873200
H 0.02710400 -3.48033200 -0.91513000
H 4.14406100 2.20503300 0.04617800
H -0.18834500 4.20511600 0.96480900
H -1.76199800 2.27356500 0.57537400
N -0.26572000 0.95027500 0.17246600
N 0.49453800 -1.52621400 -0.54126000
C 4.57338600 -2.60458400 -1.31659500
C 5.13621600 -3.71483400 -0.67529900
C 5.32779600 -1.92234300 -2.28032900
C 6.43059000 -4.12518900 -0.98010100
H 4.55845300 -4.24514000 0.07730600
C 6.61919700 -2.33888800 -2.58880300
H 4.89010000 -1.07659900 -2.80413500
C 7.17529700 -3.43819700 -1.93690000
H 6.85846200 -4.98209400 -0.46727400
H 7.18983400 -1.80617700 -3.34439400
H 8.18511000 -3.75991000 -2.17590000
C 2.49226900 4.16188500 0.82957800
C 2.29716500 5.39532400 0.19602300

C 3.53568200 4.03166300 1.75584200
C 3.13642400 6.47075200 0.47104600
H 1.49246100 5.50193400 -0.52682000
C 4.36888400 5.11062300 2.03492500
H 3.67758400 3.08720400 2.27459200
C 4.17441100 6.33106500 1.39037900
H 2.97971900 7.41909300 -0.03535500
H 5.16831600 4.99850000 2.76203200
H 4.82801000 7.17156500 1.60649800
C -2.75984500 -3.57541000 1.11001100
O -2.35002300 -3.47355000 2.36659400
O -2.27903100 -2.96280900 0.16766400
C -3.91713300 -4.51856300 0.96342600
H -4.77647700 -4.12260200 1.51578100
H -4.18104500 -4.63277100 -0.08785000
H -3.66885800 -5.48934000 1.40277500
Cu -1.51240600 -0.79774100 0.13622700
C -3.52172100 0.64645400 -1.14293200
N -2.68949700 -0.35798600 -1.38250200
H -2.78664700 -0.79388400 -2.29094900
O -3.58051200 1.21997700 -0.02587600
C -4.44846300 1.12684800 -2.23265400
C -5.62663900 1.78260200 -1.86346800
C -4.16451200 0.96703500 -3.59289200
C -6.51632800 2.24377000 -2.82841900
H -5.82550600 1.92114800 -0.80507100
C -5.04598900 1.43975300 -4.56210800
H -3.23615000 0.49217100 -3.90125600
C -6.22797800 2.07330200 -4.18235300
H -7.43457800 2.74100100 -2.52608900
H -4.80704200 1.31753800 -5.61544200
H -6.91825200 2.43842000 -4.93842200
B -1.14797400 -2.79817000 2.73900000
H -0.86925700 -2.90579100 3.89893300
H -1.10403300 -1.06852300 1.63313800
H -0.25173800 -2.82157300 1.94295400
N -2.43760200 -1.01410800 3.70225200
C -3.58476100 -0.65040800 2.88737300
H -3.26570900 -0.15571900 1.96408300
H -4.14725600 -1.55348300 2.62917300
H -4.26241000 0.03640100 3.42393500
C -2.87531100 -1.64466100 4.93595900
H -3.43597900 -2.55380800 4.69726400
H -2.00656000 -1.92363100 5.53934500

H -3.51844600 -0.97668700 5.53402700
C -1.59365800 0.13742600 3.96895000
H -0.71744400 -0.17947600 4.54462900
H -1.25119700 0.55460500 3.01702300
H -2.12644400 0.91937800 4.53707300

aTS-LC1:

O -0.62098600 0.25963800 -1.29741600
Si -1.66699800 0.02136700 -0.16042000
O -3.23649300 -0.38024200 -0.62328900
O -1.95464400 1.34394400 0.85380900
O -1.28818600 -1.25391800 0.86568800
C -4.00873200 0.56177400 -1.32583700
H -3.96060900 1.54619900 -0.83383100
H -3.61913900 0.69744800 -2.34828900
C -5.44760500 0.08892700 -1.38747000
H -6.07270000 0.80175700 -1.93912600
H -5.51082800 -0.88431900 -1.88809400
H -5.85786300 -0.02160400 -0.37679400
C -2.06145100 -1.49378500 2.01540500
H -2.15202800 -0.57711800 2.61921900
H -3.08537900 -1.79181300 1.73722500
C -1.41351300 -2.58998300 2.83771200
H -1.99684500 -2.79970400 3.74286300
H -1.33705800 -3.51485000 2.25421100
H -0.40133200 -2.29540700 3.13820300
C -0.96929400 2.34372600 0.97628000
H -1.09558600 2.81643900 1.96261300
H 0.04339500 1.91547100 0.95367300
C -1.09104200 3.38631100 -0.11931100
H -2.08285200 3.85485900 -0.09784300
H -0.33374400 4.17288300 -0.00575600
H -0.95059100 2.89657400 -1.08806100
B 1.52093800 0.62792900 -1.24866100
H 1.62366600 0.05483500 -0.18933900
H 1.32202100 1.82133200 -1.27458300
H 1.61345100 0.01107300 -2.28378100
N 3.62417500 0.96702200 -1.26173400
H 4.13715500 0.08864800 -1.25139000
H 3.93077600 1.50013500 -0.45142500
H 3.92663700 1.47908400 -2.08707200

aTS-LC3:

O -0.59026400 0.26461700 -1.30210300
Si -1.64333000 0.02938800 -0.17060100
O -3.20832200 -0.37492000 -0.64610800
O -1.93769700 1.35435700 0.83866600
O -1.27523500 -1.24395600 0.86199300
C -3.96190600 0.54772400 -1.39276800
H -3.92032900 1.54730700 -0.93125200
H -3.55138300 0.65026700 -2.41086000
C -5.40121200 0.07809300 -1.46871800
H -6.01273400 0.77510900 -2.05474200
H -5.45781500 -0.90998500 -1.94028200
H -5.83187800 -0.00034500 -0.46355400
C -2.05570100 -1.47913200 2.00751900
H -2.15635000 -0.55850000 2.60357800
H -3.07560200 -1.78572000 1.72378500
C -1.40732700 -2.56505700 2.84316100
H -1.99684300 -2.77246100 3.74483300
H -1.31954800 -3.49331100 2.26673100
H -0.39981100 -2.26126100 3.15005200
C -0.94532300 2.34466700 0.98235000
H -1.08853100 2.81853600 1.96580500
H 0.06382800 1.90697600 0.98238300
C -1.03395800 3.38811400 -0.11550600
H -2.02136500 3.86629200 -0.11493400
H -0.27151700 4.16737900 0.01313800
H -0.87856100 2.89633800 -1.08084100
B 1.55249000 0.60365000 -1.17283400
H 1.59251700 0.03652800 -0.10444500
H 1.36167000 1.79963700 -1.21954300
H 1.67530900 -0.02576300 -2.19942900
N 3.60705500 0.91946500 -1.08490900
C 3.87615300 1.70732200 0.10628400
H 3.33591400 2.65692500 0.04203100
H 3.51472600 1.16738200 0.98687600
H 4.95167700 1.91711500 0.23374300
C 4.00554600 1.63492100 -2.28544200
H 3.74480600 1.03863900 -3.16509200
H 3.46045000 2.58221800 -2.34050800
H 5.08832200 1.84540800 -2.30597200
C 4.25877500 -0.37814400 -1.01091400
H 3.90146000 -0.91301600 -0.12581100
H 3.99691800 -0.96751800 -1.89486200
H 5.35697500 -0.28949400 -0.95486000

IM8:

O -0.37438600 -0.95242600 1.54812800
Si 0.12059600 -0.03396100 0.33927400
O -0.56340800 1.47832400 0.39347100
O -0.25504500 -0.62305900 -1.16933300
O 1.74976600 0.24095200 0.40481900
C -1.94265300 1.65606500 0.13481600
H -2.21697000 1.17420200 -0.81522300
H -2.54238100 1.17988900 0.92499900
C -2.24833300 3.13724900 0.07644200
H -3.31482400 3.30576100 -0.11398400
H -1.98550400 3.62183500 1.02340600
H -1.67369000 3.61781100 -0.72354700
C 2.45225900 0.81502800 -0.68016300
H 2.14675100 0.34422600 -1.62580600
H 2.21490200 1.88722100 -0.75638700
C 3.93749400 0.62617900 -0.46038500
H 4.51118600 1.07798600 -1.27847700
H 4.24742600 1.09514300 0.48012000
H 4.18447100 -0.44003400 -0.40908000
C -0.72296700 -1.94195500 -1.39442100
H -0.51317800 -2.17556700 -2.44695700
H -0.16885000 -2.66666300 -0.78337300
C -2.20841800 -2.06911400 -1.12301400
H -2.77641100 -1.35455200 -1.73083700
H -2.55759200 -3.08113000 -1.36213600
H -2.41366600 -1.87474100 -0.06531900
B 0.09098500 -2.31621000 1.97512000
H 1.13215700 -2.66061400 1.39146600
H -0.78738600 -3.16398400 1.73446700
H 0.31058500 -2.32131100 3.19489500

bTS-LC1:

B 2.69765000 -0.09767500 0.22093900
H 2.96638700 0.73111300 -0.61165200
H 3.35640400 -0.16519000 1.23099900
H 1.96161800 -1.00693300 -0.06669900
N 4.44541700 -1.44723800 -0.83088600
C 0.24409800 1.36273300 0.22108800
O 0.30367900 2.37712900 -0.44803300
C -0.87664800 0.38867900 0.11169200
C -0.88094000 -0.85817200 0.74891200

C -1.97318800 0.76444500 -0.67245400
C -1.97103100 -1.71024300 0.60489600
H -0.03044600 -1.18689400 1.33890600
C -3.06182500 -0.08668500 -0.81141100
H -1.95368800 1.73174500 -1.16513300
C -3.06239700 -1.32585400 -0.17163300
H -1.96520600 -2.67889300 1.09687300
H -3.91082100 0.21419400 -1.41921000
H -3.91276300 -1.99387300 -0.28079400
N 1.28431800 1.04370100 1.10795200
H 1.82052900 1.87228700 1.35029000
H 1.00732600 0.53442300 1.94188400
H 4.54974600 -2.38204000 -0.44378700
H 5.36701100 -1.01754800 -0.80506800
H 4.20965100 -1.56570400 -1.81304400

bTS-LC3:

B -1.48601800 0.64360200 -0.52289500
H -1.72237300 1.48031200 0.31387500
H -2.03138100 0.70816500 -1.60053000
H -0.94659900 -0.38296700 -0.19211700
N -3.50047500 -0.42310600 0.21387100
C 1.17180900 1.58536200 -0.20385700
O 1.24527800 2.53364900 0.55433200
C 2.07524300 0.40573300 -0.11225400
C 1.88717400 -0.77097600 -0.84743500
C 3.15776100 0.49973400 0.76970900
C 2.77623900 -1.83133900 -0.70465400
H 1.03760000 -0.88321300 -1.51401200
C 4.04647400 -0.55861200 0.90689500
H 3.28719000 1.41478600 1.33946900
C 3.85657200 -1.72676200 0.16915400
H 2.61981800 -2.74421100 -1.27276000
H 4.88629700 -0.47536700 1.59132300
H 4.54963000 -2.55704200 0.27725600
N 0.16830500 1.55006500 -1.18797800
H -0.17330300 2.48680600 -1.38690400
H 0.41601900 1.06910500 -2.04784800
C -3.35599700 -0.66959800 1.63365200
H -3.21593800 0.28081900 2.15933400
H -4.23307000 -1.18291600 2.06999900
H -2.47039700 -1.28928700 1.81014300
C -3.61597500 -1.65747900 -0.53349200

H -4.52142200 -2.23553100 -0.27034200
H -3.64872200 -1.43609100 -1.60580600
H -2.73956700 -2.28586400 -0.34169400
C -4.60355500 0.47293000 -0.06241400
H -4.44899200 1.42007800 0.46557400
H -4.64561600 0.68459200 -1.13635300
H -5.58059800 0.05793200 0.24814500

IM9:

B -2.79878400 -1.17626300 0.81515700
H -3.24288700 -0.32415800 1.55625800
H -3.65193800 -1.92715600 0.38344000
H -1.84606600 -1.76113800 1.28529200
C -1.25777400 0.65224800 -0.20506500
O -1.63926700 1.78569800 -0.03908300
C 0.14991500 0.21797300 -0.10041100
C 0.56726500 -1.11263300 -0.23926000
C 1.09971000 1.22138500 0.13613100
C 1.91791200 -1.42713300 -0.14398300
H -0.14495900 -1.91626400 -0.39820100
C 2.44654300 0.90148500 0.22934500
H 0.76258100 2.24775800 0.24320100
C 2.85706500 -0.42401600 0.08840100
H 2.23672900 -2.46039300 -0.24644400
H 3.17737300 1.68414900 0.41173900
H 3.91156900 -0.67628500 0.16239700
N -2.25640700 -0.36276600 -0.51686100
H -3.06000700 0.12298800 -0.91954700
H -1.92332400 -1.03026500 -1.21417700

IM10:

C 2.13332500 -0.87922100 0.00009100
H 2.75966100 -0.72040800 0.88365700
H 2.76337200 -0.71698700 -0.88017300
H 1.75700200 -1.90352300 -0.00254400
C 1.02574000 0.13511000 -0.00014700
O -0.18121600 -0.44471800 -0.00035000
C -1.30792600 0.44882500 -0.00008300
H -1.25127100 1.09219100 0.88450400
H -1.25166600 1.09221500 -0.88467800
C -2.55668900 -0.39666400 0.00019000
H -3.44005200 0.25088900 0.00040000

H -2.59941600 -1.03466800 -0.88879200
H -2.59900800 -1.03467400 0.88919000
O 1.19305100 1.33555200 0.00011600

cTS-LC1:

B -1.86963100 -0.53451200 -0.00024800
H -1.80539500 0.04616400 -1.05245400
H -2.38098000 -1.62286800 0.02693600
H -1.79376600 0.09165500 1.02444400
N -4.36382900 0.24188900 -0.00224500
C 2.16056800 -2.06207200 0.00168000
H 2.97872000 -1.81449200 -0.67955400
H 1.71536700 -3.02045500 -0.26724400
H 2.57891200 -2.13421700 1.01249100
C 1.11468500 -0.99131400 -0.01280000
O 1.64800400 0.21549500 -0.01366500
C 0.78213400 1.37517200 0.02178800
H 0.11097400 1.33626400 -0.83913300
H 0.17963300 1.33004200 0.93213800
C 1.67037300 2.59183500 -0.00734800
H 1.04911500 3.49301200 0.02812700
H 2.34737900 2.60676500 0.85299600
H 2.26761600 2.62254700 -0.92446600
O -0.08121100 -1.25402600 -0.00100300
H -4.81643300 -0.18819400 -0.80512900
H -4.63338000 1.22301800 -0.01513800
H -4.80370300 -0.16337200 0.82036500

cTS-LC3:

B 0.87390400 -0.30868000 -0.00015500
H 1.01278800 -1.50605100 -0.00049400
H 0.95289500 0.29765500 -1.04229800
H 0.95275200 0.29707000 1.04234200
N 3.26427400 -0.18809600 0.00003200
C -1.28960000 1.98241500 0.00001100
H -2.11905900 2.69045300 0.00027200
H -0.65804600 2.14135000 -0.87951300
H -0.65765600 2.14113200 0.87929300
C -1.77445600 0.57290900 -0.00006900
O -3.09107000 0.46848700 0.00006300
C -3.64171500 -0.86869900 0.00001300
H -3.27435800 -1.39587300 -0.88589400

H -3.27425800 -1.39596900 0.88582300
 C -5.14249400 -0.73254600 0.00010100
 H -5.59753900 -1.72846700 0.00007200
 H -5.48852400 -0.19633200 0.88967600
 H -5.48861500 -0.19623800 -0.88938200
 O -1.05274000 -0.42126200 -0.00026300
 C 3.61792600 1.21589600 0.00020400
 H 3.19673000 1.70174900 -0.88670700
 H 3.19664000 1.70156000 0.88717200
 H 4.71138000 1.38233500 0.00027900
 C 3.73150000 -0.85467400 -1.19755500
 H 3.39527100 -1.89693000 -1.19222100
 H 3.30718000 -0.36441600 -2.08028300
 H 4.83356600 -0.84529100 -1.29066400
 C 3.73128500 -0.85493500 1.19755700
 H 3.30678500 -0.36491200 2.08032800
 H 3.39509300 -1.89720400 1.19190300
 H 4.83333300 -0.84554200 1.29087600

IM12:

B 2.55917600 -1.12941800 0.00061300
 H 3.03179500 -0.64275200 1.01310800
 H 2.59496900 -2.34191500 -0.00103800
 H 3.03434200 -0.63986000 -1.00926500
 C 1.39398200 1.60182300 0.00015700
 H 2.04618200 1.58988800 -0.87987500
 H 2.04849600 1.58798100 0.87841400
 H 0.77176000 2.49671000 0.00183500
 C 0.56423300 0.37682500 -0.00025500
 O -0.72248800 0.56662800 -0.00037600
 C -1.59092500 -0.60254200 -0.00065100
 H -1.35953500 -1.19622300 -0.88947300
 H -1.35831500 -1.19762900 0.88691100
 C -3.00819300 -0.09586200 0.00076500
 H -3.69304300 -0.94994000 0.00062900
 H -3.21041100 0.50690900 0.89157800
 H -3.21177200 0.50828900 -0.88880300
 O 1.01687200 -0.78610700 -0.00052300

ComA1:

B 0.29888900 -2.01787300 -0.04290600
 H 1.20292200 -2.61312700 -0.60379300

H -0.73726200 -2.05218900 -0.68457900
 H 0.13998300 -2.40313200 1.10273400
 N 0.74280900 -0.47018500 0.04224200
 H 0.88908900 -0.06384800 -0.88194000
 H 1.61403600 -0.35024600 0.55929500
 H 0.04007900 0.10352700 0.50894600

TS2-ComB1:

C -0.76776651 0.10152284 0.00000000
 C -2.05289551 0.90965784 -0.18416500
 C -1.37674251 2.09869584 0.49619000
 H -0.85552851 -0.84333816 0.54760900
 H -0.20410451 -0.07146616 -0.92753500
 H -2.49577851 1.02816184 -1.16960000
 H -1.88046251 2.51680984 1.37358400
 H -1.11015851 2.92130084 -0.18160300
 N -0.25246651 1.21556784 0.79317800
 I -3.83902551 0.06230484 1.04842600
 C 1.02985549 1.61935184 0.97810000
 O 1.33981049 2.75722884 1.28256000
 O 1.86367949 0.57702884 0.78744800
 C 3.29409849 0.73880584 0.98157100
 C 3.83232349 -0.65413916 0.68269700
 H 4.92151049 -0.66940416 0.79247100
 H 3.40040949 -1.38755316 1.37124500
 H 3.58008449 -0.95101116 -0.34066900
 C 3.58732149 1.13170884 2.42501600
 H 4.67000549 1.14015684 2.59225300
 H 3.18483749 2.12217284 2.64457900
 H 3.13900049 0.40473384 3.11089300
 C 3.84872249 1.75337284 -0.01262900
 H 3.45697749 2.75113384 0.19233500
 H 4.94191449 1.77713984 0.05586900
 H 3.57571249 1.46642484 -1.03419300
 B -4.73026051 2.91965984 0.49676000
 H -4.00498851 3.58613484 1.16912700
 H -4.75597251 2.84974684 -0.69419300
 N -6.05327151 2.47045584 1.21402200
 H -6.86299851 2.50992984 0.59616700
 H -5.95937251 1.47291584 1.53071200
 H -6.25484751 3.03112384 2.04089200

ComA2:

N 1.86508300 0.00003000 0.55215600
 H 2.11833600 -0.81481200 1.11360100
 H 2.11820900 0.81505700 1.11337700
 C 0.43658900 -0.00002900 0.31231800
 C -0.23318700 -1.21064400 0.17394800
 C -0.23317500 1.21065800 0.17391700
 C -1.59911200 -1.20560500 -0.09536200
 H 0.30975900 -2.14737800 0.27340100
 C -1.59906200 1.20562100 -0.09538800
 H 0.30985700 2.14735600 0.27339400
 C -2.28452100 -0.00000200 -0.22971500
 H -2.12685200 -2.14951400 -0.20053900
 H -2.12682700 2.14951500 -0.20056100
 H -3.35045400 0.00002300 -0.43998500
 B 2.77479300 -0.00005400 -0.80000900
 H 2.48045400 1.01121000 -1.40921900
 H 2.48061000 -1.01151100 -1.40896600
 H 3.93217400 0.00011200 -0.41786000

TS2-ComB2:

C -2.13272900 -1.00072200 0.87290400
 C -0.65965200 -0.60974000 0.97426100
 C -0.98812000 0.71668200 0.29222500
 H -2.36190100 -1.94710000 0.37060500
 H -2.67002400 -0.95914300 1.83008800
 H -0.14782900 -0.61738700 1.93291200
 H -0.41593400 0.97141700 -0.60624200
 H -0.98553600 1.58075500 0.97080900
 N -2.33096300 0.19130800 0.04607100
 I 0.74596800 -1.94143100 -0.32036800
 C -3.44621300 0.94847600 -0.10908600
 O -3.41876200 2.11997100 -0.45157600
 O -4.53863500 0.20730400 0.14476200
 C -5.87305100 0.77851300 0.01800500
 C -6.77514400 -0.38939100 0.38944100
 H -7.82521500 -0.08287500 0.34210300
 H -6.62602200 -1.22813800 -0.29909300
 H -6.56001100 -0.73462700 1.40658000
 C -6.12585800 1.21397700 -1.41978300
 H -7.17480500 1.50852500 -1.53609200
 H -5.49070800 2.05913800 -1.69247600
 H -5.92580600 0.38464600 -2.10754300

C -6.04869000 1.92479100 1.00595100
 H -5.40044200 2.76599800 0.75168900
 H -7.09011500 2.26481800 0.99263900
 H -5.81239400 1.58982800 2.02244100
 B 2.42386200 0.50234100 0.49295300
 H 1.93910000 1.51240800 0.07130200
 H 2.55607200 0.24031800 1.65400400
 N 3.55081400 -0.09084300 -0.42214900
 H 3.64241400 -1.10027600 -0.25718900
 H 3.28339000 0.00138800 -1.40609100
 C 4.82446500 0.57511400 -0.18518100
 C 5.68881800 0.06848800 0.78187000
 C 5.14068800 1.72197800 -0.90896400
 C 6.88866800 0.72940100 1.02838100
 H 5.42249300 -0.82835300 1.33543100
 C 6.34383400 2.37202800 -0.65366900
 H 4.44970400 2.10108400 -1.65753200
 C 7.21893700 1.88081200 0.31503300
 H 7.56867600 0.33840400 1.78019200
 H 6.59737600 3.26600600 -1.21666600
 H 8.15636900 2.39341500 0.51158800

ComA4:

C -2.23551900 1.33997400 -0.09872500
 C -1.60815700 3.74841100 0.00128200
 C -2.77436700 2.76402100 0.12146900
 H -2.47940500 0.95590100 -1.09261800
 H -2.61976900 0.62973200 0.63720900
 H -3.54734500 2.98752500 -0.62165200
 H -3.23782100 2.85363800 1.11093100
 C -0.17818900 2.06844800 -1.15482500
 H 0.89561100 2.15309000 -0.96844700
 H -0.31584000 1.44386200 -2.04060000
 C -0.85307000 3.44340600 -1.29508200
 H -0.09611000 4.20998500 -1.49203900
 H -1.54951300 3.44751500 -2.14161200
 H -1.97392200 4.78003000 -0.00014400
 C -0.65845200 3.51602800 1.17906300
 H 0.26082100 4.09587400 1.03644300
 H -1.11467200 3.85365700 2.11579700
 C -0.34420000 2.01221800 1.26353400
 H 0.72036100 1.81587100 1.41177600
 H -0.89062300 1.52126100 2.07309400

N -0.74524000 1.31511500 0.00436500
 B -0.20890100 -0.20022400 0.00577500
 H -0.67506800 -0.74413100 -0.98225100
 H 1.00971200 -0.14677800 -0.03647700
 H -0.60577600 -0.71713400 1.03768700

TS2-ComB4:

C 2.21412500 1.19252900 0.80676900
 C 0.76852600 0.81187800 1.11691800
 C 1.05899400 -0.60276100 0.62310500
 H 2.36950200 2.05044700 0.14265800
 H 2.84794400 1.30510700 1.69713500
 H 0.34686300 0.97344700 2.10519800
 H 0.40613600 -1.00208600 -0.16101000
 H 1.14635300 -1.34816600 1.42623000
 N 2.35560000 -0.11236500 0.15770700
 I -0.77458900 1.91807900 -0.25507300
 C 3.46776800 -0.86994300 -0.00924300
 O 3.43911000 -2.08083900 -0.16444800
 O 4.55839300 -0.08313700 0.00115200
 C 5.88545100 -0.64319100 -0.21371700
 C 6.78355600 0.58313000 -0.13650700
 H 7.82943400 0.29406100 -0.28341600
 H 6.51177300 1.30972800 -0.90980100
 H 6.69089700 1.06897000 0.84102000
 C 5.97055600 -1.28301700 -1.59358500
 H 7.00475000 -1.58339700 -1.79548100
 H 5.32951100 -2.16456800 -1.65948900
 H 5.66705400 -0.56565900 -2.36448700
 C 6.22664200 -1.62656300 0.89874400
 H 5.58764900 -2.51061800 0.85168900
 H 7.27188100 -1.94156000 0.80483700
 H 6.10041300 -1.15066300 1.87798900
 B -2.29401800 -0.29216300 1.44837000
 H -1.49065900 -1.18147500 1.51843900
 H -2.54720900 0.43892200 2.36634300
 C -3.10224200 -1.31026400 -0.71550900
 C -4.35360000 0.55430600 0.23534600
 C -4.40210100 -1.62601400 1.32032300
 C -4.30357200 -1.49683800 -1.65597300
 H -2.32500400 -0.67604600 -1.14720900
 H -2.64464600 -2.26160400 -0.43130100
 H -4.49065600 1.10891300 1.16611800

H -3.74207500 1.16453800 -0.43293600
 C -5.68821500 0.14296700 -0.40768500
 C -5.50041800 -2.19413500 0.40488900
 H -4.81286100 -1.06919800 2.16654400
 H -3.74313400 -2.40368800 1.71411500
 C -5.59159400 -1.31979700 -0.84788900
 H -4.26931000 -0.76385000 -2.47004500
 H -4.26492500 -2.49270800 -2.11001400
 H -6.51358300 0.26461500 0.30351400
 H -5.89746700 0.79160200 -1.26488800
 H -6.45595000 -2.20428800 0.94012600
 H -5.26979700 -3.22810000 0.12421900
 H -6.46325100 -1.59921900 -1.44778100
 N -3.53268100 -0.65660200 0.56502700

ComA5:

N -2.29107200 0.83408500 -0.02567100
 C -1.72232600 1.50816800 -1.23969600
 H -2.07334600 2.54043900 -1.21010700
 H -0.62952200 1.51641200 -1.12759100
 C -1.77776900 -0.57540900 0.00670800
 H -2.14581200 -1.05561500 -0.90076200
 H -0.68236400 -0.52476900 -0.05420100
 C -1.77458900 1.54654500 1.18977800
 H -2.18021100 1.01504400 2.05137900
 H -0.68281300 1.42708500 1.19992400
 C -2.14610900 3.01242900 1.30154500
 H -1.80236300 3.37273400 2.27740500
 H -1.67131100 3.63691100 0.53958900
 H -3.22836200 3.15680700 1.25194500
 C -2.11027300 0.90049900 -2.57366400
 H -1.70706100 1.54254700 -3.36453900
 H -1.69976500 -0.10160500 -2.72808600
 H -3.19579100 0.85931400 -2.69431600
 C -2.20080800 -1.40304500 1.20482500
 H -1.85683300 -2.43039000 1.04231500
 H -1.75883900 -1.05789300 2.14393500
 H -3.28810200 -1.42472100 1.31363700
 B -3.92048400 0.85655900 -0.06015700
 H -4.28626600 -0.06255100 -0.77156000
 H -4.26371800 1.93320900 -0.51618600
 H -4.31434800 0.71407600 1.08428300

TS2-ComB5:

C 2.02368400 -1.21364000 -0.85783700
C 0.57688200 -0.82621800 -1.15633600
C 0.87567900 0.58348500 -0.65367000
H 2.18092800 -2.07840200 -0.20317100
H 2.65217400 -1.31852300 -1.75294600
H 0.15017100 -0.97767100 -2.14405200
H 0.22922900 0.98043700 0.13700900
H 0.96166500 1.33430300 -1.45198400
N 2.17145300 0.08467600 -0.19735400
I -0.95031800 -1.94607800 0.21890400
C 3.28511400 0.83679600 -0.01807400
O 3.25963500 2.04705400 0.14318200
O 4.37274300 0.04590300 -0.02307800
C 5.70086900 0.60147800 0.19708500
C 6.59416600 -0.62906300 0.13251000
H 7.64064400 -0.34320400 0.28143500
H 6.31643700 -1.34854400 0.91034300
H 6.50323000 -1.12196500 -0.84159200
C 5.78231100 1.24908500 1.57366700
H 6.81775800 1.54222100 1.77985500
H 5.14798500 2.13596700 1.63089500
H 5.46869800 0.53868100 2.34696500
C 6.05124500 1.57672000 -0.91962600
H 5.41197500 2.46125300 -0.88370000
H 7.09570600 1.89249600 -0.82005200
H 5.93230500 1.09378000 -1.89633500
B -2.51897400 0.33442100 -1.37279800
H -1.67087100 1.17055700 -1.52698400
H -2.90712600 -0.35965300 -2.27258300
C -2.99624800 1.52627000 0.74397000
C -4.40480300 -0.43712400 0.05856000
C -4.53146800 1.71329800 -1.23761800
C -3.75568000 1.70211500 2.04618200
H -2.08816900 0.94994600 0.94440900
H -2.68246200 2.49130500 0.33577500
H -4.39899000 -1.10910800 -0.80324900
H -3.77360200 -0.89655600 0.82332700
C -5.83362000 -0.29177700 0.55187500
C -5.41664800 2.73340800 -0.53927500
H -5.12099500 1.05407200 -1.88103500
H -3.82956200 2.24892200 -1.88505100
H -3.96542400 0.74230200 2.52781100

H -3.10485200 2.26557200 2.72467700
H -6.50622900 0.07006300 -0.23169300
H -6.17874400 -1.29290500 0.83487600
H -5.95983400 3.27778200 -1.32041400
H -4.82852500 3.46935800 0.01666700
N -3.67421000 0.80158800 -0.39028200
H -4.68921600 2.25878800 1.94626500
H -5.93596000 0.35075100 1.42867400
H -6.15525700 2.29151800 0.13207700

ComA6:

N -1.56357200 0.33864600 0.01229000
Si -1.97838000 1.06021900 -1.63857200
Si -2.76822300 0.79290200 1.33772200
Si 0.20020000 0.58000500 0.50487800
C -3.43634000 0.19880500 -2.44590100
H -4.35582400 0.18456900 -1.85779600
H -3.64883700 0.74176200 -3.37726100
H -3.18476300 -0.83215200 -2.71209500
C -0.56072300 0.87891000 -2.85813700
H -0.92656300 1.29964700 -3.80506900
H 0.35162000 1.42267400 -2.59828200
H -0.30872600 -0.16910700 -3.04525100
C -2.34164400 2.89997700 -1.47874300
H -2.49619200 3.29156000 -2.49329000
H -3.24419600 3.13177800 -0.90530100
H -1.50754900 3.45718500 -1.04104500
C 1.36703900 -0.52896200 -0.45832000
H 1.19379900 -1.58382100 -0.22616500
H 1.33336000 -0.40769800 -1.54277800
H 2.38494500 -0.27612200 -0.13062500
C 0.71198600 2.37551500 0.26489700
H 1.74117300 2.47321700 0.63588100
H 0.71536300 2.70062500 -0.77987700
H 0.09447800 3.07324600 0.83912200
C 0.49084800 0.15633600 2.31243500
H 0.26567000 -0.89125800 2.53309700
H 1.56678200 0.30202200 2.48169600
H -0.03462000 0.79192800 3.03068500
C -2.35710800 2.48520600 2.05164200
H -3.15328200 2.73820100 2.76477100
H -1.41194500 2.51762400 2.60216200
H -2.33932900 3.27465100 1.29404000

C -4.52908500 0.87416600 0.68788000
H -4.88050000 -0.09672000 0.32559900
H -5.15246400 1.14180100 1.55243700
H -4.71281200 1.62703800 -0.08352700
C -2.81272000 -0.46770400 2.72636800
H -3.17626000 -1.43744400 2.37418300
H -1.86243400 -0.62520000 3.24020900
H -3.53057400 -0.09142000 3.46853800
B -1.73477100 -1.29956500 -0.18028300
H -1.12888500 -1.85536500 0.72087000
H -2.92372200 -1.56699700 -0.12877500
H -1.27032900 -1.60657800 -1.26541000

TS2-ComB6:

C 1.84119100 -1.02762300 -0.96692400
C 0.41306500 -0.50720900 -1.10304700
C 0.83692400 0.77861400 -0.39912500
H 1.97210000 -1.99316600 -0.46466500
H 2.40771700 -1.02985400 -1.90827100
H -0.07842500 -0.47046700 -2.07153500
H 0.26984000 1.06925400 0.49238400
H 0.92306400 1.64790600 -1.06630500
N 2.12113700 0.13735900 -0.12566600
I -1.11556600 -1.75286200 0.17809100
C 3.29513100 0.78008500 0.09145900
O 3.36789300 1.94707500 0.44372100
O 4.31851100 -0.06714400 -0.11588400
C 5.69670300 0.36187500 0.07589900
C 6.48841800 -0.89438900 -0.25795300
H 7.56149400 -0.70059700 -0.15902500
H 6.21925800 -1.71228600 0.41911100
H 6.28673400 -1.21572100 -1.28555100
C 5.92610100 0.76885200 1.52560900
H 6.99119700 0.97009000 1.68626900
H 5.35747600 1.66611700 1.77775100
H 5.62630400 -0.04116900 2.20005600
C 6.03609600 1.48349100 -0.89728800
H 5.46715700 2.38696500 -0.66856100
H 7.10535100 1.71468600 -0.83549600
H 5.81244200 1.17546700 -1.92509500
B -2.60124200 0.58106000 -1.01108300
H -1.73522800 1.40891100 -0.96399800
H -2.88833400 -0.02432500 -2.00778800

N -3.82515000 0.86955200 -0.05011000
Si -5.04242600 -0.47580700 -0.23491800
H -5.65154000 -0.28227400 -1.57257100
H -4.33041700 -1.76159400 -0.10703200
H -6.04856200 -0.28944500 0.84097200
Si -3.26033400 1.10074300 1.67360700
H -3.16727200 -0.23319500 2.30094500
H -1.97904000 1.83438800 1.62568200
H -4.31398500 1.91743500 2.33245900
Si -4.45301000 2.44227900 -0.73738300
H -3.47744600 3.48815600 -0.35653300
H -4.61010600 2.27802400 -2.19763300
H -5.77273200 2.70206400 -0.09130300

ComA7:

P -1.23945200 0.60434600 -0.02256100
B -3.05521800 -0.05072600 -0.18302800
H -2.94809200 -1.20598200 -0.54008600
H -3.57932700 0.66144000 -1.01462800
H -3.53651300 0.06777300 0.92485900
H -0.44995500 0.57799200 -1.18579100
H -1.08046100 1.94027300 0.38568400
H -0.40408900 -0.06221300 0.89032700

TS2-ComB7:

C -0.56186600 -1.16131200 0.82367700
C 0.75939200 -0.51644200 1.22359400
C 0.17883600 0.84666800 0.87634400
H -0.52084000 -1.95752500 0.07065500
H -1.16815000 -1.50022700 1.67506800
H 1.21976200 -0.70746900 2.18839200
H 0.74042900 1.46116800 0.16194600
H -0.07655000 1.46321700 1.74996600
N -0.97024600 0.14689200 0.30858600
I 2.49770200 -1.14165100 -0.28361500
C -2.21067300 0.66727700 0.13881200
O -2.43293500 1.86718300 0.09181600
O -3.10638900 -0.32634000 0.01000400
C -4.51116400 -0.03524000 -0.24638400
C -5.12957100 -1.42240900 -0.34150300
H -6.20358000 -1.34318000 -0.53935000
H -4.66835900 -1.99519000 -1.15323800

H -4.98865400 -1.97369600 0.59457100
 C -4.66077600 0.70958900 -1.56670500
 H -5.72371000 0.80955600 -1.81291100
 H -4.21741600 1.70568500 -1.50740000
 H -4.17341000 0.15212400 -2.37460500
 C -5.10753100 0.73851200 0.92259100
 H -4.66569600 1.73388700 1.00215200
 H -6.18888500 0.84354300 0.78081900
 H -4.93722300 0.19896300 1.86121400
 B 3.56175000 1.07947200 1.01038600
 H 2.73136700 1.37729600 1.81868500
 H 4.60036800 0.56959300 1.31801700
 P 3.69587200 2.27018300 -0.46030100
 H 3.92975300 1.62490500 -1.69468600
 H 4.71169500 3.25424000 -0.49702900
 H 2.54048500 3.02567800 -0.71528800

ComA8:

B -0.00503800 0.00050800 2.88127400
 H 1.16132300 -0.05524700 3.21951600
 H -0.63531500 -0.98322700 3.21664600
 H -0.54149500 1.03722600 3.22084700
 P -0.00331600 0.00120700 0.95072100
 C -1.66816400 0.19087900 0.23808300
 C -2.74391000 -0.43346800 0.88114400
 C -1.89089800 0.92179700 -0.93369400
 C -4.02606600 -0.33204500 0.35002200
 H -2.57915700 -0.99385500 1.79743200
 C -3.17656000 1.02078500 -1.45945300
 H -1.06365500 1.41638200 -1.43564600
 C -4.24359700 0.39379600 -0.81989800
 H -4.85727200 -0.81757700 0.85420300
 H -3.34354300 1.59087800 -2.36950200
 H -5.24653100 0.47423700 -1.23101800
 C 0.99671000 1.34584400 0.23795300
 C 1.74978800 1.16718600 -0.92733300
 C 0.98755700 2.59335800 0.87354000
 C 2.48089800 2.22906600 -1.45383800
 H 1.76921800 0.20051000 -1.42313300
 C 1.71853500 3.65108300 0.34149300
 H 0.41147000 2.73595700 1.78375600
 C 2.46516400 3.47040800 -0.82162700
 H 3.06573500 2.08346700 -2.35819600

H 1.70833100 4.61670100 0.83978400
 H 3.03812500 4.29713200 -1.23335600
 C 0.66632200 -1.53621200 0.24115400
 C 1.77235000 -2.12753400 0.86334200
 C 0.12239200 -2.12043100 -0.90718500
 C 2.33030600 -3.28768900 0.33561700
 H 2.19365400 -1.68237800 1.76061200
 C 0.68377300 -3.28313900 -1.42936100
 H -0.74013800 -1.67185800 -1.39260100
 C 1.78692000 -3.86652500 -0.81018100
 H 3.18798600 -3.74275600 0.82366800
 H 0.25519900 -3.73408200 -2.32046200
 H 2.22186800 -4.77511000 -1.21840600

TS2-ComB8:

C -1.75954100 0.34039600 -0.51170600
 C -1.31053300 1.44891400 -1.46302100
 C -2.77420900 1.82269100 -1.68647100
 H -1.63515700 -0.67937200 -0.90424000
 H -1.37760500 0.37084500 0.51171900
 H -3.16468100 1.56310200 -2.68004700
 H -3.05584000 2.85578900 -1.44819100
 N -3.11868700 0.85389400 -0.65257900
 C -4.29729800 0.22020000 -0.46083400
 O -5.36275000 0.60352500 -0.91985700
 O -4.09223900 -0.86063600 0.31616100
 C -5.19972000 -1.69231700 0.75758300
 C -4.50499300 -2.74094200 1.61653700
 H -5.23921100 -3.44627700 2.01825500
 H -3.77287100 -3.29809900 1.02240900
 H -3.98179900 -2.26433100 2.45222000
 C -5.87787200 -2.34211500 -0.44259600
 H -6.63414800 -3.05498900 -0.09700600
 H -6.35971200 -1.59004700 -1.06997300
 H -5.14063400 -2.88702400 -1.04240200
 C -6.17244100 -0.87077400 1.59487800
 H -6.66303300 -0.10929500 0.98590600
 H -6.93562400 -1.52931900 2.02305500
 H -5.64018500 -0.38040900 2.41717000
 C 1.09797400 -0.46759000 1.09982500
 C 0.40651800 -1.68257400 1.13088800
 C 0.86483900 0.49145600 2.09479400
 C -0.53204700 -1.92348800 2.13255000

H 0.58605100 -2.43329300 0.36726100
 C -0.06492300 0.24094200 3.09747400
 H 1.39766400 1.43784500 2.07543500
 C -0.77382100 -0.96153900 3.10964000
 H -1.07999900 -2.86141000 2.14237100
 H -0.24769100 0.99043500 3.86201300
 H -1.51366700 -1.14722800 3.88333900
 C 3.90709900 -0.13117100 0.56182700
 C 4.99074600 0.49741600 -0.06202000
 C 4.10700000 -0.84235800 1.75040900
 C 6.26124800 0.41497200 0.49955500
 H 4.83619900 1.05269500 -0.98328600
 C 5.38048600 -0.92154400 2.30785300
 H 3.26948700 -1.32955900 2.24163100
 C 6.45674300 -0.29345500 1.68409800
 H 7.09831500 0.90768000 0.01325800
 H 5.53021000 -1.47219600 3.23222700
 H 7.44889200 -0.35420100 2.12275700
 C 2.19000400 -1.48170000 -1.37760700
 C 3.13053100 -2.51661300 -1.32312800
 C 1.14994700 -1.54216100 -2.31593400
 C 3.03043200 -3.59581200 -2.19779200
 H 3.94016500 -2.48014600 -0.60010900
 C 1.05206800 -2.62523400 -3.18206300
 H 0.41900700 -0.74120500 -2.37164800
 C 1.99258200 -3.65391600 -3.12520300
 H 3.76630000 -4.39366400 -2.15154000
 H 0.24195100 -2.66438000 -3.90471600
 H 1.91629600 -4.49818800 -3.80455100
 P 2.27231800 -0.06420100 -0.24209500
 B 2.00465200 1.58836600 -1.17257900
 H 1.65149000 1.44174900 -2.30864600
 H 2.82648800 2.41079600 -0.88626600
 I -0.09383300 3.15645200 -0.33318200
 H -0.65573400 1.24242500 -2.30503600

ComA9:

P -0.08740300 0.00007500 -0.00022200
 C 0.63425000 -1.63133100 -0.35602400
 H 0.29344700 -2.35101000 0.39503200
 H 0.29469100 -1.97158200 -1.33952900
 H 1.72837700 -1.59160600 -0.34654100
 C 0.63797300 1.12333100 -1.23327900

H 0.29935300 0.83292400 -2.23291300
 H 0.29783500 2.14525000 -1.03741400
 H 1.73200200 1.09537000 -1.20083200
 C 0.63585000 0.50602100 1.59021500
 H 0.29715600 1.51692100 1.83850900
 H 0.29562400 -0.17485200 2.37695800
 H 1.72992900 0.49191800 1.55040600
 B -2.00883600 0.00213800 -0.00074800
 H -2.35433700 -0.78409500 0.86349400
 H -2.35412700 -0.35322400 -1.11382600
 H -2.35315800 1.14404400 0.24826100

TS2-ComB9:

C 1.41846900 -1.31148200 -0.71976300
 C 0.04378500 -0.85502500 -1.19508000
 C 0.42253500 0.58124200 -0.85675900
 H 1.44028400 -2.07408900 0.06807400
 H 2.09989500 -1.60810900 -1.52879800
 H -0.32874500 -1.11704800 -2.18111800
 H -0.23630600 1.12401300 -0.16955600
 H 0.61795000 1.21439300 -1.73378700
 N 1.64220000 0.05638400 -0.24521200
 I -1.68153700 -1.70874400 0.20882500
 C 2.80677100 0.74013400 -0.11745700
 O 2.87662400 1.95893000 -0.14988200
 O 3.82081300 -0.12210500 0.06998800
 C 5.18482600 0.35489400 0.25346100
 C 5.96985900 -0.93539800 0.44074200
 H 7.03164100 -0.71124400 0.58620200
 H 5.60740300 -1.48438600 1.31657500
 H 5.86846300 -1.58118300 -0.43819300
 C 5.27997300 1.22365400 1.50108300
 H 6.33002800 1.46467100 1.70090800
 H 4.72325500 2.15433300 1.37585500
 H 4.88215100 0.68669800 2.36962800
 C 5.65315600 1.08934300 -0.99606400
 H 5.09374600 2.01601400 -1.13977000
 H 6.71793900 1.33086800 -0.90461100
 H 5.52176300 0.45560300 -1.88049600
 B -2.97358100 0.36467800 -1.38740300
 H -2.04722200 0.92060000 -1.90936700
 H -3.67010400 -0.39889900 -1.99703400
 C -4.83574600 2.74577100 -0.58596500

H -5.58174100 2.40037300 -1.30856500
H -5.34328800 3.23380300 0.25426600
H -4.17853500 3.46816700 -1.08046500
C -2.71672600 2.02598100 1.23270400
H -3.27606500 2.61224000 1.96942500
H -2.18580900 1.21617900 1.74161900
H -1.98797700 2.67619800 0.73861900
C -5.01530600 0.27802000 0.90957900
H -5.75839800 -0.13089500 0.21779400
H -4.47322200 -0.55315700 1.37222400
H -5.52295500 0.85943000 1.68579400
P -3.84661900 1.32355700 -0.00661200

ComA10:

B -0.16132500 0.16364400 1.98795600
H -1.01085400 1.02009300 2.13233100
H 0.94330400 0.55517400 2.30778300
H -0.45864600 -0.89467100 2.50242700
P -0.08346200 -0.20406000 0.13703400
O -1.37590900 -0.87244600 -0.52578500
O 0.96548300 -1.32279500 -0.33136000
O 0.20740900 1.07615600 -0.79808300
C 2.36340500 -1.03692900 -0.18513000
H 2.89242900 -1.94944000 -0.46408500
H 2.66168900 -0.22590000 -0.85737900
H 2.60960900 -0.77751600 0.84978800
C 0.70638800 2.30231000 -0.24137200
H 0.75109600 3.01191800 -1.06947700
H 0.03390100 2.68472900 0.53120000
H 1.70847300 2.16803000 0.17640200
C -2.65297900 -0.26709300 -0.27255800
H -2.67622600 0.76168200 -0.64609600
H -3.38428700 -0.86555500 -0.81765600
H -2.88867400 -0.28290700 0.79565500

TS2-ComB10:

C 0.28665000 -0.37435000 -1.87168300
C 0.29608400 -1.85371700 -1.53659800
C 1.80968800 -1.78646400 -1.37227500
H 0.03868100 -0.14253200 -2.91527600
H -0.30319500 0.28250700 -1.22041500
H 2.37691000 -2.30386500 -2.15571400

H 2.21355900 -2.06520800 -0.39234100
N 1.72339600 -0.33634900 -1.59520300
C 2.30855700 0.64991900 -0.86407000
O 1.83909600 1.77403300 -0.76105100
O 3.45270300 0.20650200 -0.32356800
C 4.24609200 1.06185600 0.55119200
C 5.39577100 0.14931400 0.95534800
H 6.07775900 0.68136100 1.62577200
H 5.01783300 -0.73798300 1.47363300
H 5.95623000 -0.17548700 0.07273300
C 3.42670800 1.46355100 1.77216000
H 4.07243900 1.97539800 2.49344100
H 2.61044200 2.13288900 1.49437200
H 3.01053000 0.57282400 2.25582400
C 4.76175200 2.26871200 -0.22242800
H 5.30446800 1.94058700 -1.11538000
H 3.93851100 2.91806100 -0.52543200
H 5.45147600 2.83983700 0.40816500
P -2.75738500 0.84705800 0.06542100
B -2.73203800 -0.90441300 -0.59785400
H -3.60518000 -1.57339900 -0.12822900
H -2.43489900 -1.00363200 -1.75396800
I -0.72227600 -2.35347500 0.57350800
H -0.17691700 -2.58344200 -2.18813600
O -4.25547300 1.25580900 0.45871900
O -2.16650900 1.97959500 -0.91868800
O -1.98969200 1.23173700 1.42087800
C -2.57548200 2.02755200 -2.29116700
H -2.07276100 2.89187000 -2.72574700
H -2.27136500 1.11932300 -2.81773400
H -3.65984600 2.15285300 -2.36592900
C -4.52893700 2.52486400 1.07929500
H -4.06998400 3.33906800 0.51128400
H -5.61341700 2.63561400 1.07413600
H -4.15279000 2.52880900 2.10449500
C -0.56941600 1.43870600 1.47349700
H -0.05192100 0.47626400 1.46484500
H -0.22710400 2.05065700 0.63710100
H -0.37743900 1.95137700 2.41704100

ComA11:

P -1.10529200 0.57448300 0.10384600
C -0.29001000 1.52677500 1.44100200

H -0.42018800 0.94403300 2.36060000
 C -0.22028000 -1.03009900 0.05089500
 H -0.59550200 -1.55980300 -0.83279600
 H 0.84430500 -0.82659200 -0.12126800
 C -0.63069200 1.42902600 -1.44679100
 H -1.00676100 2.45578200 -1.36466800
 H 0.46479500 1.48731400 -1.47808600
 C -1.18253100 0.76802900 -2.70566900
 H -0.88420500 1.33957900 -3.59154700
 H -0.80733300 -0.25368700 -2.82942300
 H -2.27637800 0.72598000 -2.68546600
 C -0.42133900 -1.88358300 1.29866300
 H 0.08986000 -2.84553600 1.18182600
 H -0.01451700 -1.40032200 2.19350100
 H -1.48236300 -2.08677900 1.47674500
 C -0.85741600 2.93037700 1.62669800
 H -1.92823800 2.89941800 1.85238500
 H -0.35183200 3.43290400 2.45872900
 H -0.71763300 3.54846000 0.73325300
 H 0.78598700 1.55952000 1.22693700
 B -3.00925600 0.39757800 0.33508300
 H -3.48135800 1.51166800 0.19453100
 H -3.39651500 -0.37553800 -0.52308400
 H -3.18780500 -0.03761200 1.45887800

TS2-ComB11:

C 2.23647800 -1.36443400 -0.66152500
 C 0.84150000 -1.05249600 -1.18996700
 C 1.09269200 0.42715600 -0.92887000
 H 2.30335300 -2.08168200 0.16528300
 H 2.96092900 -1.64149700 -1.43953600
 H 0.51255900 -1.40105200 -2.16469700
 H 0.37033800 0.95438900 -0.29477400
 H 1.26498500 1.02168000 -1.83732300
 N 2.33206000 0.04034100 -0.25525700
 I -0.84591000 -1.94988500 0.23435400
 C 3.43430400 0.82373800 -0.14604100
 O 3.40607700 2.04035700 -0.24768800
 O 4.51105800 0.06029800 0.10917500
 C 5.82673400 0.66072100 0.28388300
 C 6.71217900 -0.54530100 0.56207600
 H 7.74886900 -0.22494600 0.70888100
 H 6.37906100 -1.06832000 1.46503800

H 6.68188000 -1.24990700 -0.27617000
 C 5.82267600 1.60714200 1.47767300
 H 6.84419700 1.94949000 1.67739700
 H 5.18939000 2.47614900 1.28873600
 H 5.45549700 1.08902600 2.37082200
 C 6.25683900 1.35523300 -1.00201100
 H 5.62185300 2.21795600 -1.21428400
 H 7.29408300 1.69560700 -0.90913300
 H 6.20033900 0.65835200 -1.84600900
 B -2.24749500 -0.16576600 -1.64474000
 H -1.36175600 0.54520900 -2.03397600
 H -2.67443300 -1.06150400 -2.32023500
 C -2.61835800 1.62163100 0.83008500
 C -4.49525100 -0.67008100 0.34306100
 C -4.62568600 1.79204100 -1.34729400
 C -3.34502200 1.85370900 2.15038300
 H -1.68235100 1.08216500 1.01345400
 H -2.34370100 2.57129300 0.35311500
 H -4.60932600 -1.44290900 -0.42673700
 H -3.85445200 -1.10954700 1.11816000
 C -5.85753700 -0.28248200 0.90596400
 C -5.34876600 2.85770000 -0.52961600
 H -5.33570700 1.15412700 -1.88891900
 H -3.99947500 2.26851400 -2.11159700
 H -3.55691600 0.90728200 2.65883300
 H -2.70722400 2.44714700 2.81548200
 H -6.51741000 0.11375500 0.12705200
 H -6.34320200 -1.17071500 1.32596700
 H -5.97379300 3.46529600 -1.19457100
 H -4.64129000 3.53386900 -0.03866700
 H -4.28740100 2.39421200 2.02596700
 H -5.78449100 0.46201900 1.70386400
 H -5.99996600 2.42866800 0.23670100
 P -3.48946100 0.63968800 -0.45647200

ComA12:

P -0.07525800 0.00016000 -0.00004300
 F 0.64487300 -1.19847400 -0.69554600
 F 0.64642900 -0.00378500 1.38499900
 F 0.64675200 1.20115000 -0.68971100
 B -1.93256300 0.00095700 0.00037600
 H -2.21680700 -0.00013000 -1.17461600
 H -2.21788900 -1.01603300 0.58835300

H -2.21611000 1.01895600 0.58735600

TS2-ComB12:

P 4.46277300 0.89115500 -0.11715200
F 5.81358400 1.63359300 -0.42220700
F 5.02816900 -0.34488000 0.64966800
F 3.94049700 1.79007900 1.04680700
B 3.25732200 0.53121900 -1.46119600
H 2.68917700 1.51758900 -1.82195700
H 3.64959300 -0.32594300 -2.19383100
I 1.31617100 -0.74581900 -0.13043500
C -1.54867200 -1.00720500 1.43729100
C -0.51078200 -1.92024800 0.78879900
C -1.54850900 -2.32631800 -0.25560600
H -1.83439900 -1.30127600 2.45478400
H -1.34124400 0.06720300 1.41874000
H -0.01248800 -2.68294700 1.38275300
H -1.83128000 -3.38558500 -0.21938700
H -1.34571400 -2.04450800 -1.29418900
N -2.50219400 -1.43794200 0.40906600
C -3.41128900 -0.67120600 -0.25395400
O -3.81819000 -0.93545700 -1.37306700
O -3.78250400 0.36016100 0.52053300
C -4.75038000 1.34300700 0.04659300
C -4.84893600 2.30625400 1.22059300
H -5.55453200 3.11100500 0.98963000
H -5.19726500 1.78588900 2.11932600
H -3.87206600 2.75278300 1.43590700
C -6.09311900 0.67384700 -0.21448300
H -6.84110300 1.43614000 -0.45902000
H -6.02575900 -0.03181800 -1.04493900
H -6.43150100 0.13767000 0.67937200
C -4.20954600 2.05347200 -1.18724900
H -4.13153300 1.36809100 -2.03355700
H -4.87852900 2.87680900 -1.46092600
H -3.21857500 2.47309800 -0.97987700

ComA13:

C -0.01841800 0.63764200 0.01324100
C -0.68417500 -1.58506600 -0.09007900
H -0.98103400 -1.91348500 -1.09555500
C 0.83238000 -1.52105700 0.07469800

H 1.37503600 -2.09661000 -0.68045500
N -1.06605800 -0.19105700 0.10632300
N 1.09735400 -0.09227300 -0.07497200
C -2.44785500 0.20031400 0.00320500
H -2.56128900 1.23383200 0.33103700
H -2.81023100 0.11050200 -1.02994800
H -3.05505300 -0.44626700 0.64497100
C 2.45703100 0.37714100 -0.00524900
H 3.05371700 -0.11158100 -0.78312700
H 2.48204700 1.45535000 -0.15682400
H 2.89671200 0.14019000 0.97258100
H -1.17229300 -2.23070600 0.64517400
H 1.16067600 -1.85278900 1.06892900
B -0.15525900 2.23305300 -0.01105900
H -0.82787900 2.52092100 -0.99367300
H 0.92904700 2.78387100 -0.05697600
H -0.76601600 2.57097100 0.99481900

TS2-ComB13:

C -2.82214500 1.03653600 -0.10945400
C -1.92509300 3.14892900 0.19676000
H -2.71191000 3.91286900 0.10656200
C -1.98245900 2.42954000 1.53623300
H -2.41556100 3.03287800 2.33829800
N -2.18535300 2.05516800 -0.72968000
N -2.83211300 1.28740700 1.22119700
C -2.19350600 2.30065800 -2.14897900
H -2.11107900 1.35753600 -2.69080800
H -3.10805200 2.81995100 -2.46860800
H -1.33043400 2.92355400 -2.40161800
C -3.06413900 0.29667700 2.24142400
H -3.42407500 0.79610500 3.14620800
H -3.81944500 -0.41542700 1.90783300
H -2.14086100 -0.25001000 2.47977700
H -0.95675000 3.61390700 -0.00449000
H -0.98903300 2.07599000 1.85159800
B -3.41525500 -0.21428200 -0.79735900
H -3.45504400 -0.25322700 -1.99508500
H -4.12673800 -0.93847700 -0.15864200
I -1.08904300 -1.81640000 -0.44159400
C 2.05810400 -2.25373000 -0.80281200
C 0.90873400 -2.96913600 -0.09512200
C 1.53487400 -2.55814000 1.23782700

H 2.81212500 -2.93972400 -1.21084200
 H 1.81123800 -1.49997200 -1.55447900
 H 0.68713400 -4.01359300 -0.30794700
 H 2.04871100 -3.38234200 1.74981900
 H 0.91490800 -2.01546500 1.95698300
 N 2.46806400 -1.69732200 0.49849300
 C 2.57812300 -0.36701100 0.78094100
 O 2.36115600 0.10751000 1.88415600
 O 2.98652400 0.30002300 -0.31107300
 C 3.05148700 1.75451100 -0.31438700
 C 3.44299800 2.06871500 -1.75082200
 H 3.53745400 3.15097500 -1.88771000
 H 4.40248600 1.60257400 -1.99942700
 H 2.68511000 1.69473400 -2.44799000
 C 4.12440100 2.23378000 0.65370700
 H 4.24504400 3.31919900 0.56449200
 H 3.85735300 1.99164500 1.68432900
 H 5.08545800 1.76302900 0.41804100
 C 1.67949100 2.33808800 0.00362900
 H 1.40268900 2.14805700 1.04277000
 H 1.69402800 3.42034700 -0.16738000
 H 0.91995000 1.89195900 -0.64882000

ComA14:

C -0.01042800 0.58358900 -0.00148600
 C -0.62894700 -1.57564500 0.00039200
 C 0.72656000 -1.53652500 0.00016500
 N -1.05819900 -0.26756400 -0.00055400
 N 1.08431800 -0.20547300 -0.00092900
 C -2.44136500 0.16267000 0.00016600
 H -2.64839200 0.75562000 -0.89414800
 H -3.08327200 -0.71930600 0.01126700
 H -2.64150600 0.77283400 0.88442600
 C 2.45344500 0.27629700 0.00045500
 H 3.12185000 -0.58618200 0.00526000
 H 2.64292100 0.87719100 -0.89121000
 H 2.63860300 0.88379900 0.88852600
 H -1.31890000 -2.40588200 0.00104000
 H 1.46150700 -2.32709000 0.00068800
 B -0.10204400 2.17615200 0.00018900
 H -0.76364000 2.52632000 -0.97151100
 H 1.01435800 2.66373900 -0.04036900
 H -0.69173900 2.52713700 1.01730300

TS2-ComB14:

C 3.97298200 0.80885000 0.57761200
 C 4.44227000 2.06929700 -1.22684700
 C 5.18869700 0.93680300 -1.31221700
 N 3.71041600 1.98393200 -0.06811200
 N 4.89969300 0.17893700 -0.20409700
 C 2.72942700 2.94727800 0.38119900
 H 2.97637300 3.29499100 1.38706200
 H 2.72669100 3.79401100 -0.30633100
 H 1.73764800 2.48587700 0.39848000
 C 5.42678800 -1.13829500 0.07654200
 H 6.15033400 -1.39991500 -0.69639400
 H 5.91667900 -1.14796500 1.05308100
 H 4.61358100 -1.87005200 0.08044900
 H 4.37803600 2.92132900 -1.88549600
 H 5.89822200 0.61578100 -2.05900300
 B 3.32688500 0.28555900 1.85785500
 H 2.62306700 1.02391200 2.48939200
 H 3.75632300 -0.72294800 2.34615600
 I 1.12770700 -1.01483800 0.42619400
 C -1.99377800 -1.90739100 0.18355000
 C -0.67413400 -2.03098600 -0.58848200
 C -1.30098300 -1.22021000 -1.73075900
 H -2.50749200 -2.85619000 0.37833100
 H -1.96343700 -1.32041700 1.10751400
 H -0.32248600 -3.03419100 -0.82081400
 H -1.39685800 -1.75753500 -2.68177200
 H -0.87132700 -0.23037100 -1.92080300
 N -2.54044700 -1.16544200 -0.95718700
 C -3.38261800 -0.10027200 -0.93711200
 O -3.43330200 0.73265800 -1.82927700
 O -4.13361100 -0.13601200 0.17639400
 C -5.12171200 0.89956800 0.44632700
 C -5.70422700 0.46503800 1.78429200
 H -6.47187300 1.17544900 2.10683700
 H -6.15946700 -0.52721200 1.70097200
 H -4.92147700 0.42557600 2.54887200
 C -6.19595200 0.89502100 -0.63437500
 H -6.99559000 1.59057100 -0.35816900
 H -5.78100000 1.19646900 -1.59769300
 H -6.62987200 -0.10615400 -0.73054000
 C -4.43650200 2.25475500 0.57472300

H -4.00790400 2.56740600 -0.37912200
H -5.16580500 3.00455300 0.89937700
H -3.63913300 2.20378000 1.32417800

ComA15:

C -0.02106200 1.63953500 0.00000000
N -0.01691800 0.82918500 1.08499800
N -0.01691800 0.82918500 -1.08499800
C 0.01272900 1.24569600 2.47071000
H -0.01905500 2.33253300 2.51567000
H -0.85214000 0.83288400 2.99810600
H 0.93132700 0.88689300 2.94410700
C 0.01272900 1.24569600 -2.47071000
H -0.85214000 0.83288400 -2.99810600
H -0.01905500 2.33253300 -2.51567000
H 0.93132700 0.88689300 -2.94410700
B 0.00591400 3.23786800 0.00000000
H -0.54773100 3.66264700 0.99974800
H -0.54773100 3.66264700 -0.99974800
H 1.18223400 3.58457500 0.00000000
C 0.00651900 -2.86802300 -0.70203300
C 0.00651900 -2.86802300 0.70203300
C -0.00117700 -1.68275400 1.43071800
C -0.01003600 -0.49969000 0.69871800
C -0.01003600 -0.49969000 -0.69871800
C -0.00117700 -1.68275400 -1.43071800
H 0.01414100 -3.81591300 -1.23248200
H 0.01414100 -3.81591300 1.23248200
H 0.00095800 -1.68027600 2.51639200
H 0.00095800 -1.68027600 -2.51639200

TS2-ComB15:

C 1.66683300 -2.29081000 -0.08444300
N 2.08138000 -1.62203100 1.03163500
N 2.17538000 -1.61067300 -1.15286100
C 1.70723400 -1.99701100 2.37870100
H 0.61780800 -1.99552400 2.47186700
H 2.08753500 -2.99341100 2.61445400
H 2.13100200 -1.27644100 3.07779300
C 1.93559100 -1.91616000 -2.54548400
H 2.87963700 -1.87714800 -3.09518800
H 1.51467800 -2.91679000 -2.62289900

H 1.23409100 -1.19326600 -2.97356100
B 0.75086200 -3.52570500 -0.09412700
H 0.60579800 -4.11289500 0.94041700
H 0.53833100 -4.08445400 -1.13293400
C 4.20587100 1.46078800 -0.67142400
C 4.13890900 1.46446900 0.72977900
C 3.44965300 0.47906000 1.43047500
C 2.82599300 -0.51472600 0.67940300
C 2.88788000 -0.51131400 -0.72346700
C 3.57812000 0.47361600 -1.42447500
H 4.75306100 2.24852800 -1.18028600
H 4.63574500 2.25523700 1.28369600
H 3.40634900 0.49072700 2.51446000
H 3.61854700 0.47564900 -2.50874300
I -1.59895500 -2.06074600 0.07066300
C -3.10168300 0.57720400 1.17951600
C -3.50283600 -0.64062000 0.35172000
C -3.68813900 0.28066700 -0.85177200
H -3.86643500 0.89942400 1.89862700
H -2.12802500 0.55685700 1.67681600
H -4.29908500 -1.30621000 0.67819800
H -4.73811100 0.45073100 -1.12411800
H -3.11345000 0.06423300 -1.75769500
N -3.12499600 1.37821800 -0.05424900
C -2.11072200 2.15770300 -0.52365600
O -1.94712400 2.39834100 -1.70963100
O -1.36948100 2.61880400 0.49678400
C -0.17150000 3.41076300 0.24689600
C 0.39899100 3.60420700 1.64539700
H 1.30993300 4.20914000 1.59661700
H -0.32461200 4.11212800 2.29131500
H 0.64956500 2.63628200 2.09252100
C -0.55644000 4.74759200 -0.37348800
H 0.33245000 5.38125600 -0.46298400
H -0.98859100 4.60236700 -1.36541900
H -1.28487700 5.26409900 0.26093200
C 0.80942100 2.63010700 -0.61776500
H 0.42263400 2.48994100 -1.62820300
H 1.76008800 3.16943600 -0.67126000
H 1.00769400 1.64920400 -0.17329000

ComA16:

C -0.00000800 -0.24880500 0.14673300

N -1.07237000 0.49877000 -0.21689600
 N 1.07237000 0.49879000 -0.21680600
 B -0.00002000 -1.65305500 0.91408500
 H -1.00936300 -1.71791600 1.59586400
 H 1.00913800 -1.71777300 1.59615700
 H 0.00014700 -2.56748100 0.09665100
 C -0.67484700 1.70038000 -0.77889500
 C 0.67487900 1.70040300 -0.77883500
 H -1.38873200 2.41858400 -1.15126200
 H 1.38879300 2.41861100 -1.15113800
 C 2.44171300 0.13619600 -0.05831500
 C 2.89073800 -1.10502000 -0.50238100
 C 3.32044600 1.05803200 0.50650000
 C 4.23724400 -1.42678800 -0.36649500
 H 2.19032700 -1.80509300 -0.94549600
 C 4.66744900 0.72934900 0.62708600
 H 2.94818700 2.01552000 0.86014600
 C 5.12726100 -0.51226600 0.19388100
 H 4.59105200 -2.39568500 -0.70754900
 H 5.35540200 1.44411200 1.06993300
 H 6.17855600 -0.76800600 0.29403000
 C -2.44172400 0.13618500 -0.05835800
 C -2.89079100 -1.10498300 -0.50251800
 C -3.32039200 1.05800800 0.50656100
 C -4.23729800 -1.42672500 -0.36658800
 H -2.19041400 -1.80502700 -0.94573000
 C -4.66739900 0.72934300 0.62720800
 H -2.94808500 2.01548500 0.86018700
 C -5.12725300 -0.51223000 0.19393600
 H -4.59117000 -2.39556700 -0.70773000
 H -5.35531300 1.44407200 1.07016900
 H -6.17854500 -0.76796100 0.29414300

TS2-ComB16:

C -1.98566400 1.31241800 0.21951400
 N -0.88301400 1.88778300 0.79692000
 N -2.57732700 0.61618800 1.24302200
 B -2.41031300 1.39317100 -1.25195200
 H -1.90674000 2.23728100 -1.93508400
 H -3.43600400 0.86665800 -1.57636900
 C -0.79374200 1.54865300 2.13112600
 C -1.85689800 0.75990500 2.41271800
 H 0.00493700 1.91338600 2.75759100

H -2.15958700 0.27656200 3.32812900
 I -0.50827900 -0.56237700 -2.10154800
 C 2.61633400 -1.22142900 -1.91621600
 C 1.37468100 -1.89686400 -2.50456900
 C 1.52224000 -3.00256100 -1.45619300
 H 3.51042200 -1.29518200 -2.54901300
 H 2.50806000 -0.19023700 -1.56794200
 H 1.34207000 -2.14964100 -3.56233500
 H 1.86357200 -3.96367600 -1.86222500
 H 0.67918900 -3.17800900 -0.78020100
 N 2.60436000 -2.22632900 -0.84662800
 C 2.74103200 -2.05075900 0.49098900
 O 2.32465700 -2.84997800 1.31548300
 O 3.40047600 -0.90428200 0.75112600
 C 3.83858200 -0.59596300 2.10789200
 C 4.55264500 0.73816900 1.93856400
 H 4.96757700 1.06359300 2.89762900
 H 5.37124800 0.64658400 1.21738800
 H 3.85956100 1.50815700 1.58401600
 C 4.80951400 -1.66633900 2.59111300
 H 5.22233400 -1.37570100 3.56284100
 H 4.30659900 -2.62956100 2.69684600
 H 5.63844000 -1.77171000 1.88295400
 C 2.64066900 -0.44670900 3.03872000
 H 2.12889200 -1.40003900 3.17490500
 H 2.98009400 -0.07791800 4.01264300
 H 1.92881800 0.27784000 2.62928800
 C -3.76077200 -0.17003700 1.15446100
 C -4.81140800 0.09539600 2.03085300
 C -3.84021300 -1.21315100 0.23428000
 C -5.95664800 -0.69449100 1.98288200
 H -4.73284600 0.92075000 2.73279000
 C -4.99380600 -1.98922800 0.18782800
 H -3.00314600 -1.40950300 -0.42802600
 C -6.05108400 -1.73416500 1.06012200
 H -6.77838000 -0.48933300 2.66277800
 H -5.06109400 -2.80257800 -0.52881000
 H -6.94768800 -2.34609600 1.02101900
 C 0.11211300 2.64464600 0.11332100
 C -0.19905300 3.89520400 -0.41156200
 C 1.39730200 2.11777600 0.00231800
 C 0.79254000 4.62532400 -1.06100800
 H -1.20793800 4.28245800 -0.31178000
 C 2.38445000 2.85898600 -0.64075700

H 1.61283200 1.12806100 0.39384300
C 2.08302100 4.11087400 -1.17425800
H 0.55530400 5.60074800 -1.47537900
H 3.38613300 2.44879900 -0.73387300
H 2.85348000 4.68510000 -1.68072800

ComA17:

C 0.46725300 -0.01596500 0.00000000
N -0.37493700 -0.02438900 1.06108300
N -0.37493700 -0.02438900 -1.06108300
C 0.05908500 0.01184600 2.43513600
C 0.05908500 0.01184600 -2.43513600
B 2.06062800 -0.04540100 0.00000000
H 2.46073300 0.49816400 1.00810000
H 2.46073300 0.49816400 -1.00810000
H 2.37777000 -1.22630200 0.00000000
C -1.71058700 -0.03335200 0.67231900
C -1.71058700 -0.03335200 -0.67231900
F 0.61478800 1.18014400 2.72643000
F 0.92895800 -0.95423200 2.68161600
F -1.00455500 -0.15733800 3.21514200
F 0.92895800 -0.95423200 -2.68161600
F 0.61478800 1.18014400 -2.72643000
F -1.00455500 -0.15733800 -3.21514200
H -2.52209700 -0.04101900 1.38191300
H -2.52209700 -0.04101900 -1.38191300

TS-ComB17:

C -2.25246700 0.67921100 -0.37334500
N -1.50909100 1.83069500 -0.37860500
N -2.79602800 0.66663400 0.88326500
C -0.77468600 2.31999000 -1.51319600
C -3.72324300 -0.32695700 1.35425500
B -2.39098500 -0.37952300 -1.48800700
H -2.04486600 -0.04258300 -2.58062600
H -3.27194400 -1.17557800 -1.35267500
C -1.58334700 2.49443400 0.83944600
C -2.39019500 1.76312800 1.63045800
F -1.58252600 2.55350700 -2.53806400
F 0.15379900 1.45120500 -1.89327700
F -0.17554200 3.45687600 -1.16800800
F -3.18996500 -1.53739100 1.31528000

F -4.82814100 -0.32405000 0.61822500
F -4.04544400 -0.03694500 2.61136500
H -1.06178800 3.41739600 1.02789300
H -2.71096600 1.92118100 2.64623700
I -0.35625900 -1.92294600 -0.85831400
C 2.91193700 -2.04568500 -0.99436200
C 1.84771200 -3.05514800 -0.59863000
C 2.31020500 -2.94272400 0.84573400
H 3.76884700 -2.48563500 -1.52243200
H 2.58995100 -1.14364400 -1.52171200
H 1.70191300 -4.00425800 -1.10823000
H 2.86798200 -3.81928300 1.20238100
H 1.57476900 -2.65486800 1.60370700
N 3.19074600 -1.83738200 0.43736900
C 3.16131500 -0.63686700 1.08353700
O 2.90452900 -0.52166500 2.27137300
O 3.47503800 0.35546300 0.23475400
C 3.36451900 1.74730700 0.64807600
C 3.59436800 2.50039300 -0.65547700
H 3.58488100 3.57932600 -0.47140000
H 4.56134800 2.22875900 -1.09068700
H 2.80576400 2.26271800 -1.37713900
C 4.44690600 2.06797300 1.66929600
H 4.41612100 3.13388700 1.91948800
H 4.29686700 1.48640500 2.58127400
H 5.43580600 1.83906200 1.25808200
C 1.96279100 2.03313100 1.17713000
H 1.80356800 1.58567800 2.15878100
H 1.81278800 3.11607800 1.24476200
H 1.22513400 1.62116900 0.48253000

ComA18:

C -0.11513600 -1.05730500 -0.00004700
H 0.21797400 -2.08320400 0.00007000
C -0.12894800 1.11852400 -0.00004200
H 0.29273800 2.11224200 -0.00013500
C -1.43070700 0.71277900 0.00005200
H -2.35783900 1.26485300 0.00010200
N -1.39385600 -0.65779000 0.00000800
H -2.19581000 -1.27446800 -0.00010000
N 0.67521600 0.00320100 0.00000500
B 2.25336900 -0.00919600 0.00001800
H 2.59780700 -1.17896400 -0.00090200

H 2.62876800 0.57265500 -1.00533600
H 2.62873600 0.57100300 1.00634300

TS2-ComB18:

C -1.37542400 -0.89066900 0.92328300
C -0.05095700 -0.16962100 1.15621000
C -0.63055400 1.07274800 0.48853800
H -1.33488900 -1.83362600 0.36620900
H -1.98143400 -1.03352100 1.82878400
H 0.38184900 -0.10967300 2.15070100
H -0.07479700 1.48308500 -0.36191000
H -0.87433700 1.89128700 1.18051400
N -1.79524300 0.26539900 0.12728500
I 1.73320200 -1.13346000 -0.10699400
C -3.04352300 0.74353700 -0.09320900
O -3.27768700 1.90577700 -0.38932400
O -3.94197300 -0.24850000 0.04387800
C -5.36097200 -0.00380900 -0.17096300
C -5.97905600 -1.37301900 0.07748200
H -7.06470000 -1.32254500 -0.05272400
H -5.57660400 -2.10926000 -0.62589000
H -5.76462100 -1.71210000 1.09631800
C -5.60769100 0.44204500 -1.60740800
H -6.68568700 0.50208000 -1.79170800
H -5.16128600 1.42007100 -1.79529100
H -5.17987800 -0.28515600 -2.30603800
C -5.87660400 1.00904300 0.84471700
H -5.42753800 1.98995300 0.67937000
H -6.96478800 1.09627700 0.75612100
H -5.64084000 0.67576300 1.86135400
B 2.67116300 1.73947600 -0.00767600
H 2.13272300 1.99675300 -1.04303800
H 2.29681300 2.12006300 1.06285200
N 4.05316100 1.25454700 -0.08500400
C 6.06957900 0.50870500 0.50689600
C 4.95283600 1.12694300 0.96812100
H 4.71192700 1.49691800 1.95184700
H 6.98879500 0.23974000 1.00278700
C 4.62100300 0.67463600 -1.16315100
N 5.85226800 0.24632300 -0.82446800
H 6.49545900 -0.21461100 -1.45014900
H 4.18248800 0.61914000 -2.14525400

ComA19:

C 1.50648000 0.66920600 -0.00001400
C 0.18370200 1.12415800 0.00001200
C 1.41290000 -0.71102400 -0.00000500
H -0.21434700 2.12844000 -0.00003300
H 2.16545900 -1.48672500 -0.00001900
H 2.40724400 1.26478800 -0.00002700
N 0.10694000 -1.01566400 -0.00000300
N -0.65019100 0.08596400 0.00003000
H -0.33769100 -1.92549200 0.00004200
B -2.22186700 0.01057900 -0.00002100
H -2.55786000 -0.59171000 1.00671100
H -2.55809100 -0.58956100 -1.00798900
H -2.61112100 1.16122000 0.00127800

TS2-ComB19:

C -0.30646600 3.13384200 -0.19315600
N -2.36310200 2.33782400 0.17101700
H 0.47964300 3.59182800 -0.77338400
B -3.68879500 1.84248800 -0.17313200
H -4.06982600 2.07557200 -1.28468400
H -4.36627300 1.47264700 0.73775500
I -2.36563500 -1.00234500 -0.35858000
C 0.55598600 -2.28238000 -0.63020000
C -0.73859200 -2.45835800 0.17812900
C 0.03236900 -2.02740000 1.43562400
H 0.96220000 -3.21460500 -1.03976900
H 0.54760100 -1.51794700 -1.41254900
H -1.20261400 -3.44254000 0.18093000
H 0.14182400 -2.81187400 2.19345900
H -0.29526400 -1.09998300 1.91790400
N 1.22066000 -1.84959100 0.60329800
C 2.10313000 -0.82719800 0.75519400
O 2.24022400 -0.20735300 1.79858900
O 2.78621100 -0.64459800 -0.38680300
C 3.81635500 0.38022000 -0.48814100
C 4.29866200 0.22814700 -1.92426000
H 5.09103300 0.95388200 -2.13237100
H 4.69468500 -0.77869200 -2.09144300
H 3.47533700 0.39900700 -2.62566300
C 4.94498500 0.08915700 0.49296400
H 5.76387100 0.79775100 0.32932600

H 4.59805400 0.18098500 1.52360300
H 5.33067600 -0.92381400 0.33526400
C 3.20388900 1.75865300 -0.27289400
H 2.86340800 1.87875400 0.75711800
H 3.94800600 2.53071000 -0.49533100
H 2.35086600 1.89507500 -0.94616800
C -0.35234900 2.69568900 1.11835200
C -1.64163900 2.20750900 1.31935300
H -2.10116600 1.75772300 2.18537500
H 0.45190100 2.71680600 1.83808900
N -1.52873800 2.91416400 -0.73048300
H -1.85251000 3.06209500 -1.67394100

ComA20:

C -0.01110200 0.21819500 -1.15875400
C -0.01110200 -1.16586600 -1.19688600
C -0.01200700 -1.87492700 0.00000000
C -0.01110200 -1.16586600 1.19688600
C -0.01110200 0.21819500 1.15875400
N -0.00890700 0.89832300 0.00000000
H -0.01596200 -2.96090000 0.00000000
H -0.01421100 0.82223600 -2.05878400
H -0.01487000 -1.67148500 -2.15646400
H -0.01487000 -1.67148500 2.15646400
H -0.01421100 0.82223600 2.05878400
B 0.05128700 2.49033300 0.00000000
H 1.23325000 2.79569600 0.00000000
H -0.50736100 2.87269200 1.01126500
H -0.50736100 2.87269200 -1.01126500

TS2-ComB20:

C -4.03750200 1.89775500 0.36432000
C -4.87137800 2.39506400 -0.61207000
C -5.86264500 1.57832300 -1.16133200
C -5.97501200 0.26828300 -0.68914200
C -5.11787300 -0.18277800 0.28925000
N -4.14401000 0.61450300 0.81868800
H -3.25244000 2.48942400 0.81943700
H -4.74285300 3.42234100 -0.93668000
H -6.72989500 -0.40824100 -1.07603700
H -5.16230700 -1.18965600 0.68631800
B -3.19876300 0.08502900 1.84016500

H -3.51779200 -0.95282100 2.34157800
H -2.54100800 0.90975800 2.40362000
I -1.23497600 -0.90044800 0.24688500
C 1.50644400 -0.63074900 -1.59715200
C 0.56065400 -1.73479500 -1.13434800
C 1.69972300 -2.34777600 -0.32395700
H 1.71518800 -0.62550700 -2.67464200
H 1.26691000 0.38816300 -1.27459900
H 0.02333300 -2.33589200 -1.86386400
H 2.01753500 -3.34294500 -0.66048100
H 1.58233800 -2.36009500 0.76536800
N 2.56187800 -1.26450800 -0.79865700
C 3.51890600 -0.66267400 -0.04414400
O 4.04570000 -1.19435600 0.91983400
O 3.79185400 0.55450600 -0.54410500
C 4.79258400 1.40960900 0.08014000
C 4.75409100 2.65948300 -0.78744700
H 5.47654300 3.39520800 -0.41911200
H 5.00387900 2.41674300 -1.82603700
H 3.75688400 3.11248400 -0.76782000
C 6.16376800 0.74992500 0.00964300
H 6.92691700 1.44894300 0.36952000
H 6.19760300 -0.15339300 0.62218000
H 6.40480100 0.48411600 -1.02590600
C 4.38221100 1.73834300 1.50983700
H 4.40240600 0.84734900 2.14067200
H 5.06908900 2.48245800 1.92818200
H 3.37022000 2.15874800 1.52659800
H -6.52916700 1.95214400 -1.93169600

ComA21:

C 1.46837000 -1.15063600 -0.02736700
C 0.09578100 -1.20029900 -0.01714800
C -0.65835800 0.00005500 -0.00154000
C 0.09575600 1.20043300 0.00111900
C 1.46838300 1.15089800 -0.00888200
N 2.16865800 0.00018500 -0.02115900
H 2.06044200 -2.05908100 -0.04369700
H -0.38319800 -2.17111700 -0.03077100
H -0.38295700 2.17142000 0.00983000
H 2.06046800 2.05947300 -0.00783800
B 3.75372600 -0.00023200 0.03643000
H 4.08588800 -0.01342300 1.21402000

H 4.14109800 1.01568300 -0.51623600
H 4.14169200 -1.00308000 -0.53912800
N -2.00739100 -0.00003900 0.00600900
C -2.73454100 -1.25461000 0.02508700
H -2.46797200 -1.85736200 0.90208100
H -3.80344400 -1.04570200 0.07215900
H -2.53927400 -1.84611000 -0.87849600
C -2.73501900 1.25435900 -0.00776300
H -2.47951200 1.85461800 -0.88978200
H -3.80436500 1.04506200 -0.04079100
H -2.52859600 1.84855400 0.89152200

TS2-ComB21:

I 0.23705600 1.27602100 -0.90083200
C -2.82627200 1.82369900 0.19154400
C -1.40585800 1.92229900 0.73274700
C -1.71714800 0.79461300 1.71076500
H -3.45895600 2.69746600 0.39415200
H -2.92862100 1.54485500 -0.86365800
H -1.00292200 2.86885100 1.08432400
H -1.72579100 1.09339500 2.76699700
H -1.13466700 -0.12829400 1.60778000
N -3.05523300 0.71103800 1.12127000
C -3.71001800 -0.45548100 0.88245700
O -3.47520300 -1.49305800 1.48139900
O -4.64439600 -0.26602700 -0.06501200
C -5.48556200 -1.36608400 -0.51549600
C -6.36070100 -0.70680500 -1.57189700
H -7.05127200 -1.44030700 -2.00109800
H -6.94738700 0.10756800 -1.13321800
H -5.74611100 -0.29416600 -2.37937900
C -6.33613100 -1.88463300 0.63684600
H -7.05651000 -2.61992400 0.26122900
H -5.71596700 -2.35763500 1.40078400
H -6.89593400 -1.06163400 1.09556800
C -4.62735900 -2.46041300 -1.13764700
H -3.98844800 -2.93280900 -0.38860100
H -5.27290300 -3.22559100 -1.58312400
H -3.99448100 -2.04289100 -1.92893100
C 2.99823200 -0.54180100 1.48417600
C 3.99348000 -1.34745200 1.01510600
C 4.99129100 -0.83863100 0.13484000
C 4.84690300 0.52365000 -0.23031200

C 3.82372100 1.28185200 0.27210500
N 2.89481800 0.79034800 1.16024600
H 2.22859700 -0.91762000 2.14817100
H 3.99495800 -2.38401800 1.32947500
H 5.53450800 0.99833600 -0.91982200
H 3.70278000 2.32429900 0.00320400
B 1.76104400 1.60040600 1.59035800
H 1.83238700 2.78190600 1.41978400
H 0.98878500 1.09207900 2.34941800
N 6.00592700 -1.61136100 -0.32674200
C 6.07308200 -3.01182900 0.03447500
H 5.20425800 -3.57072300 -0.33904900
H 6.97255900 -3.45057800 -0.39874500
H 6.12602300 -3.14017200 1.12290400
C 6.96355200 -1.06101400 -1.26253800
H 7.48023500 -0.19141700 -0.83662900
H 7.71302300 -1.81816600 -1.49509500
H 6.48363200 -0.75326300 -2.20164300

ComA22:

C -2.23197300 -0.30829700 -0.00004300
C -1.85893300 -1.65958700 -0.00019700
C -0.52598500 -1.97999400 -0.00002100
N -1.35984300 0.69039000 0.00005000
H -3.27596900 -0.01815400 0.00001500
H -2.63308600 -2.41902300 -0.00048200
B -1.89310000 2.19254700 0.00021200
H -3.10713700 2.13107500 0.00024800
H -1.46836000 2.73854300 -1.00407200
H -1.46837300 2.73837600 1.00460600
H -0.19484200 -3.01521100 -0.00002800
C -0.01028000 0.40747300 -0.00000100
C 0.43576100 -0.94513100 0.00012600
C 1.82540300 -1.21596200 0.00021500
C 2.73458500 -0.18762000 0.00006600
C 2.28429600 1.14966400 -0.00018700
C 0.94138600 1.44991100 -0.00020000
H 2.15221600 -2.25244600 0.00038600
H 3.80013000 -0.39833200 0.00012500
H 3.01005400 1.95821000 -0.00039100
H 0.60420900 2.47875300 -0.00035000

TS2-ComB22:

C -3.41654200 0.23945300 -0.78941100
 C -3.45319800 1.26082100 -1.72883700
 C -2.74933000 2.42440000 -1.49687300
 N -2.70206800 0.32089700 0.36349100
 H -3.95395100 -0.68900300 -0.93654500
 H -4.03426100 1.11883500 -2.63331300
 B -2.53758600 -0.97872500 1.10729900
 H -1.85018100 -0.98438000 2.08305500
 H -3.51270500 -1.67265000 1.08294800
 H -2.74923600 3.23619400 -2.21800800
 C -2.02585800 1.50333600 0.66166500
 C -2.03149800 2.57183800 -0.28099700
 C -1.33499800 3.76185200 0.02604200
 C -0.66703500 3.90548400 1.22287100
 C -0.68755700 2.85665200 2.15597500
 C -1.36024900 1.67886800 1.88644900
 H -1.34301400 4.56656900 -0.70423800
 H -0.13442100 4.82462600 1.44723800
 H -0.17817800 2.96954000 3.10836200
 H -1.38301000 0.89079300 2.62826000
 C 1.01590500 -1.07281800 1.77001900
 C 0.48657500 -2.45985700 1.47090600
 C 1.85133500 -2.85703700 0.94644900
 H 0.52024500 -0.22458600 1.28873900
 H 1.13178000 -0.85294900 2.84061000
 H -0.10347700 -3.05271700 2.16342000
 H 1.91810800 -3.20140700 -0.09229100
 H 2.39784700 -3.55944800 1.59001500
 N 2.28230900 -1.46373900 1.12609400
 C 2.89656200 -0.76893600 0.12494600
 O 3.54195200 -1.30006400 -0.76410400
 O 2.70401700 0.54812900 0.30094300
 C 3.11175600 1.50400400 -0.72093300
 C 2.66423400 2.83396900 -0.13167600
 H 2.91127800 3.64923100 -0.81925700
 H 1.58346400 2.83524800 0.03887200
 H 3.16675100 3.01926500 0.82354800
 C 2.36279400 1.21356400 -2.01600100
 H 2.57785800 1.99774800 -2.74955500
 H 2.66192000 0.24996300 -2.43363900
 H 1.28292200 1.20126500 -1.82986700
 C 4.62434200 1.47928900 -0.90325600
 H 4.95289900 0.52882300 -1.32605500

H 4.92308000 2.29183700 -1.57432800
 H 5.12192000 1.63087600 0.06081800
 I -1.09382200 -2.30781100 -0.51473800

ComA23:

C 1.19025200 1.13220000 0.00424800
 C -0.19796900 1.14877800 -0.01356500
 N -0.88797700 0.00000600 -0.01903100
 C -0.19797200 -1.14877700 -0.01355800
 C 1.19025300 -1.13220300 0.00422000
 N 1.89270700 -0.00000100 0.01243400
 H 1.74189500 2.06811200 0.00791500
 H -0.77343000 2.06663900 -0.02500500
 H -0.77343400 -2.06663500 -0.02496500
 H 1.74190500 -2.06810900 0.00795200
 B -2.47982900 -0.00001200 0.01612200
 H -2.84718100 1.01412400 -0.54303300
 H -2.84714500 -1.01461100 -0.54218500
 H -2.78396000 0.00051500 1.19682500

TS2-ComB23:

C -3.92427200 1.90417100 0.27891800
 C -4.81001900 2.34178800 -0.68522900
 C -5.87265400 0.33993600 -0.68061800
 C -5.01223900 -0.14495400 0.28356100
 N -4.01609600 0.64071900 0.77157800
 H -3.13092500 2.52505000 0.67636700
 H -4.72166000 3.35502300 -1.06782700
 H -6.66277600 -0.30264400 -1.05970200
 H -5.07951700 -1.14884800 0.68404200
 B -3.04175800 0.12344500 1.78771800
 H -3.40548100 -0.86627900 2.35126800
 H -2.40216800 0.97615400 2.32923400
 I -1.21843400 -0.89577500 0.26620700
 C 1.55568600 -0.83860900 -1.65830400
 C 0.62483300 -1.91443900 -1.12860300
 C 1.74673300 -2.44648700 -0.25425200
 H 1.79878800 -0.93136000 -2.72520600
 H 1.28582400 0.20101100 -1.44407100
 H 0.02762200 -2.55045100 -1.77592200
 H 2.09475600 -3.45209500 -0.52570800
 H 1.60262900 -2.40184800 0.83103400
 N 2.59883300 -1.37261300 -0.77189600

C 3.47264400 -0.66641900 -0.00296200
 O 3.95353600 -1.09797600 1.03177400
 O 3.72530400 0.52058300 -0.57790100
 C 4.62526300 1.47948100 0.05132200
 C 4.59615300 2.65184700 -0.91844600
 H 5.24208800 3.45705800 -0.55341200
 H 4.95031000 2.34427900 -1.90831100
 H 3.57809300 3.04308000 -1.02134500
 C 6.02941100 0.89737400 0.14725000
 H 6.72423500 1.66959000 0.49574300
 H 6.05984200 0.05701000 0.84368900
 H 6.36638100 0.55389300 -0.83734100
 C 4.07864500 1.89538700 1.41066200
 H 4.09135100 1.05945200 2.11312100
 H 4.68995100 2.70782200 1.81878700
 H 3.04916800 2.25817300 1.31170100
 N -5.79195700 1.57895800 -1.18175100

ComA24:

B -2.53062200 -0.00004100 -0.02578700
 H -2.91916400 1.01591900 -0.56416400
 H -2.91870800 -1.01572100 -0.56484300
 H -2.69737400 -0.00014700 1.18250500
 C 1.15899500 1.19188300 -0.23051800
 C -0.29045000 1.20329100 0.21540900
 C -0.29081600 -1.20310500 0.21546600
 C 1.15860100 -1.19212800 -0.23050500
 H -0.38644800 1.22605700 1.30894400
 H -0.85084100 2.03463500 -0.21537800
 H 1.19594300 1.25617400 -1.32553000
 H 1.65255200 2.08360700 0.17044100
 H -0.38694000 -1.22563100 1.30897100
 H -0.85156500 -2.03415500 -0.21539800
 H 1.65187700 -2.08399600 0.17047800
 H 1.19552600 -1.25648200 -1.32551500
 O -0.95241900 0.00027700 -0.26232900
 N 1.88501800 -0.00023800 0.18284500
 H 1.97450600 -0.00024700 1.19803100

TS2-ComB24:

C -1.76426600 -1.42670400 0.51011500
 C -0.36937100 -1.11829500 1.05448800

C -0.68323900 0.37150500 0.95218000
 H -1.81495400 -2.05845100 -0.38366800
 H -2.46925400 -1.80634100 1.26196900
 H -0.03242500 -1.54143200 1.99661100
 H 0.01940200 0.98144300 0.37349000
 H -0.86949400 0.86587500 1.91523200
 N -1.91310100 0.00623800 0.25177600
 I 1.34797100 -1.74344700 -0.39667200
 C -3.03935300 0.75751500 0.19651700
 O -3.05293500 1.96353100 0.39352500
 O -4.08967500 -0.01923700 -0.12186900
 C -5.41822700 0.55296600 -0.29065300
 C -6.26173900 -0.66143000 -0.65368300
 H -7.30346100 -0.36219300 -0.80590900
 H -5.89237100 -1.12346800 -1.57492600
 H -6.22600700 -1.40649900 0.14781900
 C -5.41447800 1.56429400 -1.43065600
 H -6.43967300 1.89338900 -1.63116200
 H -4.80586600 2.43439600 -1.17832300
 H -5.01755500 1.10352000 -2.34172900
 C -5.89505400 1.16420300 1.02162400
 H -5.28893200 2.03069300 1.29190300
 H -6.93943200 1.47870800 0.92173800
 H -5.83575100 0.42273100 1.82591200
 B 2.57619500 0.27339100 1.83968900
 H 1.78715000 1.09545400 2.20550000
 H 3.06860900 -0.58812700 2.50509000
 C 5.78124900 0.92625000 -0.13290300
 C 4.68396300 0.04390200 0.41201000
 C 3.07655800 1.79330600 -0.13348400
 C 4.21371500 2.62777300 -0.67290300
 H 4.26255400 -0.61311800 -0.35296800
 H 5.00281900 -0.53265100 1.27946700
 H 6.20892400 1.51771200 0.69680900
 H 6.56887400 0.27481400 -0.52546900
 H 2.61607400 1.16405400 -0.90100700
 H 2.32214900 2.39739000 0.36956400
 H 3.81357300 3.25762000 -1.47416300
 H 4.58060600 3.29122700 0.13107000
 N 5.23977600 1.74669700 -1.20252900
 H 5.98032600 2.29443100 -1.62904200
 O 3.59703400 0.89599400 0.89843600

ComA25:

C -3.92381900 1.54920700 0.14433600
 C -4.88915700 2.12450000 -0.65411500
 C -6.21246600 1.64440300 -0.63292400
 C -6.46043200 0.57350700 0.24879500
 C -5.44208500 0.04724200 1.01186400
 N -4.18194300 0.51739200 0.96666500
 H -2.89691800 1.89637300 0.13262300
 H -4.60476000 2.93243300 -1.31974700
 H -7.46193500 0.17262400 0.36246900
 H -5.61388500 -0.77094400 1.70249900
 B -3.03206400 -0.17654900 1.81500500
 H -3.51893700 -0.50895300 2.88236300
 H -2.13609000 0.63700800 1.95456400
 N -7.21096100 2.19199700 -1.42594900
 Si -8.26115200 1.09605500 -2.38209700
 Si -7.39723800 3.97506600 -1.48459000
 C -9.92058300 0.81628800 -1.54749800
 H -10.53708100 0.13652700 -2.14998700
 H -9.80194700 0.36264500 -0.55584400
 H -10.48111500 1.74912500 -1.42260800
 C -8.49525100 1.84942100 -4.08765500
 H -7.53243900 1.95382200 -4.60165700
 H -9.11776000 1.17316900 -4.68842500
 H -8.98864200 2.82612400 -4.08800000
 C -7.37420000 -0.54321700 -2.61782600
 H -6.33437900 -0.40052200 -2.93512400
 H -7.37073600 -1.17837100 -1.72656200
 H -7.88606800 -1.09991000 -3.41377100
 C -6.69240000 4.70619800 0.09656100
 H -7.03727600 5.74477000 0.18335400
 H -7.04872200 4.16737700 0.98265500
 H -5.59848200 4.72097800 0.12892000
 C -9.23278700 4.37390400 -1.51493000
 H -9.76948500 3.98072800 -2.38401800
 H -9.72766800 4.00054900 -0.61078800
 H -9.35313600 5.46520600 -1.52776400
 C -6.53603400 4.71230700 -2.98216900
 H -5.46856400 4.46011700 -2.99888100
 H -6.97579900 4.36134100 -3.92228600
 H -6.61568700 5.80704200 -2.96597200
 H -2.65330100 -1.15205500 1.18354100

TS2-ComB25:

I 1.54382000 -2.07957400 0.78500000
 C 4.69514500 -1.30388600 1.44273400
 C 3.36687100 -1.24535500 2.18107500
 C 3.43617300 0.27503900 2.16005600
 H 5.52835300 -1.72107600 2.02289800
 H 4.68282300 -1.76849600 0.44970100
 H 3.19798600 -1.79462600 3.10356200
 H 3.56031800 0.74268000 3.14561700
 H 2.64517500 0.80203200 1.61405400
 N 4.68807500 0.16447700 1.40728500
 C 5.01648600 0.97232200 0.36408800
 O 4.55517700 2.09213000 0.21057200
 O 5.92384500 0.36039200 -0.41552700
 C 6.43162700 1.00464900 -1.61915100
 C 7.38519300 -0.04010800 -2.18086100
 H 7.84193300 0.32637600 -3.10605400
 H 8.18296300 -0.26130900 -1.46355200
 H 6.85089300 -0.97038200 -2.40227100
 C 7.18314800 2.27877500 -1.25593400
 H 7.66248300 2.69136200 -2.15067200
 H 6.50574600 3.02827800 -0.84191600
 H 7.96471400 2.06231400 -0.51875600
 C 5.29062800 1.26517900 -2.59420900
 H 4.60006400 2.01428000 -2.20126400
 H 5.69539900 1.62354600 -3.54726400
 H 4.73637500 0.33897800 -2.78412300
 C -1.22691000 0.63865900 1.86430300
 C -2.28528200 0.98714200 1.07339400
 C -3.23113800 0.01890800 0.64814000
 C -3.00216700 -1.29706000 1.09787200
 C -1.92212900 -1.60087700 1.88925900
 N -1.02606900 -0.64579300 2.30116000
 H -0.47872900 1.35818900 2.17580000
 H -2.37014500 2.01760500 0.74351700
 H -3.68958100 -2.09407900 0.83229800
 H -1.73380100 -2.60480300 2.25009700
 B 0.20386300 -1.03864900 3.00079200
 H 0.18737100 -2.08762200 3.57439700
 H 0.94940800 -0.15253500 3.29997100
 N -4.30418200 0.34660400 -0.17953000
 Si -5.36186600 1.71274000 0.27382600
 Si -4.55248800 -0.61822900 -1.66414200
 C -4.91855100 3.28109900 -0.66382300

H -5.51816500 4.12533100 -0.29884400
 H -3.86179800 3.54392200 -0.53038000
 H -5.10432200 3.18274800 -1.73954800
 C -7.14636000 1.23154300 -0.07325600
 H -7.44148400 0.36197700 0.52594000
 H -7.80223900 2.06594100 0.20929100
 H -7.35043300 1.00412400 -1.12465700
 C -5.20161600 2.00380100 2.12425700
 H -4.25077700 2.46124000 2.41693000
 H -6.00484800 2.67991300 2.44554400
 H -5.31255800 1.06909000 2.68725400
 C -5.06519900 0.53400800 -3.05943500
 H -6.01560800 1.05165900 -2.89340400
 H -4.29281800 1.28894500 -3.24848600
 H -5.17613500 -0.05815600 -3.97779300
 C -5.86176800 -1.94443000 -1.41289000
 H -5.97503300 -2.54950400 -2.32186600
 H -5.59677800 -2.62389400 -0.59327900
 H -6.84015600 -1.50859600 -1.17954000
 C -2.91084600 -1.39450800 -2.14845300
 H -2.59865200 -2.21717200 -1.49675300
 H -2.99318800 -1.79384300 -3.16789500
 H -2.10667000 -0.64858200 -2.15047700

ComA26:

B -3.26420600 -0.00002300 0.02683900
 H -3.63665400 -1.01318100 -0.53159700
 H -3.63669100 1.01342000 -0.53105600
 N -1.67102400 0.00001000 -0.01824300
 C -0.99379100 1.15962900 -0.01548900
 C -0.99378600 -1.15961600 -0.01548600
 C 0.38813500 1.20529300 -0.00390100
 H -1.59533000 2.06073900 -0.02372300
 C 0.38813200 -1.20527700 -0.00390200
 H -1.59533400 -2.06072100 -0.02372500
 C 1.09443800 0.00001200 0.00071400
 H 0.89964300 2.16074800 -0.00322900
 H 0.89964900 -2.16072700 -0.00323000
 C 2.52546600 0.00000800 0.00710000
 N 3.68549500 -0.00002700 0.01248500
 H -3.56711600 -0.00033900 1.20844700

TS2-ComB26:

C 0.82261500 0.69118400 -1.32176200
 C -0.46760500 0.40388800 -0.58865900
 C 0.07549500 1.09479600 0.63970900
 H 1.42020700 -0.16754600 -1.65022200
 H 0.71861700 1.39053700 -2.16171700
 H -1.45647800 0.55617700 -1.00687200
 H 0.21238500 0.49501200 1.54687800
 H -0.46171200 2.01742400 0.90457700
 N 1.32550500 1.32053600 -0.09035300
 I -0.48906900 -2.20748800 -0.22086000
 C 2.55328400 1.13530200 0.47538200
 O 2.75259300 1.22321500 1.67572400
 O 3.45997000 0.88278300 -0.47874500
 C 4.85228100 0.61247700 -0.13580600
 C 5.48762700 0.36364900 -1.49664600
 H 6.55336600 0.14513200 -1.37728600
 H 5.01063700 -0.48769000 -1.99322500
 H 5.38158000 1.24516300 -2.13718100
 C 4.93863500 -0.63607900 0.73325700
 H 5.98900000 -0.91102300 0.87543900
 H 4.48331000 -0.46701800 1.71061200
 H 4.42758400 -1.47158500 0.24252100
 C 5.47320100 1.83136400 0.53456100
 H 5.00705900 2.02431700 1.50234200
 H 6.54430200 1.65886000 0.68391600
 H 5.35336000 2.71479100 -0.10181000
 B -2.64434000 -2.17782300 0.98648800
 H -3.22248700 -3.06942300 0.43633300
 H -2.29864600 -2.29417900 2.12600600
 N -3.22064100 -0.81188000 0.67830300
 C -2.95479200 0.25159200 1.49001300
 C -3.90604900 -0.59390500 -0.48339100
 C -3.31549100 1.53331500 1.15973500
 H -2.43388600 0.01863500 2.41064700
 C -4.28906300 0.66024300 -0.87954000
 H -4.10864800 -1.47573900 -1.07857900
 C -3.97402300 1.77180900 -0.06500500
 H -3.08559900 2.34668100 1.83798800
 H -4.82307400 0.78774400 -1.81379100
 C -4.32850200 3.08765800 -0.45878600
 N -4.61553600 4.16820000 -0.78475400

ComA27:

B 3.62781100 -0.00108800 0.02767900
 H 4.00054800 1.03605400 -0.48340700
 H 3.99945400 -0.98935300 -0.57339900
 N 2.03399400 0.00130600 -0.01807400
 C 1.35896300 -1.15965400 -0.03581400
 C 1.35836700 1.16153900 0.00374300
 C -0.02408800 -1.20688600 -0.02401000
 H 1.96110200 -2.05986900 -0.06031300
 C -0.02505700 1.20747300 0.01289600
 H 1.95988500 2.06238300 0.01280100
 C -0.70354200 0.00012700 -0.00157100
 H -0.54713800 -2.15481100 -0.03841400
 H -0.54865400 2.15509000 0.02821800
 N -2.17246700 -0.00045900 0.00496900
 O -2.73116600 -1.08238400 0.05632300
 O -2.73253800 1.08101300 -0.04037900
 H 3.92683400 -0.05460700 1.20883800

TS2-ComB27:

C 1.29441625 0.98984770 0.00000000
 C 0.01896225 0.64505370 0.72163400
 C 0.49659225 1.38468770 1.94170600
 H 1.94378125 0.15882570 -0.30122600
 H 1.15906625 1.66022170 -0.85983700
 H -0.97896075 0.66044370 0.29946000
 H 0.65792225 0.80836970 2.86017100
 H -0.10406375 2.27460470 2.18507600
 N 1.74055825 1.67841670 1.22269900
 I 0.21664725 -2.03894530 1.17694100
 C 2.96965025 1.57724070 1.80943000
 O 3.14384225 1.69446170 3.01033400
 O 3.90425025 1.37175970 0.87125400
 C 5.30501825 1.18466170 1.23767800
 C 5.97538725 0.95919970 -0.10962700
 H 7.05051825 0.80412270 0.02766200
 H 5.55842425 0.07633470 -0.60619100
 H 5.83027225 1.82540670 -0.76404000
 C 5.44975525 -0.04771430 2.12081000
 H 6.51206025 -0.25877030 2.28550800
 H 4.96939825 0.10083870 3.09014000
 H 4.99950325 -0.91960730 1.63264700
 C 5.84627925 2.44236770 1.90446700

H 5.36435125 2.61582270 2.86874200
 H 6.92499725 2.33620470 2.06391000
 H 5.68029325 3.31546870 1.26337900
 B -1.86295175 -2.23061730 2.38939600
 H -2.38855575 -3.16902430 1.86344800
 H -1.51640975 -2.31413830 3.53204600
 N -2.58920875 -0.91809230 2.09976100
 C -2.40775975 0.15691070 2.91003100
 C -3.33631475 -0.78040730 0.97112400
 C -2.92489975 1.39403270 2.60893800
 H -1.82219475 -0.02068130 3.80410000
 C -3.88260775 0.42393170 0.60274800
 H -3.45858075 -1.67718630 0.37580700
 C -3.65291975 1.53553070 1.42306000
 H -2.76873475 2.23471970 3.27295000
 H -4.46892175 0.51045870 -0.30329500
 N -4.17833475 2.81818070 1.05592900
 O -3.94219875 3.76865070 1.80224200
 O -4.83131975 2.89401770 0.01486300

ComA28:

B 1.55785000 -0.00612200 0.11393800
 H 2.06595800 1.00268100 -0.34722700
 H 2.05718800 -1.01974100 -0.34667100
 N 0.01206100 -0.00003700 -0.33959200
 H 0.00602600 -0.00013500 -1.36086900
 C -0.70301400 -1.21279200 0.10199300
 H -0.68399700 -1.24741300 1.19374600
 H -1.73965600 -1.19608600 -0.24888100
 H -0.19016600 -2.09110900 -0.29337700
 C -0.69284100 1.21838700 0.10198400
 H -0.17297400 2.09255900 -0.29332400
 H -1.72970800 1.21026100 -0.24842700
 H -0.67325200 1.25255600 1.19376800
 H 1.56203400 -0.00627200 1.33485700

TS2-ComB28:

C 0.93513000 -0.97611500 -0.84030500
 C -0.41717500 -0.29571900 -1.03848900
 C 0.15482400 0.97373400 -0.41141100
 H 0.93674100 -1.91362200 -0.27231100
 H 1.50855700 -1.11318800 -1.76721400

H -0.88654800 -0.25929200 -2.01785000
H -0.38326000 1.39584900 0.44444700
H 0.35780800 1.77693200 -1.13353500
N 1.34854800 0.19978000 -0.07164400
I -2.11210600 -1.23935200 0.26658300
C 2.59022900 0.71734300 0.10115000
O 2.79652000 1.88908000 0.37631900
O 3.51244800 -0.24911200 -0.05303400
C 4.93150900 0.04595000 0.09315800
C 5.58356400 -1.30522900 -0.16202200
H 6.67254400 -1.21810100 -0.08831600
H 5.24322500 -2.04362500 0.57199500
H 5.33153000 -1.67189600 -1.16300900
C 5.22723200 0.52569100 1.50861100
H 6.31025500 0.61597300 1.64830600
H 4.76596100 1.49683000 1.69910000
H 4.84807900 -0.19589600 2.24112600

C 5.36552500 1.05709600 -0.96057500
H 4.89310700 2.02694000 -0.79136900
H 6.45336100 1.18365000 -0.92550900
H 5.09523400 0.70193100 -1.96161400
B -3.21540900 1.34193700 -1.12311700
H -2.34606700 2.15781100 -0.98740800
H -3.46595300 0.80983000 -2.16896700
N -4.48181700 1.63882900 -0.24136200
H -4.91819800 2.47543100 -0.64174900
C -5.49809700 0.56219300 -0.30317000
H -5.06733500 -0.34672200 0.11934200
H -6.38591100 0.85601200 0.26395900
H -5.76165100 0.38827800 -1.34766000
C -4.13654200 1.97708700 1.16035300
H -3.42926200 2.80816400 1.15566100
H -5.04031300 2.25727600 1.70917000
H -3.66927700 1.10523200 1.62104400