Supporting Information

Theoretical Study on the Co^{II}/Co^{III} and Co^{II}/Co^{IV} Catalytic Cycles in Co^{II}(salen)-Catalyzed Radical Fluorination with Various NF-Type Fluorinating Reagents

Jingwen Li[a,c], Mong-Feng Chiou[b,*], Hongli Bao[a,c,*]

[a]College of Chemistry, Fuzhou University, Fuzhou, Fujian 350108, China.

[b]Strait Laboratory of Flexible Electronics (SLoFE), Fujian Key Laboratory of Flexible Electronics, Strait Institute of Flexible Electronics (SIFE Future Technologies), Fujian Normal University, Fuzhou, Fujian 350117, China.

[c]State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China.

*Correspondence to: ifemfchiou@fjnu.edu.cn; hlbao@fjirsm.ac.cn

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Cramer-Truhlar correction for vibrational entropy terms

In this study, structural optimization procedure inherently employs the SMD implicit solvation model including vibrational analysis. According to the report by Cramer and Truhlar et al. in *J. Phys. Chem. B*, **2011**, *115*, 14556, they assert that the free energy obtained through such a computational method is appropriate, as statement in the article: "When molecular free energies are defined to include free energy contributions from nuclear motion, it may sometimes be more consistent with parametrization history to determine these contributions from gas-phase partition functions, but it is not 'incorrect' to employ instead partition functions for structures that are stationary points in solution."

Nevertheless, following the recommended practice, we have scaled all vibrational frequencies lower than 100 cm^{-1} raised to 100 cm^{-1} for the initial reaction of Co^{II}(salen) with Me_3NFPy^+. This correction addresses the well-known breakdown of the harmonic oscillator model in the free energy calculation for low-frequency vibrational modes. The partition functions were subsequently recalculated to obtain the corrected vibrational entropy terms.

$$S_{vib,i} = R\left[\frac{x_i}{e^{xi}-1} - \ln\left(1-e^{-xi}\right)\right]; for\ frequency\ v_i$$

in which $x_i = \frac{hcv_i}{kT} \approx \frac{1.4388 v_i}{T}$; $\frac{hc}{k}$ =1.4388 (K·cm); R = 1.987 cal/(mol·K)

Based on the Cramer-Truhlar correction, the calculated relative free energies are in excellent agreement with original energy profile (Fig. S5). This are attributed to the fact that the number of vibrational modes below 100 cm^{-1} in the structures of the bimolecular reactions (e.g., **^{2}TS1**, **^{2}INT1**) does not exhibit an unreasonable increase. Therefore, we conclude that the findings of this study are reliable.

Intermediate	S_{vib} in out file (cal/mol • K)	Corrected S_{vib} (cal/mol • K)	T Δ S(Kcal/mol)	Number of freq. < 100 cm^{-1}
Co^{II}(salen)	155.80	138.97	5.02	11
Me_3NFPy^+	32.57	26.70	1.75	1
^{2}TS1	207.56	182.88	7.36	16
^{2}INT1	212.91	186.31	7.93	17
Co^{III}(salen)-F	161.72	144.38	5.16	11
Me_3NPy^+	30.67	27.03	1.09	3
$[Co^{IV}$(salen)-F$]^+$	162.27	145.14	5.11	11
Me_3NPy	29.79	24.72	1.51	3

Analysis of Counterion Dissociation Behavior and Feasibility of Fluorine Transfer Reaction

The counterions PF_6^- and OTf^- were also examined to understand their behavior in solution. The computed results are summarized in Table S3. The results show that regardless of the counterion, Me_3NFPy^+ tends to dissociate in solution.

On the other hand, according to the experimental condition screening reported by Hiroya et al. in *Org. Lett.*, **2013**, *15*, 5158, the use of Me_3NFPy·OTf (i.e., **F2**) as a fluorinating reagent yielded 0% product. This experimental result indeed provides critical support for our study, further corroborating that the reaction likely proceeds via a benzenium fluorination pathway. In addition,

the process of fluorine transfer from PF_6^- or OTf^- anions to the benzenium ion was also computationally analyzed. The results show that the reaction with the OTf^- anion exhibits a high energy barrier of 26.6 kcal/mol, and the product formation free energy is 19.6 kcal/mol, indicating that are both kinetically and thermodynamically unfavorable (see Fig. S6). Although no experimental data are available for using $Me_3NFPy{\cdot}PF_6$ as reagent, we believe that the reaction should be accessible if the counterion is PF_6^-.

Analyses of HOMO Eigenenergies, Orbital Configurations, and Electron Affinities of the fluorinating reagents at the Electronic Level

To further understand the electron affinity of the counterpart of different NF-type fluorinating reagents after fluorine transfer to Co^{II}(salen), the HOMO eigenenergies of Me_3NPy, N-tBu-amidyl anion (**15**) and $PhSO_2N(Et)^-$, as well as the β-SOMO eigenenergies corresponding to single-electron loss, were examined. The HOMO and β-SOMO eigenenergies are -0.25128, -0.12151 and -0.16397 hartree and -0.23568, -0.12232 and -0.14521 hartree, respectively. According to Koopmans' theorem, the first ionization energy of a closed-shell molecule approximates the eigenenergy of its HOMO. Although DFT may introduce errors due to inaccuracies in the exchange–correlation functional, it is still evident that the electron affinity of Me_3NPy^+ is significantly greater than that of **12** and $PhSO_2N(Et)$. This is because the HOMO of Me_3NPy is a π orbital delocalized on the pyridine ring, analogous to that of benzene, whereas the HOMOs of the other two counterparts of neutral reagents are localized on the amide moiety and even exhibit π-antibonding character with the phenyl ring of the benzyl group (see Fig. S8). Consequently, Me_3NPy^+ possesses the highest electron affinity. In addition, the electronic energy difference for each species upon gaining or losing an electron was also computationally analyzed, as listed below. Although the ligands and solvents differ in these Co(salen)-F systems, the electron binding energy is approximately ~130 kcal/mol, clearly indicating that Me_3NPy^+ is more capable to oxidize Co^{III}(salen)-F.

$Me_3NPy^+ + e^- \rightarrow Me_3NPy$	$\Delta E_{elec} = -155.9$ Kcal/mol
$Co^{III}(salen)\text{-}F - e^- \rightarrow [Co^{IV}(salen)\text{-}F]^+$	$\Delta E_{elec} = 127.9$ Kcal/mol
12 $+ e^- \rightarrow$ **15**	$\Delta E_{elec} = -82.6$ Kcal/mol
$Co^{III}(salen)\text{-}F - e^- \rightarrow [Co^{IV}(salen)\text{-}F]^+$	$\Delta E_{elec} = 137.5$ Kcal/mol
$PhSO_2N(Et) + e^- \rightarrow PhSO_2N(Et)^-$	$\Delta E_{elec} = -98.7$ Kcal/mol
$Co^{III}(salen)\text{-}F - e^- \rightarrow [Co^{IV}(salen)\text{-}F]^+$	$\Delta E_{elec} = 124.3$ Kcal/mol

The Non-innocent Behavior of the salen Ligand and Its Regulation of the Coordination Geometry of Cobalt Complexes

Due to the conjugation between the diimine moiety of the salen ligand and the phenolate groups, the structure is essentially slightly rigid. Consequently, Co^{II}(salen) adopts a nearly square-planar coordination geometry (Table S6). To further understand how the salen ligand modulates charge distribution during fluorination and oxidation, a detailed analysis was performed on the cobalt d-orbital electron populations, spin densities, and several key geometric parameters for Co^{II}(salen) versus $[Co^{III}(salen)]^+$, as well as for Co^{III}(salen)–F versus $[Co^{IV}(salen)–F]^+$. According to the ligand-field theory, the d-orbitals in a square-planar coordination field should split as shown in Table S6. Because the dxy orbital is sigma antibonding (σ*), it contains few electrons and lies at a higher energy, rendering Co^{II}(salen) a low-spin doublet state. The $dx^2–y^2$ orbital, located between all Co–

X (X = O, N) bonds, is non-bonding and therefore lowest in energy; it is always almost occupied by approximately two electrons from the cobalt d^7 configuration. Since the ONNO coordination of salen is not equivalent, the symmetric dz^2 and dxz orbitals form pi antibonding orbitals (π*) that are higher in energy than the dyz π* orbital, although all π* orbitals lie close in energy. The electron populations and spin densities listed in Table S6 reveal that the spin densities on the dz^2 and dxz orbitals increase and the total electron count decreases when CoII(salen) loses one electron to form $[Co^{III}(salen)]^+$, while the square-planar coordination geometry remains largely unchanged. Combined with the data in Table S7, it can be seen that upon oxidation to $[Co^{III}(salen)]^+$, the salen ligand itself carries only a small net positive charge but accommodates a portion of the spin density, which is primarily localized on the oxygen atoms and carbons (not listed in Table S7) of phenolic moieties. Because the antibonding π* character formed by dxz orbital loses electron density, the Co–O bond lengths shorten slightly.

On the other hand, when an F atom coordinates at the axial position to form $Co^{III}(salen)$–F, although the dz^2 orbital becomes a sigma antibonding (σ*) orbital, the pi antibonding (π*) orbitals (dxz, dyz) remain close in energy to the dz^2 σ* orbital due to the presence of the F atom with lone pairs electrons. Comparing the d-orbital electron populations and spin densities of $Co^{II}(salen)$ and $Co^{III}(salen)$−F, it can be seen that the change in the dxz orbital is minimal, whereas the electron population in the dz^2 orbital further decreases and its spin density increases. Furthermore, upon oxidation to $[Co^{IV}(salen)–F]^+$, the electron loss clearly occurs from the dyz orbital resulting in quartet state. Furthermore, comparing the structures of $Co^{III}(salen)$–F and $[Co^{IV}(salen)–F]^+$ with that of $Co^{II}(salen)$ reveals that the ∠(N2−Co−O1) angle decreases significantly, and the dihedral angle D(O1−N1−N2−O2) gradually increases. Upon the formation of $[Co^{IV}(salen)–F]^+$, the bond lengths of d(Co–O2) and d(Co–N2) are further elongated. This indicates that the coordination geometry tends to shift toward a trigonal bipyramidal rather than a square pyramidal structure, although the inherent rigidity of the salen ligand prevents a more substantial distortion. Combining the analyses of charge distribution and spin density on the ligand reveal that in both $Co^{III}(salen)$–F and $[Co^{IV}(salen)–F]^+$, the spin density on the salen ligand is no longer close to zero. Similar to the case in $[Co^{III}(salen)]^+$, a greater proportion of the unpaired electron density is delocalized onto the phenolic moieties. This disrupts the conjugation between the imine and phenolate groups, allowing rotation around the connecting C–C bond and thereby facilitating the adoption of a trigonal bipyramidal geometry. These results indicate that the salen ligand is a non-innocent ligand since the phenolate groups can accommodate spin density to adopt the trigonal bipyramidal geometry slightly.

Possible competitive pathways for the fluorination reaction of benzyl radical 17

A potential competitive pathway for the fluorination of benzyl radical **17**, namely the fluorination reaction pathway involving carbocation **19, was also computationally analyzed** (see Fig. S15 for details). The results show that although the dissociation of intermediate ^{4}**INT11** to form $[Co^{II}(salen)\text{-}F]^-$ and the nitrogen cation $PhSO_2N^+(Et)$ is slightly lower in Gibbs free energy of formation (by approximately 0.7 kcal/mol, pink pathway) compared to the formation of $[Co^{III}(salen)\text{-}F]^+$ and $PhSO_2N^{\cdot}(Et)$, the transition state ^{1}**TS25** for generating carbocation **19** in the subsequent reaction pathway has an energy barrier approximately 25.8 kcal/mol higher than that of transition state ^{2}**TS22** for generating benzyl radical **17**. This indicates that, kinetically, the radical reaction pathway remains more favorable.

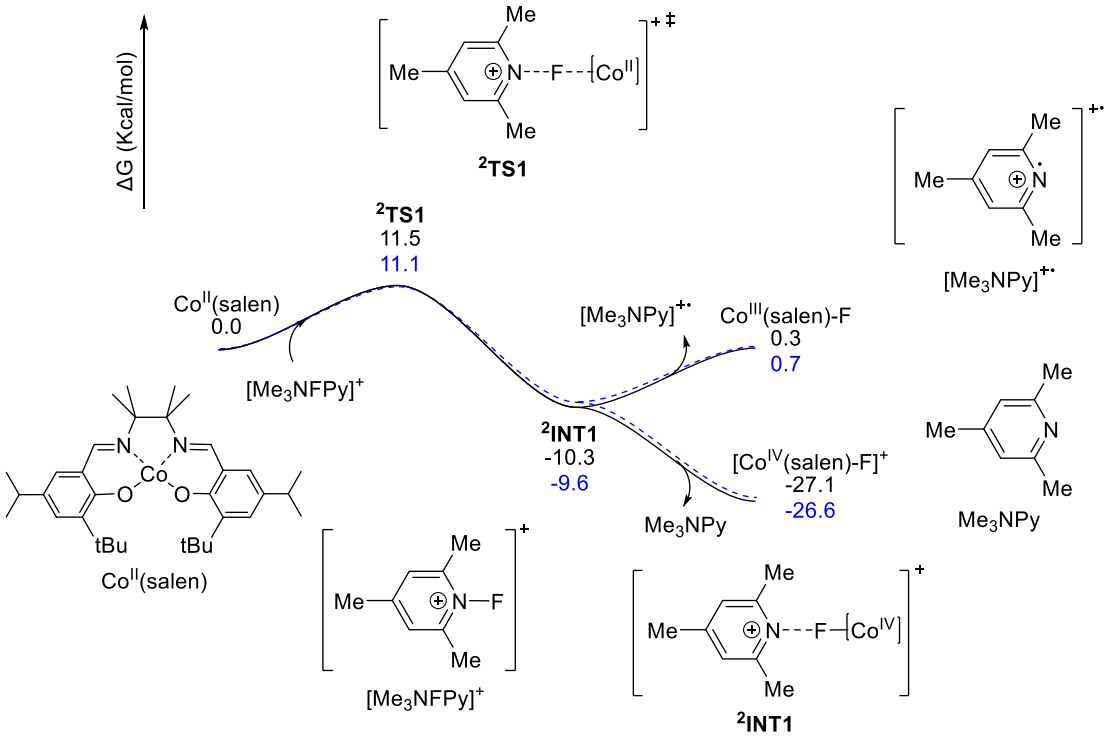


Fig. S1. Free energy profile of Co^{II}(salen) reacting with the fluorinating reagent $[Me_3NFPy]^+$ calculated by using B3LYP-D3 (black line) and M06 (blue dash line) functionals.

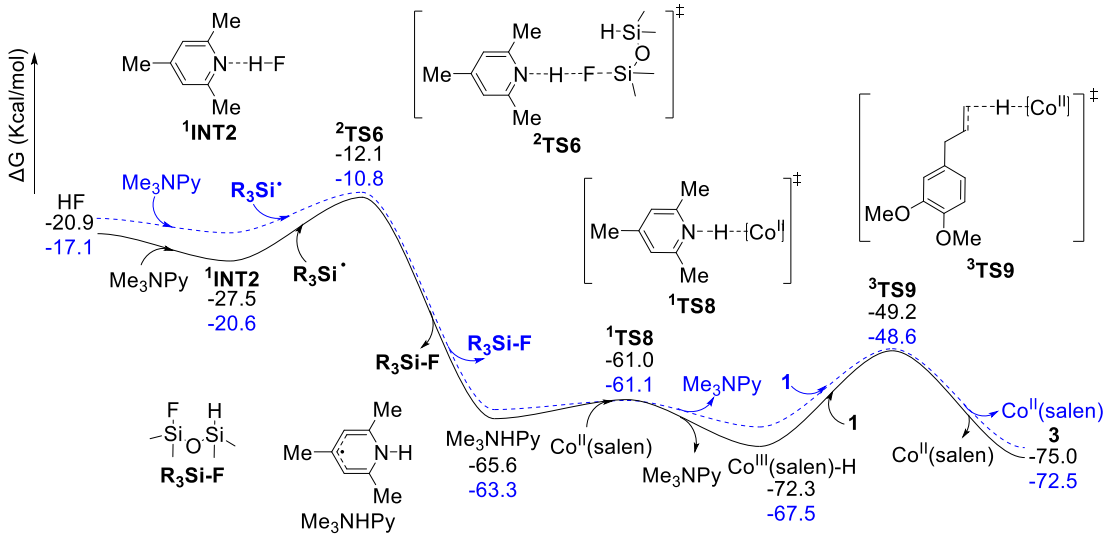


Fig. S2. Free energy profile of the formation pathway of alkyl radical **3** calculated by using B3LYP-D3 (black line) and M06 (blue dash line) functionals.

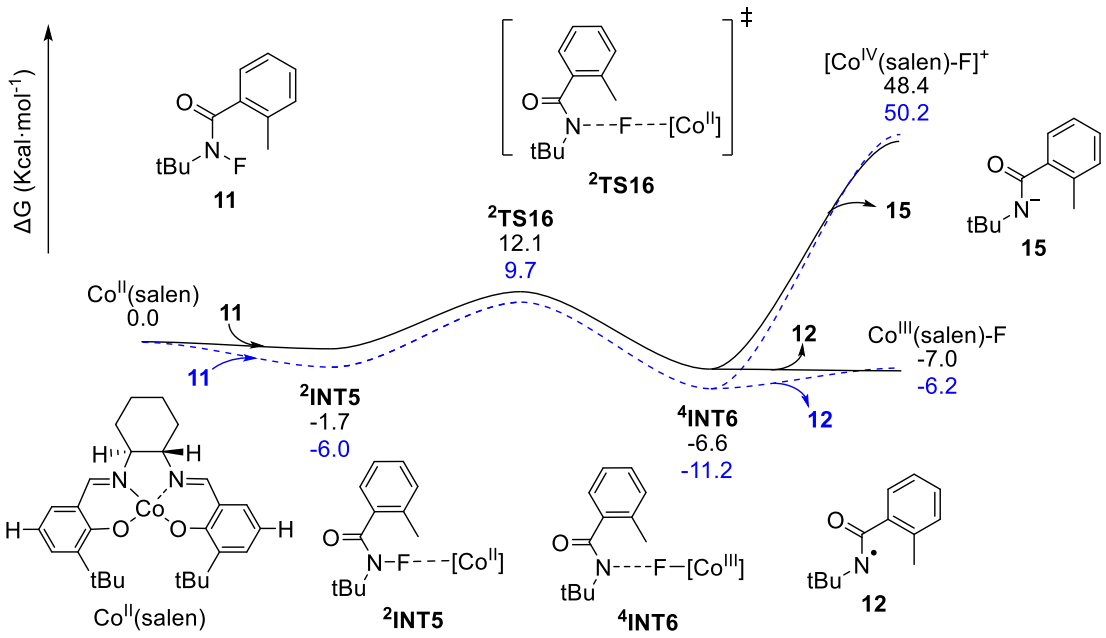


Fig. S3. Free energy profile of Co^{II}(salen) reacting with the fluorinating reagent N-tert-butylfluoramide calculated by using B3LYP-D3 (black line) and M06 (blue dash line) functionals.

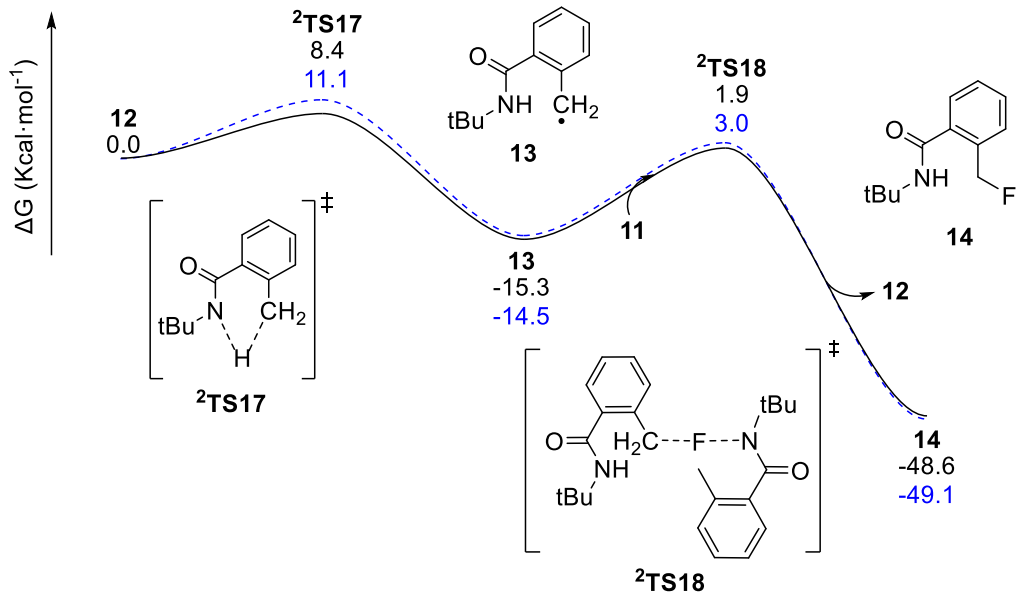


Fig. S4. Free energy profile of the formation pathway of benzyl radical **13** via 1,5-HAT and the subsequent fluorination reaction pathway calculated by using B3LYP-D3 (black line) and M06 (blue dash line) functionals.

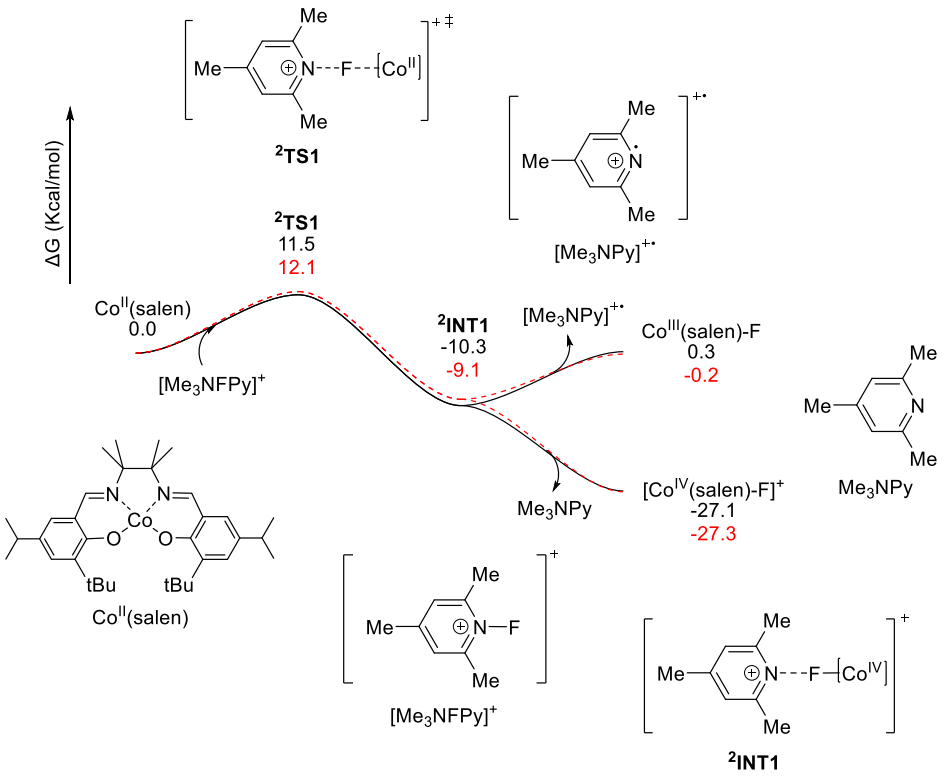


Fig. S5. Relative free energies calculated with Cramer-Truhlar correction (red dash line) for the initial reaction of Co^{II}(salen) with Me_3NFPy^+.

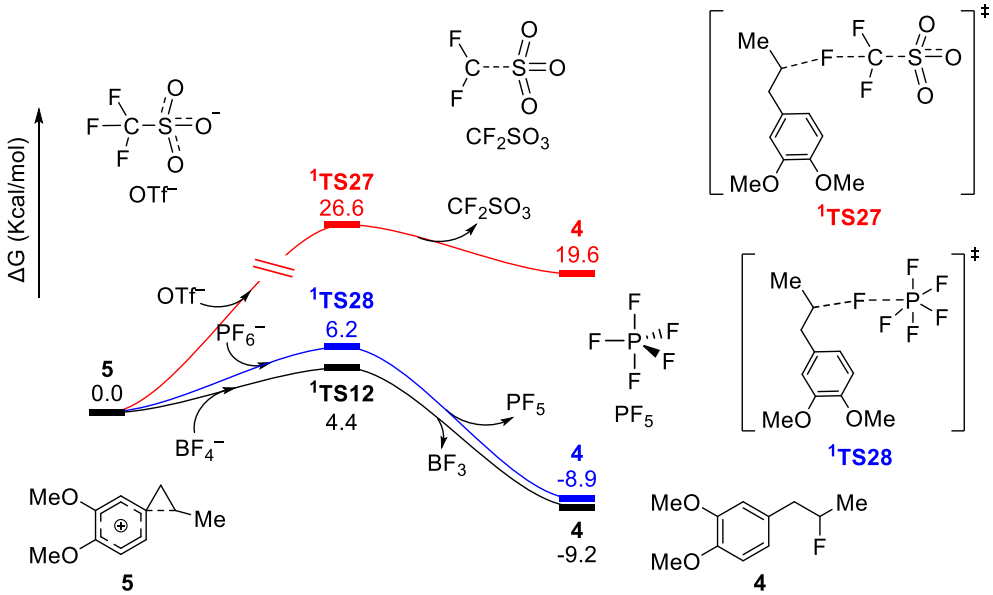


Fig. S6. Free energy profile of benzenium fluorination with BF_4^-, PF_6^- and OTf^- anions.

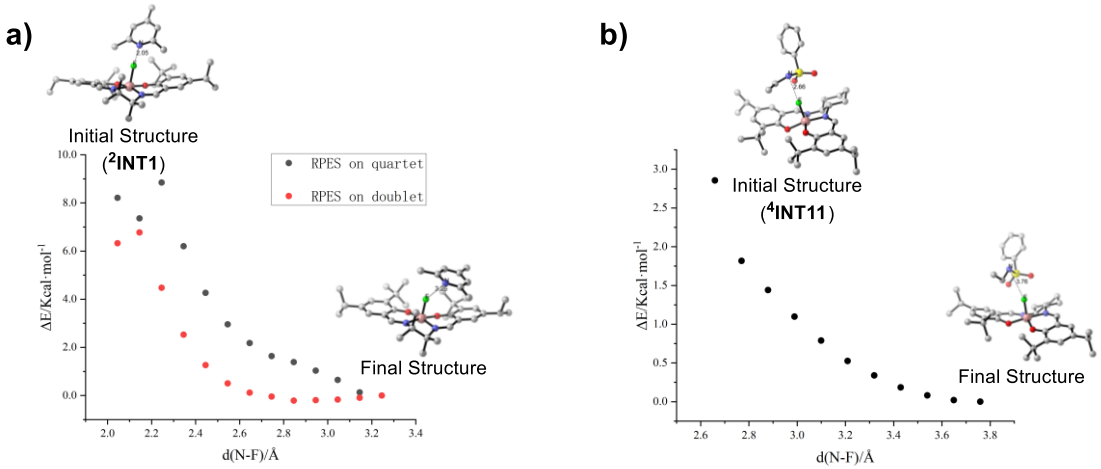


Fig. S7. RPESs of the counterpart of fluorinating reagent (a) Me_3NPy and (b) $PhSO_2N(Et)$ molecules moving away from the Co(salen)−F cluster.

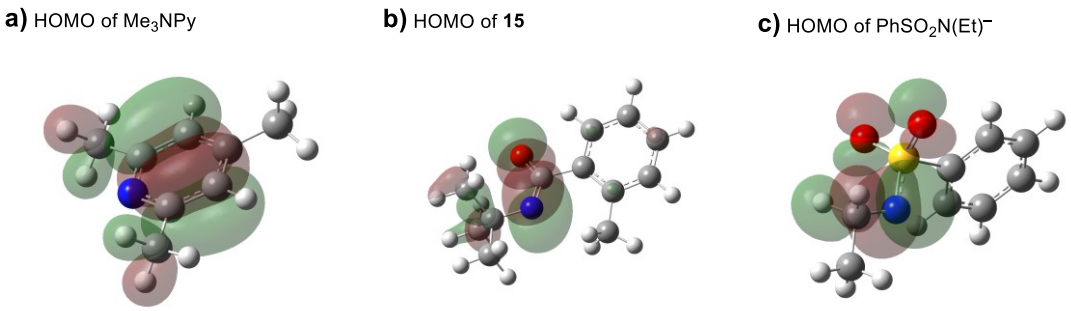


Fig. S8. Isosurfaces of HOMO (a) Me_3NPy, (b) amidyl anion **15** and (c) $PhSO_2N(Et)^-$ at 0.025 of isovalue.

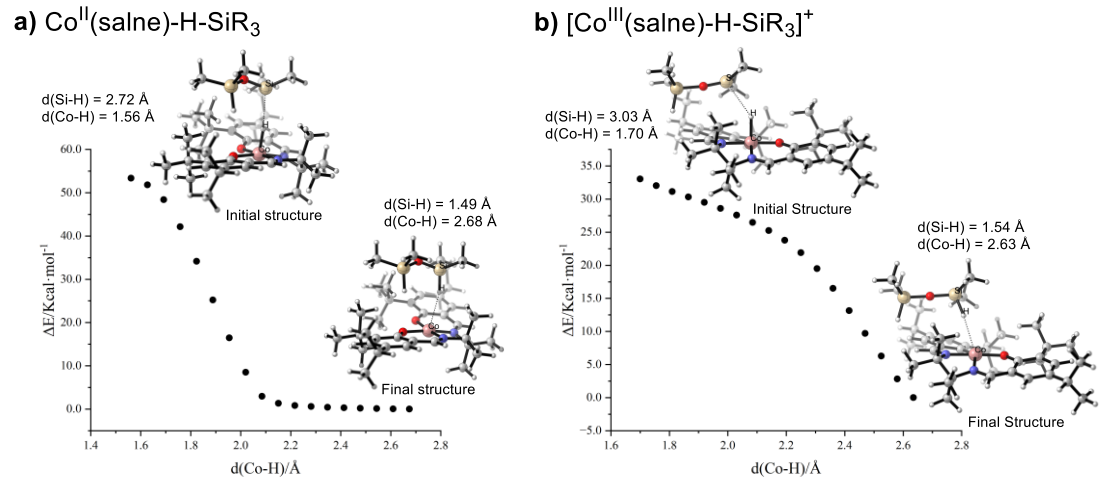


Fig. S9. The IRC paths of (a) Co^{II}(salen)−H−SiR_3 and (b) $[Co^{III}$(salen)−H−$SiR_3]^+$ corresponding to the intrinsic reaction potential surfaces of Co^{II}(salen) and $[Co^{III}$(salen)$]^+$ directly reacting with silane.

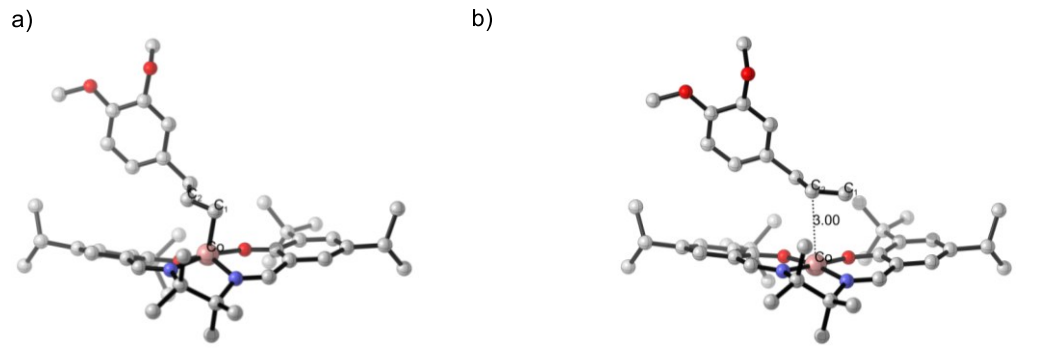


Fig. S10. a) Structure of the alkene coordinated to Co^{II}(salen) obtained from a constrained optimization fixing the Co–C1 bond length at 1.90 Å; b) Structure obtained after full unconstrained relaxation optimization of the entire molecule.

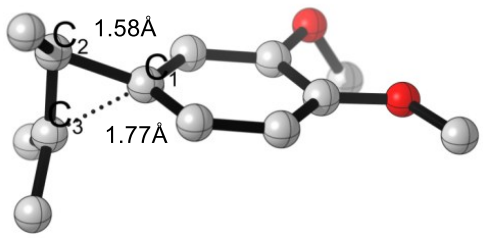
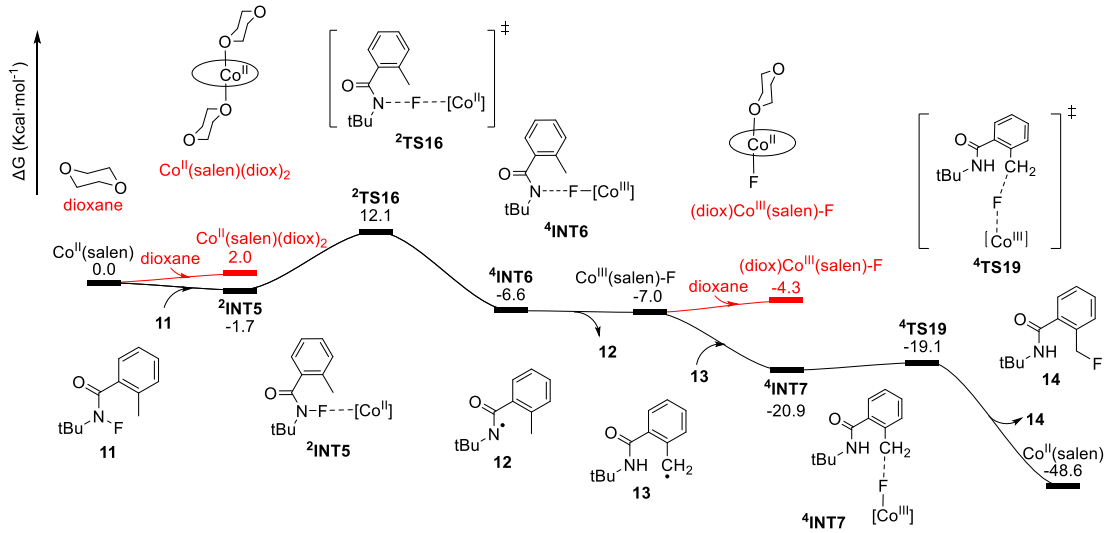


Fig. S11. Optimized structure of benzenium ion **8**.



Co(salen) species	singlet	doublet	triplet	quartet	quintet
Co^{II}(salen)(diox)$_2$	—	0.0	—	5.3	—
(diox)Co^{III}(salen)-F	0.0	—	2.1	—	6.4

Fig. S12. Relative free energy diagram of the axial coordinated Co(salen) species by solvent 1,4-dioxane.

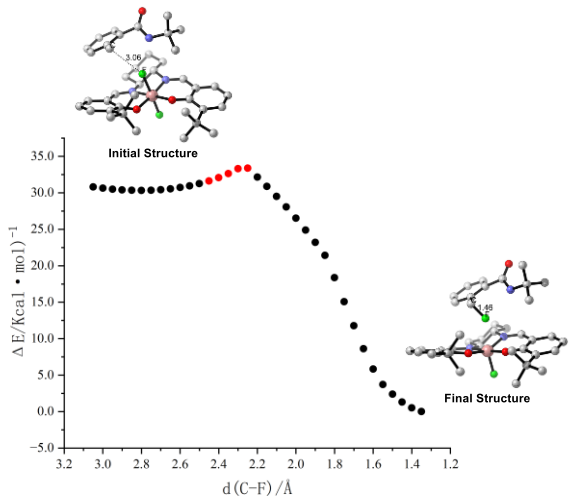


Fig. S13. IRC path scan for the process of fluorine atom abstraction from Co^{IV}(salen)-F_2 by benzyl radical **13** in the liquid phase. The results indicate a significantly low energy barrier at the saddle point for this reaction.

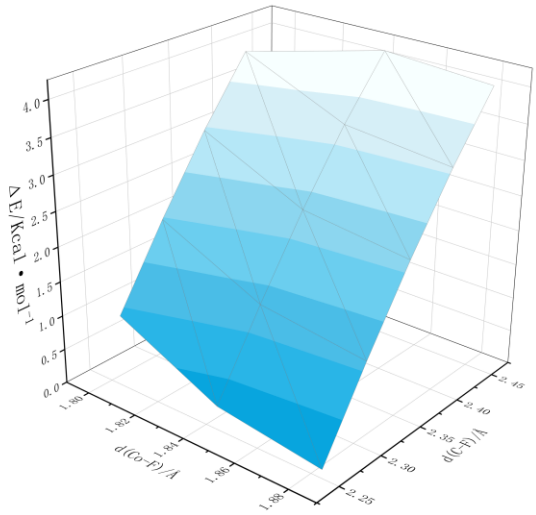


Fig. S14. 2D-RPES scan conducted on the red path segment shown in Fig. S13. The computational results indicate that although a transition state structure with a very small vibrational frequency may exist for this process, its thermodynamic and kinetic contributions can be considered negligible.

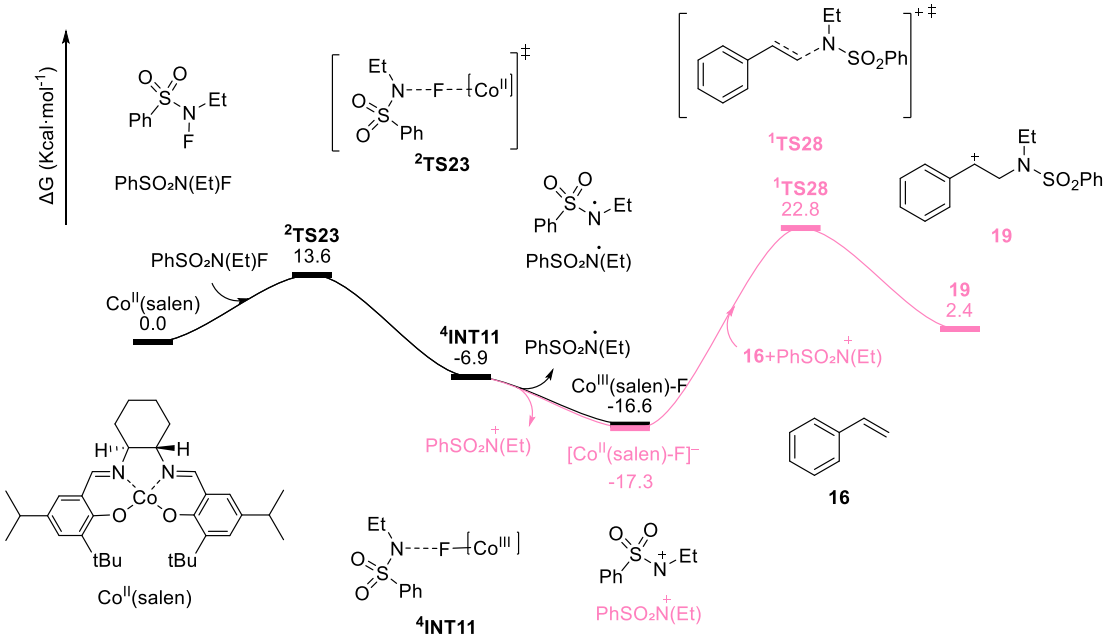


Fig. S15. Free energy profile for the ionic reaction pathway of Co^{II}(salen)-catalyzed fluorination of styrene **16**.

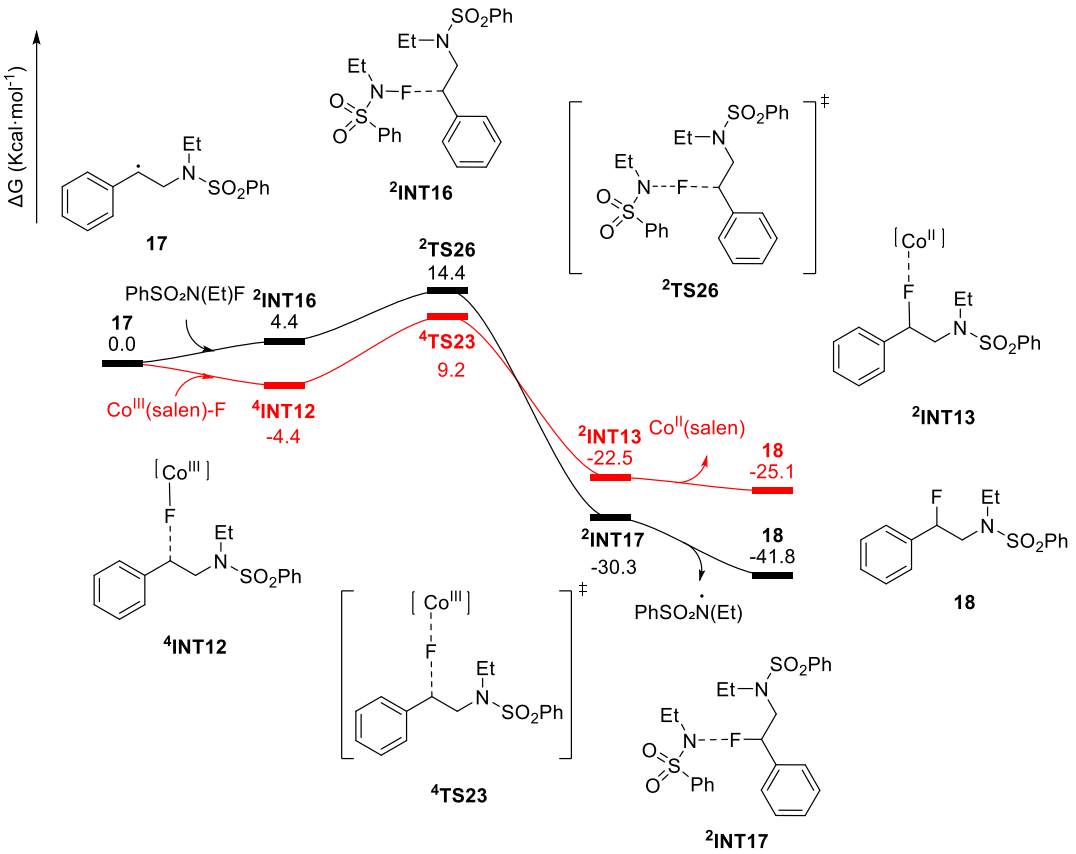


Fig. S16. Free energy profile for the two fluorination reaction pathways of benzyl radical **17**.

Table S1. The relative free energies of Co^{II}(salen), $[Co^{IV}(salen)\text{-}F]^+$, $[Co^{IV}(salen)\text{-}alkyl]^+$ and $Co^{IV}(salen)\text{-}F_2$ on each spin state.

Co(salen) species	doublet	quartet	sextet
Co^{II}(salen)	0.0	4.1	-
$[Co^{IV}(salen)\text{-}F]^+$	1.9	0.0	1.1
$[Co^{IV}(salen)\text{-}alkyl]^+$	0.0	7.6	18.9
$Co^{IV}(salen)\text{-}F_2$	0.0	15.9	14.3

Table S2. The relative free energies of $[Co^{III}(salen)]^+$, Co^{III}(salen)-F, Co^{III}(salen)-H and Co^{III}(salen)-alkyl on each spin state.

Co(salen) species	singlet	triplet	quintet
$[Co^{III}(salen)]^+$	16.5	0.0	8.7
Co^{III}(salen)-F	7.4	0.0	2.0
Co^{III}(salen)-H	0.0	14.0	24.8
Co^{III}(salen)-alkyl	0.0	6.6	10.9

Table S3. Dissociation energies of fluorinating reagents $Me_3NFPy{\cdot}BF_4$, $Me_3NFPy{\cdot}OTf$ and $Me_3NFPy{\cdot}PF_6$.

	ΔG / Kcal·mol^{-1}
$Me_3NFPy{\cdot}BF_4 \rightarrow Me_3NFPy^+ + BF_4^-$	-0.9
$Me_3NFPy{\cdot}OTf \rightarrow Me_3NFPy^+ + OTf^-$	-3.3
$Me_3NFPy{\cdot}PF_6 \rightarrow Me_3NFPy^+ + PF_6^-$	-3.1

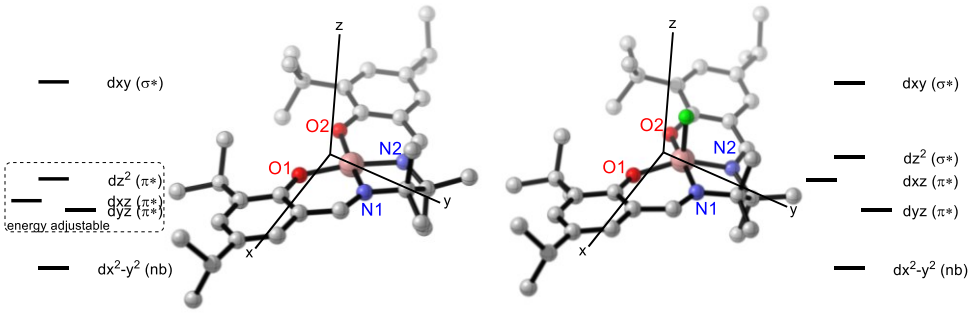
Table S4. The NBO charges on the counterpart of two different fluorinating reagents and on the Co(salen)-F.

Intermediate	^{2}TS1	^{2}INT1	6th point	Final point at doublet/quartet
Me_3NPy	1.01	0.69	0.01	0.01 / 0.00
$[Co^{IV}(salen)\text{-}F]^+$	-0.01	0.31	0.99	0.99 / 1.00
	^{2}TS21	**^{4}INT11**	6th point	Final point
$PhSO_2N(Et)\cdot$	0.10	-0.01	-0.03	-0.02
Co^{III}(salen)-F	-0.10	0.01	0.03	0.02

Table S5. The spin densities on the counterpart of two different fluorinating reagents and on the Co(salen)-F.

Intermediate	^{2}TS1	Final point of ^{2,4}INT1	^{2}TS21	Final point of ^{4}INT11
Me_3NPy	-0.16	0.00 / 0.00	-	-
$PhSO_2N(Et)\cdot$	-	-	-0.32	1.00
Co(salen)-F	1.16	1.00 / 3.00	1.32	2.00

Table S6. Electronic populations and spin densities on d-orbital of Co atom in each Co(salen) species, and geometrical parameters as well.



Geometrical parameters	Co^{II}(salen)	$[Co^{III}(salen)]^+$	Co^{III}(salen)-F	$[Co^{IV}(salen)-F]^+$
d(Co–O1/Co–O2)	1.87/1.87	1.86/1.86	1.87/1.87	1.85/1.91
d(Co–N1/Co–N2)	1.88/1.88	1.88/1.88	1.92/1.93	1.89/1.96
d(Co–F)	–	–	1.87	1.84
∠(N1–Co–O2)	170.03	173.46	173.36	175.08
∠(N2–Co–O1)	170.02	173.46	149.36	143.32
D(O1–N1–N2–O2)	13.58	8.92	16.35	21.51
Electron populations / spin densities on *d*-orbital of Co	Co^{II}(salen)	$[Co^{III}(salen)]^+$	Co^{III}(salen)-F	$[Co^{IV}(salen)-F]^+$
dxy	0.75/0.04	0.83/0.09	0.96/0.17	0.97/0.17
dz^2	1.66/0.29	1.08/0.90	1.23/0.71	1.30/0.61
dxz	1.37/0.61	1.64/0.35	1.36/0.62	1.51/0.46
dyz	1.87/0.04	1.94/0.01	1.83/0.12	1.59/0.38
dx^2-y^2	1.97/0.01	1.97/0.02	1.91/0.07	1.94/0.04

Table S7. Total charges and spin densities of selected atom and salen moiety in Co^{II}(salen), $[Co^{III}(salen)]^+$, Co^{III}(salen)-F, and $[Co^{IV}(salen)-F]^+$

Total charges / spin densities	Co	salen	F	O1	O2	N1	N2
Co^{II}(salen)	0.74 / 1.00	-0.74 / 0.00	–	-0.64 / 0.01	-0.64 / 0.01	-0.44 / 0.00	-0.44 / 0.00
$[Co^{III}(salen)]^+$	0.96 / 1.40	0.04 / 0.60	–	-0.57 / 0.13	-0.57 / 0.13	-0.42 / 0.04	-0.42 / 0.04
Co^{III}(salen)-F	0.94 / 1.69	-0.30 / 0.13	-0.64 / 0.18	-0.60 / 0.09	-0.57 / 0.00	-0.38 / -0.02	-0.43 / 0.03
$[Co^{IV}(salen)-F]^+$	0.94 / 1.66	0.65 / 1.14	-0.59 / 0.20	-0.56 / 0.15	-0.46 / 0.23	-0.36 / -0.04	-0.39 / 0.10

Table S8. Electronic potential energies and correction to zero point energies, thermal energies, enthalpies, free energies (in Hartree) and imaginary frequencies (cm^{-1}) of optimized structures calculated at the B3LYP-D3/Def2-TZVP (SMD-custom solvent-dielectric constantε=9.2) // B3LYP-D3/Def2-SVP (SMD-custom solvent-dielectric constantε=9.2).

Structure	$E_{0,Def2\text{-}TZVP}$	$E_{0,Def2\text{-}SVP}$	$cZPE_{298}$	cU_{298}	cH_{298}	cG_{298}	G	Imaginary Frequency
Co^{II}(salen)	-2969.355771	-2967.448958	0.775097	0.816557	0.817502	0.703364	-2968.652407	
R_3Si-H	-815.3897199	-814.8970932	0.168236	0.181054	0.181999	0.128373	-815.2613469	
R_3Si·	-814.7318677	-814.2407919	0.159001	0.17174	0.172684	0.118596	-814.6132717	
Co^{III}(salen)-H	-2969.925553	-2968.016821	0.784083	0.825458	0.826403	0.71384	-2969.211713	
$[Me_3NFPy]^{+\cdot}$	-466.0403106	-465.5193171	0.1749	0.18526	0.186204	0.137308	-465.9030026	
^{2}TS1	-3435.402013	-3432.982817	0.950239	1.003332	1.004276	0.864855	-3434.537158	-1027.855
^{2}INT1	-3435.435383	-3433.015859	0.950656	1.004609	1.005553	0.863597	-3434.571786	
Co^{III}(salen)-F	-3069.243091	-3067.210232	0.777709	0.820603	0.821547	0.704169	-3068.538922	
$[Me_3NPy]^+$	-366.1474339	-365.7493791	0.16861	0.178719	0.179663	0.131463	-366.0159709	
$[Co^{IV}$(salen)-F$]^+$	-3069.039208	-3067.008004	0.778337	0.821361	0.822305	0.704395	-3068.334813	
Me_3NPy	-366.3971434	-365.9957758	0.169846	0.179568	0.180512	0.133392	-366.2637514	
^{4}TS2	-3884.416	-3881.903041	0.944827	1.001741	1.002685	0.854235	-3883.561765	-1029.32
$[Co^{III}$(salen)$]^+$	-2969.174484	-2967.269191	0.776377	0.817808	0.818752	0.704201	-2968.470283	
HF	-100.4955729	-100.3578482	0.009194	0.011555	0.012499	-0.007224	-100.5027969	
R_3Si^+	-814.5849497	-814.0951108	0.16035	0.173011	0.173955	0.121171	-814.4637787	
1	-578.2462855	-577.6031919	0.225743	0.239159	0.240104	0.184329	-578.0619565	
2	-578.0365885	-577.3968095	0.226578	0.239947	0.240891	0.185411	-577.8511775	
^{3}TS3	-3548.14989	-3545.607713	1.00511	1.062081	1.063025	0.913161	-3547.236729	-671.1828
3	-578.815709	-578.1730367	0.233809	0.248274	0.249218	0.190164	-578.625545	

^{2}TS4	-1393.409248	-1392.282047	0.394674	0.421354	0.422298	0.336346	-1393.072902	-653.9432
^{4}TS5	-3648.065193	-3645.40229	1.011468	1.070245	1.07119	0.918347	-3647.146846	-181.9567
4	-678.7708369	-678.0040887	0.241682	0.256265	0.25721	0.19883	-678.5720069	
^{1}INT2	-466.9196425	-466.386344	0.182632	0.194419	0.195363	0.142662	-466.7769805	
^{2}TS6	-1281.651613	-1280.640047	0.343345	0.368157	0.369102	0.285867	-1281.365746	-110.8474
R_3Si-F	-914.7601416	-914.1365615	0.163016	0.176706	0.177651	0.121402	-914.6387396	
Me_3NHPy	-366.954612	-366.5546701	0.179052	0.189431	0.190375	0.14235	-366.812262	
^{2}TS7	-945.1746391	-944.1353108	0.401107	0.425699	0.426643	0.340752	-944.8338871	-2186.2055
^{1}TS8	-3336.329134	-3334.027538	0.954152	1.005844	1.006788	0.871725	-3335.457409	-876.9353
5	-578.6539964	-578.0137202	0.238554	0.251902	0.252846	0.199212	-578.4547844	
BF_4^-	-424.8200414	-424.2828807	0.014417	0.01876	0.019704	-0.013172	-424.8332134	
^{1}INT3	-1003.493094	-1002.328227	0.254192	0.273796	0.27474	0.204748	-1003.288346	
^{1}TS12	-1003.48464	-1002.319426	0.253125	0.272186	0.27313	0.203705	-1003.280935	-168.1318
^{1}INT4	-1003.496243	-1002.33689	0.255244	0.274913	0.275857	0.203272	-1003.292971	
BF_3	-324.7168659	-324.316148	0.012329	0.015842	0.016787	-0.01383	-324.7306959	
^{3}TS10	-3548.188335	-3545.649141	1.013328	1.068913	1.069857	0.926881	-3547.261454	-102.4296
Co^{III}(salen)-alkyl	-3548.210627	-3545.673227	1.017241	1.072178	1.073122	0.933807	-3547.27682	
$[Co^{IV}$(salen)-alkyl$]^+$	-3548.033926	-3545.496585	1.017647	1.072893	1.073837	0.933289	-3547.100637	
^{2}TS11	-3972.861931	-3969.805261	1.030534	1.091944	1.092888	0.936922	-3971.925009	-128.7074
^{1}TS13	-1003.475912	-1002.31114	0.253401	0.27241	0.273354	0.204151	-1003.271761	-297.1565
6	-657.4746866	-656.747797	0.290394	0.307199	0.308143	0.24561	-657.2290766	
7	-657.4746866	-656.747797	0.290394	0.307199	0.308143	0.24561	-657.2290766	
8	-657.3208869	-656.5964782	0.293532	0.310175	0.311119	0.250285	-657.0706019	
^{1}TS14	-1082.147708	-1080.900272	0.309116	0.330874	0.331818	0.257403	-1081.890305	-172.5981

9	-757.4302491	-756.5794404	0.297907	0.314984	0.315928	0.253591	-757.1766581	
^{1}TS15	-1082.159901	-1080.912003	0.308595	0.330358	0.331302	0.256887	-1081.903014	-101.3973
10	-757.4367735	-756.5855644	0.297393	0.314584	0.315529	0.252737	-757.1840365	
OTf^{-}	-961.9405676	-961.0324882	0.027136	0.034336	0.03528	-0.005538	-961.9461056	
^{1}TS27	-1540.571471	-1539.038142	0.266237	0.288231	0.289175	0.212942	-1540.358529	-232.5095
CF_2SO_3	-861.7866824	-861.0106925	0.022654	0.029874	0.030818	-0.01092	-861.7976024	
PF_6^{-}	-941.1008284	-940.1828738	0.01932	0.025444	0.026388	-0.007914	-941.1087424	
^{1}TS28	-1519.760249	-1518.215947	0.25816	0.279014	0.279959	0.206577	-1519.553672	-173.4015
PF_5	-840.9920903	-840.1998001	0.01633	0.021926	0.02287	-0.013587	-841.0056773	

Calculated by M06 functional at the same level of basis sets.

Co^{II}(salen)	-2967.975825	-2966.069115	0.769331	0.810999	0.811943	0.697512	-2967.278313	
R_3Si-H	-815.1294902	-814.641064	0.167544	0.180298	0.181243	0.128757	-815.0007332	
$R_3Si\cdot$	-814.4708732	-813.9848705	0.158287	0.170926	0.17187	0.119083	-814.3517902	
Co^{III}(salen)-H	-2968.539269	-2966.630579	0.777718	0.819407	0.820352	0.70701	-2967.832259	
$[Me_3NFPy]^{+\cdot}$	-465.6997583	-465.1815921	0.174389	0.184493	0.185437	0.139363	-465.5603953	
^{2}TS1	-3433.679871	-3431.262867	0.942827	0.995944	0.996888	0.858879	-3432.820992	-1157.744
^{2}INT1	-3433.710663	-3431.293358	0.94262	0.996651	0.997595	0.856708	-3432.853955	
Co^{III}(salen)-F	-3067.827214	-3065.801668	0.771887	0.815007	0.815951	0.697457	-3067.129757	
$[Me_3NPy]^{+}$	-365.8394536	-365.4405407	0.167737	0.177744	0.178688	0.131641	-365.7078126	
$[Co^{IV}$(salen)-F$]^{+}$	-3067.621989	-3065.595926	0.772089	0.815284	0.816228	0.698594	-3066.923395	
Me_3NPy	-366.0909465	-365.6924382	0.168952	0.178688	0.179632	0.13321	-365.9577365	
$[Co^{III}$(salen)$]^{+}$	-2967.788357	-2965.882652	0.769587	0.810544	0.811488	0.698112	-2967.090245	
HF	-100.4599744	-100.3304276	0.009499	0.01186	0.012804	-0.006905	-100.4668794	
^{1}INT2	-466.5736609	-466.0509059	0.182266	0.194023	0.194968	0.143431	-466.4302299	

^{2}TS6	-1281.049723	-1280.048821	0.338859	0.363724	0.364668	0.283323	-1280.7664	-652.5723
R_3Si-F	-914.4676185	-913.8551759	0.162441	0.176004	0.176949	0.122564	-914.3450545	
Me_3NHPy	-366.6455248	-366.2481817	0.177838	0.188462	0.189406	0.140583	-366.5049418	
^{1}TS8	-3334.645372	-3332.341905	0.946525	0.998227	0.999172	0.865503	-3333.779869	-460.5247
1	-577.8072609	-577.1708119	0.224554	0.238038	0.238982	0.183357	-577.6239039	
^{3}TS9	-3546.33425	-3543.794575	0.996996	1.054021	1.054965	0.907765	-3545.426485	-573.9224
3	-578.3757076	-577.739827	0.232879	0.247309	0.248253	0.189911	-578.1857966	

Table S9. Electronic potential energies and correction to zero point energies, thermal energies, enthalpies, free energies (in Hartree) and imaginary frequencies (cm^{-1}) of optimized structures calculated at the B3LYP-D3/Def2-TZVP (SMD-1,4-Dioxane) // B3LYP-D3/Def2-SVP (SMD-1,4-Dioxane).

Structure	$E_{0,Def2\text{-}TZVP}$	$E_{0,Def2\text{-}SVP}$	$cZPE_{298}$	cU_{298}	cH_{298}	cG_{298}	G	Imaginary Frequency
Co^{II}(salen)	-2732.159806	-2730.5125	0.590773	0.621168	0.622113	0.531878	-2731.6279	
11	-696.9866456	-696.20919	0.258095	0.273225	0.274169	0.216334	-696.77031	
^{2}INT5	-3429.171972	-3426.7572	0.850577	0.898041	0.898985	0.77105	-3428.4009	
^{2}TS16	-3429.152362	-3426.7386	0.849395	0.896021	0.896965	0.773427	-3428.3789	-818.7907
^{4}INT6	-3429.178047	-3426.7614	0.848756	0.896396	0.897341	0.769272	-3428.4088	
Co^{III}(salen)-F	-2832.044091	-2830.2692	0.592726	0.624785	0.625729	0.53128	-2831.5128	
12	-597.109084	-596.4533	0.253767	0.267819	0.268764	0.212452	-596.89663	
$[Co^{IV}$(salen)-F$]^{+}$	-2831.8249	-2830.0521	0.592577	0.624817	0.625761	0.530742	-2831.2942	
15	-597.2407079	-596.5778	0.253691	0.267227	0.268171	0.213764	-597.02694	
^{2}TS17	-597.0918202	-596.43745	0.248651	0.262038	0.262982	0.208647	-596.88317	-1581.2896
13	-597.1347618	-596.47899	0.254306	0.268186	0.26913	0.21377	-596.92099	
^{2}TS18	-1294.115629	-1292.686775	0.51284	0.543277	0.544221	0.451721	-1293.663908	-653.8867
14	-697.0676339	-696.28874	0.261194	0.275867	0.276811	0.219855	-696.84778	
^{4}INT7	-3429.198115	-3426.7835	0.847641	0.895718	0.896662	0.766544	-3428.4316	
^{4}TS19	-3429.195302	-3426.7822	0.847014	0.894627	0.895571	0.766683	-3428.4286	-227.7637
^{2}INT8	-3429.250187	-3426.8364	0.853869	0.900618	0.901563	0.776548	-3428.4736	
^{3}INT9	-3529.057304	-3526.5141	0.853172	0.902046	0.90299	0.771794	-3528.2855	
^{3}TS20	-3529.01956	-3526.4795	0.851691	0.89956	0.900504	0.774736	-3528.2448	-1017.3779
^{3}INT10	-3529.055441	-3526.5136	0.851676	0.900139	0.901083	0.773053	-3528.2824	
Co^{IV}(salen)-F_2	-2931.918199	-2930.017	0.595911	0.628705	0.62965	0.535183	-2931.383	

Calculated by M06 functional at the same level of basis sets.

Co^{II}(salen)	-2730.995714	-2729.350531	0.586602	0.617133	0.618077	0.527802	-2730.467912	
11	-696.4805526	-695.7120544	0.256381	0.271721	0.272665	0.214318	-696.2662346	

^{2}INT5	-3427.513044	-3425.104474	0.84509	0.892008	0.892952	0.769344	-3426.7437	
^{2}TS16	-3427.486995	-3425.080039	0.842894	0.889424	0.890368	0.768249	-3426.718746	-800.9167
^{4}INT6	-3427.517322	-3425.109219	0.842549	0.889881	0.890826	0.765261	-3426.752061	
Co^{III}(salen)-F	-2830.844561	-2829.079085	0.588712	0.620744	0.621688	0.52809	-2830.316471	
12	-596.6386999	-595.9867659	0.252143	0.266235	0.267179	0.211168	-596.4275319	
$[Co^{IV}$(salen)-F$]^{+}$	-2830.623664	-2828.857333	0.588776	0.620863	0.621807	0.528038	-2830.095626	
15	-596.7707289	-596.1151759	0.251995	0.265709	0.266653	0.212215	-596.5585139	
^{2}TS17	-596.6165831	-595.9670901	0.246766	0.260304	0.261249	0.206739	-596.4098441	-2075.836
13	-596.6618909	-596.0115326	0.25207	0.266203	0.267147	0.211175	-596.4507159	
^{2}TS18	-1293.138633	-1291.721106	0.509319	0.539592	0.540536	0.449663	-1292.68897	-747.7865
14	-696.5629479	-695.7948502	0.259754	0.274506	0.27545	0.21844	-696.3445079	

Table S10. Electronic potential energies and correction to zero point energies, thermal energies, enthalpies, free energies (in Hartree) and imaginary frequencies (cm^{-1}) of optimized structures calculated at the B3LYP-D3/Def2-TZVP (SMD-EthylEthanoate) // B3LYP-D3/Def2-SVP (SMD-EthylEthanoate).

Structure	$E_{0,Def2\text{-}TZVP}$	$E_{0,Def2\text{-}SVP}$	$cZPE_{298}$	cU_{298}	cH_{298}	cG_{298}	G	Imaginary Frequency
Co^{II}(salen)	-2968.166499	-2966.2636	0.757507	0.796733	0.797677	0.688119	-2967.47838	
$PhSO_2N(Et)F$	-1014.319944	-1013.4194	0.174622	0.187109	0.188053	0.13501	-1014.184934	
^{2}TS21	-3982.486953	-3979.6974	0.93184	0.985047	0.985991	0.845297	-3981.641656	-1230.6473
^{4}INT11	-3982.516738	-3979.7237	0.931434	0.985575	0.986519	0.842483	-3981.674255	
Co^{III}(salen)-F	-3068.056275	-3066.0246	0.759555	0.800428	0.801372	0.687742	-3067.368533	
$PhSO_2N\cdot(Et)$	-914.449467	-913.67166	0.169173	0.181152	0.182096	0.128163	-914.321304	
$[Co^{IV}$(salen)-F$]^+$	-3067.858145	-3065.8278	0.760453	0.801418	0.802363	0.688483	-3067.169662	
$PhSO_2N^-(Et)$	-914.6067209	-913.8172	0.169836	0.181405	0.182349	0.13023	-914.4764909	
16	-309.7824519	-309.44595	0.133345	0.140027	0.140971	0.102262	-309.6801899	
^{2}TS22	-1224.23397	-1223.1268	0.305388	0.32424	0.325184	0.25534	-1223.97863	-218.3675
17	-1224.271627	-1223.1697	0.308611	0.327142	0.328086	0.259188	-1224.012439	
^{4}INT12	-4292.362046	-4289.2442	1.070189	1.131249	1.132193	0.974114	-4291.387932	
^{4}TS23	-4292.335815	-4289.2196	1.067009	1.128343	1.129287	0.969593	-4291.366222	-284.7155
^{2}INT13	-4292.394608	-4289.2805	1.073752	1.134184	1.135128	0.977878	-4291.41673	
18	-1324.206971	-1322.9809	0.314632	0.333984	0.334928	0.26433	-1323.942641	
^{3}INT14	-4082.399036	-4079.4796	0.935968	0.99123	0.992174	0.846133	-4081.552903	
^{3}TS24	-4082.36688	-4079.4491	0.933932	0.988398	0.989342	0.847312	-4081.519568	-1067.0276
^{3}INT15	-4082.404537	-4079.4843	0.933968	0.9889	0.989845	0.847482	-4081.557055	
Co^{IV}(salen)-F_2	-3167.937074	-3165.7785	0.762205	0.804066	0.80501	0.690608	-3167.246466	
$[Co^{II}$(salen)-F$]^-$	-3068.191823	-3066.1559	0.755391	0.797244	0.798188	0.681608	-3067.510215	

$PhSO_2N^+(Et)$	-914.3143504	-913.54261	0.172232	0.183882	0.184826	0.133718	-914.1806324	
^{1}TS25	-1224.055307	-1222.953	0.306253	0.324992	0.325936	0.258434	-1223.796873	-268.187
19	-1224.091251	-1222.99	0.310598	0.328911	0.329855	0.261841	-1223.82941	
^{2}INT16	-2238.605016	-2236.6106	0.484655	0.517779	0.518723	0.41466	-2238.190356	
^{2}TS26	-2238.587333	-2236.5911	0.482974	0.515821	0.516765	0.412977	-2238.174356	-715.9695
^{2}INT17	-2238.661552	-2236.6677	0.485963	0.518904	0.519848	0.415851	-2238.245701	

Cartesian Coordinates of optimized Structures

Structure S1. Co^{II}(salen)

27	0.000043	0.899119	0.000415
8	-1.295777	-0.451937	0.099498
8	1.295745	-0.452032	-0.098749
7	-1.269198	2.274077	-0.225661
7	1.269362	2.274048	0.226074
6	-2.589105	-0.377307	0.046823
6	-3.384380	-1.574716	0.203296
6	-4.765495	-1.456399	0.116838
1	-5.374318	-2.353989	0.225741
6	-5.452511	-0.233836	-0.105887
6	-4.688688	0.908875	-0.235050
1	-5.176430	1.875685	-0.398612
6	-3.271026	0.868713	-0.160041
6	-2.558137	2.107961	-0.285474
1	-3.191063	2.988263	-0.449565
6	2.558335	2.107960	0.285128
1	3.191364	2.988286	0.448686
6	3.271141	0.868663	0.159584
6	4.688836	0.908814	0.233920
1	5.176675	1.875659	0.396979
6	5.452579	-0.233955	0.104752
6	4.765438	-1.456566	-0.117285
1	5.374187	-2.354208	-0.226174
6	3.384277	-1.574865	-0.203098
6	2.589106	-0.377396	-0.046645
6	-2.696070	-2.929109	0.464425
6	-1.896627	-2.853908	1.787223
1	-2.573027	-2.660211	2.636122
1	-1.144555	-2.056819	1.747565
1	-1.379797	-3.809640	1.974944
6	-1.746468	-3.273177	-0.706987
1	-0.964162	-2.514278	-0.815846
1	-2.309507	-3.343708	-1.652470
1	-1.260189	-4.246581	-0.528431
6	-3.711917	-4.078908	0.597022
1	-4.303047	-4.216707	-0.322445
1	-4.410200	-3.922005	1.434580
1	-3.173738	-5.020786	0.787979
6	2.695785	-2.929282	-0.463607
6	3.711482	-4.079226	-0.596155
1	4.302957	-4.216716	0.323137
1	4.409454	-3.922721	-1.434045
1	3.173145	-5.021130	-0.786539
6	1.746465	-3.272943	0.708159
1	0.964252	-2.513949	0.817054
1	2.309771	-3.343273	1.653498
1	1.260064	-4.246358	0.529995
6	1.896013	-2.854339	-1.786218
1	2.572249	-2.661100	-2.635352
1	1.144159	-2.057038	-1.746642
1	1.378882	-3.809996	-1.973485
6	0.642865	3.606630	0.457258
6	-0.642680	3.606686	-0.456718
6	1.582802	4.774522	0.126520
1	1.029743	5.723091	0.141519
1	2.380561	4.864987	0.877671
1	2.051339	4.663650	-0.861059
6	0.258970	3.669290	1.949505
1	1.153843	3.490799	2.563870
1	-0.145599	4.656309	2.214655
1	-0.487608	2.900756	2.197320
6	-1.582636	4.774528	-0.125815
1	-2.051449	4.663271	0.861589
1	-1.029516	5.723070	-0.140295
1	-2.380188	4.865352	-0.877134
6	-0.258754	3.669530	-1.948934
1	-1.153655	3.491351	-2.563352
1	0.146045	4.656502	-2.213914
1	0.487649	2.900855	-2.196842
6	6.971465	-0.199945	0.192589
6	7.633351	-0.656000	-1.118897
6	7.493659	-1.017587	1.386435
1	7.260486	0.852440	0.360563
1	7.290200	-0.047628	-1.970642
1	8.730862	-0.571792	-1.055771
1	7.393747	-1.709343	-1.340789
1	7.051088	-0.667835	2.332561
1	7.245960	-2.086461	1.275224
1	8.590225	-0.937693	1.468964
6	-6.971357	-0.199825	-0.194399
6	-7.633810	-0.655381	1.116976
6	-7.493061	-1.017900	-1.388161
1	-7.260282	0.852503	-0.362886
1	-7.291030	-0.046681	1.968636

1	-8.731295	-0.571205	1.053343
1	-7.394291	-1.708637	1.339372
1	-7.050042	-0.668546	-2.334225
1	-7.245484	-2.086747	-1.276425
1	-8.589585	-0.937970	-1.471215

Structure S2. R_3Si-H

8	-0.001767	-0.467554	0.067426
14	-1.588815	-0.043556	0.372826
1	-1.784068	0.015626	1.857044
14	1.593123	-0.080037	0.379936
1	1.808930	-0.133872	1.861401
6	-1.955516	1.642158	-0.371186
1	-3.006063	1.927795	-0.194497
1	-1.311422	2.420795	0.068901
1	-1.782129	1.630294	-1.460158
6	-2.689370	-1.372214	-0.360229
1	-2.453700	-2.360587	0.066568
1	-3.751320	-1.154484	-0.157888
1	-2.553229	-1.428505	-1.453013
6	1.967141	1.653732	-0.240139
1	1.772838	1.728042	-1.323080
1	1.342069	2.403665	0.271556
1	3.024423	1.912987	-0.062900
6	2.670862	-1.359693	-0.465499
1	3.737166	-1.169037	-0.258748
1	2.428727	-2.375469	-0.113162
1	2.522893	-1.330414	-1.557787

Structure S3. $R_3Si\cdot$

8	0.025930	-0.490578	-0.146968
14	1.614192	-0.043154	-0.445112
14	-1.578897	-0.081125	-0.390099
1	-1.856401	-0.129440	-1.860388
6	1.948057	1.648842	0.336417
1	3.006244	1.931106	0.212236
1	1.324359	2.437182	-0.113525
1	1.723001	1.607055	1.417761
6	2.715421	-1.365602	0.333719
1	2.512763	-2.360763	-0.092422
1	3.780069	-1.128775	0.176117
1	2.525740	-1.410188	1.421615
6	-1.904604	1.655104	0.249164
1	-1.656931	1.726447	1.321310
1	-1.297937	2.399150	-0.292174
1	-2.966733	1.924600	0.123790
6	-2.631977	-1.352348	0.497766
1	-3.704027	-1.152867	0.333110
1	-2.412089	-2.369675	0.135509
1	-2.441009	-1.325270	1.583366

Structure S4. Co^{III}(salen)-H

27	0.015233	0.896376	-0.002968
8	1.290640	-0.469940	0.194122
8	-1.282491	-0.452505	0.127516
7	1.286938	2.271078	0.242637
7	-1.253065	2.281318	-0.177873
6	2.579301	-0.392754	0.077869
6	3.360269	-1.596045	-0.105264
6	4.743929	-1.477794	-0.138012
1	5.341200	-2.380137	-0.269431
6	5.447248	-0.250147	-0.022251
6	4.695017	0.900200	0.110048
1	5.192904	1.872629	0.185732
6	3.276739	0.859773	0.147002
6	2.573329	2.101691	0.291367
1	3.209275	2.977887	0.466366
6	-2.534085	2.106866	-0.300657
1	-3.163647	2.987131	-0.477988
6	-3.247249	0.865027	-0.216408
6	-4.659821	0.906260	-0.352380
1	-5.137859	1.871093	-0.551889
6	-5.430856	-0.232623	-0.233595
6	-4.755257	-1.448402	0.049581
1	-5.369903	-2.341755	0.159634
6	-3.378928	-1.567757	0.194873
6	-2.573135	-0.377380	0.031600
6	2.653376	-2.949237	-0.313964
6	1.784894	-2.858212	-1.591859
1	2.420746	-2.687579	-2.476100
1	1.060447	-2.038046	-1.517090
1	1.229716	-3.797890	-1.746200
6	1.769715	-3.296750	0.906356
1	0.988351	-2.544066	1.054628
1	2.382479	-3.359919	1.821056

1	1.284004	-4.275152	0.755488
6	3.654355	-4.103342	-0.508108
1	4.298642	-4.244289	0.374584
1	4.302078	-3.949790	-1.385790
1	3.101145	-5.042403	-0.667358
6	-2.712509	-2.916319	0.531131
6	-3.741812	-4.052434	0.676995
1	-4.303332	-4.224556	-0.255100
1	-4.465912	-3.856729	1.483933
1	-3.217359	-4.989038	0.923793
6	-1.729142	-3.311383	-0.593412
1	-0.942489	-2.558918	-0.706122
1	-2.260902	-3.418239	-1.553426
1	-1.251118	-4.277306	-0.360259
6	-1.954208	-2.794602	1.874430
1	-2.653814	-2.558079	2.693137
1	-1.191451	-2.008396	1.824750
1	-1.455101	-3.747230	2.117567
6	-0.638208	3.627681	-0.356778
6	0.661663	3.592185	0.532037
6	-1.585008	4.762997	0.063278
1	-1.037915	5.713652	0.117393
1	-2.385440	4.904317	-0.676953
1	-2.049650	4.574823	1.040827
6	-0.285180	3.791077	-1.848390
1	-1.184767	3.616760	-2.457089
1	0.076256	4.807765	-2.057755
1	0.482646	3.067584	-2.153987
6	1.595319	4.773224	0.232331
1	2.050039	4.699509	-0.764998
1	1.039892	5.718854	0.289329
1	2.402643	4.838438	0.975761
6	0.303049	3.594178	2.032818
1	1.207599	3.390153	2.624469
1	-0.097274	4.568790	2.345594
1	-0.440370	2.816006	2.260562
6	-6.944483	-0.199688	-0.385694
6	-7.660903	-0.616745	0.910115
6	-7.418247	-1.051439	-1.575795
1	-7.223896	0.847648	-0.595992
1	-7.351628	0.015587	1.757377
1	-8.754645	-0.533021	0.799311
1	-7.433224	-1.663528	1.171888
1	-6.936168	-0.729923	-2.512558
1	-7.177632	-2.116807	-1.423156
1	-8.510266	-0.973013	-1.705900
6	6.968047	-0.216839	-0.061362
6	7.518197	-0.712444	-1.409831
6	7.588506	-1.000211	1.107997
1	7.269532	0.839482	0.050591
1	7.104804	-0.128439	-2.247292
1	8.617127	-0.628794	-1.441105
1	7.261075	-1.771276	-1.579846
1	7.226534	-0.622301	2.077257
1	7.333314	-2.071464	1.049100
1	8.688045	-0.919839	1.096075
1	0.168142	0.888796	-1.415555

Structure S5. $[Me_3NFPy]^+$

6	-0.374367	1.218618	-0.001711
6	1.014626	1.206500	-0.010826
6	1.736327	0.000463	-0.013545
6	1.015126	-1.205904	-0.010842
6	-0.373826	-1.218659	-0.001696
1	1.532896	2.166083	-0.017389
1	1.533873	-2.165230	-0.017435
6	3.234284	0.000419	0.009577
1	3.580444	-0.006509	1.057785
1	3.644460	-0.893709	-0.479991
1	3.644819	0.900350	-0.468778
6	-1.242221	-2.431750	0.000179
1	-1.896053	-2.437382	-0.885692
1	-0.620720	-3.334165	-0.001850
1	-1.891560	-2.437978	0.889256
6	-1.243333	2.431299	0.000153
1	-1.897997	2.436036	-0.885082
1	-1.891769	2.437816	0.889899
1	-0.622253	3.334005	-0.002975
7	-0.970328	-0.000150	0.003072
9	-2.324838	-0.000464	0.008113

Structure S6. ^{2}TS1

27	0.248001	1.215076	-0.476340
8	-0.982616	0.107793	-1.340042
8	1.540441	-0.074109	-0.863905
7	-0.982249	2.636733	-0.294727

7	1.465694	2.337180	0.430078	1	3.104486	-1.047331	-3.950611
6	-2.278398	0.170477	-1.285910	1	1.576110	-0.851924	-3.045103
6	-3.067755	-1.014825	-1.520769	1	1.882109	-2.345807	-3.967029
6	-4.451486	-0.885113	-1.514788	6	0.822245	3.530680	1.057440
1	-5.058597	-1.773477	-1.686830	6	-0.325209	3.929278	0.054642
6	-5.141857	0.332369	-1.277644	6	1.811784	4.684048	1.279312
6	-4.380898	1.453041	-1.010105	1	1.268968	5.596944	1.557901
1	-4.870038	2.406570	-0.787708	1	2.498079	4.463348	2.109328
6	-2.963423	1.392087	-0.979499	1	2.410233	4.897921	0.383382
6	-2.248676	2.567542	-0.583572	6	0.246624	3.089707	2.418021
1	-2.854051	3.477437	-0.496911	1	1.045862	2.635531	3.022570
6	2.732746	2.088329	0.597221	1	-0.151680	3.950400	2.972884
1	3.326000	2.798304	1.184689	1	-0.547897	2.344699	2.288465
6	3.466943	0.973126	0.081521	6	-1.302772	4.938604	0.671701
6	4.864073	0.924140	0.333167	1	-1.896529	4.497569	1.484158
1	5.318686	1.724986	0.924710	1	-0.752545	5.799216	1.074379
6	5.645852	-0.101674	-0.156946	1	-1.993202	5.334944	-0.086320
6	5.002636	-1.098596	-0.937067	6	0.255798	4.508831	-1.250447
1	5.630075	-1.895016	-1.336135	1	-0.546857	4.606834	-1.995897
6	3.643140	-1.119241	-1.221891	1	0.689560	5.504438	-1.083163
6	2.827759	-0.060873	-0.676704	1	1.031291	3.847649	-1.663709
6	-2.378014	-2.383109	-1.681093	6	7.142275	-0.169380	0.109077
6	-1.590658	-2.688678	-0.383162	6	7.959384	-0.075960	-1.190697
1	-2.279401	-2.773839	0.473781	6	7.521831	-1.425203	0.912208
1	-0.860482	-1.898706	-0.172870	1	7.399238	0.709185	0.726087
1	-1.050881	-3.644215	-0.477608	1	7.714162	0.840300	-1.750508
6	-1.422004	-2.373748	-2.895656	1	9.039944	-0.067767	-0.973433
1	-0.634958	-1.621977	-2.775989	1	7.760338	-0.936799	-1.850442
1	-1.979621	-2.159759	-3.822156	1	6.965994	-1.474375	1.861962
1	-0.943810	-3.360603	-3.007628	1	7.299904	-2.344062	0.344298
6	-3.392342	-3.522079	-1.891814	1	8.599400	-1.430757	1.144020
1	-3.985823	-3.381049	-2.808970	6	-6.662376	0.374203	-1.271730
1	-4.087619	-3.623079	-1.043362	6	-7.243229	-0.469411	-0.123483
1	-2.852278	-4.476670	-1.990205	6	-7.257001	-0.047072	-2.625612
6	3.012498	-2.218038	-2.099686	1	-6.954670	1.423421	-1.092460
6	4.060674	-3.228766	-2.600695	1	-6.844196	-0.143080	0.850300
1	4.550315	-3.763315	-1.771161	1	-8.341805	-0.385838	-0.090846
1	4.842053	-2.748629	-3.210658	1	-6.994431	-1.536505	-0.248617
1	3.565740	-3.982913	-3.232228	1	-6.865424	0.576877	-3.444352
6	1.954030	-2.999452	-1.289447	1	-7.016711	-1.097687	-2.858727
1	1.135154	-2.343361	-0.980402	1	-8.355086	0.047106	-2.616131
1	2.405990	-3.454452	-0.392734	6	-2.205272	-0.946702	2.798976
1	1.526505	-3.809249	-1.902828	6	-2.489704	-1.949422	3.726797
6	2.350895	-1.570271	-3.339481	6	-1.478486	-2.793509	4.215306

6	-0.165489	-2.596879	3.754998
6	0.127055	-1.597471	2.827770
1	-3.522616	-2.062931	4.059874
1	0.652151	-3.225095	4.111206
6	-1.797600	-3.898278	5.179310
1	-0.935162	-4.139594	5.816298
1	-2.657877	-3.643535	5.813959
1	-2.059801	-4.810024	4.615351
6	1.473628	-1.315615	2.247724
1	1.755717	-0.266735	2.422155
1	2.225896	-1.978780	2.689467
1	1.444523	-1.458418	1.158464
6	-3.215792	-0.028989	2.192067
1	-2.846521	1.004914	2.170607
1	-3.410819	-0.327112	1.150139
1	-4.155162	-0.079997	2.754997
7	-0.917451	-0.851243	2.438260
9	-0.584345	0.185778	1.336624

Structure S7. ^{2}INT1

27	0.298207	1.251358	-0.245436
8	-0.942363	0.234447	-1.183871
8	1.574156	0.008094	-0.797542
7	-0.836749	2.769881	-0.183793
7	1.590238	2.380870	0.564916
6	-2.237521	0.336848	-1.123533
6	-3.060183	-0.798715	-1.458158
6	-4.438177	-0.629523	-1.407395
1	-5.074857	-1.482288	-1.639605
6	-5.087409	0.583425	-1.057169
6	-4.291369	1.667664	-0.743762
1	-4.748424	2.620301	-0.460823
6	-2.877844	1.564535	-0.750482
6	-2.117253	2.722235	-0.394316
1	-2.691659	3.650472	-0.298601
6	2.838392	2.065924	0.741388
1	3.465905	2.767292	1.302641
6	3.521196	0.908695	0.249408
6	4.903325	0.778190	0.540225
1	5.379324	1.525245	1.182236
6	5.645320	-0.265133	0.022812
6	4.981925	-1.178800	-0.836636
1	5.581058	-1.984907	-1.258445
6	3.634643	-1.110265	-1.172002
6	2.858548	-0.052953	-0.577844
6	-2.418061	-2.157940	-1.792702
6	-1.632716	-2.650067	-0.554958
1	-2.318559	-2.839634	0.285008
1	-0.890900	-1.909740	-0.235718
1	-1.108237	-3.590872	-0.784162
6	-1.474393	-2.025485	-3.010657
1	-0.650279	-1.333521	-2.807098
1	-2.029375	-1.666119	-3.892596
1	-1.043303	-3.008910	-3.258731
6	-3.473555	-3.225801	-2.134257
1	-4.069471	-2.949808	-3.018648
1	-4.163412	-3.412639	-1.296275
1	-2.966478	-4.176786	-2.359269
6	2.983357	-2.119133	-2.137308
6	4.005227	-3.133002	-2.684520
1	4.450096	-3.746004	-1.884823
1	4.820835	-2.642451	-3.238903
1	3.497903	-3.818778	-3.380536
6	1.878043	-2.910231	-1.403730
1	1.085684	-2.245210	-1.049217
1	2.294280	-3.455249	-0.541000
1	1.423153	-3.646919	-2.085492
6	2.378489	-1.362239	-3.343903
1	3.165024	-0.823924	-3.897314
1	1.618061	-0.639871	-3.022932
1	1.903421	-2.076211	-4.035975
6	1.014355	3.647939	1.114441
6	-0.105347	4.042779	0.079516
6	2.073314	4.751208	1.252141
1	1.586176	5.711234	1.467543
1	2.747719	4.547247	2.095799
1	2.678362	4.867108	0.342776
6	0.420670	3.328862	2.499488
1	1.211278	2.915310	3.143143
1	0.037290	4.241277	2.976380
1	-0.375002	2.578491	2.422620
6	-1.026156	5.146093	0.614913
1	-1.637271	4.804124	1.461025
1	-0.426547	6.003023	0.948441
1	-1.695889	5.518140	-0.173485
6	0.505946	4.491382	-1.263690
1	-0.290045	4.571625	-2.017944

1	0.984962	5.475217	-1.166387
1	1.253399	3.770533	-1.626536
6	7.122589	-0.433372	0.342205
6	7.996309	-0.336831	-0.919825
6	7.389431	-1.742995	1.103751
1	7.404862	0.401358	1.006649
1	7.827785	0.613433	-1.450408
1	9.064861	-0.399830	-0.657903
1	7.778396	-1.158670	-1.621798
1	6.792381	-1.796247	2.027748
1	7.135926	-2.621258	0.487123
1	8.453950	-1.824664	1.376781
6	-6.604585	0.660663	-0.999853
6	-7.167273	-0.250215	0.105374
6	-7.250055	0.350519	-2.360532
1	-6.864118	1.700611	-0.737359
1	-6.727909	-0.004721	1.085253
1	-8.261296	-0.141979	0.181361
1	-6.951307	-1.310994	-0.104684
1	-6.867531	1.021137	-3.145884
1	-7.047191	-0.686797	-2.674135
1	-8.343952	0.472012	-2.307340
6	-2.358254	-1.214169	2.643078
6	-2.816141	-2.458761	3.106758
6	-1.917789	-3.517871	3.289528
6	-0.555995	-3.297376	3.010067
6	-0.120524	-2.047405	2.560908
1	-3.882330	-2.584347	3.306088
1	0.176093	-4.097473	3.137065
6	-2.382896	-4.870237	3.755212
1	-1.820506	-5.187618	4.647475
1	-3.454620	-4.875500	3.995723
1	-2.199013	-5.625363	2.973595
6	1.294535	-1.702337	2.213828
1	1.640366	-0.858440	2.829035
1	1.957634	-2.563551	2.361796
1	1.339956	-1.371316	1.168547
6	-3.255249	-0.050934	2.344907
1	-2.675035	0.877560	2.307789
1	-3.721504	-0.195648	1.357568
1	-4.058430	0.020335	3.091414
7	-1.055267	-1.108270	2.432757
9	-0.372932	0.558421	1.462892

Structure S8. Co^{III}(salen)-F

27	-0.032545	0.823376	0.122776
8	-1.280082	-0.520958	-0.249874
8	1.298749	-0.426069	-0.301842
7	-1.242191	2.213880	-0.440976
7	1.239428	2.247486	0.287558
6	-2.568379	-0.418022	-0.147660
6	-3.353023	-1.597302	0.122593
6	-4.735494	-1.468364	0.120539
1	-5.341064	-2.352135	0.321530
6	-5.427298	-0.249631	-0.112870
6	-4.668326	0.882802	-0.329584
1	-5.158401	1.847886	-0.492048
6	-3.249298	0.831127	-0.332127
6	-2.526600	2.047696	-0.547072
1	-3.141612	2.914507	-0.817533
6	2.520058	2.084177	0.367147
1	3.144662	2.971756	0.522416
6	3.246648	0.850633	0.235299
6	4.653602	0.886150	0.402196
1	5.126090	1.833557	0.680043
6	5.427426	-0.244991	0.221104
6	4.760749	-1.439333	-0.150316
1	5.375722	-2.328001	-0.290852
6	3.386660	-1.545679	-0.340529
6	2.589777	-0.364446	-0.134837
6	-2.646151	-2.926635	0.445032
6	-1.768607	-2.730559	1.707391
1	-2.407426	-2.546437	2.586893
1	-1.082517	-1.880624	1.602805
1	-1.176737	-3.639851	1.902489
6	-1.779522	-3.379039	-0.753971
1	-0.994411	-2.649273	-0.979141
1	-2.405445	-3.515003	-1.651609
1	-1.298015	-4.344478	-0.527529
6	-3.650647	-4.055470	0.742018
1	-4.292742	-4.276728	-0.125699
1	-4.299800	-3.819122	1.599961
1	-3.099976	-4.976598	0.989465
6	2.713593	-2.877615	-0.725432
6	3.741281	-4.009699	-0.909167
1	4.302331	-4.215098	0.016244
1	4.465288	-3.786184	-1.709031

1	3.215826	-4.936540	-1.187777
6	1.737445	-3.300703	0.397507
1	0.952220	-2.551496	0.547575
1	2.278988	-3.440336	1.347430
1	1.253125	-4.256488	0.138665
6	1.946881	-2.719150	-2.060139
1	2.638390	-2.445110	-2.874040
1	1.171848	-1.947419	-1.982114
1	1.463272	-3.671851	-2.332204
6	0.582810	3.583962	0.363207
6	-0.558196	3.503920	-0.727103
6	1.556801	4.737245	0.091616
1	1.005724	5.685255	0.037567
1	2.278901	4.840885	0.914154
1	2.115570	4.608798	-0.845659
6	-0.001079	3.729383	1.782209
1	0.819381	3.670280	2.512653
1	-0.495498	4.703414	1.901989
1	-0.697794	2.912450	2.004289
6	-1.508191	4.705701	-0.667571
1	-2.078732	4.740022	0.270541
1	-0.938536	5.639550	-0.760408
1	-2.218910	4.686054	-1.506295
6	0.032907	3.386660	-2.146457
1	-0.774984	3.169426	-2.860478
1	0.517683	4.323821	-2.453361
1	0.768232	2.570590	-2.202344
6	6.937689	-0.221099	0.404883
6	7.677262	-0.547736	-0.903710
6	7.389826	-1.151874	1.542881
1	7.210443	0.809517	0.691498
1	7.382982	0.141712	-1.710752
1	8.768390	-0.471419	-0.766644
1	7.455965	-1.574018	-1.241052
1	6.887788	-0.897106	2.489509
1	7.157973	-2.205000	1.312335
1	8.478489	-1.078344	1.699627
6	-6.948024	-0.205715	-0.098362
6	-7.517496	-0.582075	1.280210
6	-7.555125	-1.083470	-1.205956
1	-7.241451	0.838415	-0.304188
1	-7.110960	0.068701	2.070308
1	-8.615905	-0.489276	1.288626
1	-7.270470	-1.624156	1.543004
1	-7.177195	-0.791386	-2.198458
1	-7.308393	-2.147170	-1.051974
1	-8.653935	-0.996022	-1.216613
9	-0.316155	0.702944	1.963454

Structure S9. $[Me_3MPy]^{+\cdot}$

6	-0.706973	1.214048	0.001197
6	0.700692	1.211742	-0.008817
6	1.414863	0.001882	-0.012635
6	0.703725	-1.209807	-0.009155
6	-0.703864	-1.215750	0.001079
1	1.208368	2.178794	-0.016228
1	1.213987	-2.175498	-0.015878
6	2.917677	0.003406	0.005758
1	3.268768	-0.001110	1.051678
1	3.326005	-0.889950	-0.486393
1	3.324447	0.901747	-0.478453
6	-1.576041	-2.436383	0.000064
1	-2.220592	-2.438446	-0.891966
1	-0.953231	-3.338352	0.000589
1	-2.223457	-2.438354	0.889854
6	-1.582235	2.432486	-0.000162
1	-2.234657	2.427648	-0.886374
1	-2.221736	2.438228	0.895387
1	-0.961605	3.335906	-0.010137
7	-1.219052	-0.001479	0.011992

Structure S10. $[Co^{IV}(salen)\text{-}F]^+$

27	0.005796	0.842430	0.165175
8	-1.289040	-0.530227	-0.154145
8	1.288335	-0.372255	-0.376199
7	-1.210870	2.235614	-0.480841
7	1.251107	2.254671	0.332282
6	-2.549764	-0.425555	-0.105900
6	-3.355282	-1.623788	0.139823
6	-4.733664	-1.483032	0.110558
1	-5.356561	-2.357079	0.290735
6	-5.390655	-0.253015	-0.131261
6	-4.605415	0.902548	-0.337696
1	-5.104379	1.857294	-0.522239
6	-3.218182	0.852037	-0.312508
6	-2.487198	2.085648	-0.543037

1	-3.115466	2.951796	-0.782785
6	2.535816	2.092338	0.354359
1	3.161379	2.981387	0.487318
6	3.253288	0.860049	0.193705
6	4.657728	0.876204	0.358595
1	5.146259	1.813706	0.638660
6	5.410056	-0.271866	0.178200
6	4.723327	-1.459290	-0.178641
1	5.323058	-2.359282	-0.308480
6	3.347135	-1.547942	-0.363779
6	2.581108	-0.345974	-0.182497
6	-2.664099	-2.949704	0.465669
6	-1.809951	-2.767593	1.749928
1	-2.462976	-2.575161	2.616018
1	-1.098669	-1.936627	1.670329
1	-1.247406	-3.693215	1.947219
6	-1.781452	-3.389746	-0.730380
1	-0.978149	-2.675432	-0.936660
1	-2.394007	-3.508143	-1.638437
1	-1.322071	-4.363915	-0.502561
6	-3.683584	-4.072041	0.733621
1	-4.309811	-4.281648	-0.147639
1	-4.342599	-3.840457	1.584681
1	-3.141137	-4.996817	0.980371
6	2.650367	-2.876941	-0.709687
6	3.659174	-4.030301	-0.863176
1	4.221843	-4.215932	0.065089
1	4.380272	-3.844267	-1.674767
1	3.116188	-4.955888	-1.108767
6	1.679631	-3.246836	0.436900
1	0.912548	-2.478043	0.581009
1	2.229971	-3.372995	1.383038
1	1.171487	-4.197489	0.209933
6	1.880451	-2.747479	-2.045564
1	2.573077	-2.513121	-2.870220
1	1.117825	-1.960981	-1.997384
1	1.380478	-3.700443	-2.282823
6	0.585806	3.592062	0.403228
6	-0.514253	3.528162	-0.734596
6	1.568495	4.746959	0.181229
1	1.018159	5.695988	0.148306
1	2.273335	4.821960	1.021420
1	2.142123	4.648200	-0.750093
6	-0.046779	3.724027	1.801847
1	0.744114	3.631296	2.559892
1	-0.519136	4.708550	1.918998
1	-0.777820	2.929368	1.991516
6	-1.461302	4.730031	-0.707149
1	-2.042040	4.787397	0.223615
1	-0.885593	5.658327	-0.812066
1	-2.159203	4.696250	-1.556334
6	0.123577	3.400387	-2.132860
1	-0.662119	3.200566	-2.875405
1	0.629005	4.333850	-2.414277
1	0.850295	2.576339	-2.170990
6	6.919082	-0.274004	0.361287
6	7.648825	-0.646776	-0.940546
6	7.346965	-1.189616	1.521178
1	7.212861	0.756472	0.624693
1	7.367544	0.028255	-1.763996
1	8.740357	-0.585675	-0.803089
1	7.410664	-1.677227	-1.251985
1	6.849806	-0.902538	2.460911
1	7.094300	-2.242429	1.313155
1	8.436366	-1.133702	1.676727
6	-6.899975	-0.175564	-0.157424
6	-7.501646	-0.558940	1.208854
6	-7.482889	-1.042192	-1.290484
1	-7.171287	0.872861	-0.361594
1	-7.098131	0.071051	2.016084
1	-8.594713	-0.429373	1.183453
1	-7.294419	-1.611640	1.458985
1	-7.071258	-0.752774	-2.269405
1	-7.268784	-2.111021	-1.130596
1	-8.576648	-0.921263	-1.326824
9	-0.361098	0.682484	1.959937

Structure S11. Me_3MPy

6	-0.704642	1.155926	0.000672
6	0.697293	1.195908	-0.010298
6	1.428830	0.000984	-0.013439
6	0.698837	-1.194917	-0.010158
6	-0.703120	-1.156755	0.000807
1	1.215465	2.158355	-0.018392
1	1.218267	-2.156692	-0.018178
6	2.935216	0.001718	0.008926
1	3.302903	-0.004549	1.049717

1	3.347417	-0.889185	-0.488422
1	3.346627	0.898815	-0.477744
6	-1.525491	-2.421611	0.002596
1	-2.177889	-2.453245	-0.885415
1	-0.898276	-3.324360	0.009577
1	-2.186771	-2.444678	0.884082
6	-1.528646	2.419712	0.002653
1	-2.183440	2.449100	-0.883644
1	-2.187606	2.443308	0.885882
1	-0.902589	3.323283	0.006695
7	-1.383397	-0.000849	0.006468

Structure S12. ^{4}TS2

27	-0.268916	-1.232144	0.582679
8	-1.534644	-0.009457	1.156696
8	1.039344	-0.136486	1.392280
7	-1.553642	-2.587125	0.281154
7	1.004521	-2.528562	0.017695
6	-2.807065	0.022117	0.891796
6	-3.530838	1.260366	1.029851
6	-4.902644	1.224631	0.820047
1	-5.467599	2.150506	0.922513
6	-5.632815	0.058617	0.464811
6	-4.924377	-1.114111	0.294399
1	-5.442243	-2.031253	-0.000554
6	-3.518753	-1.153664	0.482029
6	-2.841422	-2.393851	0.280462
1	-3.489524	-3.259798	0.107796
6	2.276411	-2.305963	-0.048152
1	2.910830	-3.063152	-0.523194
6	2.980534	-1.152557	0.448263
6	4.375703	-1.101602	0.249564
1	4.858051	-1.894424	-0.328709
6	5.140266	-0.073674	0.780568
6	4.478392	0.913977	1.559884
1	5.094553	1.708115	1.977816
6	3.114720	0.934185	1.804536
6	2.313973	-0.121306	1.211847
6	-2.779307	2.567452	1.337324
6	-1.782058	2.839251	0.184342
1	-2.325439	3.008404	-0.758157
1	-1.093123	1.999735	0.030563
1	-1.187213	3.741148	0.399340
6	-2.040566	2.461468	2.692242
1	-1.291542	1.662234	2.684404
1	-2.757618	2.264986	3.506027
1	-1.527937	3.410903	2.914897
6	-3.734122	3.772613	1.423063
1	-4.468765	3.660872	2.236280
1	-4.281498	3.937256	0.481729
1	-3.150187	4.683359	1.627172
6	2.452990	2.038959	2.644394
6	3.490319	3.027505	3.207934
1	4.039675	3.552095	2.410621
1	4.220948	2.531412	3.866179
1	2.971518	3.792291	3.805579
6	1.472797	2.834496	1.752347
1	0.699591	2.186249	1.329015
1	2.011766	3.327702	0.928429
1	0.974412	3.616413	2.346351
6	1.697734	1.414940	3.842986
1	2.391093	0.851697	4.488367
1	0.899260	0.740445	3.512148
1	1.243252	2.214335	4.449654
6	0.384829	-3.733658	-0.614242
6	-0.950049	-3.951454	0.186613
6	1.310616	-4.955265	-0.541975
1	0.760539	-5.861246	-0.827884
1	2.145147	-4.861010	-1.250863
1	1.724037	-5.102280	0.465050
6	0.104445	-3.371141	-2.086271
1	1.047351	-3.087263	-2.575627
1	-0.310537	-4.233630	-2.624615
1	-0.582624	-2.518855	-2.160808
6	-1.880067	-4.955236	-0.506738
1	-2.268741	-4.573096	-1.460227
1	-1.338630	-5.889453	-0.704986
1	-2.730704	-5.216643	0.138257
6	-0.672898	-4.422459	1.629602
1	-1.609575	-4.405898	2.205643
1	-0.287767	-5.451229	1.636234
1	0.054531	-3.772584	2.139642
6	6.633788	0.014807	0.528925
6	7.440929	0.027504	1.838008
6	6.970275	1.233891	-0.349817
1	6.920857	-0.889931	-0.032850
1	7.210944	-0.852824	2.458131

1	8.520562	0.022308	1.620007
1	7.228773	0.928960	2.435495
1	6.429548	1.197607	-1.308276
1	6.701208	2.176313	0.154907
1	8.050070	1.265509	-0.565500
6	-7.138561	0.120522	0.264201
6	-7.520072	1.055897	-0.895918
6	-7.866570	0.516283	1.560167
1	-7.469230	-0.897001	-0.006297
1	-7.022718	0.755147	-1.831378
1	-8.608926	1.040356	-1.064449
1	-7.232706	2.098318	-0.680494
1	-7.622195	-0.174431	2.382410
1	-7.587946	1.533912	1.880352
1	-8.958366	0.502133	1.411680
9	-0.145664	-0.355593	-1.182566
8	1.062484	1.374889	-3.583292
14	-0.294894	2.387338	-3.564776
1	-0.114306	3.342959	-2.431377
14	2.196248	0.758372	-2.551395
1	1.242637	0.073671	-1.441168
6	-0.310553	3.305567	-5.196885
1	-1.169657	3.995511	-5.239964
1	0.611328	3.893908	-5.330764
1	-0.396231	2.598607	-6.038321
6	-1.828636	1.346475	-3.306532
1	-1.724943	0.767941	-2.376720
1	-2.725399	1.984127	-3.238535
1	-1.965317	0.644263	-4.145404
6	3.225685	2.104231	-1.765590
1	3.852106	2.573129	-2.543470
1	2.577064	2.874160	-1.322683
1	3.881583	1.700648	-0.981988
6	3.153204	-0.609966	-3.387938
1	3.861051	-1.078308	-2.687763
1	2.471452	-1.380205	-3.779337
1	3.725190	-0.187690	-4.231450

Structure S13. $[Co^{III}(salen)]^{+}$

27	-0.000006	0.912577	-0.000041
8	-1.282651	-0.432635	-0.009317
8	1.282649	-0.432626	0.009172
7	-1.268887	2.283590	-0.221828
7	1.268863	2.283592	0.221786
6	-2.575519	-0.373175	-0.006988
6	-3.350223	-1.581473	0.168181
6	-4.730956	-1.466441	0.102628
1	-5.334474	-2.364984	0.222718
6	-5.427281	-0.245466	-0.107148
6	-4.678805	0.911507	-0.237898
1	-5.178517	1.873542	-0.382003
6	-3.266527	0.877665	-0.181460
6	-2.556466	2.114293	-0.302878
1	-3.182945	2.994612	-0.482104
6	2.556438	2.114290	0.302921
1	3.182904	2.994608	0.482196
6	3.266509	0.877667	0.181526
6	4.678784	0.911511	0.238070
1	5.178482	1.873542	0.382253
6	5.427271	-0.245454	0.107324
6	4.730964	-1.466422	-0.102559
1	5.334494	-2.364957	-0.222645
6	3.350237	-1.581455	-0.168220
6	2.575517	-0.373166	0.006948
6	-2.654224	-2.926372	0.440848
6	-1.843513	-2.817829	1.755160
1	-2.513735	-2.614434	2.605872
1	-1.094497	-2.018421	1.701977
1	-1.319048	-3.766139	1.953223
6	-1.722767	-3.290498	-0.738331
1	-0.937117	-2.540956	-0.875242
1	-2.298423	-3.375773	-1.674231
1	-1.238624	-4.261677	-0.548022
6	-3.667743	-4.073423	0.609392
1	-4.268341	-4.231616	-0.300201
1	-4.354319	-3.901370	1.453124
1	-3.124056	-5.008771	0.812389
6	2.654261	-2.926347	-0.440979
6	3.667795	-4.073390	-0.609488
1	4.268326	-4.231615	0.300143
1	4.354433	-3.901303	-1.453164
1	3.124126	-5.008732	-0.812559
6	1.722728	-3.290501	0.738130
1	0.937080	-2.540952	0.875014
1	2.298324	-3.375813	1.674063
1	1.238582	-4.261667	0.547760
6	1.843631	-2.817775	-1.755340

1	2.513903	-2.614347	-2.606004
1	1.094600	-2.018380	-1.702181
1	1.319194	-3.766089	-1.953462
6	0.639105	3.618907	0.459770
6	-0.639126	3.618893	-0.459858
6	1.585627	4.780693	0.132309
1	1.033024	5.728994	0.145113
1	2.377777	4.871212	0.888779
1	2.056759	4.668736	-0.853619
6	0.254835	3.670879	1.952691
1	1.150625	3.498834	2.566852
1	-0.153932	4.655923	2.215983
1	-0.488969	2.900490	2.206391
6	-1.585642	4.780698	-0.132447
1	-2.056766	4.668797	0.853490
1	-1.033035	5.728996	-0.145307
1	-2.377797	4.871178	-0.888916
6	-0.254855	3.670806	-1.952782
1	-1.150645	3.498727	-2.566933
1	0.153903	4.655843	-2.216113
1	0.488956	2.900415	-2.206454
6	6.944651	-0.223962	0.170774
6	7.574060	-0.680762	-1.156939
6	7.472515	-1.055579	1.352890
1	7.245579	0.823993	0.339341
1	7.220526	-0.065819	-1.999277
1	8.671956	-0.601520	-1.109935
1	7.325890	-1.732005	-1.377498
1	7.045750	-0.709622	2.307281
1	7.220674	-2.122523	1.236307
1	8.569606	-0.978463	1.418434
6	-6.944665	-0.223974	-0.170490
6	-7.573982	-0.680850	1.157240
6	-7.472607	-1.055524	-1.352618
1	-7.245607	0.823990	-0.338977
1	-7.220389	-0.065957	1.999589
1	-8.671882	-0.601602	1.110316
1	-7.325800	-1.732107	1.377721
1	-7.045912	-0.709510	-2.307018
1	-7.220752	-2.122474	-1.236114
1	-8.569704	-0.978411	-1.418080

Structure S14. HF

9	0.000000	0.000000	0.092769
1	0.000000	0.000000	-0.834923

Structure S15. R_3Si^+

8	0.032529	-0.356475	-0.216825
14	1.575355	-0.046691	-0.011579
14	-1.658209	-0.041970	-0.418378
1	-1.843511	-0.056033	-1.892440
6	2.113993	1.703162	0.086690
1	3.210141	1.782519	0.065512
1	1.673555	2.275505	-0.745567
1	1.735872	2.136534	1.028926
6	2.713809	-1.473554	0.114160
1	2.162277	-2.423455	0.127697
1	3.400161	-1.452052	-0.750427
1	3.328513	-1.372505	1.024118
6	-2.008014	1.634760	0.321688
1	-1.769819	1.644469	1.397780
1	-1.422637	2.423586	-0.176796
1	-3.077030	1.879302	0.207430
6	-2.539036	-1.451341	0.423248
1	-3.628811	-1.345617	0.294476
1	-2.233430	-2.419127	-0.004585
1	-2.320082	-1.458214	1.503147

Structure S16. 1

6	1.308212	0.570092	-0.053265
6	0.291669	1.475139	0.284902
6	-1.025857	1.033427	0.451139
6	-1.367126	-0.315130	0.294323
6	-0.343100	-1.216413	-0.034931
6	0.977017	-0.798252	-0.209215
1	0.517455	2.534111	0.410984
1	-1.803119	1.760575	0.701124
1	-0.552870	-2.280770	-0.168266
8	1.919756	-1.719470	-0.579803
8	2.607733	0.904943	-0.261716
6	2.927414	-2.017433	0.382454
1	2.480406	-2.400741	1.317834
1	3.563488	-2.800035	-0.054725
1	3.545153	-1.134911	0.612738
6	3.003550	2.256325	-0.117152

1	2.824504	2.627663	0.907546
1	4.080755	2.289758	-0.326553
1	2.477856	2.913878	-0.831913
6	-2.803849	-0.778018	0.472103
1	-2.837503	-1.877181	0.378606
1	-3.153643	-0.534588	1.490286
6	-3.740004	-0.164681	-0.537809
6	-4.791013	0.608053	-0.245757
1	-3.501677	-0.375438	-1.588446
1	-5.428513	1.028957	-1.028884
1	-5.053690	0.846262	0.791068

Structure S17. 2

6	1.266238	0.549313	0.049851
6	0.220317	1.484169	0.206276
6	-1.077997	1.046836	0.362450
6	-1.412496	-0.350985	0.381832
6	-0.402988	-1.277190	0.223113
6	0.944774	-0.877059	0.053733
1	0.439091	2.550700	0.204461
1	-1.881122	1.778390	0.474251
1	-0.603296	-2.349600	0.227439
8	1.810353	-1.850722	-0.084871
8	2.533767	0.862568	-0.101094
6	3.235825	-1.735645	-0.267845
1	3.690194	-1.232698	0.595524
1	3.590006	-2.769001	-0.346247
1	3.457466	-1.176843	-1.186194
6	2.979574	2.230076	-0.114730
1	2.730465	2.717093	0.839368
1	4.065600	2.182908	-0.244886
1	2.518297	2.769267	-0.954971
6	-2.856734	-0.753405	0.552887
1	-2.923687	-1.850116	0.628999
1	-3.232920	-0.331475	1.500815
6	-3.702046	-0.255132	-0.596272
6	-4.683782	0.645245	-0.484424
1	-3.454091	-0.672626	-1.579416
1	-5.262304	0.966545	-1.354993
1	-4.950776	1.085352	0.482350

Structure S18. ^{3}TS3

27	1.402034	1.096566	-0.235218
8	2.309813	-0.579416	-0.113996
8	-0.140161	0.937681	0.970571
7	3.157656	2.126977	-0.344500
7	0.680131	2.854867	-0.893054
6	3.568601	-0.847028	0.061424
6	3.977751	-2.217943	0.272118
6	5.328376	-2.481689	0.466666
1	5.641890	-3.511858	0.636050
6	6.341410	-1.491060	0.459211
6	5.946028	-0.183986	0.246358
1	6.698357	0.611917	0.228763
6	4.586119	0.171606	0.051520
6	4.314827	1.575116	-0.175509
1	5.219319	2.201667	-0.204169
6	-0.569347	3.176830	-0.842750
1	-0.911454	4.085298	-1.359720
6	-1.608619	2.494601	-0.098481
6	-2.925047	2.998034	-0.236372
1	-3.107049	3.785421	-0.975992
6	-3.970293	2.544384	0.549152
6	-3.662738	1.577188	1.535641
1	-4.478913	1.245989	2.176086
6	-2.394862	1.037095	1.736285
6	-1.323957	1.462568	0.864757
6	2.922182	-3.343474	0.279867
6	2.217627	-3.399632	-1.096288
1	2.939999	-3.640938	-1.893115
1	1.748770	-2.436826	-1.329207
1	1.437249	-4.179227	-1.096723
6	1.879705	-3.088067	1.394615
1	1.369142	-2.129347	1.248236
1	2.366494	-3.077124	2.383707
1	1.122550	-3.890107	1.399143
6	3.549161	-4.726301	0.538769
1	4.048915	-4.776400	1.519230
1	4.282683	-5.001131	-0.235762
1	2.758316	-5.493010	0.531213
6	-2.119216	0.035649	2.879433
6	-3.386864	-0.263115	3.702275
1	-4.174356	-0.729054	3.089088
1	-3.804819	0.643107	4.168248
1	-3.140010	-0.967754	4.511813
6	-1.600190	-1.311304	2.327103

1	-0.653497	-1.178489	1.791744
1	-2.333519	-1.760916	1.639579
1	-1.431932	-2.019680	3.155377
6	-1.067652	0.640367	3.839868
1	-1.437817	1.581764	4.278215
1	-0.127550	0.845742	3.312100
1	-0.858821	-0.059861	4.666152
6	1.716028	3.697084	-1.532727
6	2.982709	3.578497	-0.569138
6	1.267197	5.153976	-1.715130
1	2.100680	5.771077	-2.075238
1	0.473224	5.224539	-2.473114
1	0.888036	5.594349	-0.782471
6	2.030829	3.095858	-2.916597
1	1.107065	3.045329	-3.511844
1	2.751746	3.720258	-3.462646
1	2.439758	2.080526	-2.824655
6	4.225125	4.249538	-1.171971
1	4.585162	3.723943	-2.067672
1	4.011075	5.291757	-1.442955
1	5.046980	4.278509	-0.441612
6	2.676727	4.207643	0.805210
1	3.508963	3.999944	1.494369
1	2.559909	5.298199	0.730641
1	1.759837	3.778815	1.234424
6	-5.363782	3.147951	0.432690
6	-5.586740	4.215576	1.519848
6	-6.485985	2.100545	0.461449
1	-5.409879	3.657526	-0.546084
1	-4.820919	5.005542	1.466897
1	-6.578027	4.687921	1.416161
1	-5.531690	3.761988	2.524038
1	-6.320880	1.301028	-0.274942
1	-6.560897	1.622862	1.452384
1	-7.460287	2.573921	0.257222
6	7.800906	-1.864568	0.674554
6	8.324251	-2.795069	-0.432990
6	8.036687	-2.477740	2.065484
1	8.383878	-0.928180	0.622702
1	8.192765	-2.342195	-1.428494
1	9.396178	-3.011497	-0.292085
1	7.787786	-3.758645	-0.429404
1	7.698217	-1.797514	2.863012
1	7.487887	-3.427509	2.179669
1	9.106486	-2.691135	2.225842
1	0.797708	0.710414	-1.595546
6	-5.254805	-3.256132	-1.234447
6	-4.148263	-3.997104	-1.665763
6	-2.873386	-3.413828	-1.694240
6	-2.668617	-2.092503	-1.289241
6	-3.782354	-1.355203	-0.847963
6	-5.057097	-1.914273	-0.820044
1	-4.267675	-5.030798	-1.990376
1	-2.025327	-4.011698	-2.039073
1	-3.671617	-0.325611	-0.500302
8	-6.121974	-1.144876	-0.428892
8	-6.530407	-3.719097	-1.181893
6	-6.685851	-1.459501	0.840339
1	-5.939408	-1.334298	1.644942
1	-7.509288	-0.752252	1.007987
1	-7.077783	-2.488800	0.863909
6	-6.793163	-5.054611	-1.569744
1	-6.248450	-5.778575	-0.937879
1	-7.872598	-5.210020	-1.442873
1	-6.526085	-5.232417	-2.626548
6	-1.294466	-1.463194	-1.320681
1	-1.076912	-0.998531	-0.340807
1	-0.520730	-2.233269	-1.458442
6	-1.120768	-0.370731	-2.331134
6	0.082236	-0.066482	-2.888008
1	-1.968073	0.309260	-2.476079
1	0.180302	0.760270	-3.595305
1	0.908812	-0.782132	-2.852844

Structure S19. 3

6	1.462498	0.529093	-0.065900
6	0.593744	1.568910	0.293041
6	-0.761654	1.310701	0.534344
6	-1.286508	0.017572	0.432058
6	-0.407510	-1.020054	0.082374
6	0.945239	-0.786232	-0.166039
1	0.964316	2.590362	0.380785
1	-1.419608	2.140916	0.805741
1	-0.763769	-2.049392	-0.008679
8	1.739525	-1.833406	-0.550905
8	2.784255	0.680803	-0.341510
6	2.740411	-2.242775	0.376567

1	2.288380	-2.545660	1.338712
1	3.249360	-3.110613	-0.066238
1	3.477591	-1.444848	0.559580
6	3.360966	1.970716	-0.261194
1	3.283767	2.391221	0.757299
1	4.421509	1.855089	-0.520656
1	2.891211	2.672423	-0.973053
6	-2.761971	-0.246152	0.646579
1	-2.900841	-1.303470	0.962808
1	-3.131534	0.353446	1.500667
6	-3.607821	0.038329	-0.557748
1	-3.145322	-0.068436	-1.545157
6	-5.093140	0.098097	-0.450148
1	-5.559215	0.516145	-1.356408
1	-5.537008	-0.909944	-0.296273
1	-5.414601	0.704360	0.416590

Structure S20. ^{2}TS4

6	-3.103185	-0.290854	-0.319292
6	-3.264097	0.851523	-1.120692
6	-2.652730	2.050387	-0.769045
6	-1.891672	2.155279	0.416312
6	-1.753152	1.022815	1.232138
6	-2.354717	-0.190453	0.901887
1	-3.843760	0.795781	-2.041001
1	-2.761376	2.919152	-1.421961
1	-1.180360	1.064785	2.160329
8	-2.118138	-1.231905	1.721474
8	-3.561351	-1.508353	-0.633884
6	-3.094531	-2.249966	1.979523
1	-3.051390	-3.042467	1.220917
1	-2.842502	-2.661060	2.965989
1	-4.109215	-1.825380	2.005949
6	-4.290402	-1.715666	-1.841165
1	-3.674803	-1.465608	-2.720446
1	-4.544342	-2.781921	-1.861982
1	-5.215146	-1.116555	-1.851746
6	-1.105430	3.419418	0.708826
1	-1.660853	4.322610	0.422778
1	-0.822828	3.481867	1.768837
6	0.069895	3.180749	-0.184475
6	1.196852	2.460672	0.195574
1	-0.036688	3.463957	-1.236727
1	2.058926	2.429818	-0.475208
1	1.403644	2.300184	1.258283
8	2.800876	-0.455990	-0.934267
14	4.456370	-0.395722	-0.608561
1	5.120146	-0.314441	-1.940168
14	1.292142	-0.610992	-0.289762
1	0.885923	0.915050	-0.011514
6	4.817501	1.141098	0.404854
1	5.892178	1.202741	0.643625
1	4.538256	2.057752	-0.139161
1	4.259136	1.117413	1.355682
6	4.961389	-1.961295	0.289369
1	4.680559	-2.855959	-0.289510
1	6.052963	-1.981639	0.444202
1	4.475472	-2.021906	1.276954
6	1.285140	-1.467883	1.367116
1	1.652572	-2.500758	1.242850
1	1.943035	-0.949566	2.081915
1	0.263273	-1.506098	1.774683
6	0.094974	-1.265158	-1.562790
1	-0.852192	-1.559253	-1.087820
1	-0.114230	-0.515603	-2.340883
1	0.538330	-2.152908	-2.043770

Structure S21. ^{4}TS5

27	-1.104275	0.692549	-0.323958
8	-2.450012	-0.666035	-0.571612
8	0.158775	-0.332849	-1.342209
7	-2.544049	2.077433	-0.876184
7	0.073741	2.350838	-0.782755
6	-3.703210	-0.609514	-0.237403
6	-4.384470	-1.793430	0.220138
6	-5.745337	-1.695018	0.486886
1	-6.276310	-2.583083	0.830230
6	-6.501600	-0.503220	0.345132
6	-5.830282	0.635900	-0.060702
1	-6.374191	1.580110	-0.167774
6	-4.439201	0.617704	-0.333076
6	-3.813909	1.851266	-0.739168
1	-4.521153	2.666827	-0.944161
6	1.325817	2.282746	-1.098047
1	1.904329	3.210452	-1.211437
6	2.080535	1.077492	-1.348420

6	3.475470	1.195154	-1.539733	1	-3.361089	4.647730	-0.252114
1	3.937565	2.182731	-1.442600	1	-2.545638	5.458484	-1.613057
6	4.259815	0.095506	-1.846971	1	-3.896731	4.375607	-1.928336
6	3.612715	-1.158730	-1.970304	6	-1.773519	3.089910	-2.933326
1	4.236007	-2.017901	-2.215099	1	-2.714391	2.783638	-3.414052
6	2.246549	-1.352566	-1.796411	1	-1.409538	3.993909	-3.441635
6	1.443319	-0.200520	-1.481981	1	-1.041082	2.281847	-3.071169
6	-3.590761	-3.096980	0.430711	6	5.750885	0.244383	-2.113325
6	-2.480111	-2.850572	1.482601	6	6.034279	0.240853	-3.626763
1	-2.928410	-2.628190	2.465063	6	6.604865	-0.810193	-1.395042
1	-1.831452	-2.009606	1.207412	1	6.047688	1.232811	-1.720834
1	-1.855759	-3.752935	1.592416	1	5.470753	1.035373	-4.140733
6	-2.967009	-3.565577	-0.905474	1	7.107693	0.392855	-3.827952
1	-2.274184	-2.817086	-1.305704	1	5.739660	-0.723488	-4.074054
1	-3.754363	-3.754530	-1.653875	1	6.394942	-0.835437	-0.317491
1	-2.411378	-4.505869	-0.753113	1	6.424538	-1.820009	-1.798884
6	-4.484869	-4.237408	0.951738	1	7.676840	-0.594412	-1.531559
1	-5.284140	-4.495052	0.238431	6	-7.993726	-0.489803	0.643625
1	-4.952394	-3.989432	1.917856	6	-8.286583	-0.825170	2.116053
1	-3.873230	-5.140719	1.103524	6	-8.773152	-1.421222	-0.300345
6	1.585445	-2.739823	-1.929718	1	-8.349015	0.539503	0.461516
6	2.623777	-3.842802	-2.207308	1	-7.757849	-0.136966	2.794273
1	3.367170	-3.922139	-1.397840	1	-9.366336	-0.754764	2.327030
1	3.162714	-3.678627	-3.153752	1	-7.966544	-1.851278	2.362340
1	2.113402	-4.815604	-2.282475	1	-8.595145	-1.159249	-1.355301
6	0.841319	-3.115311	-0.624655	1	-8.472042	-2.472769	-0.160042
1	0.070214	-2.379663	-0.371077	1	-9.856775	-1.357583	-0.107884
1	1.542473	-3.193234	0.220651	9	-0.798543	0.393087	1.453744
1	0.352549	-4.096100	-0.742031	6	4.733242	-1.042465	1.991550
6	0.583075	-2.725070	-3.108871	6	3.427049	-1.302049	1.557570
1	1.098110	-2.485461	-4.053656	6	2.399420	-0.383892	1.787350
1	-0.210115	-1.985156	-2.944195	6	2.649827	0.819440	2.459656
1	0.114333	-3.717076	-3.219244	6	3.962538	1.084739	2.873489
6	-0.665398	3.628491	-0.668809	6	5.003850	0.180905	2.646782
6	-2.029562	3.353829	-1.434591	1	3.204454	-2.221983	1.021920
6	0.095890	4.825507	-1.253495	1	1.387720	-0.592877	1.433070
1	-0.524873	5.729688	-1.211940	1	4.210952	2.013658	3.393276
1	0.997678	5.036383	-0.660106	8	6.251396	0.493408	3.120423
1	0.402143	4.664727	-2.296518	8	5.782212	-1.897369	1.826586
6	-0.922777	3.884850	0.828463	6	7.295322	0.632032	2.162437
1	0.036323	3.979460	1.355724	1	6.988302	1.291772	1.330504
1	-1.484247	4.817253	0.977402	1	8.146930	1.091175	2.684701
1	-1.477400	3.056572	1.287696	1	7.603296	-0.340574	1.748730
6	-3.015246	4.521421	-1.287531	6	5.549075	-3.153781	1.217821

1	5.185658	-3.044028	0.181595
1	6.514201	-3.676686	1.202072
1	4.820232	-3.753851	1.790500
6	1.521349	1.789071	2.722374
1	1.921287	2.769148	3.050636
1	0.999386	1.986115	1.767893
6	0.500863	1.299231	3.697201
1	0.557927	0.260951	4.036932
6	-0.694335	2.107808	4.053403
1	-1.037872	1.910934	5.083158
1	-0.509809	3.190123	3.945754
1	-1.535927	1.853102	3.378569

Structure S22. 4

6	1.733607	0.517400	-0.028150
6	0.812073	1.485552	0.394767
6	-0.519858	1.137427	0.648391
6	-0.969233	-0.179212	0.492441
6	-0.038010	-1.145398	0.077625
6	1.293535	-0.820538	-0.181371
1	1.123378	2.522392	0.522502
1	-1.223643	1.911358	0.960973
1	-0.333506	-2.189101	-0.057427
8	2.140399	-1.799722	-0.627957
8	3.037530	0.761077	-0.319166
6	3.182459	-2.189296	0.262037
1	2.768939	-2.559545	1.217906
1	3.731391	-3.005744	-0.228210
1	3.875938	-1.358132	0.466612
6	3.538777	2.078286	-0.186772
1	3.457971	2.444407	0.852162
1	4.598611	2.038626	-0.470571
1	3.013590	2.783310	-0.855153
6	-2.418300	-0.540989	0.720974
1	-2.522774	-1.629551	0.853359
1	-2.792787	-0.066725	1.644344
6	-4.789923	-0.517286	-0.217080
1	-5.411791	-0.129702	-1.037902
1	-4.887436	-1.613438	-0.192886
1	-5.169895	-0.110560	0.733556
6	-3.341671	-0.117032	-0.421736
1	-2.959210	-0.522879	-1.375529
9	-3.288104	1.282329	-0.535945

Structure S23. ^{1}INT2

6	-0.201580	1.168555	0.036240
6	1.196255	1.198618	0.006640
6	1.923314	0.000028	-0.009787
6	1.196253	-1.198586	0.006664
6	-0.201559	-1.168541	0.036245
1	1.714860	2.160290	-0.006428
1	1.714865	-2.160258	-0.006371
6	3.427103	-0.000035	-0.079542
1	3.853731	-0.894084	0.398749
1	3.757335	-0.001036	-1.132665
1	3.853775	0.894849	0.397140
6	-1.032347	-2.424553	0.073211
1	-2.065744	-2.201251	-0.224878
1	-0.615790	-3.201871	-0.584457
1	-1.056586	-2.836931	1.096466
6	-1.032339	2.424585	0.073216
1	-2.065747	2.201301	-0.224849
1	-1.056543	2.836953	1.096477
1	-0.615766	3.201892	-0.584452
7	-0.866098	0.000016	0.049993
1	-2.418066	-0.000014	-0.038149
9	-3.398693	-0.000042	-0.154873

Structure S24. ^{2}TS6

6	1.998449	-1.157677	0.166588
6	3.326301	-1.420610	0.479679
6	4.337404	-0.504076	0.136082
6	3.960225	0.672009	-0.522584
6	2.618366	0.913795	-0.820960
1	3.576679	-2.349408	0.995408
1	4.707979	1.414303	-0.807727
6	5.771903	-0.793828	0.477159
1	6.446543	-0.002892	0.122319
1	5.892875	-0.893171	1.568184
1	6.087636	-1.751140	0.032003
6	2.136930	2.160209	-1.504361
1	1.056766	2.099536	-1.686887
1	2.342974	3.038284	-0.871332
1	2.671133	2.307475	-2.455453
6	0.863272	-2.079240	0.489380

1	0.080938	-1.548819	1.055972
1	0.385922	-2.438979	-0.435431
1	1.210856	-2.943172	1.069660
7	1.694594	-0.002290	-0.471119
1	0.632485	0.239242	-0.710664
9	-0.625473	0.695526	-0.988006
8	-2.413395	-0.320528	0.711655
14	-1.461379	1.054619	1.034680
14	-2.932690	-1.119213	-0.655425
1	-1.851973	-2.009274	-1.186892
6	-2.352033	2.599774	0.380270
1	-1.870583	3.516769	0.761269
1	-2.346972	2.634522	-0.718188
1	-3.400699	2.602586	0.730066
6	-1.669897	1.159770	2.950998
1	-1.252993	0.270607	3.453133
1	-1.155838	2.049337	3.353922
1	-2.742286	1.229087	3.217871
6	-3.487056	0.053138	-2.015519
1	-4.278874	0.731248	-1.656253
1	-2.619663	0.655028	-2.322593
1	-3.875054	-0.501968	-2.886183
6	-4.359129	-2.227888	-0.118959
1	-4.721003	-2.838787	-0.963530
1	-4.048852	-2.911918	0.688375
1	-5.205185	-1.625921	0.253392

Structure S25. R_3Si-F

9	-1.901887	-0.642321	1.465076
8	0.184069	-0.439691	-0.148340
14	-1.416527	-0.060805	0.005518
14	1.732445	-0.008704	0.336464
1	1.725803	0.155745	1.823318
6	-1.681329	1.783323	0.046128
1	-2.749680	2.026729	0.163870
1	-1.131556	2.238644	0.886060
1	-1.324845	2.247701	-0.887695
6	-2.384587	-0.960688	-1.302150
1	-2.192761	-2.044471	-1.250218
1	-3.466310	-0.792542	-1.176412
1	-2.096904	-0.609276	-2.306345
6	2.204210	1.616086	-0.475776
1	2.182345	1.520294	-1.574072
1	1.508560	2.420772	-0.187383
1	3.221600	1.920703	-0.178519
6	2.887798	-1.397856	-0.155220
1	3.920197	-1.175628	0.162098
1	2.581841	-2.348765	0.310106
1	2.886727	-1.533552	-1.249409

Structure S26. Me_3NHPy

6	-0.615793	1.240369	-0.001524
6	0.753610	1.193010	-0.010785
6	1.475130	-0.045362	-0.022562
6	0.689286	-1.235150	-0.009002
6	-0.684348	-1.209588	-0.000627
1	1.300536	2.140162	-0.012585
1	1.182849	-2.211354	-0.008506
6	2.977147	-0.071593	0.016851
1	3.381952	0.187935	1.016236
1	3.370751	-1.068772	-0.238213
1	3.420223	0.651901	-0.691303
6	-1.577025	-2.409970	0.006347
1	-2.231952	-2.431416	-0.885017
1	-0.989663	-3.338303	0.023473
1	-2.245658	-2.410083	0.888069
6	-1.440372	2.489573	0.007306
1	-2.094740	2.544329	-0.882450
1	-2.104953	2.524615	0.890830
1	-0.802858	3.384040	0.022347
7	-1.331016	0.036337	-0.020975
1	-2.335186	0.064852	0.107923

Structure S27. ^{2}TS7

6	-4.800240	-0.357653	-0.070748
6	-4.041983	-1.342379	-0.722026
6	-2.652458	-1.388720	-0.563424
6	-1.979148	-0.467137	0.248466
6	-2.743507	0.521525	0.886278
6	-4.130644	0.589821	0.740062
1	-4.530993	-2.085648	-1.352113
1	-2.081744	-2.161350	-1.085836
1	-2.269558	1.269248	1.527598
8	-4.822745	1.550529	1.429804
8	-6.152911	-0.242977	-0.145733

6	-5.433059	2.572830	0.648145
1	-6.207824	2.166554	-0.021594
1	-5.897438	3.278208	1.351885
1	-4.680549	3.112907	0.044839
6	-6.877959	-1.156320	-0.947015
1	-6.755135	-2.195879	-0.594607
1	-7.935688	-0.873839	-0.863277
1	-6.574367	-1.101877	-2.007751
6	-0.468118	-0.526901	0.403652
1	-0.167344	0.216858	1.167647
1	-0.177712	-1.511823	0.811234
6	0.267222	-0.289654	-0.885233
6	1.355124	-1.073881	-1.319882
1	0.030921	0.642729	-1.411950
1	1.684852	-0.964129	-2.362086
1	1.411404	-2.109520	-0.953402
6	4.128258	-0.739065	0.862960
6	5.510881	-0.668567	0.969414
6	6.253525	0.234662	0.181826
6	5.522887	1.058390	-0.696794
6	4.139804	0.960420	-0.784247
1	6.019678	-1.310441	1.693512
1	6.040653	1.801496	-1.309140
6	7.754215	0.298377	0.260472
1	8.220016	-0.420031	-0.438646
1	8.130934	1.298364	-0.005312
1	8.116830	0.046284	1.269431
6	3.312201	1.804420	-1.709479
1	2.452138	2.240359	-1.173984
1	3.906113	2.610466	-2.161525
1	2.892393	1.187805	-2.522778
6	3.285901	-1.670316	1.686610
1	2.513167	-1.111992	2.240471
1	2.752406	-2.384612	1.036686
1	3.894445	-2.239933	2.401917
7	3.449758	0.064212	-0.013410
1	2.451930	-0.469232	-0.594151

Structure S28. ^{1}TS8

27	0.104225	1.087599	-0.205587
8	-1.208680	-0.221556	-0.631378
8	1.398869	-0.268123	-0.525330
7	-1.122360	2.505994	-0.263072
7	1.395764	2.391103	0.170250
6	-2.485731	-0.094168	-0.786907
6	-3.323990	-1.261428	-0.984421
6	-4.692037	-1.072433	-1.136885
1	-5.327859	-1.946748	-1.277379
6	-5.330856	0.194711	-1.132217
6	-4.527047	1.306329	-0.967990
1	-4.975975	2.305754	-0.963686
6	-3.124996	1.195244	-0.785773
6	-2.381021	2.408486	-0.589935
1	-2.962991	3.329710	-0.719104
6	2.682946	2.255824	0.030909
1	3.331971	3.112719	0.244719
6	3.379830	1.058319	-0.356676
6	4.794349	1.119857	-0.437056
1	5.286800	2.077284	-0.233694
6	5.556797	0.011330	-0.753062
6	4.864463	-1.201785	-1.000143
1	5.467258	-2.075310	-1.249524
6	3.482818	-1.339325	-0.945151
6	2.686124	-0.175270	-0.612003
6	-2.694508	-2.667355	-1.049663
6	-1.947692	-2.981040	0.265908
1	-2.653895	-3.015342	1.110221
1	-1.189291	-2.220998	0.481869
1	-1.449842	-3.963132	0.199717
6	-1.710173	-2.724024	-2.238986
1	-0.924875	-1.969470	-2.127176
1	-2.240562	-2.546291	-3.189212
1	-1.231580	-3.716056	-2.296200
6	-3.746923	-3.772143	-1.259297
1	-4.297677	-3.647754	-2.205193
1	-4.479812	-3.807800	-0.437253
1	-3.244070	-4.751726	-1.296660
6	2.792567	-2.681302	-1.256087
6	3.801166	-3.806418	-1.553572
1	4.468690	-3.999717	-0.698428
1	4.425832	-3.584194	-2.433238
1	3.254634	-4.739367	-1.765139
6	1.931519	-3.135348	-0.053777
1	1.192676	-2.372118	0.212830
1	2.568607	-3.330875	0.825074
1	1.398489	-4.069906	-0.296529
6	1.905370	-2.501342	-2.508935

1	2.525079	-2.241624	-3.382991
1	1.169899	-1.704683	-2.349875
1	1.363625	-3.433742	-2.738322
6	0.808242	3.662293	0.672978
6	-0.497553	3.859986	-0.184235
6	1.754895	4.866621	0.555301
1	1.213253	5.794920	0.782607
1	2.576062	4.793067	1.283167
1	2.193202	4.964038	-0.447087
6	0.472273	3.453795	2.164398
1	1.370970	3.101065	2.692063
1	0.145754	4.393239	2.632777
1	-0.312100	2.699043	2.293493
6	-1.436972	4.900192	0.448853
1	-1.907456	4.516991	1.364789
1	-0.884901	5.816876	0.698178
1	-2.234883	5.194733	-0.247484
6	-0.147386	4.287060	-1.623090
1	-1.053153	4.254184	-2.246510
1	0.248364	5.312206	-1.655065
1	0.594150	3.601759	-2.059321
6	7.075066	0.074810	-0.834178
6	7.589459	-0.241804	-2.249068
6	7.744862	-0.835354	0.209758
1	7.366890	1.114318	-0.601731
1	7.142859	0.434610	-2.995018
1	8.686074	-0.138808	-2.303695
1	7.337944	-1.275116	-2.541197
1	7.409936	-0.584862	1.228941
1	7.500395	-1.895310	0.027927
1	8.842689	-0.737185	0.174386
6	-6.838466	0.309726	-1.304058
6	-7.599158	-0.365447	-0.149680
6	-7.308489	-0.234901	-2.663815
1	-7.084540	1.386047	-1.276637
1	-7.296412	0.052269	0.823768
1	-8.687981	-0.228898	-0.259104
1	-7.401074	-1.450137	-0.124926
1	-6.793608	0.272711	-3.494861
1	-7.103148	-1.314804	-2.752453
1	-8.394326	-0.092024	-2.792828
6	-1.493716	-0.346537	2.780266
6	-1.797592	-1.568885	3.370719
6	-0.784762	-2.503955	3.631577
6	0.532117	-2.125510	3.341787
6	0.801460	-0.881112	2.772075
1	-2.837444	-1.797288	3.613745
1	1.364528	-2.796335	3.565608
6	-1.111590	-3.868723	4.168309
1	-1.407862	-4.530589	3.335786
1	-0.247601	-4.329517	4.668539
1	-1.956657	-3.834061	4.872296
6	2.197152	-0.391019	2.540563
1	2.185764	0.511398	1.925021
1	2.667328	-0.150967	3.508642
1	2.812848	-1.151515	2.042286
6	-2.523895	0.706038	2.512708
1	-2.225895	1.301972	1.645762
1	-3.513356	0.267656	2.328420
1	-2.597979	1.385193	3.379111
7	-0.212805	-0.043676	2.465583
1	-0.047074	0.664838	1.394253

Structure S29. ^{3}TS9

27	1.402034	1.096566	-0.235218
8	2.309813	-0.579416	-0.113996
8	-0.140161	0.937681	0.970571
7	3.157656	2.126977	-0.344500
7	0.680131	2.854867	-0.893054
6	3.568601	-0.847028	0.061424
6	3.977751	-2.217943	0.272118
6	5.328376	-2.481689	0.466666
1	5.641890	-3.511858	0.636050
6	6.341410	-1.491060	0.459211
6	5.946028	-0.183986	0.246358
1	6.698357	0.611917	0.228763
6	4.586119	0.171606	0.051520
6	4.314827	1.575116	-0.175509
1	5.219319	2.201667	-0.204169
6	-0.569347	3.176830	-0.842750
1	-0.911454	4.085298	-1.359720
6	-1.608619	2.494601	-0.098481
6	-2.925047	2.998034	-0.236372
1	-3.107049	3.785421	-0.975992
6	-3.970293	2.544384	0.549152
6	-3.662738	1.577188	1.535641
1	-4.478913	1.245989	2.176086

6	-2.394862	1.037095	1.736285	1	2.559909	5.298199	0.730641
6	-1.323957	1.462568	0.864757	1	1.759837	3.778815	1.234424
6	2.922182	-3.343474	0.279867	6	-5.363782	3.147951	0.432690
6	2.217627	-3.399632	-1.096288	6	-5.586740	4.215576	1.519848
1	2.939999	-3.640938	-1.893115	6	-6.485985	2.100545	0.461449
1	1.748770	-2.436826	-1.329207	1	-5.409879	3.657526	-0.546084
1	1.437249	-4.179227	-1.096723	1	-4.820919	5.005542	1.466897
6	1.879705	-3.088067	1.394615	1	-6.578027	4.687921	1.416161
1	1.369142	-2.129347	1.248236	1	-5.531690	3.761988	2.524038
1	2.366494	-3.077124	2.383707	1	-6.320880	1.301028	-0.274942
1	1.122550	-3.890107	1.399143	1	-6.560897	1.622862	1.452384
6	3.549161	-4.726301	0.538769	1	-7.460287	2.573921	0.257222
1	4.048915	-4.776400	1.519230	6	7.800906	-1.864568	0.674554
1	4.282683	-5.001131	-0.235762	6	8.324251	-2.795069	-0.432990
1	2.758316	-5.493010	0.531213	6	8.036687	-2.477740	2.065484
6	-2.119216	0.035649	2.879433	1	8.383878	-0.928180	0.622702
6	-3.386864	-0.263115	3.702275	1	8.192765	-2.342195	-1.428494
1	-4.174356	-0.729054	3.089088	1	9.396178	-3.011497	-0.292085
1	-3.804819	0.643107	4.168248	1	7.787786	-3.758645	-0.429404
1	-3.140010	-0.967754	4.511813	1	7.698217	-1.797514	2.863012
6	-1.600190	-1.311304	2.327103	1	7.487887	-3.427509	2.179669
1	-0.653497	-1.178489	1.791744	1	9.106486	-2.691135	2.225842
1	-2.333519	-1.760916	1.639579	1	0.797708	0.710414	-1.595546
1	-1.431932	-2.019680	3.155377	6	-5.254805	-3.256132	-1.234447
6	-1.067652	0.640367	3.839868	6	-4.148263	-3.997104	-1.665763
1	-1.437817	1.581764	4.278215	6	-2.873386	-3.413828	-1.694240
1	-0.127550	0.845742	3.312100	6	-2.668617	-2.092503	-1.289241
1	-0.858821	-0.059861	4.666152	6	-3.782354	-1.355203	-0.847963
6	1.716028	3.697084	-1.532727	6	-5.057097	-1.914273	-0.820044
6	2.982709	3.578497	-0.569138	1	-4.267675	-5.030798	-1.990376
6	1.267197	5.153976	-1.715130	1	-2.025327	-4.011698	-2.039073
1	2.100680	5.771077	-2.075238	1	-3.671617	-0.325611	-0.500302
1	0.473224	5.224539	-2.473114	8	-6.121974	-1.144876	-0.428892
1	0.888036	5.594349	-0.782471	8	-6.530407	-3.719097	-1.181893
6	2.030829	3.095858	-2.916597	6	-6.685851	-1.459501	0.840339
1	1.107065	3.045329	-3.511844	1	-5.939408	-1.334298	1.644942
1	2.751746	3.720258	-3.462646	1	-7.509288	-0.752252	1.007987
1	2.439758	2.080526	-2.824655	1	-7.077783	-2.488800	0.863909
6	4.225125	4.249538	-1.171971	6	-6.793163	-5.054611	-1.569744
1	4.585162	3.723943	-2.067672	1	-6.248450	-5.778575	-0.937879
1	4.011075	5.291757	-1.442955	1	-7.872598	-5.210020	-1.442873
1	5.046980	4.278509	-0.441612	1	-6.526085	-5.232417	-2.626548
6	2.676727	4.207643	0.805210	6	-1.294466	-1.463194	-1.320681
1	3.508963	3.999944	1.494369	1	-1.076912	-0.998531	-0.340807

1	-0.520730	-2.233269	-1.458442
6	-1.120768	-0.370731	-2.331134
6	0.082236	-0.066482	-2.888008
1	-1.968073	0.309260	-2.476079
1	0.180302	0.760270	-3.595305
1	0.908812	-0.782132	-2.852844

Structure S30. 5

6	-1.186658	-0.563648	-0.014054
6	-0.217274	-1.520618	0.389319
6	1.094198	-1.146183	0.549493
6	1.514468	0.205079	0.317425
6	0.508978	1.166023	-0.054912
6	-0.804967	0.809641	-0.225477
1	-0.508178	-2.555468	0.562161
1	1.828317	-1.893308	0.854145
1	0.785014	2.208053	-0.228438
8	-1.710438	1.718785	-0.653267
8	-2.450430	-0.840680	-0.233029
6	-2.729758	2.120829	0.271936
1	-2.278168	2.553954	1.180434
1	-3.324052	2.888567	-0.239470
1	-3.381546	1.278252	0.547806
6	-2.970890	-2.170344	-0.073804
1	-2.857492	-2.505901	0.967742
1	-4.033545	-2.103405	-0.330304
1	-2.463484	-2.866007	-0.758569
6	2.818323	0.728422	1.037878
1	2.735789	1.763167	1.377362
1	3.216553	0.026659	1.775294
6	2.994250	0.438948	-0.367785
1	2.924714	1.287083	-1.055173
6	3.762471	-0.739876	-0.900852
1	3.312227	-1.127119	-1.826240
1	4.781368	-0.393627	-1.140547
1	3.850581	-1.555390	-0.170838

Structure S31. BF_4^-

5	-0.000120	0.000083	0.000231
9	-1.074255	0.824353	0.377388
9	1.198710	0.530266	0.507853
9	-0.196881	-1.292383	0.516657
9	0.072493	-0.062282	-1.402027

Structure S32. ^{1}INT3

6	-2.697415	-0.034433	-0.050831
6	-2.583976	-1.404102	0.303055
6	-1.342241	-1.960286	0.505817
6	-0.152934	-1.179450	0.369347
6	-0.285648	0.209301	0.029827
6	-1.519598	0.774590	-0.185392
1	-3.475662	-2.019721	0.409949
1	-1.267087	-3.014527	0.775986
1	0.608455	0.823582	-0.077318
8	-1.624666	2.069944	-0.576695
8	-3.841207	0.577539	-0.287779
6	-2.115139	2.996142	0.397488
1	-1.455933	3.015935	1.282252
1	-2.108736	3.984556	-0.080098
1	-3.142547	2.749334	0.708891
6	-5.091278	-0.116212	-0.191649
1	-5.252045	-0.488398	0.831804
1	-5.861190	0.622024	-0.441982
1	-5.129361	-0.950228	-0.908949
6	1.155408	-1.638460	1.140176
1	1.727166	-0.790851	1.521461
1	0.965542	-2.456942	1.839705
6	1.195206	-1.923029	-0.269886
1	1.711400	-1.186706	-0.890768
6	1.062480	-3.297911	-0.861332
1	0.521996	-3.277272	-1.818774
1	2.082660	-3.666374	-1.061131
1	0.576470	-4.012786	-0.183314
5	3.372538	0.856356	-0.052047
9	2.557381	0.826675	-1.211158
9	4.376642	1.808371	-0.200388
9	2.551307	1.188855	1.054116
9	3.916222	-0.418366	0.151718

Structure S33. ^{1}TS12

6	-3.003311	-0.254023	-0.003170
6	-2.551448	-1.506293	0.451225
6	-1.206283	-1.702973	0.756260
6	-0.287644	-0.646625	0.644623

6	-0.739376	0.608684	0.181202
6	-2.074331	0.819540	-0.133768
1	-3.248202	-2.336614	0.559625
1	-0.872371	-2.685256	1.097588
1	-0.040782	1.439652	0.060287
8	-2.461921	2.029601	-0.620304
8	-4.269419	0.018551	-0.352485
6	-3.316427	2.818166	0.210334
1	-2.831245	3.031977	1.178892
1	-3.485656	3.763393	-0.322676
1	-4.282843	2.321213	0.386840
6	-5.263910	-0.995286	-0.269955
1	-5.385233	-1.354172	0.765734
1	-6.200266	-0.533184	-0.605654
1	-5.021459	-1.846995	-0.927176
6	1.195938	-0.837143	0.979498
1	1.655127	0.086245	1.346791
1	1.367354	-1.675060	1.665593
6	1.524092	-1.135754	-0.409619
1	1.550216	-0.284315	-1.091660
6	1.550242	-2.485073	-0.999934
1	0.750600	-2.583430	-1.752584
1	2.499340	-2.568318	-1.555359
1	1.478650	-3.287915	-0.255616
5	3.947098	0.622698	-0.020837
9	2.911173	1.396515	-0.567763
9	5.168428	0.954795	-0.573068
9	3.947950	0.740683	1.365919
9	3.663198	-0.768131	-0.347789

Structure S34. ^{1}INT4

6	-3.093260	-0.277251	0.024107
6	-2.594009	-1.484600	0.529501
6	-1.224734	-1.636042	0.786061
6	-0.325037	-0.592054	0.553286
6	-0.833560	0.621735	0.058248
6	-2.190316	0.793007	-0.207335
1	-3.265441	-2.321558	0.720576
1	-0.860837	-2.590501	1.175188
1	-0.170782	1.469517	-0.134135
8	-2.618637	1.980307	-0.733388
8	-4.393841	-0.042268	-0.279175
6	-3.442001	2.787365	0.105258
1	-2.915727	3.048540	1.041209
1	-3.655837	3.709651	-0.452783
1	-4.390214	2.283871	0.351416
6	-5.349144	-1.065894	-0.065204
1	-5.403086	-1.357517	0.998550
1	-6.319339	-0.655565	-0.373998
1	-5.127572	-1.961891	-0.671260
6	1.161323	-0.753003	0.779423
1	1.576628	0.163832	1.223113
1	1.366371	-1.578926	1.478537
6	1.904610	-1.017841	-0.525710
1	1.715635	-0.209255	-1.246167
6	1.691333	-2.376774	-1.143194
1	0.631503	-2.489038	-1.415547
1	2.300537	-2.490335	-2.051348
1	1.954362	-3.171657	-0.428550
5	4.153854	0.851519	0.121389
9	3.272293	1.573830	-0.570267
9	5.325307	0.564609	-0.432961
9	4.041576	0.822726	1.446542
9	3.323395	-0.917052	-0.230856

Structure S35. BF_3

5	0.000000	0.000433	0.000091
9	-1.139194	0.656956	-0.000017
9	1.138892	0.657479	-0.000017
9	0.000302	-1.314676	-0.000017

Structure S36. ^{3}TS10

27	-0.861762	0.834171	-0.267587
8	-2.172895	-0.514303	-0.112391
8	0.386391	-0.551439	-0.604698
7	-2.137176	2.163591	-0.757287
7	0.424571	2.202280	-0.499196
6	-3.461333	-0.428713	-0.117237
6	-4.264274	-1.599458	0.170900
6	-5.644439	-1.456346	0.176988
1	-6.257510	-2.329098	0.401237
6	-6.329844	-0.240369	-0.090666
6	-5.562425	0.868119	-0.380427
1	-6.046460	1.825226	-0.601146
6	-4.142705	0.806606	-0.398700

6	-3.429027	2.000280	-0.738701	6	-0.425473	4.006052	0.937904
1	-4.064822	2.846673	-1.026509	1	0.514350	3.960315	1.505671
6	1.684955	2.005522	-0.748463	1	-0.796704	5.039096	0.980818
1	2.329862	2.881766	-0.875086	1	-1.155350	3.345199	1.418835
6	2.351197	0.750673	-0.951829	6	-2.428662	4.634548	-1.159905
6	3.717665	0.790794	-1.325100	1	-2.828112	4.735589	-0.141380
1	4.214184	1.765002	-1.378027	1	-1.872382	5.548888	-1.405582
6	4.413785	-0.355139	-1.656886	1	-3.275991	4.586593	-1.858837
6	3.706730	-1.583272	-1.597905	6	-1.256519	3.138072	-2.801451
1	4.257466	-2.485116	-1.865774	1	-2.198772	2.852858	-3.292328
6	2.364768	-1.698765	-1.252862	1	-0.868311	4.034805	-3.304512
6	1.645721	-0.493771	-0.910120	1	-0.539328	2.314686	-2.931609
6	-3.587033	-2.953035	0.463895	6	5.854679	-0.299127	-2.146258
6	-2.686571	-2.834229	1.715961	6	5.956263	-0.704105	-3.627572
1	-3.278834	-2.533390	2.595723	6	6.811764	-1.132666	-1.280933
1	-1.893361	-2.094880	1.560301	1	6.177068	0.754712	-2.071256
1	-2.215430	-3.806189	1.937688	1	5.304195	-0.078652	-4.257645
6	-2.733032	-3.380469	-0.751525	1	6.991110	-0.602829	-3.994775
1	-1.947427	-2.645686	-0.955960	1	5.652624	-1.754666	-3.770644
1	-3.362793	-3.488811	-1.650059	1	6.776317	-0.807180	-0.232626
1	-2.251118	-4.352616	-0.555451	1	6.547758	-2.202691	-1.311028
6	-4.615557	-4.067394	0.732983	1	7.848673	-1.038426	-1.643396
1	-5.279964	-4.234548	-0.129706	6	-7.849848	-0.181552	-0.057253
1	-5.241669	-3.851132	1.613305	6	-8.403723	-0.500154	1.342103
1	-4.085411	-5.012562	0.929447	6	-8.483270	-1.093627	-1.121749
6	1.623802	-3.049998	-1.308809	1	-8.136796	0.857086	-0.298167
6	2.573914	-4.217695	-1.633739	1	-7.981368	0.177262	2.101092
1	3.368083	-4.322072	-0.876629	1	-9.501423	-0.399289	1.363209
1	3.052217	-4.106196	-2.619564	1	-8.159580	-1.533152	1.641330
1	2.003792	-5.160037	-1.649983	1	-8.117592	-0.842317	-2.129914
6	0.938188	-3.372681	0.039370	1	-8.243669	-2.153289	-0.932383
1	0.233912	-2.584077	0.324915	1	-9.581498	-0.996491	-1.119736
1	1.687829	-3.485011	0.837718	6	4.332085	-0.501663	2.125493
1	0.385175	-4.323015	-0.039639	6	3.196214	-1.318680	2.156965
6	0.560306	-2.976094	-2.431016	6	1.928797	-0.786721	2.401867
1	1.042542	-2.806795	-3.407750	6	1.751663	0.583876	2.610048
1	-0.148192	-2.159906	-2.242725	6	2.887099	1.403674	2.538838
1	-0.006117	-3.920398	-2.487635	6	4.167457	0.892911	2.304454
6	-0.164441	3.574574	-0.513786	1	3.295775	-2.390724	1.997163
6	-1.521008	3.404258	-1.305560	1	1.073953	-1.463203	2.420591
6	0.750108	4.617398	-1.173070	1	2.803689	2.484950	2.675601
1	0.212437	5.568422	-1.284416	8	5.202867	1.785074	2.329526
1	1.626848	4.823384	-0.541962	8	5.600959	-0.971946	1.954607
1	1.105174	4.307056	-2.164914	6	6.239019	1.704075	1.356433

1	5.843972	1.404418	0.373851
1	6.674177	2.711508	1.277652
1	7.021553	0.989349	1.651342
6	5.794601	-2.366700	1.817899
1	5.274897	-2.765081	0.929479
1	6.874460	-2.521365	1.695817
1	5.449121	-2.913333	2.713277
6	0.401426	1.166475	2.965753
1	0.237979	0.992608	4.055481
1	0.436971	2.263246	2.874983
6	-0.796839	0.619360	2.240174
1	-0.752832	-0.445303	1.998387
6	-2.136274	1.094452	2.723359
1	-2.346477	0.707340	3.743353
1	-2.186945	2.194087	2.797815
1	-2.958157	0.758825	2.077372

Structure S37. Co^{III}(salen)-alkyl

27	0.853036	0.847040	0.207603
8	2.161461	-0.536634	0.252385
8	-0.403788	-0.535239	0.487255
7	2.154827	2.194048	0.565121
7	-0.418552	2.235176	0.491297
6	3.447711	-0.455672	0.140711
6	4.234009	-1.638529	-0.138934
6	5.614443	-1.502494	-0.212280
1	6.214173	-2.387167	-0.425608
6	6.313735	-0.280628	-0.030164
6	5.560081	0.846778	0.227942
1	6.054393	1.812991	0.373834
6	4.144258	0.791539	0.301433
6	3.440383	2.003536	0.603604
1	4.079448	2.835813	0.923750
6	-1.680913	2.032058	0.732736
1	-2.327652	2.905654	0.872590
6	-2.346830	0.776638	0.920387
6	-3.715966	0.812218	1.288610
1	-4.217751	1.784350	1.331300
6	-4.408789	-0.335270	1.618138
6	-3.688578	-1.557335	1.590119
1	-4.230782	-2.457129	1.880511
6	-2.349248	-1.671311	1.241438
6	-1.643363	-0.469378	0.852596
6	3.542637	-2.997060	-0.366396
6	2.572227	-2.892534	-1.566574
1	3.116402	-2.613387	-2.483711
1	1.796772	-2.142111	-1.377064
1	2.079565	-3.862855	-1.743165
6	2.761330	-3.403693	0.902639
1	1.995077	-2.660045	1.142596
1	3.443579	-3.503555	1.763125
1	2.262270	-4.375001	0.749641
6	4.552131	-4.117666	-0.678088
1	5.261894	-4.277845	0.149085
1	5.130231	-3.913452	-1.593446
1	4.009246	-5.063189	-0.834247
6	-1.597509	-3.013012	1.350061
6	-2.533730	-4.172286	1.739533
1	-3.329973	-4.324401	0.992792
1	-3.008653	-4.015698	2.720813
1	-1.952826	-5.106097	1.801198
6	-0.917982	-3.395028	0.015745
1	-0.205236	-2.625711	-0.296573
1	-1.669490	-3.526907	-0.778202
1	-0.375821	-4.348062	0.129992
6	-0.527588	-2.873679	2.459682
1	-1.004956	-2.657545	3.429498
1	0.173554	-2.063304	2.223849
1	0.047646	-3.808627	2.561141
6	0.155885	3.614427	0.549470
6	1.577806	3.419257	1.198889
6	-0.708743	4.578942	1.380221
1	-0.156869	5.509927	1.567926
1	-1.620689	4.859035	0.833438
1	-1.005698	4.154900	2.348647
6	0.277071	4.193884	-0.868954
1	-0.702725	4.162788	-1.366046
1	0.597478	5.243843	-0.831842
1	0.997787	3.630764	-1.471540
6	2.468615	4.657172	1.005961
1	2.802726	4.763575	-0.035036
1	1.923583	5.567236	1.290761
1	3.358147	4.612492	1.649969
6	1.454431	3.111601	2.707157
1	2.437311	2.814010	3.100859
1	1.116722	3.993016	3.269759
1	0.750219	2.284881	2.885232

6	-5.863923	-0.296464	2.063121
6	-6.007601	-0.665424	3.550182
6	-6.769564	-1.177083	1.187467
1	-6.207409	0.747142	1.949148
1	-5.395898	-0.005333	4.185369
1	-7.057274	-0.584215	3.878359
1	-5.680290	-1.702806	3.732142
1	-6.689746	-0.894514	0.128796
1	-6.493332	-2.241167	1.272815
1	-7.823666	-1.084732	1.497068
6	7.831612	-0.230769	-0.122368
6	8.333208	-0.619188	-1.523811
6	8.500620	-1.093648	0.961191
1	8.130483	0.816887	0.057322
1	7.885256	0.022569	-2.298939
1	9.429695	-0.524425	-1.589676
1	8.075443	-1.664344	-1.763354
1	8.172850	-0.792407	1.968739
1	8.250394	-2.159861	0.831816
1	9.598390	-1.002402	0.914705
6	-4.318339	-0.555038	-2.188518
6	-3.163485	-1.346939	-2.177618
6	-1.893691	-0.773695	-2.281004
6	-1.735077	0.610744	-2.373751
6	-2.895203	1.398994	-2.374983
6	-4.175842	0.849146	-2.291626
1	-3.248090	-2.428935	-2.089395
1	-1.021274	-1.426416	-2.257831
1	-2.828095	2.488076	-2.438467
8	-5.234538	1.712498	-2.373813
8	-5.586466	-1.052617	-2.123025
6	-6.290914	1.621328	-1.423809
1	-5.904355	1.399764	-0.416704
1	-6.786288	2.603466	-1.409569
1	-7.022355	0.846502	-1.697394
6	-5.764476	-2.451299	-2.006586
1	-5.287177	-2.848228	-1.093754
1	-6.846973	-2.623732	-1.945160
1	-5.362277	-2.986771	-2.884845
6	-0.383009	1.261161	-2.543347
1	-0.121012	1.169784	-3.618718
1	-0.481680	2.339013	-2.378771
6	0.822693	0.707703	-1.784641
1	0.811812	-0.389419	-1.825116
6	2.113954	1.215634	-2.407051
1	2.167200	0.898277	-3.465874
1	2.177412	2.314777	-2.400160
1	3.009060	0.825711	-1.912189

Structure S38. $[Co^{IV}(salen)\text{-}alkyl]^{+}$

27	0.844961	0.867528	0.226707
8	2.126403	-0.497447	0.222845
8	-0.391958	-0.472607	0.480878
7	2.124298	2.185425	0.601727
7	-0.424036	2.243528	0.456194
6	3.420024	-0.442007	0.137108
6	4.187686	-1.633790	-0.138622
6	5.567473	-1.501821	-0.196030
1	6.163301	-2.388331	-0.408184
6	6.276704	-0.284780	0.001861
6	5.538932	0.849253	0.264214
1	6.039055	1.808832	0.422885
6	4.120881	0.800287	0.322108
6	3.418625	2.001067	0.620079
1	4.048988	2.847584	0.911441
6	-1.695864	2.048300	0.668828
1	-2.336917	2.929529	0.768100
6	-2.361267	0.802348	0.876051
6	-3.728668	0.834516	1.242672
1	-4.242242	1.799472	1.268020
6	-4.398138	-0.320090	1.598286
6	-3.664137	-1.533622	1.584644
1	-4.194635	-2.434482	1.889417
6	-2.322945	-1.641105	1.236876
6	-1.646347	-0.433633	0.838292
6	3.495863	-2.990541	-0.365001
6	2.531183	-2.893978	-1.569868
1	3.072591	-2.597897	-2.482595
1	1.735281	-2.165170	-1.383330
1	2.057388	-3.871209	-1.753539
6	2.717932	-3.387415	0.908722
1	1.954629	-2.642970	1.154081
1	3.402887	-3.487189	1.766187
1	2.214860	-4.356273	0.760177
6	4.508833	-4.110006	-0.669459
1	5.216067	-4.265506	0.160187
1	5.086675	-3.909916	-1.585586

1	3.966693	-5.055982	-0.820757
6	-1.559824	-2.972141	1.369194
6	-2.491192	-4.132335	1.767507
1	-3.282939	-4.297739	1.019252
1	-2.968751	-3.969077	2.746003
1	-1.903433	-5.060233	1.840811
6	-0.872545	-3.364994	0.042968
1	-0.163335	-2.599003	-0.283128
1	-1.619192	-3.516704	-0.751194
1	-0.321548	-4.309560	0.173508
6	-0.504640	-2.803450	2.489216
1	-0.995953	-2.578823	3.449483
1	0.194907	-1.990273	2.257085
1	0.076113	-3.731687	2.610140
6	0.155552	3.627511	0.509413
6	1.545769	3.427510	1.212814
6	-0.735880	4.602894	1.293703
1	-0.187961	5.536355	1.477960
1	-1.629453	4.873348	0.713532
1	-1.058230	4.198311	2.262016
6	0.327407	4.172014	-0.916834
1	-0.634928	4.142306	-1.446553
1	0.654804	5.219295	-0.889734
1	1.067678	3.596286	-1.483408
6	2.459489	4.648734	1.030203
1	2.819228	4.747547	-0.002790
1	1.915538	5.564631	1.295994
1	3.329447	4.599607	1.699488
6	1.380535	3.132271	2.718617
1	2.351299	2.832743	3.139446
1	1.038824	4.025234	3.258981
1	0.666282	2.314050	2.895161
6	-5.845503	-0.293624	2.065153
6	-5.946685	-0.626141	3.564519
6	-6.749485	-1.213410	1.229639
1	-6.207917	0.740533	1.932139
1	-5.331616	0.059533	4.168186
1	-6.990097	-0.549038	3.910589
1	-5.602527	-1.654148	3.765924
1	-6.700299	-0.953562	0.163538
1	-6.453405	-2.270063	1.334419
1	-7.796442	-1.130268	1.562466
6	7.794182	-0.254508	-0.078274
6	8.296041	-0.648179	-1.478062
6	8.436880	-1.130451	1.010740
1	8.104969	0.788030	0.106111
1	7.860344	-0.000905	-2.255318
1	9.393100	-0.562474	-1.534187
1	8.032148	-1.691070	-1.719628
1	8.103098	-0.827517	2.015543
1	8.177592	-2.193415	0.874676
1	9.535153	-1.049706	0.974065
6	-4.278564	-0.589314	-2.150685
6	-3.123596	-1.382118	-2.179016
6	-1.857605	-0.813454	-2.330767
6	-1.707324	0.571272	-2.427923
6	-2.862477	1.364405	-2.393478
6	-4.141548	0.817523	-2.264737
1	-3.208539	-2.464013	-2.094235
1	-0.989790	-1.473379	-2.354935
1	-2.796263	2.452626	-2.464476
8	-5.185868	1.690810	-2.319460
8	-5.536654	-1.090555	-2.041331
6	-6.305194	1.550756	-1.449033
1	-5.989084	1.266893	-0.434012
1	-6.790061	2.536678	-1.410426
1	-7.020960	0.802762	-1.818442
6	-5.712544	-2.493154	-1.939207
1	-5.205607	-2.901654	-1.048079
1	-6.792390	-2.663679	-1.844600
1	-5.340043	-3.013148	-2.838738
6	-0.364253	1.222567	-2.633429
1	-0.102975	1.118345	-3.709590
1	-0.433951	2.305498	-2.485337
6	0.851107	0.662978	-1.946126
1	0.836471	-0.423593	-1.827371
6	2.157407	1.183524	-2.468585
1	2.300785	0.747800	-3.475710
1	2.164828	2.276234	-2.581896
1	3.025612	0.874034	-1.878976

Structure S39. ^{2}TS11

27	0.661713	1.407067	0.357526
8	2.011779	0.222161	0.905691
8	-0.570156	0.130575	0.928406
7	1.891689	2.782865	-0.010307
7	-0.661025	2.657466	-0.135256

6	3.295951	0.283592	0.739297	1	0.093148	-0.904868	2.833447
6	4.140797	-0.816086	1.150343	1	-0.101089	-2.366422	3.829974
6	5.487602	-0.745918	0.827872	6	-0.124672	3.886893	-0.791824
1	6.130788	-1.580695	1.103870	6	1.259355	4.132126	-0.083733
6	6.106707	0.351998	0.167789	6	-1.062487	5.094306	-0.651640
6	5.315045	1.436307	-0.139876	1	-0.555276	6.005608	-0.994891
1	5.753131	2.322877	-0.608643	1	-1.955152	4.974949	-1.282341
6	3.920007	1.431357	0.136555	1	-1.390291	5.252014	0.384600
6	3.180550	2.628504	-0.122784	6	0.077224	3.589169	-2.288300
1	3.786761	3.491664	-0.418881	1	-0.865726	3.230570	-2.725352
6	-1.932705	2.520862	0.109830	1	0.371696	4.495567	-2.834351
1	-2.609116	3.327022	-0.193807	1	0.856738	2.829630	-2.439899
6	-2.568829	1.429556	0.779352	6	2.119180	5.160798	-0.830310
6	-3.951809	1.560373	1.063869	1	2.461274	4.794438	-1.807835
1	-4.475810	2.454060	0.713315	1	1.545675	6.083153	-0.991331
6	-4.632747	0.594670	1.774075	1	3.002272	5.440084	-0.237941
6	-3.895552	-0.540721	2.196932	6	1.063376	4.599296	1.373354
1	-4.436886	-1.295962	2.766097	1	2.031476	4.581522	1.895038
6	-2.541435	-0.741663	1.948938	1	0.674794	5.626578	1.409250
6	-1.839888	0.269894	1.195821	1	0.370716	3.936406	1.911742
6	3.560434	-1.990635	1.959407	6	-6.105709	0.752277	2.122407
6	2.407526	-2.672105	1.193486	6	-6.334305	0.779316	3.643048
1	2.728841	-3.011387	0.199828	6	-6.974366	-0.319773	1.446974
1	1.559571	-1.993520	1.068112	1	-6.423036	1.731639	1.723307
1	2.051909	-3.552739	1.752896	1	-5.737629	1.571008	4.123565
6	3.050095	-1.439501	3.311653	1	-7.396689	0.959770	3.876116
1	2.292112	-0.660642	3.160948	1	-6.052727	-0.181095	4.106117
1	3.880809	-1.013940	3.898253	1	-6.826044	-0.308492	0.358584
1	2.591931	-2.248664	3.903560	1	-6.711088	-1.327673	1.809422
6	4.623147	-3.064941	2.256135	1	-8.042456	-0.155887	1.666344
1	5.469414	-2.670110	2.840566	6	7.592905	0.323660	-0.152841
1	5.018941	-3.514387	1.331495	6	7.937675	-0.807782	-1.136310
1	4.164962	-3.873353	2.846830	6	8.452744	0.233106	1.119464
6	-1.794198	-1.970684	2.504546	1	7.833316	1.280289	-0.648470
6	-2.710143	-2.866945	3.359111	1	7.349358	-0.723274	-2.063572
1	-3.554080	-3.271332	2.777627	1	9.006875	-0.781662	-1.402872
1	-3.117497	-2.333012	4.232552	1	7.728843	-1.796574	-0.695330
1	-2.130163	-3.724562	3.734729	1	8.230424	1.061202	1.810850
6	-1.245778	-2.833436	1.349415	1	8.272841	-0.712362	1.657462
1	-0.614631	-2.252560	0.671743	1	9.525368	0.272539	0.868854
1	-2.069663	-3.261503	0.760338	6	-4.309261	-1.223894	-1.640415
1	-0.640363	-3.664069	1.745670	6	-3.261548	-2.149242	-1.565852
6	-0.629280	-1.497254	3.405122	6	-1.952109	-1.777544	-1.880694
1	-1.007949	-0.887004	4.242087	6	-1.658499	-0.470029	-2.277207

6	-2.712056	0.452457	-2.366959
6	-4.021512	0.100482	-2.048789
1	-3.455123	-3.173749	-1.251060
1	-1.158408	-2.518045	-1.805237
1	-2.534939	1.486684	-2.668307
8	-4.990896	1.067343	-2.071409
8	-5.601417	-1.502059	-1.336425
6	-6.000727	0.931021	-3.067661
1	-6.579152	0.003084	-2.936161
1	-6.672353	1.794353	-2.959611
1	-5.560054	0.943294	-4.081088
6	-5.925951	-2.778582	-0.814859
1	-5.371910	-2.984303	0.117273
1	-7.000800	-2.759612	-0.595135
1	-5.718892	-3.580818	-1.544088
6	-0.265734	-0.063793	-2.680528
1	-0.047463	-0.386656	-3.719158
1	-0.164916	1.033138	-2.747521
6	0.883505	-0.545780	-1.902087
1	0.723641	-1.121526	-0.985586
6	2.256557	-0.296674	-2.326923
1	2.808823	-1.250315	-2.283975
1	2.330243	0.169399	-3.317438
1	2.761394	0.341460	-1.577261
5	1.338272	-3.703913	-2.345501
9	0.629910	-3.795696	-1.143813
9	1.186095	-4.852637	-3.107640
9	0.811669	-2.583753	-3.077536
9	2.697668	-3.448263	-2.095835

Structure S40. ^{1}TS13

6	3.078875	-0.326086	-0.024937
6	2.457776	-1.544432	-0.353794
6	1.086003	-1.704841	-0.182064
6	0.298209	-0.660614	0.341846
6	0.922355	0.577302	0.633576
6	2.286175	0.753623	0.470157
1	3.046175	-2.376787	-0.737655
1	0.630154	-2.661732	-0.439899
1	0.341259	1.418511	1.017344
8	2.857393	1.931345	0.838648
8	4.390938	-0.087925	-0.130128
6	3.386404	2.749586	-0.207595
1	2.597159	3.015608	-0.932424
1	3.758974	3.665515	0.270094
1	4.214378	2.250480	-0.734220
6	5.265105	-1.102075	-0.615983
1	5.002828	-1.394221	-1.646192
1	6.271615	-0.666935	-0.606165
1	5.244344	-1.990624	0.036081
6	-1.383967	-0.409916	-0.784226
1	-1.341614	0.647448	-1.041282
1	-1.276967	-1.138070	-1.590240
6	-1.217615	-0.827872	0.596195
1	-1.551662	-0.052504	1.295655
6	-1.731089	-2.201998	0.991714
1	-1.298643	-2.509016	1.955005
1	-2.822876	-2.138550	1.090817
1	-1.496971	-2.969645	0.239545
5	-4.082371	0.528923	-0.190470
9	-4.225619	-0.135498	1.022005
9	-5.297651	0.841352	-0.761959
9	-3.264741	1.648557	-0.048365
9	-3.387805	-0.388579	-1.109637

Structure S41. 6

6	1.746541	-0.516891	0.038650
6	0.827403	-1.552025	-0.179851
6	-0.548555	-1.318699	-0.063855
6	-1.048187	-0.053489	0.269839
6	-0.119743	0.981482	0.470398
6	1.254732	0.771799	0.364500
1	1.175902	-2.553581	-0.431973
1	-1.233155	-2.153205	-0.233704
1	-0.453213	1.990131	0.726965
8	2.105303	1.810463	0.630337
8	3.095513	-0.650931	-0.022206
6	2.853458	2.316197	-0.472175
1	2.182572	2.673324	-1.274608
1	3.440822	3.165186	-0.095037
1	3.536860	1.556761	-0.883978
6	3.649965	-1.913159	-0.345239
1	3.333106	-2.254336	-1.346715
1	4.740270	-1.785271	-0.339029
1	3.373466	-2.681487	0.398119
6	-3.172113	0.147589	-1.016837

1	-2.679578	0.856334	-1.703928
1	-3.089129	-0.869487	-1.439477
6	-2.541002	0.213117	0.374481
1	-2.676246	1.249454	0.727714
6	-3.266034	-0.721180	1.352815
1	-2.847116	-0.629212	2.366411
1	-4.336841	-0.471442	1.391984
1	-3.178140	-1.774889	1.042071
9	-4.523879	0.475223	-0.947358

Structure S42. 7

6	-1.917589	-0.592120	-0.090184
6	-0.968849	-1.590981	0.169932
6	0.394322	-1.280069	0.214821
6	0.863650	0.025147	0.008202
6	-0.097122	1.018396	-0.240266
6	-1.462568	0.731780	-0.292811
1	-1.283879	-2.622484	0.328889
1	1.110088	-2.082646	0.409906
1	0.180652	2.058672	-0.409822
8	-2.336276	1.743953	-0.594253
8	-3.257986	-0.795788	-0.179984
6	-3.213407	2.151954	0.451059
1	-2.644439	2.497330	1.333655
1	-3.807358	2.990423	0.060416
1	-3.891431	1.338529	0.755122
6	-3.769951	-2.100489	0.016265
1	-3.537266	-2.484183	1.025615
1	-4.859729	-2.028497	-0.096338
1	-3.377384	-2.809959	-0.733643
6	2.371267	0.315858	0.105807
6	3.128461	-0.693986	-0.732408
1	2.702403	-0.922269	-1.715091
6	4.535326	-1.098196	-0.446499
1	4.919280	-1.792593	-1.208864
1	5.223751	-0.227084	-0.419013
1	4.640286	-1.588778	0.538989
6	2.786435	0.239286	1.596140
1	2.609508	-0.765726	2.009037
1	3.853116	0.480721	1.726337
1	2.201255	0.959061	2.189302
6	2.724148	1.731079	-0.419010
1	2.394196	1.866916	-1.460298
1	2.262215	2.520051	0.196646
1	3.814093	1.881241	-0.383240

Structure S43. 8

6	-1.726290	-0.578984	-0.037075
6	-0.794801	-1.607346	0.239818
6	0.557031	-1.379663	0.091474
6	1.057016	-0.112357	-0.328932
6	0.097424	0.914947	-0.605592
6	-1.255353	0.707584	-0.467397
1	-1.139358	-2.590509	0.556623
1	1.242308	-2.200366	0.296060
1	0.413722	1.896932	-0.956879
8	-2.128778	1.684976	-0.810192
8	-3.035244	-0.711754	0.051952
6	-2.875999	2.296764	0.248368
1	-2.197013	2.756436	0.986679
1	-3.487928	3.079852	-0.217339
1	-3.532992	1.571612	0.752024
6	-3.631067	-1.952841	0.450828
1	-3.311313	-2.228703	1.467294
1	-4.713044	-1.781622	0.436389
1	-3.371593	-2.752672	-0.259213
6	2.534193	0.415487	0.486867
6	2.521974	0.028569	-0.912068
1	2.536187	0.874581	-1.607610
6	3.212994	-1.193531	-1.476077
1	2.725997	-1.506509	-2.410704
1	4.257738	-0.930053	-1.703349
1	3.227431	-2.048368	-0.788955
6	3.023339	-0.499268	1.581843
1	3.037576	-1.560512	1.314978
1	4.061737	-0.202392	1.806441
1	2.433938	-0.364734	2.500102
6	2.523785	1.872794	0.879194
1	2.236914	2.544611	0.062011
1	1.872804	2.050373	1.747277
1	3.553589	2.133321	1.176597

Structure S44. ^{1}TS14

6	-3.244945	-0.245771	-0.299958
6	-2.695123	-1.526143	-0.115005

6	-1.379352	-1.678944	0.316061
6	-0.573228	-0.562456	0.603632
6	-1.131349	0.721515	0.409385
6	-2.438734	0.893349	-0.026971
1	-3.291793	-2.415297	-0.315348
1	-0.991250	-2.690121	0.431719
1	-0.558319	1.628687	0.598083
8	-2.905323	2.155463	-0.238196
8	-4.490546	-0.002958	-0.736770
6	-3.931844	2.618466	0.640925
1	-3.586140	2.601764	1.689646
1	-4.148832	3.655486	0.351335
1	-4.848260	2.015234	0.548828
6	-5.362502	-1.087800	-1.030081
1	-5.544714	-1.708395	-0.136688
1	-6.308028	-0.640141	-1.359755
1	-4.957474	-1.719548	-1.838072
6	0.901029	-0.721198	1.093180
6	1.395544	-0.599271	-0.290889
1	1.442400	0.424440	-0.672926
6	1.528477	-1.666508	-1.302752
1	0.675730	-1.600946	-1.999391
1	2.427835	-1.438769	-1.893787
1	1.584549	-2.676223	-0.880886
5	4.064098	0.651151	-0.554878
9	4.065898	0.308165	-1.903978
9	5.337404	0.824133	-0.055420
9	3.258228	1.770395	-0.333853
9	3.448927	-0.466298	0.166796
6	1.353086	0.440175	1.993524
1	0.685325	0.518994	2.863629
1	2.377068	0.247143	2.337564
1	1.373786	1.400823	1.463745
6	1.193038	-2.058539	1.780047
1	2.273131	-2.126971	1.971774
1	0.657753	-2.105593	2.739331
1	0.905009	-2.935163	1.186804

Structure S45. 9

6	-2.162712	-0.493220	-0.069737
6	-1.391118	-1.607865	0.274351
6	-0.008265	-1.488661	0.477113
6	0.650695	-0.261087	0.349632
6	-0.142411	0.856625	0.019936
6	-1.514859	0.761745	-0.192470
1	-1.855678	-2.588261	0.380144
1	0.544285	-2.391684	0.735191
1	0.291873	1.852117	-0.089114
8	-2.206178	1.883766	-0.563195
8	-3.497771	-0.512259	-0.311261
6	-3.132906	2.398725	0.389151
1	-2.623870	2.659294	1.334947
1	-3.563417	3.311184	-0.046837
1	-3.941710	1.681148	0.599965
6	-4.200030	-1.736712	-0.199276
1	-4.136854	-2.151719	0.822229
1	-5.250013	-1.516404	-0.432106
1	-3.822974	-2.489049	-0.914312
6	2.164255	-0.095454	0.549916
6	2.782902	0.432027	-0.775786
1	2.362326	1.429871	-0.988416
6	2.622056	-0.454675	-1.996221
1	1.557711	-0.605278	-2.226317
1	3.103663	0.021278	-2.863371
1	3.090233	-1.437475	-1.839523
9	4.159070	0.632619	-0.567215
6	2.435972	0.950065	1.656205
1	2.005997	0.615492	2.612762
1	3.518869	1.090533	1.787671
1	1.998089	1.929613	1.411526
6	2.860093	-1.406507	0.954494
1	3.943471	-1.236728	1.028426
1	2.499730	-1.753357	1.934635
1	2.696219	-2.216250	0.229232

Structure S46. ^{1}TS15

6	-3.509841	-0.423897	0.006827
6	-2.713485	-1.555135	0.235973
6	-1.345829	-1.532040	-0.053133
6	-0.741156	-0.388452	-0.588992
6	-1.539667	0.751676	-0.799984
6	-2.901598	0.749885	-0.518752
1	-3.154350	-2.469222	0.632153
1	-0.765170	-2.437462	0.131067
1	-1.116602	1.668195	-1.216024
8	-3.638193	1.857831	-0.814005

8	-4.837173	-0.358315	0.229624
6	-4.194113	2.575471	0.288217
1	-3.399086	2.917116	0.974806
1	-4.704276	3.452380	-0.132983
1	-4.920277	1.964860	0.846656
6	-5.517653	-1.490970	0.750001
1	-5.128795	-1.774240	1.743106
1	-6.571556	-1.200896	0.844196
1	-5.438653	-2.355488	0.069066
6	1.350445	-0.064609	0.427523
6	0.763728	-0.335133	-0.914614
1	0.932124	0.564706	-1.522058
6	1.319754	-1.555173	-1.647076
1	0.851169	-1.631016	-2.638569
1	2.405721	-1.441207	-1.767849
1	1.129100	-2.495889	-1.111873
6	1.877977	-1.169921	1.249802
1	2.722303	-1.636966	0.718483
1	2.207118	-0.839182	2.240282
1	1.102900	-1.948097	1.343591
6	1.211447	1.261674	1.055716
1	0.864005	2.042907	0.370845
1	0.512106	1.165739	1.906073
1	2.191137	1.518462	1.488868
5	4.518813	0.292000	0.078382
9	5.528935	1.034679	-0.505042
9	4.344899	0.633684	1.425598
9	3.278085	0.584451	-0.603187
9	4.751403	-1.081824	-0.049119

Structure S47. 10

6	-2.184323	-0.526953	-0.037859
6	-1.306041	-1.594892	0.186596
6	0.064327	-1.457549	-0.070205
6	0.602227	-0.257807	-0.551835
6	-0.288421	0.808379	-0.768153
6	-1.655450	0.695279	-0.522281
1	-1.682631	-2.549763	0.553330
1	0.712036	-2.317214	0.110740
1	0.071471	1.768518	-1.145376
8	-2.470952	1.757655	-0.805721
8	-3.526866	-0.569963	0.155492
6	-3.072637	2.406848	0.310798
1	-2.304147	2.794264	1.004410
1	-3.652185	3.252060	-0.086461
1	-3.747354	1.731150	0.860226
6	-4.116012	-1.763748	0.637789
1	-3.723640	-2.040215	1.632512
1	-5.193296	-1.568826	0.719454
1	-3.954564	-2.606949	-0.056788
6	2.889204	0.299061	0.466557
6	2.089779	-0.074684	-0.816348
1	2.197085	0.812107	-1.462894
6	2.720839	-1.253277	-1.571771
1	2.216623	-1.396620	-2.539469
1	3.785923	-1.055657	-1.757601
1	2.646759	-2.199902	-1.016016
6	2.986393	-0.813908	1.502330
1	3.412353	-1.728301	1.065974
1	3.639823	-0.490822	2.326526
1	1.995401	-1.048888	1.915096
6	2.402174	1.601491	1.090546
1	2.380231	2.405688	0.339441
1	1.391097	1.485327	1.505257
1	3.083641	1.899571	1.901408
9	4.212840	0.549278	0.021676

Structure S48. Co^{II}(salen)

27	-0.649678	0.000057	-0.000014
8	0.684544	1.309226	-0.053179
8	0.684302	-1.309359	0.053138
7	-2.019662	1.262437	0.295468
7	-2.019900	-1.262070	-0.295479
6	0.609697	2.599673	0.032758
6	1.807791	3.394850	-0.123029
6	1.692730	4.774421	0.000562
1	2.581666	5.396725	-0.105381
6	0.468460	5.432508	0.258480
6	-0.682044	4.687220	0.386935
1	-1.643600	5.174560	0.575760
6	-0.639585	3.273252	0.273420
6	-1.872123	2.551392	0.390235
1	-2.760961	3.167381	0.578093
6	-3.319159	0.598124	0.484068
1	-3.306926	0.174895	1.506913
6	-3.319271	-0.597512	-0.484079

1	-3.306954	-0.174284	-1.506924
6	-4.575544	-1.454468	-0.326061
1	-4.565770	-1.932235	0.669666
1	-4.586121	-2.263032	-1.073650
6	-5.835309	-0.592446	-0.484165
1	-5.888748	-0.216173	-1.521627
1	-6.732309	-1.213747	-0.330403
6	-5.835199	0.593536	0.484138
1	-5.888718	0.217272	1.521599
1	-6.732080	1.215008	0.330369
6	-4.575269	1.455318	0.326043
1	-4.585699	2.263881	1.073634
1	-4.565396	1.933085	-0.669683
6	-1.872607	-2.551055	-0.390213
1	-2.761564	-3.166880	-0.578045
6	-0.640204	-3.273146	-0.273389
6	-0.682932	-4.687109	-0.386852
1	-1.644583	-5.174274	-0.575649
6	0.467432	-5.432612	-0.258380
6	1.691828	-4.774747	-0.000496
1	2.580647	-5.397215	0.105462
6	1.807152	-3.395192	0.123036
6	0.609208	-2.599795	-0.032766
6	3.154742	2.708268	-0.423945
6	3.053479	1.937718	-1.761297
1	2.840003	2.629721	-2.593077
1	2.259891	1.181435	-1.727325
1	4.006157	1.428870	-1.983750
6	3.519245	1.735463	0.721179
1	2.762684	0.951205	0.832880
1	3.606425	2.276554	1.678181
1	4.489874	1.253352	0.518155
6	4.302870	3.724732	-0.557636
1	4.463656	4.297053	0.370235
1	4.134335	4.440442	-1.378465
1	5.241177	3.191302	-0.778643
6	3.154227	-2.708843	0.423923
6	4.302125	-3.725524	0.557965
1	4.462869	-4.298106	-0.369753
1	4.133363	-4.440996	1.378953
1	5.240527	-3.192243	0.778924
6	3.519061	-1.736379	-0.721384
1	2.762683	-0.951982	-0.833341
1	3.606222	-2.277707	-1.678253
1	4.489775	-1.254433	-0.518369
6	3.052985	-1.937960	1.761083
1	2.839263	-2.629721	2.593001
1	2.259562	-1.181512	1.726842
1	4.005747	-1.429264	1.983524
1	0.443210	-6.521090	-0.347312
1	0.444446	6.520988	0.347452

Structure S49. 11

6	3.388858	-1.347258	-0.470826
6	3.997348	-0.094406	-0.360219
6	2.029946	-1.470167	-0.188075
6	1.263253	-0.350776	0.174574
6	1.871490	0.919757	0.308886
6	3.245684	1.013737	0.035942
1	3.970036	-2.223920	-0.767025
1	5.063966	0.020395	-0.571085
1	1.539061	-2.443954	-0.247868
6	-0.175821	-0.639425	0.495219
6	1.119797	2.152566	0.747457
1	3.737867	1.984273	0.145302
8	-0.507411	-1.588725	1.185550
7	-1.127051	0.247521	0.000195
9	-0.667251	0.873431	-1.175262
6	-2.587479	-0.027950	-0.112363
1	0.363753	1.926261	1.513487
1	0.585070	2.609758	-0.100035
1	1.809974	2.904555	1.157968
6	-3.140999	-0.240684	1.306096
6	-2.821376	-1.256104	-1.003928
6	-3.244937	1.221505	-0.719083
1	-2.735644	-1.146228	1.770477
1	-4.236788	-0.331278	1.248575
1	-2.901130	0.620621	1.949067
1	-3.011931	2.118584	-0.124626
1	-4.336519	1.084098	-0.722058
1	-2.919424	1.395906	-1.753225
1	-2.380022	-2.155964	-0.551682
1	-2.369142	-1.101309	-1.996134
1	-3.899808	-1.430283	-1.141630

Structure S50. ^{2}INT5

9	0.815954	-0.347355	1.164778	1	1.290104	-1.630287	-3.295723
7	1.006114	-0.570415	2.552814	6	3.297250	-1.558172	-2.503167
6	-0.187957	-1.270394	3.105193	1	3.796492	-1.249348	-1.570276
6	-0.140441	-1.156747	4.637063	1	3.663029	-0.894611	-3.302370
1	0.686683	-1.731668	5.067658	6	3.662233	-3.010323	-2.836494
1	-0.035070	-0.104859	4.944883	1	3.259406	-3.270829	-3.832054
1	-1.090449	-1.537095	5.043126	1	4.757706	-3.108255	-2.907364
6	-0.186153	-2.734440	2.644621	6	3.106864	-3.986983	-1.796394
1	0.698165	-3.264823	3.027600	1	3.587012	-3.792087	-0.820633
1	-1.087682	-3.250388	3.008060	1	3.358542	-5.024576	-2.069096
1	-0.189237	-2.786067	1.546614	6	1.586706	-3.844324	-1.644861
6	-1.430335	-0.531507	2.585955	1	1.227873	-4.526410	-0.858078
1	-2.330177	-1.012284	2.995909	1	1.082749	-4.136843	-2.583236
1	-1.421963	0.521396	2.904651	6	1.995581	1.002275	-2.051450
1	-1.498665	-0.557413	1.493544	1	2.999400	0.925204	-2.486883
6	2.336555	-0.893117	2.799493	6	1.595540	2.325220	-1.665222
8	2.651639	-1.560299	3.769883	6	2.530957	3.377583	-1.832555
6	3.355853	-0.350015	1.836799	1	3.491315	3.160314	-2.309931
6	3.388719	0.990627	1.383111	6	2.240800	4.649811	-1.389694
6	4.363220	-1.254078	1.462031	6	1.006821	4.890132	-0.742983
6	4.442482	1.359268	0.530452	1	0.821667	5.900536	-0.377178
6	5.391430	-0.866193	0.604018	6	0.043343	3.907428	-0.550261
6	5.426342	0.450034	0.135235	6	0.317067	2.580354	-1.056653
1	4.486763	2.391289	0.174221	6	-5.029589	0.210421	-0.200687
1	6.161213	-1.583321	0.308924	6	-4.866315	0.942478	-1.553019
1	6.227632	0.774606	-0.534073	1	-5.412935	0.412740	-2.351048
27	-0.453969	-0.199926	-1.194494	1	-3.811533	1.014198	-1.844019
8	-2.283228	-0.340119	-0.780460	1	-5.275415	1.964421	-1.486305
8	-0.576816	1.654234	-0.924087	6	-4.313392	1.004570	0.916601
7	-0.200253	-2.071064	-1.158472	1	-3.245607	1.116145	0.702764
7	1.296431	-0.082195	-1.906581	1	-4.426907	0.498303	1.889404
6	-3.030735	-1.383575	-0.600531	1	-4.753880	2.010950	1.009908
6	-4.433562	-1.208353	-0.299478	6	-6.531540	0.182249	0.134953
6	-5.203622	-2.349040	-0.101586	1	-6.732738	-0.292154	1.109113
1	-6.263830	-2.245122	0.130416	1	-7.122076	-0.343515	-0.632660
6	-4.683844	-3.660478	-0.181991	1	-6.914199	1.213930	0.190008
6	-3.348606	-3.838491	-0.469955	6	-1.262713	4.175440	0.222607
1	-2.922412	-4.844352	-0.535141	6	-1.355566	5.631509	0.711722
6	-2.502514	-2.720058	-0.681288	1	-1.359349	6.352490	-0.121873
6	-1.115350	-2.970345	-0.953601	1	-0.530101	5.896931	1.391824
1	-0.821378	-4.027912	-0.958467	1	-2.295028	5.771999	1.269869
6	1.225756	-2.400315	-1.301994	6	-2.487237	3.901935	-0.680840
1	1.693819	-2.140359	-0.334427	1	-2.511505	2.858172	-1.012524
6	1.786344	-1.403532	-2.332176	1	-2.466243	4.551226	-1.572034

1	-3.420464	4.114421	-0.133296
6	-1.308442	3.258274	1.469117
1	-0.477480	3.491831	2.155211
1	-1.238301	2.201864	1.186881
1	-2.251918	3.405659	2.020478
1	-5.340252	-4.517339	-0.014587
1	2.956020	5.465341	-1.518315
6	2.363789	2.020907	1.783698
1	1.427064	1.872863	1.231077
1	2.116045	1.959174	2.853936
1	2.720428	3.036765	1.564484
1	4.328020	-2.271684	1.857630

Structure S51. ^{2}TS16

9	0.412629	-0.427109	1.017969
7	0.706692	-0.546480	2.722858
6	-0.484296	-1.227249	3.239938
6	-0.389679	-1.178430	4.782916
1	0.449189	-1.781452	5.150718
1	-0.261642	-0.142106	5.132621
1	-1.328734	-1.569560	5.205923
6	-0.588318	-2.673878	2.735264
1	0.266328	-3.274300	3.076451
1	-1.515501	-3.141857	3.100605
1	-0.613898	-2.678399	1.637481
6	-1.710117	-0.414820	2.793456
1	-2.621437	-0.847073	3.233699
1	-1.627044	0.632701	3.120451
1	-1.806899	-0.423833	1.702821
6	1.988585	-1.036509	2.811490
8	2.294133	-1.908286	3.622428
6	3.036088	-0.406447	1.934384
6	3.067218	0.958711	1.553501
6	4.086515	-1.263721	1.561961
6	4.164987	1.394531	0.791012
6	5.159565	-0.809252	0.797784
6	5.195868	0.533051	0.409992
1	4.207207	2.445833	0.495482
1	5.961977	-1.494253	0.512642
1	6.030791	0.913737	-0.184734
27	-0.222469	-0.184229	-0.969980
8	-2.065071	-0.420007	-0.776506
8	-0.486853	1.655027	-0.787832
7	0.088157	-2.045455	-1.120110
7	1.454831	0.043007	-1.824982
6	-2.788776	-1.500305	-0.709456
6	-4.216321	-1.383212	-0.546166
6	-4.952039	-2.560102	-0.436267
1	-6.031599	-2.504170	-0.296424
6	-4.373156	-3.845487	-0.498031
6	-3.013197	-3.964507	-0.689669
1	-2.543172	-4.950334	-0.754819
6	-2.203633	-2.807591	-0.799991
6	-0.794158	-2.987240	-1.016538
1	-0.457032	-4.028841	-1.090007
6	1.524673	-2.290912	-1.294808
1	1.994073	-2.024133	-0.330974
6	1.994287	-1.238576	-2.314989
1	1.471456	-1.458810	-3.265218
6	3.502956	-1.304249	-2.548649
1	4.018460	-0.988517	-1.627840
1	3.798238	-0.605970	-3.347664
6	3.933144	-2.727557	-2.926865
1	3.505699	-2.991767	-3.911153
1	5.028537	-2.761539	-3.042772
6	3.474981	-3.752525	-1.885805
1	3.975537	-3.544940	-0.923542
1	3.777212	-4.768481	-2.186698
6	1.955111	-3.703367	-1.682372
1	1.659466	-4.419613	-0.899507
1	1.441719	-4.004594	-2.612992
6	2.089594	1.170408	-1.959061
1	3.078826	1.155935	-2.432006
6	1.632326	2.458157	-1.538891
6	2.508177	3.563046	-1.699354
1	3.488470	3.398839	-2.156317
6	2.130413	4.816724	-1.275613
6	0.859808	4.993299	-0.677681
1	0.600513	5.998255	-0.344167
6	-0.049826	3.960040	-0.495989
6	0.335210	2.639999	-0.944500
6	-4.884618	0.006474	-0.515203
6	-4.612647	0.735108	-1.852260
1	-5.049032	0.176723	-2.696999
1	-3.536953	0.851352	-2.033241
1	-5.068538	1.738891	-1.839669
6	-4.333228	0.846009	0.660061

1	-3.258007	1.021158	0.556919
1	-4.515097	0.341460	1.622677
1	-4.839301	1.824786	0.693730
6	-6.410888	-0.094067	-0.340762
1	-6.691111	-0.573389	0.611218
1	-6.891338	-0.650995	-1.161347
1	-6.845674	0.918067	-0.336382
6	-1.413376	4.171778	0.189873
6	-1.622457	5.636949	0.611748
1	-1.610488	6.325676	-0.248610
1	-0.862984	5.976090	1.334669
1	-2.604798	5.741748	1.099086
6	-2.553551	3.793524	-0.783394
1	-2.496387	2.739251	-1.075082
1	-2.509115	4.411105	-1.695944
1	-3.533320	3.966768	-0.308607
6	-1.494332	3.298959	1.465779
1	-0.716310	3.592168	2.189468
1	-1.365818	2.235748	1.235267
1	-2.474653	3.427686	1.954016
1	-5.004377	-4.731673	-0.402223
1	2.799135	5.672465	-1.391370
6	2.004093	1.955858	1.935106
1	1.067807	1.736694	1.409291
1	1.771075	1.912440	3.009267
1	2.317806	2.978184	1.681071
1	4.048384	-2.302123	1.897667

Structure S52. ^{4}INT6

9	0.482364	-0.390218	0.731706
7	0.928583	-0.542765	3.466478
6	-0.422013	-1.077729	3.589672
6	-0.628386	-1.374166	5.091955
1	0.065889	-2.159538	5.427711
1	-0.452599	-0.472434	5.698456
1	-1.659973	-1.721065	5.266446
6	-0.714904	-2.332425	2.748540
1	-0.112921	-3.188129	3.080158
1	-1.781863	-2.592514	2.837081
1	-0.491242	-2.125250	1.694821
6	-1.372812	0.058655	3.148178
1	-2.414315	-0.236886	3.349271
1	-1.163791	0.991752	3.692448
1	-1.251506	0.233953	2.072923
6	1.989479	-1.192170	2.908911
8	2.186470	-2.378136	3.195343
6	2.993907	-0.418108	2.092659
6	2.924085	0.964338	1.780169
6	4.065236	-1.185993	1.601703
6	3.949952	1.506132	0.985343
6	5.069682	-0.626624	0.814385
6	5.008903	0.734594	0.503814
1	3.904674	2.568505	0.732884
1	5.892915	-1.246683	0.449845
1	5.784980	1.198288	-0.111910
27	-0.207341	-0.203644	-0.998604
8	-2.055112	-0.447622	-0.946029
8	-0.506996	1.641277	-0.904421
7	0.099945	-2.078044	-1.208721
7	1.443694	0.013187	-1.965737
6	-2.772976	-1.530058	-0.806664
6	-4.191197	-1.406558	-0.601125
6	-4.924115	-2.582108	-0.446329
1	-5.998726	-2.521062	-0.274783
6	-4.347493	-3.867097	-0.493920
6	-2.989260	-3.990402	-0.702893
1	-2.517726	-4.976408	-0.743684
6	-2.186517	-2.836067	-0.857906
6	-0.777242	-3.015503	-1.081180
1	-0.434391	-4.056200	-1.140217
6	1.541627	-2.300640	-1.363300
1	1.986350	-1.994100	-0.399913
6	2.001625	-1.275187	-2.415469
1	1.492555	-1.531173	-3.363919
6	3.514735	-1.324499	-2.625876
1	4.011058	-0.979424	-1.703767
1	3.812248	-0.642796	-3.438377
6	3.967801	-2.752249	-2.958772
1	3.553699	-3.050487	-3.939077
1	5.064548	-2.773324	-3.063225
6	3.514377	-3.751974	-1.891422
1	4.002030	-3.509053	-0.931162
1	3.832563	-4.772129	-2.159501
6	1.992184	-3.718802	-1.702190
1	1.700285	-4.410852	-0.896772
1	1.490855	-4.056542	-2.627018
6	2.089556	1.136135	-2.049454

1	3.086741	1.123566	-2.505847
6	1.646279	2.418416	-1.597313
6	2.546150	3.507871	-1.724687
1	3.532358	3.330744	-2.163036
6	2.183660	4.762253	-1.290875
6	0.904455	4.952816	-0.720424
1	0.654392	5.957978	-0.381391
6	-0.028552	3.933865	-0.568369
6	0.344736	2.612319	-1.018852
6	-4.849897	-0.014542	-0.535438
6	-4.632776	0.731120	-1.872543
1	-5.105571	0.184308	-2.705221
1	-3.566233	0.850256	-2.098182
1	-5.088138	1.734040	-1.826782
6	-4.237583	0.796538	0.630235
1	-3.161582	0.946229	0.494113
1	-4.397158	0.279982	1.590653
1	-4.717381	1.786563	0.696843
6	-6.367563	-0.107325	-0.295787
1	-6.610371	-0.595671	0.661687
1	-6.886466	-0.650843	-1.101961
1	-6.794030	0.907657	-0.260528
6	-1.403142	4.174184	0.086458
6	-1.600109	5.647811	0.484973
1	-1.560112	6.325195	-0.383565
1	-0.853607	5.986303	1.221364
1	-2.591446	5.771200	0.948991
6	-2.532650	3.800937	-0.901005
1	-2.496371	2.740045	-1.170913
1	-2.457931	4.398493	-1.824838
1	-3.516186	4.007084	-0.447687
6	-1.515970	3.319620	1.370218
1	-0.754025	3.618252	2.107718
1	-1.383982	2.254809	1.155048
1	-2.506792	3.453880	1.834805
1	-4.975429	-4.751028	-0.363724
1	2.871099	5.606292	-1.378115
6	1.800311	1.867719	2.210911
1	0.871034	1.533313	1.732567
1	1.637641	1.831192	3.297853
1	1.997930	2.908173	1.914326
1	4.090979	-2.245511	1.862786
27	-0.576547	-0.098976	0.200929
8	0.461670	1.403875	-0.214274
8	0.943231	-1.137057	-0.094864
7	-2.158677	0.967425	0.320543
7	-1.756851	-1.453004	-0.541551
6	0.203635	2.677289	-0.115237
6	1.276260	3.622958	-0.280108
6	0.961402	4.977281	-0.190753
1	1.753686	5.717402	-0.305139
6	-0.343349	5.455337	0.049397
6	-1.373288	4.552562	0.216253
1	-2.392937	4.898496	0.409767
6	-1.119350	3.162307	0.145192
6	-2.224158	2.256215	0.309849
1	-3.208820	2.726756	0.428667
6	-3.309595	0.072875	0.463487
1	-3.150400	-0.447325	1.424521
6	-3.147550	-0.982155	-0.651481
1	-3.236803	-0.447179	-1.616051
6	-4.237605	-2.052255	-0.568386
1	-4.093565	-2.633425	0.359318
1	-4.153279	-2.756492	-1.410823
6	-5.630737	-1.409005	-0.572139
1	-5.804672	-0.923226	-1.549226
1	-6.398614	-2.192917	-0.471958
6	-5.777834	-0.370455	0.543353
1	-5.701390	-0.872458	1.524069
1	-6.775063	0.096306	0.504874
6	-4.695567	0.712626	0.446710
1	-4.794551	1.423509	1.282399
1	-4.827154	1.284798	-0.489063
6	-1.400544	-2.683315	-0.756197
1	-2.167374	-3.396113	-1.087340
6	-0.092284	-3.236902	-0.586158
6	0.071798	-4.632755	-0.784803
1	-0.794633	-5.230848	-1.082196
6	1.300428	-5.222636	-0.592597
6	2.394556	-4.427301	-0.180055
1	3.346042	-4.932725	-0.012507
6	2.306993	-3.056502	0.028779
6	1.031429	-2.422872	-0.207240
6	2.716052	3.124400	-0.512055
6	2.786571	2.302828	-1.820535

Structure S53. Co^{III}(salen)-F

1	2.529586	2.932351	-2.688909
1	2.098864	1.449142	-1.796652
1	3.807979	1.917069	-1.974480
6	3.159046	2.256417	0.690257
1	2.520154	1.374169	0.812391
1	3.124387	2.841293	1.624255
1	4.196336	1.911427	0.548849
6	3.713429	4.289771	-0.640368
1	3.755180	4.906720	0.271746
1	3.479246	4.948793	-1.492016
1	4.725417	3.888092	-0.807987
6	3.499467	-2.212137	0.516563
6	4.753518	-3.072939	0.751080
1	5.107090	-3.556254	-0.174238
1	4.588293	-3.857352	1.507210
1	5.572274	-2.434451	1.119354
6	3.858861	-1.144733	-0.543190
1	3.024193	-0.459513	-0.723006
1	4.130946	-1.621408	-1.499864
1	4.725206	-0.552055	-0.206479
6	3.134755	-1.536306	1.861968
1	2.998274	-2.296199	2.649265
1	2.207967	-0.952167	1.798812
1	3.948071	-0.863786	2.181928
9	-0.689888	-0.465659	2.004235
1	-0.527421	6.530313	0.106986
1	1.434711	-6.296541	-0.739039

Structure S54. 12

6	3.518200	-1.086115	0.063093
6	3.914163	0.254001	0.091202
6	2.163434	-1.392098	-0.028883
6	1.189097	-0.380110	-0.104461
6	1.581384	0.982178	-0.066096
6	2.953844	1.265296	0.031046
1	4.261042	-1.886161	0.111389
1	4.973411	0.515096	0.163722
1	1.826184	-2.429994	-0.050154
6	-0.231381	-0.853562	-0.195494
6	0.602095	2.128009	-0.108675
1	3.274408	2.310211	0.062761
8	-0.532580	-2.041959	-0.060130
7	-1.200220	0.040807	-0.572583
6	-2.517858	0.115780	0.044648
1	-0.125548	2.069685	0.716395
1	0.023317	2.131545	-1.045261
1	1.124062	3.092875	-0.021182
6	-2.489823	-0.169376	1.555759
6	-3.408370	-0.922845	-0.685735
6	-3.064014	1.528841	-0.228637
1	-2.124213	-1.185185	1.760796
1	-3.500466	-0.073831	1.982450
1	-1.833476	0.547931	2.074565
1	-2.462591	2.294255	0.284924
1	-4.100030	1.609490	0.135501
1	-3.053223	1.749995	-1.306714
1	-3.031535	-1.938038	-0.506094
1	-3.412506	-0.736506	-1.770441
1	-4.441274	-0.841344	-0.310143

Structure S55. $[Co^{IV}(salen)\text{-}F]^{+}$

27	-0.593374	-0.106837	0.238537
8	0.383520	1.399468	-0.207040
8	0.988133	-1.107140	-0.047755
7	-2.197750	0.866762	0.379868
7	-1.717458	-1.510674	-0.586524
6	0.097981	2.665815	-0.078465
6	1.142168	3.640002	-0.257299
6	0.784679	4.980749	-0.130501
1	1.546874	5.749380	-0.253943
6	-0.526770	5.408796	0.159182
6	-1.531282	4.476042	0.336064
1	-2.552377	4.791988	0.564641
6	-1.238031	3.099843	0.226973
6	-2.306919	2.155690	0.387257
1	-3.307827	2.584723	0.515109
6	-3.325822	-0.071117	0.464146
1	-3.176576	-0.626725	1.406086
6	-3.117773	-1.072357	-0.699279
1	-3.179721	-0.487962	-1.635455
6	-4.183478	-2.164820	-0.704684
1	-4.062295	-2.787846	0.198753
1	-4.052021	-2.820051	-1.580451
6	-5.587779	-1.545913	-0.720747
1	-5.741137	-1.013272	-1.676066
1	-6.341071	-2.348307	-0.685475

6	-5.785820	-0.573343	0.444471
1	-5.727404	-1.123655	1.399893
1	-6.789234	-0.122293	0.401702
6	-4.726916	0.536578	0.433105
1	-4.865730	1.204001	1.297833
1	-4.842858	1.146520	-0.480238
6	-1.340441	-2.738053	-0.676436
1	-2.079814	-3.510769	-0.924489
6	0.007346	-3.236201	-0.474631
6	0.225351	-4.603498	-0.620127
1	-0.608025	-5.261064	-0.879306
6	1.507740	-5.141231	-0.439362
6	2.593186	-4.314671	-0.108610
1	3.565275	-4.784989	0.031495
6	2.463384	-2.936781	0.047191
6	1.130519	-2.365546	-0.148166
6	2.587091	3.197787	-0.549572
6	2.637818	2.398295	-1.872922
1	2.322281	3.028286	-2.720620
1	1.990904	1.513184	-1.844249
1	3.668642	2.062716	-2.070554
6	3.103804	2.335734	0.627181
1	2.505900	1.428155	0.766528
1	3.085649	2.910527	1.567243
1	4.146299	2.032946	0.440984
6	3.534389	4.401706	-0.698738
1	3.588170	5.007612	0.219588
1	3.245605	5.060369	-1.533304
1	4.552557	4.038913	-0.908092
6	3.636302	-2.034007	0.436327
6	4.936435	-2.837250	0.614775
1	5.249055	-3.337095	-0.315910
1	4.855653	-3.596411	1.408713
1	5.747154	-2.151589	0.903518
6	3.876901	-0.987561	-0.681541
1	3.022782	-0.316038	-0.810105
1	4.084297	-1.483096	-1.643798
1	4.755928	-0.376332	-0.425489
6	3.321603	-1.333134	1.784543
1	3.241420	-2.073312	2.596549
1	2.386778	-0.760288	1.756206
1	4.141453	-0.643214	2.038307
9	-0.704448	-0.687890	1.958486
1	-0.740566	6.475963	0.245501
1	1.664375	-6.215910	-0.553814

Structure S56. 15

6	3.426460	-1.259001	-0.188873
6	3.985455	0.021140	-0.171718
6	2.044118	-1.400371	-0.067971
6	1.176680	-0.299217	0.051710
6	1.745596	1.003324	0.076787
6	3.143751	1.127356	-0.032781
1	4.064239	-2.142964	-0.290960
1	5.067526	0.161462	-0.258378
1	1.573727	-2.385474	-0.050645
6	-0.319541	-0.645068	0.159003
6	0.930607	2.263713	0.229503
1	3.583932	2.130047	-0.005736
8	-0.590213	-1.840346	0.470551
7	-1.140031	0.349769	-0.129324
6	-2.579520	0.104046	-0.102866
1	0.265177	2.202647	1.102948
1	0.246545	2.394998	-0.620427
1	1.585797	3.146419	0.328503
6	-3.064621	-0.313491	1.304285
6	-2.999336	-0.972867	-1.130296
6	-3.258430	1.434254	-0.481635
1	-2.581380	-1.256412	1.594375
1	-4.162546	-0.439680	1.340176
1	-2.784158	0.458011	2.041891
1	-2.977834	2.224472	0.234943
1	-4.360453	1.350429	-0.492875
1	-2.923527	1.763665	-1.479657
1	-2.527572	-1.931303	-0.873088
1	-2.658150	-0.680830	-2.138398
1	-4.096721	-1.104010	-1.162700

Structure S57. ^{2}TS17

6	3.583771	-1.005253	-0.054804
6	3.927810	0.352398	-0.054435
6	2.240631	-1.378513	-0.034426
6	1.234990	-0.402880	-0.010186
6	1.576801	0.967407	0.023561
6	2.931916	1.330814	-0.019707
1	4.364700	-1.769437	-0.080669

1	4.979510	0.650297	-0.078172
1	1.942961	-2.429062	-0.047997
6	-0.201783	-0.855408	-0.043043
6	0.483868	1.975795	0.119193
1	3.203697	2.389874	-0.009416
8	-0.518720	-2.023889	0.171724
7	-1.104408	0.105515	-0.414575
6	-2.524243	0.117904	-0.032661
1	0.182901	2.234837	1.145560
1	-0.490317	1.279547	-0.314905
1	0.592349	2.867198	-0.514565
6	-2.707998	-0.149745	1.470337
6	-3.247842	-0.960587	-0.867794
6	-3.077402	1.503916	-0.400032
1	-2.305876	-1.135318	1.743576
1	-3.775940	-0.124769	1.739211
1	-2.188014	0.616803	2.067810
1	-2.588238	2.297472	0.188154
1	-4.157867	1.549323	-0.195488
1	-2.915994	1.719110	-1.467971
1	-2.858811	-1.957678	-0.624688
1	-3.098732	-0.779973	-1.943622
1	-4.328824	-0.930798	-0.654603

Structure S58. 13

6	3.388079	-1.263472	-0.384036
6	3.960020	0.020009	-0.401911
6	2.025480	-1.405787	-0.103052
6	1.208397	-0.300642	0.144702
6	1.785284	1.020977	0.184416
6	3.181356	1.130107	-0.120496
1	3.999549	-2.144836	-0.591496
1	5.022988	0.143474	-0.625569
1	1.567858	-2.397188	-0.082369
6	-0.253806	-0.608909	0.375669
6	1.079507	2.181808	0.560539
1	3.636651	2.124124	-0.103891
8	-0.591481	-1.586534	1.035751
7	-1.137142	0.227228	-0.237878
6	-2.610182	0.095942	-0.218335
1	0.044749	2.152682	0.900348
1	-0.750840	0.924146	-0.864416
1	1.592402	3.146659	0.577904
6	-3.122869	0.180036	1.228918
6	-3.031588	-1.235158	-0.864896
6	-3.162529	1.272718	-1.033416
1	-2.710490	-0.638072	1.834031
1	-4.222222	0.113212	1.248145
1	-2.828565	1.136620	1.690035
1	-2.857100	2.238268	-0.597495
1	-4.262362	1.242498	-1.049579
1	-2.810452	1.236669	-2.078174
1	-2.623413	-2.083510	-0.299168
1	-2.660138	-1.296913	-1.900677
1	-4.129668	-1.321933	-0.887099

Structure S59. ^{2}TS18

6	4.044881	-2.258354	-0.118997
6	3.190752	-3.187617	-0.731299
6	3.744865	-0.895487	-0.176367
6	2.607919	-0.421879	-0.836627
6	1.764408	-1.353529	-1.528092
6	2.073476	-2.740701	-1.420795
1	4.935186	-2.598065	0.415897
1	3.409044	-4.257002	-0.677197
1	4.391235	-0.164618	0.312005
6	2.382035	1.075361	-0.744278
6	0.670372	-0.975895	-2.352147
1	1.422654	-3.459274	-1.925967
8	3.346480	1.830744	-0.648828
7	1.089682	1.488232	-0.739508
6	0.643829	2.892904	-0.616207
1	0.115771	-1.752514	-2.880141
1	0.560906	0.043731	-2.713870
6	1.296433	3.762502	-1.703576
6	0.991532	3.427747	0.783397
6	-0.876703	2.882251	-0.824031
1	2.385708	3.801110	-1.579662
1	0.896527	4.787682	-1.651772
1	1.075537	3.359603	-2.705483
1	-1.130568	2.540055	-1.839613
1	-1.285221	3.895825	-0.692926
1	-1.380492	2.211333	-0.112740
1	2.078076	3.391032	0.946338
1	0.503825	2.819945	1.560334
1	0.654928	4.471011	0.895166

1	0.364069	0.780459	-0.638297
6	1.297728	-1.648672	2.127185
6	1.584914	-0.598851	3.002378
6	0.063250	-1.685858	1.477685
6	-0.891175	-0.691841	1.717900
6	-0.626899	0.360096	2.619378
6	0.630178	0.393023	3.241143
1	2.038889	-2.425045	1.930809
1	2.556779	-0.549033	3.500076
1	-0.158417	-2.485144	0.768337
6	-2.255884	-0.789258	1.089502
6	-1.672347	1.405658	2.914315
1	0.860590	1.210883	3.929389
8	-3.220046	-1.190343	1.728134
7	-2.402940	-0.268684	-0.177817
6	-3.476959	-0.616831	-1.118894
1	-1.280249	2.195910	3.570771
1	-2.547533	0.952469	3.406932
6	-4.800253	-0.079823	-0.522458
6	-3.544300	-2.133462	-1.345304
6	-3.214500	0.123750	-2.440199
1	-5.074562	-0.615822	0.392785
1	-5.599380	-0.205027	-1.270394
1	-4.713030	0.992782	-0.288875
1	-3.123606	1.206768	-2.268671
1	-4.055420	-0.048144	-3.129169
1	-2.293023	-0.228971	-2.920478
1	-3.758647	-2.661464	-0.404706
1	-2.584660	-2.497961	-1.742111
1	-4.336546	-2.381087	-2.068811
1	-2.043236	1.882566	1.993152
9	-0.941014	-0.593939	-1.031772

Structure S60. 14

6	3.402690	-1.440905	-0.409112
6	3.961244	-0.170313	-0.248637
6	2.031190	-1.620784	-0.232407
6	1.190667	-0.542183	0.081502
6	1.755042	0.743265	0.264443
6	3.139283	0.904400	0.092921
1	4.036059	-2.293948	-0.665620
1	5.035378	-0.016889	-0.379347
1	1.582896	-2.611243	-0.330401
6	-0.277162	-0.886932	0.256077
6	0.943993	1.947614	0.663210
1	3.579055	1.894743	0.240645
8	-0.600899	-1.957423	0.762560
7	-1.162660	0.033604	-0.202276
6	-2.635476	-0.073563	-0.136491
1	1.595626	2.747911	1.045046
1	0.189991	1.703948	1.426656
6	-3.088592	-0.206719	1.327070
6	-3.114803	-1.280948	-0.959315
6	-3.184095	1.228513	-0.736055
1	-2.672687	-1.115455	1.782364
1	-4.187642	-0.257872	1.381707
1	-2.757517	0.663047	1.917589
1	-2.810619	2.107023	-0.184919
1	-4.283648	1.237001	-0.694253
1	-2.886439	1.337355	-1.792337
1	-2.702317	-2.212968	-0.549185
1	-2.789539	-1.188958	-2.008233
1	-4.214586	-1.345077	-0.943856
1	-0.792843	0.838085	-0.697469
9	0.253417	2.480976	-0.445797

Structure S61. ^{4}INT7

27	-0.479724	0.275719	-0.749916
8	-2.261612	-0.328359	-0.900205
8	-0.801496	2.136194	-0.885871
7	0.078417	-1.652860	-1.330954
7	1.285235	0.653047	-1.807174
6	-2.854603	-1.486459	-0.909486
6	-4.239466	-1.578480	-0.535303
6	-4.846495	-2.828639	-0.633547
1	-5.898438	-2.936032	-0.368780
6	-4.160641	-3.986642	-1.054429
6	-2.816403	-3.909547	-1.362752
1	-2.259152	-4.803821	-1.656559
6	-2.138105	-2.672498	-1.278251
6	-0.714065	-2.659578	-1.505442
1	-0.293045	-3.626772	-1.814198
6	1.522826	-1.732030	-1.549533
1	1.984561	-1.543135	-0.563960
6	1.886425	-0.525754	-2.445131
1	1.349258	-0.673884	-3.401666

6	3.389465	-0.454439	-2.725016
1	3.912740	-0.205435	-1.788155
1	3.603367	0.351434	-3.445255
6	3.922504	-1.784972	-3.268467
1	3.485395	-1.980093	-4.264621
1	5.012332	-1.710164	-3.414373
6	3.585768	-2.945941	-2.330296
1	4.091117	-2.793897	-1.361130
1	3.963935	-3.896592	-2.739154
6	2.074134	-3.045963	-2.101555
1	1.850746	-3.866009	-1.400584
1	1.574400	-3.285058	-3.057517
6	1.886891	1.798768	-1.762179
1	2.894050	1.886883	-2.191316
6	1.384004	3.010969	-1.166528
6	2.263949	4.110873	-1.040610
1	3.281852	4.026259	-1.432280
6	1.845046	5.265404	-0.409247
6	0.539993	5.333042	0.123457
1	0.257238	6.247141	0.646035
6	-0.380669	4.293027	0.019071
6	0.037238	3.110620	-0.684613
6	-4.978106	-0.333946	-0.007529
6	-5.008218	0.773986	-1.085418
1	-5.542310	0.428401	-1.986111
1	-3.996551	1.078153	-1.378790
1	-5.535954	1.662351	-0.700618
6	-4.257198	0.181979	1.262038
1	-3.219794	0.471060	1.056423
1	-4.248728	-0.591091	2.047852
1	-4.783575	1.064092	1.662510
6	-6.433774	-0.653742	0.376138
1	-6.498116	-1.410916	1.174018
1	-7.023554	-1.007587	-0.484841
1	-6.922330	0.258882	0.752526
6	-1.771307	4.342690	0.679613
6	-2.027881	5.691856	1.374760
1	-2.013555	6.534195	0.664144
1	-1.295077	5.899392	2.170802
1	-3.023028	5.677092	1.846854
6	-2.887114	4.140047	-0.371331
1	-2.816453	3.157483	-0.851204
1	-2.833977	4.914450	-1.154681
1	-3.876010	4.217364	0.110346
6	-1.846034	3.231649	1.755990
1	-1.153850	3.451840	2.585563
1	-1.578955	2.243872	1.360414
1	-2.863958	3.175003	2.175797
9	-0.146620	0.296291	1.066558
1	-4.691414	-4.939330	-1.114110
1	2.519227	6.117969	-0.301978
6	5.346344	-0.085073	0.415221
6	4.969453	1.267940	0.484782
6	4.539478	-1.052636	1.021576
6	3.362694	-0.718252	1.699315
6	3.003788	0.671390	1.849370
6	3.830639	1.634045	1.182354
1	6.253014	-0.382264	-0.117255
1	5.581013	2.034359	0.000465
1	4.812782	-2.108736	0.972982
6	2.570794	-1.897391	2.233208
6	1.944345	1.139051	2.648240
1	3.554509	2.688557	1.259478
8	3.165314	-2.894005	2.646587
7	1.221763	-1.800936	2.148557
6	0.262416	-2.831084	2.601151
1	1.335889	0.477982	3.260925
1	0.806351	-0.966757	1.718690
1	1.707665	2.205093	2.665450
6	0.458566	-3.115312	4.099972
6	0.449417	-4.122163	1.784354
6	-1.145267	-2.262917	2.362705
1	1.466884	-3.504518	4.294550
1	-0.279151	-3.856015	4.448523
1	0.320582	-2.193228	4.687230
1	-1.310414	-1.345905	2.948008
1	-1.906027	-3.004030	2.650996
1	-1.298860	-2.005061	1.307133
1	1.469202	-4.511777	1.907311
1	0.272529	-3.927604	0.715353
1	-0.266761	-4.893283	2.110479

Structure S62. ^{4}TS19

27	0.437384	-0.272984	-0.731832
8	2.276502	0.241002	-0.779118
8	0.704368	-2.166048	-0.920073
7	-0.012978	1.651368	-1.356583

7	-1.358621	-0.594123	-1.783974	1	4.289587	0.598254	2.120072
6	2.916967	1.365930	-0.881174	1	4.767471	-1.094793	1.839938
6	4.310008	1.426742	-0.521259	6	6.470782	0.469399	0.440039
6	4.973282	2.636092	-0.711165	1	6.572966	1.275499	1.184465
1	6.031566	2.711662	-0.460203	1	7.070744	0.739465	-0.444079
6	4.340335	3.794172	-1.210606	1	6.922994	-0.436139	0.874845
6	2.993544	3.754883	-1.507041	6	1.590838	-4.406360	0.643550
1	2.475704	4.650215	-1.864360	6	1.791172	-5.756563	1.354787
6	2.256587	2.558238	-1.334964	1	1.741215	-6.606341	0.654721
6	0.834028	2.609103	-1.559411	1	1.050315	-5.924377	2.153036
1	0.463237	3.588114	-1.895365	1	2.786420	-5.778427	1.826558
6	-1.455099	1.806112	-1.545245	6	2.709048	-4.265779	-0.415175
1	-1.901852	1.656110	-0.545817	1	2.669788	-3.290030	-0.911977
6	-1.913904	0.610942	-2.412794	1	2.622675	-5.051534	-1.184207
1	-1.405507	0.722101	-3.390225	1	3.697273	-4.371322	0.062706
6	-3.429170	0.620451	-2.637581	6	1.723183	-3.287118	1.705961
1	-3.927065	0.399050	-1.680104	1	1.020579	-3.460077	2.538414
1	-3.714033	-0.175063	-3.344335	1	1.512797	-2.292873	1.294368
6	-3.914447	1.973867	-3.168740	1	2.742651	-3.279120	2.126063
1	-3.510609	2.138751	-4.184131	9	-0.028896	-0.387973	1.083675
1	-5.012060	1.956394	-3.268350	1	4.914372	4.714200	-1.341040
6	-3.476402	3.122663	-2.257845	1	-2.748663	-6.038945	-0.372081
1	-3.946991	3.005777	-1.265696	6	-5.330847	0.148612	0.542850
1	-3.821906	4.088781	-2.659420	6	-4.925552	-1.195993	0.561056
6	-1.953178	3.142326	-2.094017	6	-4.518877	1.126206	1.127962
1	-1.657034	3.956802	-1.413823	6	-3.305890	0.803782	1.740953
1	-1.480563	3.343083	-3.072289	6	-2.913449	-0.579731	1.833868
6	-1.982068	-1.726414	-1.790402	6	-3.742855	-1.550602	1.189920
1	-2.980725	-1.786950	-2.246353	1	-6.268400	0.436013	0.060789
6	-1.513127	-2.961912	-1.211020	1	-5.544065	-1.963963	0.089317
6	-2.424749	-4.036783	-1.099046	1	-4.814930	2.176875	1.108030
1	-3.436336	-3.920138	-1.499779	6	-2.495242	1.985658	2.244499
6	-2.048229	-5.206300	-0.467905	6	-1.794321	-1.036894	2.555444
6	-0.750300	-5.315027	0.078090	1	-3.436634	-2.598377	1.226831
1	-0.501082	-6.239582	0.599653	8	-3.072631	2.988708	2.663273
6	0.202411	-4.304712	-0.016237	7	-1.151655	1.869501	2.126324
6	-0.167149	-3.103993	-0.724634	6	-0.157330	2.882495	2.537391
6	5.000577	0.187915	0.082795	1	-1.235526	-0.395734	3.232187
6	4.977283	-0.984888	-0.924096	1	-0.767214	1.025142	1.688401
1	5.521264	-0.719412	-1.845794	1	-1.522140	-2.093143	2.523659
1	3.950877	-1.259793	-1.194395	6	-0.319447	3.210355	4.030825
1	5.468279	-1.870876	-0.487846	6	-0.322247	4.155641	1.689251
6	4.269482	-0.222648	1.384230	6	1.223430	2.256591	2.288178
1	3.223023	-0.490214	1.194517	1	-1.309406	3.640981	4.232199

1	0.451111	3.931364	4.347485
1	-0.204777	2.299056	4.639637
1	1.372083	1.359240	2.907989
1	2.019673	2.978325	2.523847
1	1.339640	1.951503	1.240107
1	-1.333990	4.568124	1.807675
1	-0.152713	3.932583	0.625100
1	0.408994	4.920833	1.994667

Structure S63. ^{2}INT18

27	-0.166234	0.226737	-1.127789
8	-1.830422	-0.606029	-0.777873
8	-0.975379	1.905314	-0.789567
7	0.669631	-1.435337	-1.507839
7	1.488429	1.028512	-1.628872
6	-2.222501	-1.811219	-1.023277
6	-3.576898	-2.203076	-0.692246
6	-3.983338	-3.489800	-1.022901
1	-5.003720	-3.801670	-0.798217
6	-3.133945	-4.443201	-1.630542
6	-1.824627	-4.104749	-1.889549
1	-1.134746	-4.837584	-2.319698
6	-1.342857	-2.805058	-1.587855
6	0.059441	-2.554973	-1.754763
1	0.654907	-3.415591	-2.084565
6	2.127790	-1.286958	-1.569384
1	2.461874	-1.159651	-0.524552
6	2.388656	0.055958	-2.273383
1	2.034714	-0.060300	-3.316289
6	3.879392	0.398677	-2.295080
1	4.211170	0.599105	-1.263029
1	4.055589	1.316641	-2.877282
6	4.695080	-0.753127	-2.897385
1	4.437904	-0.861580	-3.966636
1	5.768173	-0.504937	-2.858882
6	4.427109	-2.078350	-2.178297
1	4.774993	-2.006716	-1.132281
1	5.003659	-2.892977	-2.645206
6	2.933515	-2.427813	-2.185433
1	2.764698	-3.357794	-1.619794
1	2.594200	-2.606399	-3.221456
6	1.791982	2.284737	-1.515540
1	2.782012	2.618586	-1.851166
6	0.953193	3.310249	-0.963374
6	1.524730	4.591262	-0.762684
1	2.563357	4.758832	-1.064198
6	0.793246	5.603049	-0.179462
6	-0.544995	5.351327	0.200220
1	-1.097357	6.171887	0.659067
6	-1.176982	4.127876	0.009169
6	-0.414872	3.052264	-0.593009
6	-4.497640	-1.218260	0.053632
6	-4.679821	0.081793	-0.761893
1	-5.116369	-0.136269	-1.751115
1	-3.722798	0.592284	-0.908972
1	-5.365932	0.767347	-0.237332
6	-3.868884	-0.895159	1.431072
1	-2.860298	-0.476734	1.328514
1	-3.806856	-1.806325	2.049255
1	-4.491057	-0.163596	1.973598
6	-5.895223	-1.811795	0.305443
1	-5.859421	-2.725164	0.920835
1	-6.420924	-2.050387	-0.633468
1	-6.512655	-1.078325	0.848389
6	-2.647917	3.896282	0.405686
6	-3.271431	5.135189	1.073354
1	-3.283399	6.011570	0.405528
1	-2.746850	5.417880	2.000690
1	-4.317461	4.918168	1.343047
6	-3.471350	3.584165	-0.865455
1	-3.078531	2.703721	-1.387410
1	-3.448523	4.439357	-1.561325
1	-4.524823	3.388752	-0.605074
6	-2.751920	2.722532	1.407947
1	-2.215836	2.965541	2.341575
1	-2.334161	1.800233	0.991425
1	-3.806367	2.540265	1.673004
9	-0.434848	0.215873	1.540876
1	-3.513670	-5.439882	-1.866089
1	1.231516	6.589471	-0.012213
6	4.422984	1.549170	1.362298
6	3.501309	2.588061	1.500544
6	4.021863	0.233920	1.598222
6	2.702479	-0.075997	1.962015
6	1.769259	0.981098	2.119071
6	2.189860	2.297885	1.878240
1	5.456150	1.760601	1.074975

1	3.794334	3.623861	1.314973
1	4.735265	-0.587770	1.516302
6	2.441730	-1.551765	2.223648
6	0.351203	0.780338	2.575374
1	1.471523	3.113283	1.986365
8	3.362707	-2.266657	2.612364
7	1.185270	-2.007989	1.991701
6	0.702340	-3.378581	2.275039
1	0.278453	0.092345	3.430422
1	0.530661	-1.398194	1.512150
1	-0.122375	1.737436	2.831054
6	0.987354	-3.750992	3.739122
6	1.378855	-4.377420	1.321235
6	-0.813657	-3.356022	2.039408
1	2.065461	-3.774676	3.942360
1	0.563239	-4.742792	3.961564
1	0.521057	-3.020246	4.419757
1	-1.308928	-2.640670	2.714507
1	-1.243602	-4.352597	2.219334
1	-1.056960	-3.073647	1.005627
1	2.471053	-4.341040	1.440431
1	1.127295	-4.141043	0.275969
1	1.036666	-5.403770	1.528262

Structure S64. ^{3}INT9

6	5.333951	-0.934204	0.439498
6	5.405440	0.382718	-0.023310
6	4.340010	-1.279197	1.354362
6	3.400990	-0.330935	1.791849
6	3.472441	1.009863	1.345027
6	4.491367	1.334699	0.434116
1	6.050037	-1.684762	0.096455
1	6.182212	0.674324	-0.735270
1	4.280545	-2.296688	1.747036
6	2.418712	-0.827580	2.816402
6	2.523637	2.082876	1.814784
1	4.566319	2.366602	0.083007
8	2.766618	-1.496360	3.775100
7	1.088868	-0.465479	2.644688
9	0.816312	-0.222115	1.279352
6	-0.083932	-1.120120	3.294329
1	2.358898	2.037014	2.901921
1	1.540588	1.970044	1.339644
1	2.903256	3.082396	1.561486
6	0.038471	-0.904209	4.811408
6	-0.109328	-2.613289	2.937770
6	-1.348213	-0.411255	2.788400
1	0.901874	-1.431298	5.233111
1	-0.877586	-1.279823	5.292999
1	0.131289	0.168072	5.043089
1	-1.329329	0.657007	3.048480
1	-2.226464	-0.868258	3.266999
1	-1.464227	-0.495525	1.702767
1	0.781803	-3.125033	3.328731
1	-0.146280	-2.742327	1.847045
1	-1.003460	-3.092783	3.364239
27	-0.546430	-0.201133	-1.303602
8	-0.510322	1.592496	-0.763830
8	-2.250572	-0.320381	-0.545781
7	1.261053	-0.114544	-1.908108
7	-0.144662	-2.049458	-0.876487
6	0.368872	2.532100	-0.962921
6	0.098788	3.858114	-0.469575
6	1.053662	4.843392	-0.707959
1	0.871775	5.858917	-0.355777
6	2.264553	4.599018	-1.388601
6	2.540447	3.323505	-1.836909
1	3.480406	3.104503	-2.351415
6	1.609559	2.278573	-1.631514
6	1.984136	0.946879	-2.024553
1	2.996641	0.842858	-2.433018
6	1.701862	-1.462908	-2.278526
1	1.077045	-1.746156	-3.143767
6	1.273036	-2.363035	-1.101049
1	1.819389	-2.003543	-0.210514
6	1.622248	-3.829492	-1.347181
1	1.014425	-4.209745	-2.187037
1	1.372969	-4.435227	-0.461393
6	3.113439	-3.976208	-1.676379
1	3.711001	-3.681829	-0.795229
1	3.345703	-5.034472	-1.876569
6	3.511079	-3.104845	-2.871106
1	2.977385	-3.453851	-3.772991
1	4.587506	-3.210927	-3.081730
6	3.179615	-1.628326	-2.621580
1	3.429009	-1.029620	-3.512121
1	3.790676	-1.249832	-1.785663

6	-1.047272	-2.939408	-0.603905
1	-0.733949	-3.987812	-0.514084
6	-2.442024	-2.699883	-0.381378
6	-3.279033	-3.817435	-0.131179
1	-2.840211	-4.819418	-0.131139
6	-4.623810	-3.639990	0.105709
6	-5.163571	-2.333793	0.091471
1	-6.234117	-2.232123	0.271216
6	-4.402049	-1.195189	-0.144849
6	-2.990177	-1.371556	-0.381731
6	-1.201893	4.142215	0.305430
6	-1.249713	3.250832	1.569219
1	-0.415478	3.490899	2.249372
1	-1.188205	2.189252	1.306877
1	-2.190856	3.415959	2.119304
6	-2.425213	3.853377	-0.595789
1	-2.454375	2.805202	-0.914028
1	-2.403257	4.488150	-1.496986
1	-3.358185	4.074352	-0.051804
6	-1.290414	5.608395	0.763880
1	-1.297873	6.312178	-0.084083
1	-0.461699	5.886557	1.434980
1	-2.227349	5.761126	1.322697
6	-5.009352	0.220096	-0.171055
6	-6.528676	0.196816	0.073285
1	-6.786281	-0.209102	1.065157
1	-7.065263	-0.390140	-0.689446
1	-6.922370	1.224747	0.028903
6	-4.370194	1.084374	0.941558
1	-3.290992	1.195694	0.794345
1	-4.543627	0.634150	1.933277
1	-4.821549	2.090096	0.947064
6	-4.766546	0.862714	-1.558725
1	-5.309532	0.306551	-2.340635
1	-3.703704	0.872983	-1.830223
1	-5.136620	1.901375	-1.566094
9	-1.111204	-0.417337	-3.047827
1	2.973499	5.414221	-1.548675
1	-5.275810	-4.495166	0.296147

Structure S65. ^{3}TS20

6	5.295600	-0.675604	0.542616
6	5.339676	0.660609	0.135403
6	4.242112	-1.101228	1.347981
6	3.219452	-0.221617	1.747561
6	3.260133	1.139342	1.349035
6	4.337784	1.543926	0.541794
1	6.074985	-1.378309	0.238001
1	6.158579	1.019703	-0.493943
1	4.197791	-2.135243	1.695880
6	2.203765	-0.823589	2.674240
6	2.239669	2.168012	1.761789
1	4.387132	2.589730	0.229701
8	2.510414	-1.744960	3.428044
7	0.956084	-0.236766	2.737915
9	0.507164	-0.199724	0.934645
6	-0.212351	-0.837625	3.367572
1	2.125774	2.206758	2.855719
1	1.252681	1.918129	1.358963
1	2.526524	3.166173	1.402145
6	0.069027	-0.790848	4.895354
6	-0.485001	-2.271586	2.897864
6	-1.416712	0.066416	3.065695
1	0.885702	-1.469027	5.169908
1	-0.850584	-1.094131	5.420178
1	0.327968	0.229843	5.215876
1	-1.224651	1.096742	3.398852
1	-2.306098	-0.312659	3.591706
1	-1.619216	0.073967	1.989821
1	0.365152	-2.932477	3.114178
1	-0.672498	-2.264418	1.817985
1	-1.378731	-2.672303	3.400068
27	-0.340920	-0.309873	-0.898004
8	-0.551428	1.556105	-0.828357
8	-2.052155	-0.476293	-0.157325
7	1.384201	-0.190522	-1.685720
7	-0.012065	-2.188876	-0.774524
6	0.312609	2.495976	-1.041379
6	-0.013363	3.855227	-0.664830
6	0.912945	4.847185	-0.962212
1	0.690016	5.880825	-0.698049
6	2.151663	4.591548	-1.591180
6	2.487628	3.295819	-1.916847
1	3.449752	3.069662	-2.384526
6	1.593678	2.234237	-1.637970
6	2.023293	0.902306	-1.942088
1	2.999425	0.822862	-2.435429

6	1.841507	-1.519770	-2.104314
1	1.231214	-1.779452	-2.987526
6	1.408062	-2.471938	-0.972263
1	1.922080	-2.133875	-0.056156
6	1.786818	-3.922372	-1.260381
1	1.212668	-4.284531	-2.131406
1	1.522032	-4.560941	-0.402604
6	3.288542	-4.027521	-1.554350
1	3.857910	-3.744507	-0.651305
1	3.549584	-5.074432	-1.777324
6	3.691685	-3.115599	-2.716451
1	3.184228	-3.452751	-3.638004
1	4.774082	-3.192963	-2.908134
6	3.326118	-1.652222	-2.438275
1	3.574074	-1.034243	-3.315537
1	3.918137	-1.274273	-1.590006
6	-0.931394	-3.085622	-0.639297
1	-0.634412	-4.142006	-0.658422
6	-2.329054	-2.834748	-0.447947
6	-3.207678	-3.944033	-0.412648
1	-2.795974	-4.951976	-0.516464
6	-4.563655	-3.749875	-0.259484
6	-5.071507	-2.434016	-0.185613
1	-6.153389	-2.317634	-0.121053
6	-4.265475	-1.301554	-0.217231
6	-2.837164	-1.499471	-0.281676
6	-1.331302	4.163476	0.067895
6	-1.372722	3.365886	1.392376
1	-0.556975	3.678853	2.064436
1	-1.275446	2.290465	1.213006
1	-2.327275	3.540591	1.915398
6	-2.530734	3.775703	-0.824605
1	-2.520259	2.708435	-1.064187
1	-2.513827	4.343569	-1.769599
1	-3.478004	4.006451	-0.310312
6	-1.465169	5.656992	0.412849
1	-1.483283	6.293655	-0.486414
1	-0.653783	6.010122	1.069617
1	-2.413579	5.823280	0.947791
6	-4.847856	0.121588	-0.290015
6	-6.386418	0.113664	-0.244539
1	-6.772590	-0.293856	0.704219
1	-6.828744	-0.461756	-1.073202
1	-6.759677	1.146306	-0.332363
6	-4.354754	0.997614	0.884025
1	-3.273155	1.151930	0.845702
1	-4.607297	0.534787	1.852396
1	-4.844506	1.984379	0.846631
6	-4.414761	0.735870	-1.644613
1	-4.865519	0.174632	-2.479433
1	-3.325103	0.712314	-1.779597
1	-4.755854	1.781322	-1.718213
9	-1.084619	-0.557885	-2.577753
1	2.834345	5.417262	-1.803051
1	-5.249827	-4.598957	-0.227498

Structure S66. ^{3}INT10

6	5.264279	-0.465276	0.650145
6	5.278053	0.924712	0.508934
6	4.192788	-1.068359	1.306369
6	3.131207	-0.314664	1.836963
6	3.142055	1.097169	1.705151
6	4.228257	1.682356	1.031641
1	6.081358	-1.074748	0.255491
1	6.106309	1.421679	-0.004046
1	4.157826	-2.152153	1.428361
6	2.046295	-1.122328	2.502791
6	2.033127	1.981905	2.203649
1	4.240123	2.768492	0.910648
8	2.027780	-2.355511	2.399970
7	1.216848	-0.508128	3.390374
9	0.439032	0.010667	0.619217
6	-0.180126	-0.824161	3.650849
1	1.878507	1.861285	3.286690
1	1.098828	1.697347	1.702112
1	2.246777	3.040448	1.994158
6	-0.247924	-1.298038	5.117848
6	-0.815858	-1.862161	2.712302
6	-0.946173	0.512269	3.495645
1	0.316760	-2.234704	5.245700
1	-1.295449	-1.482369	5.406401
1	0.177991	-0.542654	5.796017
1	-0.509241	1.303596	4.122817
1	-1.995133	0.365886	3.797063
1	-0.918185	0.822293	2.445035
1	-0.334292	-2.842953	2.811437
1	-0.718536	-1.518245	1.678195

1	-1.885798	-1.962852	2.955346
27	-0.298474	-0.289254	-1.046284
8	-0.557904	1.599594	-1.150843
8	-2.061217	-0.427692	-0.347960
7	1.433143	-0.184759	-1.805904
7	0.027919	-2.145552	-0.846016
6	0.349853	2.499523	-1.150215
6	0.021906	3.854860	-0.725443
6	1.008062	4.825269	-0.840875
1	0.791114	5.850000	-0.540626
6	2.305978	4.549772	-1.321070
6	2.649284	3.253825	-1.671896
1	3.661532	3.022726	-2.013169
6	1.706066	2.217129	-1.576152
6	2.133479	0.886756	-1.923526
1	3.154568	0.808632	-2.315436
6	1.902499	-1.517793	-2.175110
1	1.304659	-1.806041	-3.057445
6	1.449233	-2.433400	-1.014727
1	1.939442	-2.070011	-0.097365
6	1.832117	-3.892144	-1.247446
1	1.262579	-4.289483	-2.106549
1	1.567541	-4.493761	-0.363809
6	3.335477	-4.009534	-1.527566
1	3.896788	-3.702820	-0.627731
1	3.594781	-5.063385	-1.717566
6	3.753784	-3.133508	-2.711695
1	3.252245	-3.492082	-3.628528
1	4.837353	-3.221902	-2.891492
6	3.392161	-1.661992	-2.475043
1	3.660066	-1.061505	-3.359201
1	3.969688	-1.272438	-1.620617
6	-0.872817	-3.042723	-0.656599
1	-0.566600	-4.094996	-0.613021
6	-2.280316	-2.799732	-0.471972
6	-3.133279	-3.910743	-0.369442
1	-2.709735	-4.916810	-0.431050
6	-4.498041	-3.734970	-0.198136
6	-5.037908	-2.432699	-0.146547
1	-6.118601	-2.339760	-0.042598
6	-4.257412	-1.287925	-0.233974
6	-2.816808	-1.457570	-0.362031
6	-1.352176	4.155405	-0.109816
6	-1.536882	3.250540	1.131269
1	-0.767078	3.466358	1.888836
1	-1.466942	2.191720	0.861202
1	-2.522288	3.428503	1.590622
6	-2.471252	3.888381	-1.141626
1	-2.472365	2.844983	-1.471829
1	-2.346894	4.533450	-2.027047
1	-3.454866	4.112616	-0.697261
6	-1.472810	5.618638	0.350399
1	-1.379197	6.330397	-0.485779
1	-0.722762	5.879163	1.114290
1	-2.465169	5.776820	0.801309
6	-4.863195	0.121669	-0.254375
6	-6.399446	0.091971	-0.165562
1	-6.754773	-0.355223	0.776960
1	-6.857404	-0.457259	-1.003692
1	-6.785519	1.122833	-0.202466
6	-4.341247	0.941110	0.948374
1	-3.251054	1.023194	0.938892
1	-4.644487	0.472172	1.899217
1	-4.766253	1.957762	0.924393
6	-4.480465	0.802859	-1.592123
1	-4.937131	0.265130	-2.439113
1	-3.395619	0.821242	-1.754235
1	-4.855909	1.838491	-1.609012
9	-0.999578	-0.622448	-2.692824
1	3.039521	5.355732	-1.393361
1	-5.160947	-4.599351	-0.119690

Structure S67. Co^{IV}(salen)-F_2

27	-0.596686	0.000268	0.000381
8	0.774459	1.269805	0.315805
8	0.773694	-1.269801	-0.314801
7	-1.971856	1.228713	0.431131
7	-1.972334	-1.227364	-0.431024
6	0.674717	2.537881	0.216362
6	1.865128	3.326638	-0.065374
6	1.749145	4.708957	-0.017584
1	2.624668	5.329724	-0.207337
6	0.529091	5.367195	0.249193
6	-0.628848	4.627958	0.434669
1	-1.585052	5.131878	0.601343
6	-0.589482	3.223294	0.395901
6	-1.826857	2.501993	0.541388

1	-2.709029	3.117501	0.758776
6	-3.244471	0.527219	0.568408
1	-3.172581	-0.032600	1.517313
6	-3.244787	-0.525420	-0.567890
1	-3.173309	0.034333	-1.516871
6	-4.508000	-1.383859	-0.550718
1	-4.510649	-2.003605	0.363520
1	-4.513645	-2.070659	-1.412249
6	-5.761813	-0.501222	-0.576665
1	-5.804727	0.044003	-1.536488
1	-6.661570	-1.135816	-0.535069
6	-5.761377	0.503501	0.578762
1	-5.803689	-0.041697	1.538625
1	-6.661096	1.138190	0.537764
6	-4.507458	1.385947	0.551903
1	-4.512337	2.072876	1.413340
1	-4.510633	2.005541	-0.362443
6	-1.827764	-2.500568	-0.543394
1	-2.710221	-3.115253	-0.761942
6	-0.590915	-3.222658	-0.398402
6	-0.630947	-4.627356	-0.438940
1	-1.587330	-5.130503	-0.606912
6	0.526407	-5.367321	-0.253360
6	1.746495	-4.709846	0.015336
1	2.621597	-5.331197	0.205154
6	1.863050	-3.327633	0.064851
6	0.673330	-2.538071	-0.217005
6	3.165108	2.616904	-0.468320
6	2.889808	1.797038	-1.755492
1	2.664100	2.473135	-2.596569
1	2.039391	1.111694	-1.644025
1	3.781998	1.209750	-2.027119
6	3.656704	1.697953	0.674043
1	2.932204	0.909887	0.897774
1	3.831048	2.281439	1.593332
1	4.610530	1.224464	0.390941
6	4.292861	3.617038	-0.778756
1	4.571995	4.217597	0.102349
1	4.029801	4.304902	-1.598190
1	5.192125	3.065036	-1.094753
6	3.163086	-2.618957	0.469584
6	4.289958	-3.619965	0.780361
1	4.569650	-4.219974	-0.100946
1	4.025676	-4.308346	1.598969
1	5.189228	-3.068714	1.097652
6	3.656174	-1.699495	-0.671687
1	2.932054	-0.911173	-0.895662
1	3.831310	-2.282434	-1.591178
1	4.609825	-1.226409	-0.387315
6	2.887191	-1.799676	1.756978
1	2.660163	-2.476043	2.597488
1	2.037404	-1.113611	1.645108
1	3.779570	-1.213226	2.029818
9	-0.629087	-0.610668	1.727836
1	0.498706	6.458602	0.279906
1	0.495662	-6.458676	-0.285404
9	-0.627736	0.611542	-1.727022

Structure S68. Co^{II}(salen)

27	0.000005	0.788728	0.000015
8	-1.307254	-0.553547	0.081346
8	1.307257	-0.553557	-0.081292
7	-1.272977	2.160343	-0.254193
7	1.272996	2.160340	0.254207
6	-2.600726	-0.470596	0.034242
6	-3.400842	-1.662762	0.207113
6	-4.781908	-1.541762	0.119931
1	-5.394460	-2.435370	0.239995
6	-5.464904	-0.319591	-0.116914
6	-4.697778	0.820116	-0.255745
1	-5.181733	1.787527	-0.426956
6	-3.280293	0.776726	-0.180090
6	-2.563239	2.013636	-0.312974
1	-3.185030	2.902024	-0.481801
6	-0.613824	3.460665	-0.463218
1	-0.226933	3.448715	-1.500163
6	0.613848	3.460664	0.463225
1	0.226957	3.448720	1.500170
6	1.465589	4.715847	0.274592
1	1.906141	4.704876	-0.738050
1	2.299941	4.724902	0.992999
6	0.609658	5.975537	0.463175
1	0.269405	6.027458	1.513110
1	1.225810	6.872197	0.287011
6	-0.609626	5.975537	-0.463176
1	-0.269373	6.027453	-1.513111
1	-1.225775	6.872200	-0.287016

6	-1.465561	4.715851	-0.274589
1	-2.299913	4.724907	-0.992997
1	-1.906113	4.704884	0.738053
6	2.563258	2.013630	0.312969
1	3.185054	2.902017	0.481782
6	3.280305	0.776716	0.180084
6	4.697792	0.820099	0.255716
1	5.181755	1.787510	0.426912
6	5.464910	-0.319614	0.116888
6	4.781905	-1.541781	-0.119944
1	5.394451	-2.435394	-0.240009
6	3.400837	-1.662772	-0.207110
6	2.600730	-0.470605	-0.034223
6	-2.717560	-3.016917	0.486478
6	-1.910511	-2.924849	1.803091
1	-2.579412	-2.710063	2.653398
1	-1.151467	-2.134524	1.749508
1	-1.401975	-3.881697	2.008717
6	-1.776394	-3.385874	-0.683591
1	-0.991037	-2.632448	-0.811771
1	-2.342022	-3.467280	-1.627047
1	-1.296370	-4.360622	-0.494777
6	-3.738698	-4.158094	0.645000
1	-4.337333	-4.311295	-0.267346
1	-4.431515	-3.983586	1.483874
1	-3.206292	-5.100617	0.850449
6	2.717530	-3.016914	-0.486468
6	3.738638	-4.158120	-0.644993
1	4.337300	-4.311311	0.267337
1	4.431432	-3.983652	-1.483895
1	3.206204	-5.100636	-0.850399
6	1.776353	-3.385843	0.683600
1	0.991033	-2.632382	0.811792
1	2.341980	-3.467286	1.627053
1	1.296283	-4.360567	0.494778
6	1.910480	-2.924814	-1.803077
1	2.579388	-2.710067	-2.653387
1	1.151476	-2.134450	-1.749495
1	1.401895	-3.881638	-2.008693
6	6.984322	-0.283372	0.204216
6	7.645550	-0.721413	-1.113107
6	7.509235	-1.117420	1.384222
1	7.271457	0.766972	0.387154
1	7.304252	-0.102680	-1.958856
1	8.743695	-0.637647	-1.050847
1	7.407716	-1.772128	-1.350251
1	7.072182	-0.781497	2.338440
1	7.262065	-2.185263	1.260502
1	8.606498	-1.039351	1.465656
6	-6.984314	-0.283342	-0.204258
6	-7.645558	-0.721347	1.113069
6	-7.509220	-1.117415	-1.384250
1	-7.271440	0.767000	-0.387224
1	-7.304271	-0.102592	1.958806
1	-8.743703	-0.637583	1.050793
1	-7.407728	-1.772056	1.350244
1	-7.072149	-0.781522	-2.338470
1	-7.262066	-2.185257	-1.260497
1	-8.606482	-1.039334	-1.465702

Structure S69. $PhSO_2N(Et)F$

16	-0.572181	-1.043987	-0.247160
8	-0.886534	-1.190107	-1.673728
8	-0.728769	-2.168106	0.672241
6	1.042346	-0.308348	-0.060965
6	1.697326	0.192752	-1.189576
6	1.615486	-0.272696	1.215381
6	2.966411	0.754597	-1.027895
1	1.221739	0.138469	-2.170218
6	2.882201	0.295005	1.358866
1	1.080269	-0.683034	2.073551
6	3.553780	0.806697	0.241042
1	3.497220	1.150529	-1.896853
1	3.348934	0.334371	2.345846
1	4.546374	1.248169	0.360884
7	-1.536096	0.270220	0.478822
9	-2.783663	-0.355284	0.756882
6	-1.827073	1.364415	-0.452283
6	-2.621670	2.459607	0.243068
1	-2.350325	0.976926	-1.343673
1	-0.842298	1.741719	-0.773409
1	-2.795805	3.292293	-0.455826
1	-3.598673	2.080087	0.576843
1	-2.077315	2.843804	1.119795

Structure S70. ^{2}**TS21**

27	-0.730245	-0.113845	0.967537	1	-0.577880	-3.052688	-1.177569
8	0.060365	-1.791594	0.648719	1	-0.785133	-4.739358	-1.712023
8	-2.224059	-0.731463	0.018584	6	-0.304528	-4.771357	1.001410
7	0.669208	0.413759	2.133679	1	-0.833867	-3.856962	1.297964
7	-1.585174	1.506329	1.445422	1	0.209152	-5.178965	1.888063
6	1.294409	-2.150580	0.809540	1	-1.054020	-5.511958	0.675926
6	1.732919	-3.451709	0.353409	6	1.372857	-5.831708	-0.504251
6	3.092573	-3.731652	0.409167	1	1.906250	-6.280764	0.348967
1	3.444964	-4.691752	0.032282	1	2.086272	-5.726908	-1.337500
6	4.071416	-2.849392	0.939107	1	0.600484	-6.549383	-0.824004
6	3.627296	-1.659480	1.482977	6	-4.070874	-2.284399	-1.524447
1	4.337815	-0.968839	1.947886	6	-5.280200	-2.903334	-2.249241
6	2.257578	-1.296939	1.447352	1	-5.678566	-2.244483	-3.037536
6	1.862762	-0.088903	2.118495	1	-6.102230	-3.143050	-1.555449
1	2.653762	0.412618	2.686131	1	-4.973814	-3.844411	-2.733746
6	0.305997	1.594630	2.932840	6	-2.971622	-2.025101	-2.582437
1	-0.305594	1.215991	3.774172	1	-2.079991	-1.572679	-2.131143
6	-0.623459	2.440537	2.046178	1	-3.343429	-1.345227	-3.367155
1	-0.013806	2.808167	1.205695	1	-2.672576	-2.969244	-3.067413
6	-1.183540	3.643151	2.803096	6	-3.575725	-3.312382	-0.480058
1	-1.834429	3.295568	3.625519	1	-4.359847	-3.511367	0.269842
1	-1.802563	4.261545	2.134336	1	-2.680572	-2.951490	0.038359
6	-0.029929	4.488342	3.360949	1	-3.332146	-4.268756	-0.971554
1	0.543513	4.909748	2.516710	6	-7.502979	1.345925	-0.427891
1	-0.434052	5.341484	3.929823	6	-8.530397	0.385750	0.193296
6	0.907103	3.655599	4.240366	6	-7.859091	1.661688	-1.889969
1	0.358362	3.314420	5.136932	1	-7.549878	2.293120	0.137634
1	1.744989	4.274295	4.600931	1	-8.298891	0.180205	1.251013
6	1.455650	2.434998	3.489475	1	-9.547528	0.809540	0.142916
1	2.078167	1.831408	4.168986	1	-8.548618	-0.580268	-0.338994
1	2.095666	2.755192	2.650633	1	-7.149313	2.382054	-2.327855
6	-2.824325	1.815518	1.222858	1	-7.837192	0.750712	-2.511614
1	-3.193030	2.783660	1.584290	1	-8.872363	2.091009	-1.966693
6	-3.783815	1.015686	0.513656	6	5.546402	-3.222533	0.922577
6	-5.107078	1.513672	0.396025	6	6.086890	-3.321580	-0.513858
1	-5.347711	2.472356	0.867290	6	5.827412	-4.514314	1.706885
6	-6.080950	0.819540	-0.295554	1	6.090124	-2.404031	1.425817
6	-5.703700	-0.408824	-0.897955	1	5.931496	-2.380117	-1.065539
1	-6.473754	-0.944672	-1.453115	1	7.167531	-3.542884	-0.514966
6	-4.428610	-0.956887	-0.827051	1	5.582500	-4.125795	-1.075860
6	-3.419547	-0.235314	-0.085870	1	5.465857	-4.438786	2.745216
6	0.705752	-4.493459	-0.137420	1	5.331899	-5.383362	1.242414
6	-0.048010	-3.986922	-1.386489	1	6.908891	-4.728667	1.736779
1	0.648018	-3.817963	-2.223370	16	2.322076	2.605792	-0.697348

8	3.120466	2.004840	0.385716
8	1.333068	3.642611	-0.383993
6	3.429634	3.223024	-1.956716
6	4.779861	2.861378	-1.917145
6	2.907922	4.050801	-2.958419
6	5.629947	3.345709	-2.914632
1	5.151626	2.219409	-1.116780
6	3.770552	4.523120	-3.948444
1	1.849588	4.317800	-2.956808
6	5.126341	4.171068	-3.926547
1	6.689313	3.078691	-2.899270
1	3.383863	5.170553	-4.739037
1	5.796203	4.545185	-4.704907
7	1.506274	1.415631	-1.650807
9	0.266061	0.980004	-0.557682
6	2.223728	0.163178	-1.796206
6	1.351217	-0.876271	-2.480323
1	2.598965	-0.202831	-0.825398
1	3.109008	0.398584	-2.418898
1	1.939752	-1.786530	-2.666083
1	0.505092	-1.133152	-1.830709
1	0.964610	-0.501695	-3.441020

Structure S71. ^{4}INT11

27	0.906743	-0.041530	0.749942
8	0.447752	1.766044	0.890903
8	2.517098	0.479295	-0.072625
7	-0.487722	-0.524720	1.995945
7	1.522714	-1.823040	0.996394
6	-0.773368	2.223110	0.976675
6	-1.079632	3.544984	0.494075
6	-2.404412	3.967793	0.558946
1	-2.658111	4.951142	0.163839
6	-3.462803	3.198550	1.101976
6	-3.146459	1.955470	1.619018
1	-3.927315	1.324226	2.052456
6	-1.825416	1.454206	1.566318
6	-1.579521	0.151273	2.121761
1	-2.400935	-0.278776	2.703281
6	-0.292044	-1.870244	2.556155
1	0.432639	-1.770270	3.385900
6	0.404192	-2.665314	1.436574
1	-0.294552	-2.687983	0.584867
6	0.730997	-4.093310	1.861661
1	1.474152	-4.080258	2.679516
1	1.177154	-4.644522	1.018633
6	-0.549439	-4.796300	2.333012
1	-1.250135	-4.869801	1.483690
1	-0.313016	-5.824943	2.650175
6	-1.217878	-4.024077	3.474262
1	-0.545587	-4.012098	4.351387
1	-2.142247	-4.532959	3.792450
6	-1.547174	-2.583960	3.060595
1	-1.977438	-2.036199	3.914355
1	-2.297649	-2.586615	2.255028
6	2.721514	-2.261175	0.778175
1	2.931313	-3.316762	0.991815
6	3.823791	-1.500172	0.265209
6	5.085097	-2.141938	0.167406
1	5.171096	-3.180173	0.503068
6	6.187875	-1.483886	-0.340326
6	6.005292	-0.146847	-0.777902
1	6.875615	0.359291	-1.194710
6	4.800689	0.543853	-0.716251
6	3.658088	-0.141866	-0.161185
6	0.032570	4.439701	-0.084825
6	0.689759	3.746449	-1.299863
1	-0.045507	3.596515	-2.106521
1	1.104604	2.770429	-1.027566
1	1.503962	4.373082	-1.699144
6	1.087708	4.709392	1.013237
1	1.525395	3.775432	1.386883
1	0.633387	5.244438	1.863950
1	1.902705	5.337236	0.616566
6	-0.505309	5.802753	-0.556600
1	-0.963756	6.378314	0.263635
1	-1.250116	5.700850	-1.362304
1	0.326821	6.404892	-0.955225
6	4.660386	1.982576	-1.250553
6	5.999594	2.541906	-1.764668
1	6.404031	1.953649	-2.603754
1	6.764569	2.581851	-0.972460
1	5.849635	3.570492	-2.129942
6	3.666497	1.981363	-2.436195
1	2.683762	1.594856	-2.139332
1	4.049948	1.356045	-3.259349
1	3.531415	3.004319	-2.824844

6	4.160352	2.923218	-0.129837
1	4.878582	2.945329	0.707070
1	3.186172	2.603977	0.255145
1	4.062404	3.952129	-0.513347
6	7.547153	-2.159099	-0.452260
6	8.626157	-1.416521	0.352513
6	7.974771	-2.330122	-1.919264
1	7.442989	-3.167964	-0.016292
1	8.337320	-1.311766	1.410835
1	9.586319	-1.957693	0.313324
1	8.800929	-0.404273	-0.049211
1	7.223208	-2.897676	-2.491475
1	8.103859	-1.352662	-2.413996
1	8.935084	-2.867960	-1.990055
6	-4.892062	3.719726	1.092287
6	-5.423526	3.872611	-0.342703
6	-5.037685	5.032763	1.877381
1	-5.513438	2.959535	1.596992
1	-5.355926	2.922284	-0.896939
1	-6.479101	4.192511	-0.340910
1	-4.847902	4.628539	-0.903302
1	-4.684363	4.921055	2.915214
1	-4.456815	5.846494	1.411635
1	-6.091629	5.355994	1.908604
16	-3.063369	-2.039808	-0.728309
8	-3.445618	-1.256917	0.464439
8	-2.148549	-3.181901	-0.577298
6	-4.564502	-2.618719	-1.514692
6	-5.775030	-1.979467	-1.226634
6	-4.484828	-3.687516	-2.415395
6	-6.936265	-2.427885	-1.860445
1	-5.801691	-1.155009	-0.512000
6	-5.654186	-4.123302	-3.040941
1	-3.524549	-4.167692	-2.612400
6	-6.874993	-3.494486	-2.765224
1	-7.892118	-1.944144	-1.645164
1	-5.613074	-4.957390	-3.745659
1	-7.786634	-3.840199	-3.259238
7	-2.480564	-1.083249	-2.008383
9	-0.241715	-0.480085	-0.705911
6	-2.691807	0.333993	-1.869936
6	-1.794204	1.115683	-2.818116
1	-2.551531	0.658449	-0.826547
1	-3.764894	0.519135	-2.106678
1	-2.049161	2.185996	-2.777240
1	-0.751203	0.982435	-2.501179
1	-1.907492	0.767748	-3.857378

Structure S72. Co^{III}(salen)-F

27	-0.016061	0.720084	0.192167
8	1.304276	-0.536716	-0.230764
8	-1.275220	-0.625162	-0.102407
7	1.274617	2.126715	0.309177
7	-1.210502	2.094742	-0.464610
6	2.605102	-0.466353	-0.145217
6	3.387219	-1.659389	-0.332005
6	4.772106	-1.546244	-0.245076
1	5.378504	-2.442398	-0.375277
6	5.459897	-0.334370	0.009985
6	4.697672	0.806312	0.187866
1	5.184468	1.765989	0.388308
6	3.283702	0.763581	0.121248
6	2.558734	1.995481	0.291722
1	3.175336	2.895852	0.407417
6	0.572164	3.406314	0.453414
1	0.063457	3.351521	1.432157
6	-0.529753	3.391470	-0.625198
1	-0.019531	3.370092	-1.606175
6	-1.412394	4.637137	-0.544768
1	-1.979859	4.609541	0.401988
1	-2.145197	4.641971	-1.366770
6	-0.556500	5.909152	-0.604932
1	-0.077393	5.978827	-1.598031
1	-1.205997	6.793647	-0.505718
6	0.524050	5.914913	0.479990
1	0.044309	5.940613	1.474467
1	1.141904	6.823971	0.402500
6	1.420675	4.673563	0.385739
1	2.160161	4.678111	1.202111
1	1.979788	4.688684	-0.566789
6	-2.490570	1.936180	-0.618578
1	-3.089877	2.806843	-0.914589
6	-3.226549	0.723917	-0.417379
6	-4.642398	0.774449	-0.518293
1	-5.115378	1.730051	-0.765831
6	-5.418967	-0.345147	-0.295704
6	-4.751447	-1.548940	0.055892

1	-5.374879	-2.419391	0.261105
6	-3.373152	-1.675446	0.167493
6	-2.566569	-0.512843	-0.112149
6	2.690089	-3.011538	-0.583863
6	1.850411	-2.940768	-1.880988
1	2.498065	-2.744860	-2.752051
1	1.093812	-2.148653	-1.825130
1	1.335416	-3.900548	-2.053337
6	1.780320	-3.353425	0.620262
1	1.000232	-2.596748	0.764961
1	2.373145	-3.422931	1.547465
1	1.289860	-4.327928	0.461852
6	3.703414	-4.158865	-0.747599
1	4.319743	-4.302756	0.154248
1	4.379099	-3.997550	-1.602957
1	3.162951	-5.101507	-0.929041
6	-2.694618	-2.986638	0.607707
6	-3.721785	-4.093178	0.907606
1	-4.309100	-4.368640	0.016607
1	-4.423280	-3.805364	1.706998
1	-3.194420	-4.999784	1.245095
6	-1.764439	-3.505041	-0.513538
1	-0.966397	-2.788179	-0.734973
1	-2.337140	-3.687128	-1.438492
1	-1.300902	-4.458936	-0.212128
6	-1.887099	-2.730680	1.905198
1	-2.569021	-2.495051	2.739322
1	-1.183699	-1.894799	1.800025
1	-1.316768	-3.632885	2.182679
6	-6.936893	-0.304957	-0.399033
6	-7.611548	-0.621230	0.945849
6	-7.455676	-1.238060	-1.505497
1	-7.214166	0.727292	-0.675676
1	-7.271407	0.066063	1.737138
1	-8.708005	-0.533150	0.865532
1	-7.385868	-1.649241	1.275644
1	-7.007258	-0.992805	-2.481758
1	-7.217873	-2.292087	-1.283741
1	-8.551303	-1.160194	-1.604661
6	6.979686	-0.304781	0.089741
6	7.630865	-0.724856	-1.238152
6	7.505622	-1.159774	1.254143
1	7.271168	0.741399	0.287884
1	7.287957	-0.091643	-2.072431
1	8.729407	-0.646143	-1.179831
1	7.387872	-1.770974	-1.489741
1	7.073508	-0.838185	2.215380
1	7.254975	-2.224640	1.113586
1	8.603267	-1.085628	1.331863
9	-0.306617	0.805905	2.027595

Structure S73. $PhSO_2N^{\cdot}(Et)$

16	0.683615	-0.752451	-0.261487
8	0.930406	-1.839022	0.699279
8	0.953908	-0.961257	-1.693984
6	-0.992933	-0.172055	-0.063023
6	-1.641215	-0.383266	1.157384
6	-1.613064	0.481217	-1.132122
6	-2.949027	0.083974	1.308637
1	-1.131297	-0.909068	1.966558
6	-2.920901	0.942087	-0.964979
1	-1.082067	0.616410	-2.076015
6	-3.585110	0.745179	0.251563
1	-3.473863	-0.072929	2.254099
1	-3.424094	1.452825	-1.789470
1	-4.609164	1.106708	0.375205
7	1.571037	0.616078	0.207992
6	2.992806	0.373127	0.276199
6	3.762292	1.669520	0.480620
1	3.334649	-0.160528	-0.634413
1	3.179281	-0.338718	1.108480
1	4.841515	1.463012	0.555319
1	3.598903	2.357047	-0.364033
1	3.439423	2.175449	1.404075

Structure S74. $[Co^{IV}(salen)\text{-}F]^+$

27	0.014941	0.742034	0.212403
8	1.287023	-0.507508	-0.253458
8	-1.288660	-0.626380	-0.056077
7	1.277296	2.133164	0.339814
7	-1.192437	2.122087	-0.515269
6	2.591960	-0.460591	-0.149976
6	3.353143	-1.665106	-0.329184
6	4.738255	-1.564443	-0.231831
1	5.336963	-2.465312	-0.360650
6	5.436896	-0.360325	0.031139

6	4.690055	0.792349	0.206449
1	5.186927	1.744055	0.415080
6	3.278677	0.763762	0.127852
6	2.563070	1.996006	0.303277
1	3.180031	2.896320	0.407797
6	0.575121	3.419546	0.459787
1	0.045415	3.380365	1.427106
6	-0.500725	3.415059	-0.651288
1	0.036144	3.374541	-1.616183
6	-1.373089	4.666416	-0.599060
1	-1.957521	4.654874	0.337717
1	-2.089646	4.667912	-1.435871
6	-0.499528	5.926458	-0.654164
1	0.001503	5.979424	-1.636999
1	-1.140473	6.818758	-0.577483
6	0.555128	5.928307	0.455559
1	0.054226	5.971582	1.438652
1	1.188082	6.826616	0.382250
6	1.439471	4.676368	0.394822
1	2.159539	4.679528	1.228125
1	2.018050	4.672176	-0.545770
6	-2.469017	1.982913	-0.591014
1	-3.089826	2.855774	-0.829649
6	-3.206680	0.749633	-0.374949
6	-4.591450	0.796995	-0.462616
1	-5.082082	1.745815	-0.695864
6	-5.384771	-0.351722	-0.251708
6	-4.742316	-1.573711	0.060522
1	-5.377598	-2.439118	0.241488
6	-3.366981	-1.711074	0.157580
6	-2.550642	-0.519521	-0.086995
6	2.646846	-3.009177	-0.591325
6	1.821481	-2.927944	-1.896999
1	2.478957	-2.726589	-2.758909
1	1.061716	-2.138118	-1.850297
1	1.310622	-3.887288	-2.080741
6	1.728940	-3.346141	0.607615
1	0.952095	-2.586713	0.753904
1	2.316953	-3.423295	1.536797
1	1.232575	-4.316034	0.443285
6	3.653995	-4.162379	-0.750575
1	4.262080	-4.313160	0.155355
1	4.335970	-4.003176	-1.600933
1	3.107700	-5.099916	-0.938402
6	-2.692729	-3.028815	0.550724
6	-3.726177	-4.141048	0.800658
1	-4.312365	-4.374124	-0.102318
1	-4.423420	-3.885237	1.613655
1	-3.200161	-5.061000	1.097852
6	-1.756678	-3.500130	-0.589823
1	-0.939541	-2.794660	-0.770858
1	-2.321741	-3.632682	-1.526814
1	-1.316428	-4.473275	-0.321944
6	-1.894609	-2.819035	1.864696
1	-2.578216	-2.578151	2.694908
1	-1.156576	-2.010882	1.788289
1	-1.364619	-3.749127	2.123915
6	-6.891146	-0.276825	-0.347943
6	-7.555254	-0.631415	0.995603
6	-7.419116	-1.174065	-1.482946
1	-7.151964	0.766276	-0.590700
1	-7.194452	0.018186	1.808478
1	-8.647045	-0.507083	0.917437
1	-7.356612	-1.677547	1.279790
1	-6.969297	-0.906885	-2.452052
1	-7.204270	-2.237193	-1.287752
1	-8.511573	-1.063082	-1.570830
6	6.954494	-0.350332	0.122650
6	7.606150	-0.777227	-1.202781
6	7.455763	-1.216680	1.289576
1	7.257297	0.691115	0.325634
1	7.276969	-0.138344	-2.038151
1	8.704479	-0.710631	-1.135217
1	7.353463	-1.820389	-1.456274
1	7.020848	-0.891088	2.248085
1	7.192663	-2.277596	1.143196
1	8.553166	-1.156346	1.375221
9	-0.448282	0.841501	1.985136

Structure S75. $PhSO_2N^-(Et)$

16	-0.733145	-0.743890	0.230306
8	-0.791406	-2.005097	-0.577017
8	-0.872224	-0.999862	1.700123
6	0.946272	-0.091422	0.010548
6	1.920887	-0.904279	-0.571849
6	1.279888	1.175358	0.505290
6	3.240435	-0.446061	-0.667307

1	1.624835	-1.885314	-0.949092
6	2.596833	1.630210	0.405098
1	0.498695	1.796369	0.948323
6	3.580301	0.820026	-0.179771
1	4.004239	-1.079909	-1.127146
1	2.859776	2.622159	0.783802
1	4.610739	1.178456	-0.255755
7	-1.585272	0.466962	-0.325744
6	-3.020725	0.327421	-0.151391
6	-3.718079	1.596706	-0.634371
1	-3.309071	0.147504	0.909942
1	-3.442921	-0.538806	-0.713972
1	-4.814011	1.531739	-0.518653
1	-3.359249	2.471985	-0.065946
1	-3.491633	1.781230	-1.698509

Structure S76. 16

6	-1.786535	-1.045916	0.000005
6	-0.409847	-1.286937	0.000003
6	0.516752	-0.225320	-0.000013
6	0.013041	1.092505	-0.000006
6	-1.360469	1.333991	0.000000
6	-2.268371	0.266383	0.000001
1	-2.485376	-1.886835	0.000015
1	-0.040805	-2.316762	0.000009
1	0.703211	1.939196	-0.000002
1	-1.728343	2.363718	0.000005
1	-3.344411	0.459525	0.000003
6	1.959150	-0.534177	-0.000008
6	2.978712	0.338744	0.000011
1	2.196694	-1.605065	-0.000022
1	4.014549	-0.012449	0.000013
1	2.829888	1.423040	0.000024

Structure S77. ^{2}TS22

6	4.670228	-0.928497	-1.336776
6	3.329121	-1.139229	-1.023251
6	2.850728	-0.929809	0.292059
6	3.775696	-0.510537	1.275337
6	5.117784	-0.301071	0.959163
6	5.571425	-0.506997	-0.349120
1	5.019057	-1.094063	-2.359588
1	2.643928	-1.470558	-1.806221
1	3.424347	-0.341050	2.297008
1	5.814202	0.027311	1.735144
1	6.622514	-0.341625	-0.599569
6	1.453791	-1.108918	0.666810
6	0.417815	-1.408804	-0.171958
1	1.212382	-0.916236	1.716578
1	0.573800	-1.669839	-1.219721
1	-0.564050	-1.646555	0.237816
7	-0.359562	0.642896	-0.854560
16	-1.424070	1.156931	0.331672
6	0.752727	1.537509	-1.158267
8	-1.887662	2.504595	-0.061107
8	-0.913871	0.966275	1.702841
6	-2.780565	0.007854	0.081243
6	1.416042	2.316532	-0.022835
1	0.377194	2.247332	-1.922418
1	1.497469	0.911957	-1.677623
6	-3.432928	-0.012894	-1.156431
6	-3.187987	-0.804073	1.141148
1	2.273156	2.883452	-0.420035
1	0.715016	3.030390	0.433542
1	1.783339	1.644668	0.764609
6	-4.509255	-0.883219	-1.334348
1	-3.096948	0.636992	-1.966685
6	-4.271033	-1.669208	0.951113
1	-2.659814	-0.755860	2.094889
6	-4.927424	-1.709871	-0.282696
1	-5.026288	-0.916083	-2.296554
1	-4.600504	-2.312040	1.771160
1	-5.771470	-2.388946	-0.428180

Structure S78. 17

6	-4.779001	1.248467	-1.283486
6	-3.426957	1.022923	-1.050533
6	-2.960936	0.586279	0.228978
6	-3.948576	0.393629	1.246927
6	-5.295955	0.622053	1.001267
6	-5.726187	1.052850	-0.265395
1	-5.106218	1.581207	-2.272609
1	-2.714567	1.180628	-1.862613
1	-3.622628	0.057710	2.235366
1	-6.026197	0.465022	1.800060

1	-6.787048	1.232565	-0.456941
6	-1.598903	0.334150	0.525479
6	-0.439821	0.474435	-0.412787
1	-1.344535	-0.019608	1.528417
1	-0.751185	0.806770	-1.413526
1	0.249468	1.254762	-0.041769
7	0.352859	-0.755230	-0.600569
16	1.544075	-1.059392	0.538032
6	-0.251938	-1.904342	-1.294413
8	2.101417	-2.380869	0.215504
8	1.056439	-0.790993	1.902247
6	2.776945	0.191611	0.158679
6	-1.127837	-2.811285	-0.432655
1	0.561415	-2.490593	-1.746165
1	-0.837542	-1.474719	-2.123155
6	3.437325	0.131027	-1.073992
6	3.074881	1.173428	1.105624
1	-1.521543	-3.642341	-1.040967
1	-0.540361	-3.243805	0.391933
1	-1.982463	-2.266647	-0.004404
6	4.412743	1.086327	-1.361468
1	3.189971	-0.650180	-1.795592
6	4.055284	2.125167	0.804666
1	2.544480	1.185735	2.059030
6	4.720582	2.082051	-0.424143
1	4.937366	1.053998	-2.319528
1	4.297975	2.901063	1.534865
1	5.485662	2.827594	-0.655433

Structure S79. ^{4}INT12

6	3.976946	2.523055	-0.421872
6	2.637561	2.672626	-0.767966
6	1.955933	3.905836	-0.523182
6	2.689567	4.944766	0.129232
6	4.022618	4.774102	0.481239
6	4.683099	3.565393	0.198990
1	4.476293	1.572396	-0.622354
1	2.092746	1.821139	-1.181087
1	2.184477	5.891187	0.342308
1	4.560624	5.586936	0.977156
1	5.734294	3.435158	0.469065
6	0.608894	4.115942	-0.909403
6	-0.190467	3.117403	-1.685509
1	0.122925	5.061230	-0.653706
1	0.320904	2.862757	-2.633142
1	-0.226628	2.158316	-1.142269
7	-1.538460	3.580907	-2.022764
16	-2.815636	3.095377	-1.081008
6	-1.802127	4.094921	-3.370191
8	-3.906508	4.061515	-1.267996
8	-2.265681	2.863344	0.263927
6	-3.378344	1.514098	-1.728346
6	-1.172447	5.464742	-3.597367
1	-2.890775	4.162895	-3.503086
1	-1.428119	3.367328	-4.113789
6	-2.532519	0.399437	-1.658256
6	-4.654623	1.433470	-2.295405
1	-1.385635	5.816560	-4.619969
1	-1.579815	6.197245	-2.882391
1	-0.078186	5.432117	-3.472596
6	-2.985566	-0.813522	-2.180938
1	-1.533963	0.445787	-1.215758
6	-5.093763	0.208329	-2.806051
1	-5.290545	2.319276	-2.328102
6	-4.260593	-0.914034	-2.748155
1	-2.335230	-1.687038	-2.125737
1	-6.091130	0.132506	-3.246177
1	-4.608310	-1.873170	-3.140289
27	0.510332	-0.662475	0.958381
8	-0.817704	-1.973564	0.888282
8	1.708015	-1.963116	0.348491
7	-0.676327	0.599869	1.759125
7	1.899037	0.291435	1.888740
6	-2.112438	-1.880187	1.043165
6	-2.940610	-3.020113	0.755793
6	-4.319254	-2.860282	0.872004
1	-4.965114	-3.703225	0.626919
6	-4.952308	-1.662533	1.283584
6	-4.140430	-0.589528	1.605718
1	-4.582449	0.354858	1.937223
6	-2.733228	-0.676383	1.496672
6	-1.956221	0.474656	1.871441
1	-2.521205	1.314283	2.287163
6	0.061239	1.810770	2.140996
1	0.336105	2.301488	1.192945
6	1.358952	1.318200	2.799600
1	1.074466	0.798945	3.734110

6	2.293822	2.480861	3.134123
1	2.636606	2.941783	2.194093
1	3.186125	2.117286	3.666823
6	1.568835	3.523487	3.995243
1	1.339599	3.085315	4.983495
1	2.242024	4.377313	4.176304
6	0.269577	3.997043	3.337913
1	0.507901	4.527282	2.399176
1	-0.248981	4.719653	3.988703
6	-0.667510	2.824207	3.019930
1	-1.559602	3.192060	2.496210
1	-0.994264	2.334293	3.954611
6	3.172035	0.088246	1.727492
1	3.870661	0.720181	2.288921
6	3.773127	-0.869978	0.851138
6	5.181342	-0.830151	0.676362
1	5.758141	-0.093710	1.244502
6	5.817813	-1.676451	-0.209722
6	5.010673	-2.583572	-0.948296
1	5.517835	-3.224048	-1.670013
6	3.632593	-2.690185	-0.816386
6	2.981248	-1.830630	0.141082
6	-2.307556	-4.354617	0.310945
6	-1.320729	-4.852647	1.393132
1	-1.843481	-5.016536	2.350326
1	-0.511050	-4.131521	1.559373
1	-0.871862	-5.811737	1.085235
6	-1.563463	-4.165487	-1.031233
1	-0.799115	-3.382699	-0.962467
1	-2.271803	-3.901135	-1.833023
1	-1.067174	-5.104612	-1.325288
6	-3.366920	-5.453226	0.107005
1	-4.089858	-5.192933	-0.682498
1	-3.928418	-5.666738	1.030822
1	-2.870383	-6.387342	-0.200613
6	2.789346	-3.652543	-1.673589
6	3.654863	-4.442291	-2.671968
1	4.388611	-5.090554	-2.166042
1	4.201023	-3.781306	-3.363853
1	3.007926	-5.092217	-3.282742
6	2.069381	-4.677342	-0.766089
1	1.377629	-4.184721	-0.073497
1	2.801695	-5.254839	-0.177134
1	1.495581	-5.390626	-1.380382
6	1.758258	-2.833225	-2.490097
1	2.274017	-2.198046	-3.229629
1	1.150345	-2.178935	-1.852516
1	1.084062	-3.510353	-3.040711
6	7.322705	-1.621745	-0.429516
6	7.667004	-1.139729	-1.848780
6	7.999806	-2.967605	-0.124884
1	7.724458	-0.878812	0.281316
1	7.222059	-0.152989	-2.055801
1	8.758454	-1.057047	-1.983939
1	7.290584	-1.842950	-2.610707
1	7.775811	-3.307198	0.899301
1	7.661925	-3.754212	-0.820337
1	9.095086	-2.887145	-0.224979
6	-6.469056	-1.567721	1.357315
6	-7.063869	-2.586386	2.342734
6	-7.110442	-1.702846	-0.033001
1	-6.709171	-0.559063	1.735617
1	-6.628539	-2.473410	3.348900
1	-8.155889	-2.457842	2.427476
1	-6.878457	-3.621975	2.011326
1	-6.713664	-0.948129	-0.729415
1	-6.912291	-2.696468	-0.469812
1	-8.204742	-1.576701	0.024834
9	0.451646	0.239387	-0.726198

Structure S80. ^{4}TS23

6	3.765899	2.286361	-3.150493
6	2.455680	2.619309	-2.826527
6	2.011046	2.599198	-1.471974
6	2.951705	2.207442	-0.473710
6	4.254419	1.866626	-0.810058
6	4.673521	1.908378	-2.148549
1	4.086916	2.310312	-4.195198
1	1.766705	2.900542	-3.625118
1	2.620181	2.147609	0.565227
1	4.949357	1.543399	-0.033343
1	5.698327	1.632451	-2.408654
6	0.683703	2.894047	-1.077480
6	-0.451692	3.145417	-2.011368
1	0.457983	2.953043	-0.014532
1	-0.097189	3.604344	-2.944713
1	-0.871910	2.167180	-2.320888

7	-1.497786	4.036887	-1.482798	6	0.729160	2.493243	5.287831
16	-2.592194	3.400157	-0.374949	1	0.441219	1.777542	6.079317
6	-1.953511	5.111936	-2.379992	1	1.300070	3.295951	5.782967
8	-3.559502	4.460857	-0.065991	6	-0.534908	3.057218	4.633996
8	-1.800032	2.800078	0.706184	1	-0.254281	3.840264	3.906647
6	-3.453542	2.066092	-1.206699	1	-1.175590	3.542307	5.388441
6	-0.942836	6.251864	-2.437211	6	-1.321017	1.960779	3.907877
1	-2.908190	5.491692	-1.996388	1	-2.187515	2.397652	3.388566
1	-2.144819	4.702487	-3.389465	1	-1.702598	1.226604	4.640262
6	-2.854617	0.801485	-1.268177	6	2.879266	-0.160921	2.488909
6	-4.691702	2.328082	-1.805926	1	3.432346	0.221766	3.359803
1	-1.304700	7.044978	-3.111635	6	3.706205	-0.773824	1.479494
1	-0.796493	6.683676	-1.434452	6	5.111780	-0.639611	1.605079
1	0.037738	5.915488	-2.811332	1	5.512992	-0.149676	2.498666
6	-3.515412	-0.215403	-1.962588	6	5.971319	-1.073668	0.611741
1	-1.890958	0.615487	-0.791087	6	5.394592	-1.649441	-0.550797
6	-5.340305	1.296734	-2.488943	1	6.076391	-1.944877	-1.348671
1	-5.141043	3.319092	-1.722267	6	4.030348	-1.843202	-0.728530
6	-4.750711	0.028638	-2.569915	6	3.146669	-1.442852	0.338212
1	-3.062576	-1.205961	-2.009516	6	-2.030027	-4.228708	-0.888066
1	-6.311963	1.482025	-2.953766	6	-1.037249	-5.001414	0.012271
1	-5.262857	-0.777568	-3.100450	1	-1.573334	-5.547838	0.806403
27	0.383217	-0.615842	0.852267	1	-0.317412	-4.320794	0.483441
8	-0.837499	-2.107185	0.608507	1	-0.477083	-5.740235	-0.585413
8	1.880631	-1.694549	0.258876	6	-1.253108	-3.490196	-2.005106
7	-1.031279	0.168315	2.120638	1	-0.598053	-2.711015	-1.596289
7	1.596119	0.015635	2.431502	1	-1.948444	-3.025975	-2.723967
6	-2.132213	-2.169624	0.669460	1	-0.626701	-4.203091	-2.566840
6	-2.828331	-3.214560	-0.041888	6	-2.948296	-5.262462	-1.564957
6	-4.215954	-3.253774	0.050876	1	-3.671638	-4.791762	-2.250209
1	-4.757271	-4.031536	-0.488007	1	-3.511637	-5.861925	-0.831764
6	-4.987252	-2.332992	0.802901	1	-2.338900	-5.959680	-2.162123
6	-4.309707	-1.335155	1.483886	6	3.432297	-2.418267	-2.027252
1	-4.869580	-0.597842	2.068463	6	4.521018	-2.728264	-3.070300
6	-2.901568	-1.225972	1.431817	1	5.231775	-3.493079	-2.717312
6	-2.282672	-0.139330	2.158901	1	5.093958	-1.829256	-3.349271
1	-2.969952	0.457530	2.775944	1	4.051138	-3.115202	-3.988847
6	-0.433191	1.253999	2.887187	6	2.671323	-3.732664	-1.733484
1	-0.116682	1.999606	2.138626	1	1.836380	-3.564498	-1.042596
6	0.858694	0.685513	3.516999	1	3.346201	-4.483918	-1.289493
1	0.552694	-0.097285	4.237242	1	2.269234	-4.155825	-2.669714
6	1.625753	1.781108	4.267519	6	2.471526	-1.375603	-2.651290
1	2.006995	2.509256	3.529151	1	3.026486	-0.473871	-2.954308
1	2.500937	1.356743	4.783159	1	1.683875	-1.061959	-1.954499

1	1.990676	-1.795230	-3.551560
6	7.478285	-0.891415	0.721268
6	8.003628	0.100426	-0.330819
6	8.231572	-2.228664	0.641045
1	7.678879	-0.456514	1.716034
1	7.499410	1.076814	-0.247663
1	9.087488	0.267363	-0.211952
1	7.836880	-0.278697	-1.353158
1	7.877176	-2.934981	1.409069
1	8.095074	-2.708523	-0.342696
1	9.314462	-2.079914	0.788345
6	-6.505857	-2.433643	0.839441
6	-6.984993	-3.786623	1.389683
6	-7.126877	-2.148097	-0.538324
1	-6.863033	-1.650270	1.530404
1	-6.564965	-3.985627	2.388857
1	-8.084636	-3.808426	1.472211
1	-6.687619	-4.618468	0.729351
1	-6.838524	-1.151051	-0.905779
1	-6.797245	-2.889828	-1.285628
1	-8.228282	-2.189858	-0.491066
9	0.239186	0.547704	-0.587644

Structure S81. ^{2}INT13

6	1.696508	3.417899	-2.393374
6	1.222633	2.142071	-2.068708
6	-0.088863	1.973870	-1.604237
6	-0.922016	3.094431	-1.464457
6	-0.447536	4.367129	-1.792665
6	0.862764	4.533102	-2.258715
1	2.724322	3.540056	-2.745390
1	1.879229	1.274161	-2.151840
1	-1.939193	2.961631	-1.092289
1	-1.101428	5.235449	-1.676504
1	1.233960	5.530487	-2.508577
6	-0.607192	0.605215	-1.248872
6	-1.409757	-0.092617	-2.356652
1	-1.199196	0.650566	-0.327319
1	-0.708740	-0.313154	-3.173385
1	-1.761297	-1.064935	-1.966736
7	-2.499164	0.701223	-2.918698
16	-3.917495	0.806009	-2.032818
6	-2.559694	0.847858	-4.383229
8	-4.813503	1.720053	-2.749070
8	-3.520229	1.094008	-0.645286
6	-4.645893	-0.831625	-2.050003
6	-1.520959	1.836231	-4.900279
1	-3.563377	1.206328	-4.643790
1	-2.430871	-0.142909	-4.856299
6	-4.346543	-1.726297	-1.016889
6	-5.463949	-1.195430	-3.126450
1	-1.585281	1.904704	-5.998446
1	-1.691543	2.836214	-4.473259
1	-0.495925	1.528569	-4.640729
6	-4.874557	-3.019443	-1.075112
1	-3.729780	-1.409859	-0.174795
6	-5.984227	-2.490683	-3.169006
1	-5.699845	-0.470431	-3.907434
6	-5.687547	-3.401460	-2.147430
1	-4.652421	-3.728132	-0.274462
1	-6.628877	-2.787611	-3.999917
1	-6.098095	-4.413602	-2.184925
27	1.445143	0.391763	1.428813
8	0.023999	-0.782282	1.863237
8	2.465654	-1.116596	0.893928
7	0.400072	1.941748	1.781672
7	2.923426	1.573355	1.257318
6	-1.209291	-0.526405	2.161118
6	-2.147217	-1.613726	2.339945
6	-3.476471	-1.299700	2.600176
1	-4.195041	-2.112995	2.703369
6	-3.975630	0.022706	2.719945
6	-3.069595	1.055366	2.586676
1	-3.412143	2.092743	2.657817
6	-1.700066	0.816388	2.312103
6	-0.851089	1.960320	2.129399
1	-1.341048	2.931802	2.270165
6	1.147412	3.177354	1.492708
1	1.106589	3.309996	0.399139
6	2.615674	2.890200	1.840307
1	2.668664	2.762466	2.938850
6	3.517760	4.058383	1.440325
1	3.508504	4.155787	0.340400
1	4.558512	3.865552	1.743039
6	3.027058	5.359470	2.089323
1	3.144230	5.282382	3.185415
1	3.662690	6.199037	1.763628

6	1.559285	5.640981	1.756619
1	1.460610	5.822525	0.671561
1	1.219483	6.558812	2.263576
6	0.651686	4.466819	2.146886
1	-0.380286	4.684092	1.831209
1	0.639177	4.339024	3.244077
6	4.095991	1.273795	0.790233
1	4.867476	2.054384	0.764514
6	4.504509	-0.010733	0.291245
6	5.809791	-0.117804	-0.256807
1	6.441927	0.776708	-0.273664
6	6.289903	-1.309851	-0.762620
6	5.416095	-2.428463	-0.727995
1	5.792964	-3.361963	-1.146215
6	4.127264	-2.402061	-0.211097
6	3.638990	-1.159522	0.354418
6	-1.664805	-3.071783	2.205441
6	-0.548781	-3.355091	3.237949
1	-0.926375	-3.218416	4.265311
1	0.306733	-2.685528	3.089116
1	-0.196187	-4.396098	3.144925
6	-1.128211	-3.305741	0.774201
1	-0.310960	-2.613392	0.544413
1	-1.929805	-3.163250	0.030256
1	-0.753743	-4.337532	0.668314
6	-2.795985	-4.084275	2.458385
1	-3.620589	-3.978072	1.736180
1	-3.218304	-3.993043	3.472159
1	-2.401954	-5.108167	2.355199
6	3.201103	-3.633038	-0.280875
6	3.908300	-4.859946	-0.885851
1	4.777150	-5.177235	-0.286461
1	4.251410	-4.680022	-1.917307
1	3.205060	-5.707692	-0.920289
6	2.705681	-4.029224	1.128859
1	2.124080	-3.220569	1.584665
1	3.557578	-4.264127	1.789385
1	2.070951	-4.929338	1.069479
6	1.995502	-3.289351	-1.187524
1	2.334402	-3.083336	-2.217006
1	1.457890	-2.407221	-0.821289
1	1.289225	-4.135683	-1.228539
6	7.690502	-1.434412	-1.345473
6	7.662710	-1.826276	-2.832101
6	8.559611	-2.412531	-0.538002
1	8.159915	-0.437271	-1.274669
1	7.068635	-1.111412	-3.424353
1	8.681974	-1.853636	-3.253139
1	7.220014	-2.826571	-2.974638
1	8.615358	-2.116853	0.522156
1	8.150612	-3.436342	-0.578160
1	9.587908	-2.451093	-0.935851
6	-5.464173	0.289516	2.890265
6	-6.072276	-0.442723	4.095402
6	-6.227433	-0.039935	1.595210
1	-5.575928	1.373339	3.069870
1	-5.541713	-0.191281	5.028237
1	-7.133893	-0.172490	4.224310
1	-6.027487	-1.537650	3.969219
1	-5.793299	0.495162	0.736862
1	-6.179463	-1.119077	1.371380
1	-7.292678	0.235903	1.679107
9	0.476777	-0.252569	-0.999254

Structure S82.18

6	-3.974023	-2.291852	-0.513763
6	-2.946462	-1.376484	-0.754981
6	-2.967109	-0.110803	-0.147987
6	-4.030620	0.228903	0.698388
6	-5.061689	-0.687009	0.935048
6	-5.035390	-1.948763	0.332630
1	-3.950827	-3.273745	-0.993997
1	-2.122442	-1.640351	-1.424377
1	-4.052271	1.216990	1.162091
1	-5.890676	-0.411671	1.592739
1	-5.842294	-2.662796	0.517590
6	-0.604962	0.495241	0.481514
1	-0.862031	0.680053	1.535829
1	-0.410824	-0.585675	0.392032
7	0.588982	1.271529	0.156472
16	1.600241	0.659056	-1.022528
6	1.111061	2.252482	1.119037
8	2.527969	1.728977	-1.403843
8	0.734597	0.015304	-2.021662
6	2.552932	-0.641291	-0.229239
6	0.345830	3.569215	1.077830
1	2.167078	2.434937	0.879707

1	1.080954	1.809859	2.130774
6	3.729277	-0.305543	0.451851
6	2.080044	-1.958145	-0.267435
1	0.776727	4.281325	1.800818
1	0.406114	4.010143	0.070361
1	-0.716431	3.423126	1.320581
6	4.432989	-1.310137	1.120077
1	4.094462	0.722767	0.442560
6	2.794725	-2.952884	0.406125
1	1.178042	-2.198863	-0.832082
6	3.965257	-2.629741	1.100960
1	5.355151	-1.062493	1.651667
1	2.438485	-3.985623	0.380290
1	4.521623	-3.412012	1.623505
6	-1.819529	0.843368	-0.382156
1	-1.514366	0.831263	-1.439014
9	-2.213080	2.151507	-0.078809

Structure S83. ^{3}INT14

27	0.074149	-0.328289	-1.642078
8	1.202525	0.975263	-0.903619
8	-1.362462	0.834721	-1.339087
7	1.520101	-1.563707	-1.796357
7	-0.951957	-1.881421	-1.127495
6	2.499638	1.007897	-0.750773
6	3.120502	2.201052	-0.240023
6	4.502039	2.188712	-0.061395
1	4.985916	3.082856	0.330791
6	5.333792	1.081990	-0.355375
6	4.726939	-0.054336	-0.860775
1	5.328382	-0.937230	-1.099323
6	3.329135	-0.110969	-1.066685
6	2.763439	-1.348519	-1.537025
1	3.470956	-2.177253	-1.664874
6	0.963955	-2.858041	-2.196439
1	0.499692	-2.682425	-3.182442
6	-0.166819	-3.129019	-1.191734
1	0.294126	-3.266229	-0.201492
6	-0.946899	-4.390395	-1.564701
1	-1.475279	-4.214289	-2.518336
1	-1.708441	-4.611660	-0.802009
6	0.007851	-5.585378	-1.694095
1	0.432174	-5.813675	-0.699853
1	-0.557742	-6.477569	-2.008226
6	1.149620	-5.304506	-2.676514
1	0.736857	-5.178274	-3.693208
1	1.838961	-6.163283	-2.718499
6	1.925773	-4.038084	-2.288911
1	2.715479	-3.829699	-3.028348
1	2.415730	-4.188924	-1.311035
6	-2.175824	-1.857839	-0.690259
1	-2.619257	-2.801569	-0.351819
6	-3.035548	-0.716131	-0.621348
6	-4.358344	-0.899230	-0.139021
1	-4.652198	-1.892535	0.214300
6	-5.261124	0.144265	-0.105419
6	-4.842476	1.393183	-0.639560
1	-5.580048	2.195790	-0.660941
6	-3.570181	1.644338	-1.134715
6	-2.599148	0.580354	-1.050942
6	2.268223	3.447047	0.071188
6	1.194753	3.103651	1.129437
1	1.663789	2.772387	2.071270
1	0.533910	2.306290	0.775805
1	0.579630	3.990895	1.354551
6	1.593904	3.936931	-1.232236
1	0.962846	3.157822	-1.677692
1	2.355160	4.231971	-1.973266
1	0.962809	4.817631	-1.028291
6	3.116475	4.606002	0.624519
1	3.886891	4.938497	-0.089343
1	3.616278	4.340841	1.570256
1	2.464396	5.470347	0.828354
6	-3.177553	2.990976	-1.774547
6	-4.380888	3.944697	-1.885572
1	-4.792493	4.214206	-0.899593
1	-5.195684	3.516315	-2.491268
1	-4.063009	4.880194	-2.372924
6	-2.092477	3.696432	-0.929455
1	-1.210990	3.059503	-0.800389
1	-2.484833	3.967265	0.064962
1	-1.773490	4.629253	-1.423317
6	-2.646577	2.737560	-3.207725
1	-3.435187	2.293566	-3.838053
1	-1.782906	2.059596	-3.217089
1	-2.342956	3.690722	-3.672331
6	-6.660905	-0.024518	0.466316

6	-7.752532	0.228661	-0.585413
6	-6.868438	0.863676	1.704238
1	-6.750496	-1.075637	0.791556
1	-7.623723	-0.427707	-1.461183
1	-8.754764	0.042939	-0.164195
1	-7.733082	1.272014	-0.942679
1	-6.104319	0.663050	2.472713
1	-6.806568	1.933403	1.441670
1	-7.860447	0.689913	2.154020
6	6.832001	1.140887	-0.095200
6	7.135412	1.262807	1.407380
6	7.514202	2.265674	-0.889473
1	7.256995	0.183322	-0.443032
1	6.684074	0.433057	1.974999
1	8.222581	1.252015	1.593211
1	6.736884	2.205492	1.819110
1	7.317433	2.169977	-1.969465
1	7.154874	3.258419	-0.570393
1	8.606435	2.246570	-0.738169
9	-0.003545	-0.184948	-3.491048
16	-0.133860	-2.113594	2.859745
8	0.144219	-2.737858	4.158801
8	-0.801168	-2.892201	1.815290
6	-0.954456	-0.551870	3.104808
6	-1.465274	-0.267731	4.375859
6	-1.131346	0.309783	2.017080
6	-2.185086	0.915665	4.554133
1	-1.299486	-0.960828	5.202069
6	-1.845423	1.491179	2.217095
1	-0.708710	0.081999	1.040115
6	-2.375109	1.789902	3.477437
1	-2.596270	1.154835	5.537674
1	-1.986022	2.175323	1.381248
1	-2.938053	2.715357	3.621835
7	1.369793	-1.498242	2.111812
9	1.923892	-2.641441	1.461544
6	2.351102	-1.080541	3.120217
6	3.615711	-0.539044	2.475817
1	2.563939	-1.916971	3.807897
1	1.840456	-0.290839	3.695909
1	4.308142	-0.206079	3.264033
1	4.118248	-1.315204	1.882357
1	3.396344	0.314233	1.820099

Structure S84. ^{3}TS24

27	-0.088511	0.447177	-1.046242
8	-1.272874	-1.004374	-1.131773
8	1.233201	-0.736071	-0.463199
7	-1.417823	1.698637	-1.598461
7	1.031114	1.966658	-0.760345
6	-2.561164	-0.949068	-1.003521
6	-3.268724	-2.067476	-0.429083
6	-4.657222	-2.027962	-0.440130
1	-5.207832	-2.868674	-0.018831
6	-5.421760	-0.943473	-0.943560
6	-4.734956	0.162253	-1.410151
1	-5.284506	1.046222	-1.748762
6	-3.319078	0.197618	-1.416498
6	-2.676185	1.438508	-1.741909
1	-3.336697	2.238080	-2.100392
6	-0.805108	3.001151	-1.876383
1	-0.249639	2.886042	-2.823611
6	0.243606	3.197616	-0.760121
1	-0.289653	3.212362	0.203817
6	1.015350	4.504685	-0.920301
1	1.622641	4.461832	-1.841526
1	1.706091	4.638039	-0.073158
6	0.041703	5.687192	-0.997768
1	-0.493697	5.780823	-0.035987
1	0.606430	6.622938	-1.138382
6	-0.973018	5.500338	-2.129257
1	-0.442691	5.491562	-3.098242
1	-1.675811	6.348542	-2.160852
6	-1.758347	4.191874	-1.972611
1	-2.444793	4.062752	-2.823792
1	-2.373406	4.234163	-1.056233
6	2.320403	1.913900	-0.729446
1	2.882900	2.853835	-0.664344
6	3.107751	0.715451	-0.768438
6	4.515387	0.845503	-0.835066
1	4.947966	1.850504	-0.858984
6	5.338310	-0.265323	-0.874555
6	4.717352	-1.541352	-0.892512
1	5.370874	-2.408891	-0.979656
6	3.345142	-1.743986	-0.827303
6	2.500442	-0.582182	-0.687920
6	-2.484036	-3.216060	0.232258

6	-1.596085	-2.628344	1.358293
1	-2.220423	-2.155439	2.133578
1	-0.898294	-1.872471	0.980312
1	-1.012396	-3.431771	1.837100
6	-1.610724	-3.942847	-0.813888
1	-0.878133	-3.262396	-1.258695
1	-2.235491	-4.361654	-1.620592
1	-1.067160	-4.777822	-0.341708
6	-3.420710	-4.257970	0.869631
1	-4.066486	-4.750080	0.124481
1	-4.066001	-3.817960	1.647005
1	-2.817400	-5.044478	1.350383
6	2.716324	-3.142109	-0.971222
6	3.779798	-4.231303	-1.202131
1	4.474517	-4.322180	-0.351367
1	4.373061	-4.049926	-2.112543
1	3.281472	-5.206360	-1.323420
6	1.929679	-3.522579	0.302133
1	1.145287	-2.792388	0.523738
1	2.605293	-3.580934	1.169780
1	1.459973	-4.511684	0.174577
6	1.780468	-3.130891	-2.205235
1	2.359770	-2.936788	-3.123018
1	1.004815	-2.358767	-2.128039
1	1.289019	-4.111274	-2.317755
6	6.853418	-0.141317	-0.921878
6	7.437198	-0.718422	-2.221840
6	7.509272	-0.785399	0.310855
1	7.090592	0.936571	-0.900850
1	6.992174	-0.238568	-3.108290
1	8.528567	-0.565044	-2.262220
1	7.251804	-1.802902	-2.298863
1	7.117137	-0.353671	1.246297
1	7.324098	-1.872380	0.340242
1	8.601701	-0.634961	0.299256
6	-6.941507	-0.978399	-0.888638
6	-7.447690	-0.990048	0.563904
6	-7.521027	-2.157549	-1.685663
1	-7.303837	-0.048183	-1.359592
1	-7.063489	-0.124789	1.128069
1	-8.549601	-0.958787	0.597609
1	-7.124695	-1.902712	1.092328
1	-7.184657	-2.136269	-2.734818
1	-7.212907	-3.124824	-1.254501
1	-8.623463	-2.129912	-1.680043
9	0.583028	0.321071	-2.786901
16	-0.109271	1.704832	3.194993
8	-0.504162	1.823937	4.609171
8	0.252348	2.926592	2.462115
6	1.179437	0.489251	3.031959
6	0.950128	-0.812943	3.491705
6	2.418114	0.895777	2.537053
6	1.998390	-1.730208	3.435147
1	-0.030626	-1.105811	3.868802
6	3.462007	-0.032558	2.500850
1	2.556769	1.917020	2.181843
6	3.251923	-1.339596	2.945822
1	1.834522	-2.757324	3.768592
1	4.433782	0.263089	2.101033
1	4.067533	-2.064955	2.899149
7	-1.451140	0.871667	2.522101
9	-0.816130	0.699700	0.839377
6	-2.623601	1.706562	2.338738
6	-3.861867	0.856957	2.101810
1	-2.450585	2.430680	1.523238
1	-2.731606	2.304140	3.265226
1	-4.733314	1.504984	1.920444
1	-3.726250	0.206468	1.229342
1	-4.073127	0.223326	2.976831

Structure S85. ^{3}INT15

27	0.011232	0.329711	-1.116048
8	-1.154288	-1.155974	-1.107402
8	1.384440	-0.860441	-0.527552
7	-1.308736	1.510720	-1.792498
7	1.156126	1.840966	-1.008559
6	-2.431567	-1.096052	-0.985080
6	-3.141177	-2.179659	-0.336042
6	-4.527158	-2.171358	-0.390246
1	-5.076178	-2.988714	0.076768
6	-5.293294	-1.138254	-0.991930
6	-4.610207	-0.045587	-1.503285
1	-5.167960	0.802478	-1.912988
6	-3.199563	0.017762	-1.479849
6	-2.564787	1.236685	-1.903870
1	-3.235669	2.003972	-2.310224
6	-0.712930	2.800383	-2.145116

1	-0.174766	2.648773	-3.097412	1	1.213481	-2.763047	0.729036
6	0.359819	3.062616	-1.061290	1	2.655192	-3.371412	1.580960
1	-0.157155	3.103133	-0.086664	1	1.613437	-4.498410	0.679188
6	1.114121	4.366870	-1.300468	6	2.035549	-3.449258	-1.872003
1	1.701428	4.286409	-2.232407	1	2.671237	-3.400587	-2.771613
1	1.824052	4.547556	-0.478013	1	1.264782	-2.673427	-1.961620
6	0.126822	5.535455	-1.407659	1	1.540377	-4.433486	-1.860863
1	-0.387171	5.664481	-0.438673	6	6.974741	-0.205332	-0.646892
1	0.677730	6.469689	-1.602784	6	7.689248	-0.999899	-1.752853
6	-0.910832	5.287237	-2.505920	6	7.508709	-0.588482	0.745550
1	-0.402333	5.241564	-3.485644	1	7.193233	0.863651	-0.807913
1	-1.623993	6.125663	-2.558559	1	7.319122	-0.720597	-2.752152
6	-1.677411	3.979003	-2.273863	1	8.773408	-0.803269	-1.723867
1	-2.379682	3.807557	-3.104426	1	7.546726	-2.086059	-1.630063
1	-2.272272	4.054247	-1.346592	1	7.027975	0.006968	1.538353
6	2.437615	1.806822	-0.944931	1	7.323652	-1.653393	0.963660
1	3.000716	2.748522	-0.944262	1	8.596204	-0.417886	0.802271
6	3.236725	0.606425	-0.840439	6	-6.811826	-1.205391	-0.995758
6	4.628011	0.740529	-0.839966	6	-7.382984	-1.181572	0.432585
1	5.063282	1.739194	-0.937997	6	-7.327503	-2.425665	-1.775678
6	5.468687	-0.367347	-0.704246	1	-7.175034	-0.300951	-1.514005
6	4.876850	-1.654815	-0.608675	1	-7.041885	-0.292420	0.986339
1	5.550337	-2.508055	-0.543983	1	-8.485630	-1.169766	0.413373
6	3.510537	-1.873204	-0.604178	1	-7.071093	-2.071231	1.004825
6	2.635833	-0.704695	-0.659279	1	-6.950581	-2.428114	-2.811152
6	-2.349441	-3.234391	0.455140	1	-7.009933	-3.368868	-1.300343
6	-1.525074	-2.502425	1.546772	1	-8.429722	-2.428326	-1.813329
1	-2.197537	-2.014093	2.270607	9	0.620252	0.018583	-2.817264
1	-0.874004	-1.725035	1.128045	16	-0.678048	2.103526	3.126935
1	-0.902172	-3.225879	2.098799	8	-0.920817	2.415105	4.549437
6	-1.419005	-4.032800	-0.485005	8	-0.511754	3.245775	2.206797
1	-0.682968	-3.379443	-0.963221	6	0.750549	1.033296	3.008819
1	-2.003488	-4.536388	-1.273333	6	0.688725	-0.275804	3.495313
1	-0.881551	-4.810335	0.082420	6	1.931029	1.573276	2.497063
6	-3.277598	-4.239031	1.160866	6	1.841316	-1.062409	3.449649
1	-3.876982	-4.826366	0.446361	1	-0.248463	-0.679114	3.880249
1	-3.967112	-3.745902	1.864705	6	3.081444	0.780935	2.476293
1	-2.669952	-4.950879	1.742239	1	1.941487	2.593894	2.112836
6	2.896782	-3.279531	-0.594264	6	3.036373	-0.535971	2.945075
6	3.975994	-4.376488	-0.606633	1	1.802430	-2.094509	3.805005
1	4.611329	-4.346205	0.293329	1	4.012653	1.188772	2.078369
1	4.627950	-4.312348	-1.492369	1	3.935003	-1.156553	2.909694
1	3.488102	-5.363524	-0.629783	7	-1.964266	1.072003	2.742744
6	2.036998	-3.481436	0.675749	9	-0.578631	0.679795	0.594529

6	-2.988717	1.671572	1.927950
6	-4.272542	0.857758	1.967962
1	-2.567525	1.693728	0.903568
1	-3.163779	2.730027	2.205573
1	-5.032024	1.321863	1.320436
1	-4.095224	-0.165597	1.606291
1	-4.676247	0.803863	2.991633

Structure S86. Co^{IV}(salen)-F_2

27	0.000010	0.733755	0.000165
8	1.276383	-0.640308	0.297949
8	-1.276429	-0.640274	-0.297878
7	1.236857	2.110773	0.408477
7	-1.236810	2.110865	-0.408030
6	2.543757	-0.535657	0.180345
6	3.335759	-1.719740	-0.114411
6	4.715451	-1.596992	-0.093767
1	5.326711	-2.475240	-0.299435
6	5.398627	-0.378558	0.161801
6	4.636169	0.768062	0.360662
1	5.134486	1.729188	0.520009
6	3.231051	0.726709	0.346776
6	2.512283	1.966591	0.501831
1	3.130662	2.848939	0.708320
6	0.539550	3.386897	0.555032
1	0.001708	3.325136	1.517068
6	-0.539376	3.386889	-0.554738
1	-0.001533	3.324916	-1.516756
6	-1.399767	4.647846	-0.512902
1	-1.993064	4.646884	0.418473
1	-2.109556	4.651705	-1.355289
6	-0.518548	5.902075	-0.563047
1	-0.000566	5.944542	-1.537797
1	-1.153066	6.800876	-0.502103
6	0.518924	5.902078	0.563092
1	0.000946	5.944661	1.537840
1	1.153515	6.800822	0.502080
6	1.400046	4.647777	0.513042
1	2.109868	4.651658	1.355402
1	1.993302	4.646683	-0.418359
6	-2.512197	1.966711	-0.501827
1	-3.130496	2.849049	-0.708607
6	-3.231025	0.726842	-0.346811
6	-4.636109	0.768193	-0.360956
1	-5.134411	1.729305	-0.520417
6	-5.398622	-0.378439	-0.162185
6	-4.715529	-1.596870	0.093586
1	-5.326851	-2.475092	0.299180
6	-3.335849	-1.719638	0.114489
6	-2.543775	-0.535571	-0.180261
6	2.628785	-3.026900	-0.503915
6	1.784123	-2.760157	-1.776427
1	2.443341	-2.524676	-2.628418
1	1.090801	-1.918895	-1.646535
1	1.202207	-3.658486	-2.039583
6	1.730714	-3.523919	0.652609
1	0.940847	-2.803743	0.885922
1	2.329904	-3.692685	1.562946
1	1.259602	-4.481603	0.377779
6	3.631884	-4.147851	-0.829511
1	4.250241	-4.417628	0.041937
1	4.304130	-3.879613	-1.660008
1	3.081151	-5.052083	-1.133673
6	-2.628961	-3.026776	0.504195
6	-3.632165	-4.147610	0.829855
1	-4.250441	-4.417472	-0.041625
1	-4.304484	-3.879207	1.660239
1	-3.081525	-5.051837	1.134196
6	-1.730796	-3.523990	-0.652163
1	-0.940865	-2.803890	-0.885465
1	-2.329870	-3.692839	-1.562564
1	-1.259779	-4.481664	-0.377146
6	-1.784355	-2.759932	1.776734
1	-2.443582	-2.524230	2.628658
1	-1.090898	-1.918795	1.646767
1	-1.202597	-3.658315	2.040052
6	-6.916114	-0.333783	-0.179841
6	-7.510791	-0.708610	1.188852
6	-7.495256	-1.221406	-1.294695
1	-7.206662	0.708385	-0.396640
1	-7.123524	-0.055714	1.987339
1	-8.609248	-0.614767	1.173349
1	-7.270507	-1.750280	1.459230
1	-7.099754	-0.936333	-2.282703
1	-7.252185	-2.283999	-1.128295
1	-8.593792	-1.133401	-1.328493
6	6.916132	-0.333925	0.179113

6	7.510484	-0.708790	-1.189701
6	7.495529	-1.221511	1.293863
1	7.206738	0.708248	0.395816
1	7.123038	-0.055905	-1.988110
1	8.608949	-0.614975	-1.174470
1	7.270119	-1.750461	-1.460009
1	7.100251	-0.936394	2.281949
1	7.252409	-2.284109	1.127557
1	8.594074	-1.133517	1.327409
9	-0.578801	0.754714	1.746154
9	0.578785	0.755105	-1.745874

Structure S87. $[Co^{II}(salen)\text{-}F]^-$

27	0.019706	0.777266	0.974132
8	1.321307	-0.590530	0.289817
8	-1.565232	-0.457434	0.956653
7	1.531759	2.166092	0.347643
7	-1.098073	2.172799	-0.075035
6	2.576320	-0.581988	-0.005143
6	3.280386	-1.836763	-0.199890
6	4.631035	-1.806693	-0.533936
1	5.158712	-2.750524	-0.677460
6	5.379572	-0.617269	-0.702663
6	4.707770	0.581411	-0.515887
1	5.248937	1.527459	-0.637019
6	3.338124	0.634411	-0.170290
6	2.743274	1.953677	-0.009734
1	3.423280	2.798619	-0.223372
6	0.907573	3.464001	0.487085
1	0.587106	3.494728	1.545051
6	-0.398174	3.435511	-0.351996
1	-0.099513	3.440016	-1.419545
6	-1.224313	4.698512	-0.065691
1	-1.539769	4.668188	0.992273
1	-2.142702	4.704061	-0.673571
6	-0.409703	5.968487	-0.340435
1	-0.190484	6.028529	-1.422485
1	-1.009851	6.860066	-0.091814
6	0.909314	5.978675	0.440734
1	0.688948	6.037593	1.521760
1	1.497924	6.876802	0.188275
6	1.732622	4.712445	0.171781
1	2.650669	4.720466	0.781956
1	2.049952	4.690498	-0.886851
6	-2.258736	1.945342	-0.599215
1	-2.710145	2.720736	-1.243456
6	-3.072944	0.758591	-0.459192
6	-4.318103	0.765484	-1.141090
1	-4.585313	1.657150	-1.719954
6	-5.192347	-0.304186	-1.098800
6	-4.796646	-1.434120	-0.335909
1	-5.487159	-2.277883	-0.304284
6	-3.597725	-1.523351	0.357424
6	-2.677202	-0.396453	0.319535
6	2.515931	-3.167137	-0.035367
6	1.371101	-3.240048	-1.073094
1	1.776880	-3.220153	-2.098982
1	0.682131	-2.395176	-0.954885
1	0.801234	-4.177591	-0.954488
6	1.937294	-3.268789	1.396061
1	1.270798	-2.425339	1.613122
1	2.749730	-3.271572	2.142544
1	1.366418	-4.205629	1.515618
6	3.421024	-4.393166	-0.256883
1	4.254116	-4.431997	0.463714
1	3.847727	-4.419596	-1.272806
1	2.830945	-5.315139	-0.126303
6	-3.216014	-2.783205	1.162191
6	-4.296118	-3.877467	1.078968
1	-4.464472	-4.218586	0.044420
1	-5.262898	-3.543058	1.489288
1	-3.977710	-4.754968	1.665272
6	-1.900331	-3.377238	0.606517
1	-1.081548	-2.652962	0.681815
1	-2.017751	-3.661442	-0.452595
1	-1.619117	-4.284465	1.168755
6	-3.032168	-2.419019	2.654248
1	-3.972442	-2.029572	3.080228
1	-2.252612	-1.656930	2.779891
1	-2.744796	-3.312489	3.235404
6	-6.526444	-0.282847	-1.832162
6	-7.718970	-0.367167	-0.864279
6	-6.615627	-1.382343	-2.903882
1	-6.592151	0.689753	-2.351475
1	-7.686318	0.442316	-0.117135
1	-8.677107	-0.292297	-1.406763
1	-7.722851	-1.324855	-0.316539

1	-5.789903	-1.303000	-3.629504
1	-6.565040	-2.387270	-2.451727
1	-7.566331	-1.317639	-3.460470
6	6.855319	-0.664664	-1.074534
6	7.080777	-1.298325	-2.457662
6	7.698231	-1.378040	-0.004597
1	7.208154	0.380786	-1.128721
1	6.513777	-0.765266	-3.238203
1	8.148351	-1.278152	-2.736917
1	6.754609	-2.352172	-2.471137
1	7.574114	-0.904557	0.982870
1	7.404971	-2.436864	0.095162
1	8.771297	-1.355258	-0.261630
9	0.208458	1.448036	2.745312

Structure S88. $PhSO_2N^+(Et)$

16	-0.653826	-1.010360	-0.274943
8	-1.139549	-0.950519	-1.645788
8	-0.772402	-2.185765	0.568851
6	0.924445	-0.242137	-0.098284
6	1.363273	0.626834	-1.105725
6	1.681347	-0.531186	1.045110
6	2.610481	1.231002	-0.949298
1	0.752563	0.814666	-1.990426
6	2.923361	0.089772	1.179720
1	1.315415	-1.228864	1.800453
6	3.382880	0.965735	0.188649
1	2.982996	1.907141	-1.721776
1	3.536682	-0.117759	2.059169
1	4.358374	1.444751	0.302065
7	-1.724046	0.215295	0.589871
6	-2.619853	0.918011	-0.006205
6	-3.519232	1.863830	0.667420
1	-2.697302	0.779454	-1.094522
1	-1.595418	0.278632	1.608965
1	-3.402974	2.850714	0.184590
1	-4.558973	1.552324	0.459118
1	-3.346434	1.936737	1.749534

Structure S89. ^{1}TS25

6	3.633071	-1.667574	-0.410357
6	2.371114	-1.500278	0.364508
6	2.053576	-0.109805	0.844263
6	2.919961	0.954655	0.435350
6	4.040188	0.713527	-0.316124
6	4.415577	-0.614755	-0.739647
1	3.893322	-2.682407	-0.723617
1	2.356380	-2.220789	1.203660
1	2.674109	1.973582	0.743327
1	4.679958	1.552666	-0.603869
1	5.328746	-0.750119	-1.323161
6	0.924030	0.173604	1.607504
6	0.017368	-0.795209	2.074281
1	0.700143	1.223332	1.809654
1	0.352911	-1.826795	2.200555
1	-0.764011	-0.475926	2.767006
7	-1.295093	-1.386252	0.682913
16	-1.405774	-0.571637	-0.885171
6	-1.907362	-2.487248	0.923598
8	-2.748114	-0.808436	-1.419996
8	-0.213806	-0.986306	-1.629064
6	-1.267252	1.133436	-0.405997
6	-2.808062	-3.295827	0.057766
1	-1.732881	-2.879498	1.939940
1	1.532420	-1.831662	-0.281419
6	-2.249357	1.680068	0.427103
6	-0.216732	1.890645	-0.929388
1	-2.796769	-4.338866	0.402848
1	-3.838198	-2.913825	0.179464
1	-2.558005	-3.234675	-1.008143
6	-2.148187	3.028755	0.770477
1	-3.072091	1.068453	0.803551
6	-0.142400	3.243092	-0.588909
1	0.531396	1.428245	-1.574181
6	-1.098498	3.806310	0.263258
1	-2.895943	3.477146	1.428460
1	0.669852	3.855327	-0.987149
1	-1.030148	4.863329	0.531782

Structure S90. 19

6	4.676755	-1.652226	-1.111182
6	3.398444	-1.133950	-1.060391
6	3.016178	-0.283177	0.029388
6	3.978076	0.023756	1.049251
6	5.255414	-0.502730	0.982752

6	5.601279	-1.336676	-0.093953
1	4.977872	-2.300280	-1.936388
1	2.682335	-1.370749	-1.848559
1	3.683747	0.674719	1.875981
1	5.990615	-0.273936	1.756197
1	6.612635	-1.748504	-0.147749
6	1.736925	0.251784	0.156902
6	0.569539	0.014146	-0.734004
1	1.542916	0.885839	1.027462
1	0.875724	-0.064677	-1.790188
1	0.193433	-1.001102	-0.486041
7	-0.491484	0.994668	-0.628511
16	-1.496602	0.891166	0.723792
6	-0.354837	2.273289	-1.346076
8	-2.189426	2.177286	0.834250
8	-0.690541	0.366690	1.840718
6	-2.679303	-0.374037	0.276893
6	0.662107	3.231996	-0.737539
1	-1.346521	2.743272	-1.379354
1	-0.085956	2.020703	-2.384884
6	-3.771628	-0.016520	-0.522272
6	-2.486071	-1.685195	0.723251
1	0.697099	4.167211	-1.319508
1	0.387357	3.482676	0.298793
1	1.681805	2.809175	-0.739848
6	-4.681548	-1.007059	-0.893614
1	-3.910408	1.019783	-0.835813
6	-3.405433	-2.666436	0.339384
1	-1.641814	-1.925807	1.371244
6	-4.496814	-2.328875	-0.467186
1	-5.543206	-0.745473	-1.512380
1	-3.271814	-3.695613	0.681113
1	-5.214553	-3.098900	-0.760543

Structure S91. ^{2}INT16

6	-1.262623	3.493907	1.935007
6	-0.391406	2.689944	1.208569
6	0.383244	3.228902	0.132222
6	0.219500	4.621738	-0.152586
6	-0.654037	5.412500	0.582364
6	-1.404988	4.858202	1.633182
1	-1.842323	3.054137	2.751787
1	-0.314661	1.630583	1.455286
1	0.798237	5.061868	-0.969603
1	-0.756848	6.474046	0.340455
1	-2.091638	5.482839	2.210013
6	1.272477	2.454571	-0.652739
6	1.541983	0.992142	-0.511865
1	1.834163	2.962613	-1.443334
1	0.939410	0.528339	0.285427
1	1.265050	0.484954	-1.448160
7	2.978208	0.745718	-0.295722
16	3.614283	-0.682880	-0.894754
6	3.592627	1.280593	0.934272
8	5.072895	-0.589004	-0.747840
8	3.006983	-0.909814	-2.211488
6	3.033095	-1.972013	0.214754
6	4.624633	2.360673	0.639813
1	4.051423	0.461821	1.513280
1	2.778517	1.678121	1.559866
6	3.891537	-2.462699	1.204728
6	1.707519	-2.411307	0.109250
1	5.073229	2.735186	1.574932
1	5.424050	1.950843	0.004859
1	4.161897	3.210579	0.113218
6	3.406005	-3.408610	2.112280
1	4.924024	-2.112859	1.250227
6	1.233542	-3.349502	1.029000
1	1.053669	-2.033168	-0.677104
6	2.079567	-3.846153	2.027549
1	4.067828	-3.804114	2.887008
1	0.196348	-3.679397	0.955497
1	1.702511	-4.581793	2.742862
16	-1.968574	-1.383086	-0.108846
8	-1.211661	-0.616565	0.891479
8	-1.615543	-2.773531	-0.396573
6	-3.711665	-1.236573	0.214836
6	-4.152557	-0.294726	1.150073
6	-4.590112	-2.075926	-0.479864
6	-5.524374	-0.192355	1.390876
1	-3.436285	0.342321	1.671624
6	-5.957662	-1.955565	-0.228850
1	-4.208806	-2.805673	-1.196166
6	-6.421120	-1.017774	0.702504
1	-5.893033	0.534366	2.118371
1	-6.663709	-2.598815	-0.759043
1	-7.493401	-0.931145	0.895161

7	-1.916527	-0.581093	-1.697466
9	-0.588761	-0.861277	-2.143532
6	-2.035838	0.879963	-1.627454
6	-1.898817	1.506362	-3.006005
1	-1.303868	1.298112	-0.920856
1	-3.042532	1.060785	-1.218748
1	-2.059115	2.592532	-2.925470
1	-0.893271	1.339304	-3.418593
1	-2.639707	1.091742	-3.707211

Structure S92. ^{2}TS26

6	0.867072	3.912357	2.169176
6	0.961602	2.798194	1.341400
6	1.308654	2.940527	-0.030464
6	1.545036	4.252813	-0.524458
6	1.452406	5.360715	0.311312
6	1.112573	5.197837	1.662777
1	0.595461	3.783801	3.220235
1	0.750111	1.807911	1.746825
1	1.802824	4.381845	-1.578965
1	1.642404	6.360609	-0.087390
1	1.037138	6.068945	2.318564
6	1.368159	1.831334	-0.929060
6	1.426008	0.385702	-0.544016
1	1.639027	2.045871	-1.967065
1	0.932796	0.193279	0.420612
1	0.868976	-0.173865	-1.303387
7	2.813442	-0.100182	-0.540575
16	3.067470	-1.647415	-1.138035
6	3.721964	0.363010	0.524611
8	4.521140	-1.857345	-1.152764
8	2.278624	-1.775487	-2.367459
6	2.357755	-2.750239	0.092139
6	4.859816	1.214032	-0.021744
1	4.122667	-0.502249	1.078385
1	3.119912	0.935142	1.246576
6	3.199397	-3.393473	1.005746
6	0.964870	-2.887617	0.152531
1	5.520823	1.550527	0.794111
1	5.454864	0.628771	-0.738410
1	4.467747	2.104528	-0.539012
6	2.629490	-4.186938	2.006085
1	4.281427	-3.279288	0.922226
6	0.411168	-3.675021	1.164298
1	0.317855	-2.387540	-0.569016
6	1.239203	-4.323203	2.088593
1	3.275643	-4.700329	2.722653
1	-0.675046	-3.776750	1.228154
1	0.798520	-4.940103	2.876076
16	-2.104367	-0.357181	-0.268459
8	-1.471199	-0.333031	1.061538
8	-1.478164	-1.106646	-1.363695
6	-3.801045	-0.886568	-0.095722
6	-4.376455	-0.932231	1.178033
6	-4.512498	-1.236990	-1.249471
6	-5.707853	-1.339592	1.294078
1	-3.786855	-0.660851	2.055321
6	-5.842510	-1.638118	-1.115505
1	-4.029089	-1.199925	-2.227246
6	-6.437542	-1.687887	0.151611
1	-6.175361	-1.386730	2.280470
1	-6.415840	-1.916019	-2.003073
1	-7.479310	-2.003762	0.248923
7	-2.380470	1.243593	-0.879857
9	-0.758749	1.629755	-1.180827
6	-2.711341	2.227361	0.139975
6	-2.772826	3.621822	-0.466143
1	-1.996487	2.183107	0.980015
1	-3.703042	1.934357	0.535355
1	-3.074656	4.350042	0.302673
1	-1.785757	3.912392	-0.852945
1	-3.500293	3.661252	-1.291936

Structure S93. ^{2}INT17

6	1.826640	3.526125	2.250152
6	1.355199	2.677682	1.246435
6	2.071194	2.535743	0.044482
6	3.256305	3.259783	-0.135658
6	3.734210	4.102932	0.874390
6	3.020033	4.237637	2.068138
1	1.264155	3.631429	3.181760
1	0.430695	2.113938	1.395665
1	3.811055	3.161792	-1.072768
1	4.663923	4.658098	0.724489
1	3.390384	4.897504	2.857320
6	1.556239	1.617211	-1.034363

6	1.354024	0.152673	-0.638778
1	2.204399	1.659155	-1.923529
1	0.768505	0.086340	0.291604
1	0.740698	-0.277334	-1.437624
7	2.604023	-0.599806	-0.543217
16	2.546008	-2.162962	-1.171713
6	3.443523	-0.427398	0.662339
8	3.908122	-2.704155	-1.085720
8	1.851565	-2.090085	-2.461306
6	1.510793	-3.091700	-0.029821
6	4.872379	-0.022326	0.329093
1	3.437372	-1.351592	1.266645
1	2.961043	0.340697	1.282160
6	2.114188	-3.924222	0.918742
6	0.122077	-2.911473	-0.070407
1	5.453300	0.124432	1.254594
1	5.359408	-0.802247	-0.273058
1	4.889197	0.919849	-0.239648
6	1.306917	-4.584595	1.850123
1	3.197268	-4.055816	0.915466
6	-0.669385	-3.570264	0.872984
1	-0.342639	-2.262874	-0.813084
6	-0.080460	-4.404410	1.830938
1	1.765643	-5.242184	2.592829
1	-1.752797	-3.426480	0.855675
1	-0.706382	-4.918604	2.564888
16	-2.262255	0.410552	-0.319557
8	-1.522772	0.606540	0.943465
8	-1.721459	-0.487953	-1.350781
6	-3.929242	-0.093475	0.071200
6	-4.412438	0.095208	1.370748
6	-4.713781	-0.659046	-0.942206
6	-5.720553	-0.299045	1.659646
1	-3.768861	0.531795	2.136307
6	-6.019733	-1.044414	-0.636498
1	-4.303100	-0.797929	-1.943902
6	-6.520576	-0.864142	0.659187
1	-6.115206	-0.167516	2.669934
1	-6.648086	-1.490056	-1.411265
1	-7.544155	-1.168570	0.891711
7	-2.606597	1.873368	-1.125336
9	0.276828	2.074263	-1.426609
6	-2.315871	3.086405	-0.412239
6	-2.085731	4.243615	-1.377865
1	-1.473262	2.969491	0.290173
1	-3.209319	3.291331	0.222062
1	-1.948788	5.179880	-0.814434
1	-1.178432	4.057764	-1.971136
1	-2.938845	4.367168	-2.063012

Structure S94. OTf^-

16	0.922097	0.000193	0.000000
8	1.244660	-0.722206	1.251375
8	1.244663	-0.723151	-1.250828
8	1.245876	1.444803	-0.000545
6	-0.955040	0.000409	-0.000001
9	-1.440294	-1.251436	0.000455
9	-1.441236	0.626051	1.083510
9	-1.441237	0.625262	-1.083966

Structure S95. ^{1}**TS27**

6	4.022746	-0.527805	0.088086
6	3.095193	-1.578149	0.070454
6	1.729367	-1.317532	-0.096634
6	1.258875	-0.010794	-0.257166
6	2.193398	1.038913	-0.250418
6	3.555901	0.801850	-0.082187
1	3.427370	-2.608770	0.193348
1	1.025249	-2.153379	-0.102654
1	1.876056	2.076723	-0.380040
8	4.412847	1.865348	-0.036068
8	5.356883	-0.676009	0.267994
6	5.331135	1.992255	-1.120142
1	4.795080	2.079659	-2.082347
1	5.902510	2.914383	-0.944768
1	6.025016	1.138388	-1.167984
6	5.893077	-1.977069	0.436094
1	5.699876	-2.613885	-0.444903
1	6.976734	-1.852863	0.558608
1	5.482976	-2.472055	1.333678
6	-0.222702	0.275920	-0.400302
1	-0.394870	1.083059	-1.126901
1	-0.763434	-0.613387	-0.745519
6	-0.779483	0.716690	0.935309
1	-0.308610	1.638691	1.300245
6	-0.964231	-0.314272	2.005902

1	0.038836	-0.674649	2.282380
1	-1.432951	0.116955	2.900690
1	-1.549336	-1.165663	1.633738
16	-3.692660	-0.727673	-0.879989
8	-5.133532	-1.014858	-0.941050
8	-3.112070	0.037689	-1.986241
8	-2.844227	-1.758260	-0.263436
6	-3.789640	0.596923	0.511646
9	-4.419639	1.683882	0.262529
9	-3.959070	0.210918	1.724868
9	-2.187841	1.320389	0.623581

Structure S96. CF_2SO_3

16	0.872151	-0.000040	0.013103
8	0.836972	-0.000495	1.482331
8	1.184808	-1.253981	-0.658425
8	1.183765	1.254597	-0.657658
6	-1.126365	-0.000255	-0.107021
9	-1.824952	-1.047797	-0.049932
9	-1.824002	1.047930	-0.049791

Structure S97. PF_6^-

15	0.000000	0.000000	0.000000
9	0.000000	0.000000	1.637608
9	0.000000	1.637608	0.000000
9	-1.637608	0.000000	0.000000
9	0.000000	0.000000	-1.637608
9	0.000000	-1.637608	0.000000
9	1.637608	0.000000	0.000000

Structure S98. ^{1}**TS28**

6	4.019184	-0.440271	-0.074735
6	3.203293	-1.496563	-0.514342
6	1.827358	-1.315696	-0.658518
6	1.237733	-0.071928	-0.391823
6	2.054518	0.986106	0.051876
6	3.426819	0.822697	0.206160
1	3.637094	-2.469998	-0.740468
1	1.210974	-2.152964	-0.993421
1	1.632248	1.967563	0.278250
8	4.169354	1.862841	0.677630
8	5.347236	-0.528541	0.121604
6	5.109368	2.447459	-0.225375
1	4.599897	2.830555	-1.127230
1	5.575248	3.287589	0.307228
1	5.887846	1.728456	-0.523643
6	6.019148	-1.753955	-0.135820
1	5.920533	-2.052725	-1.193226
1	7.077535	-1.577653	0.092711
1	5.638514	-2.563894	0.509091
6	-0.272048	0.125287	-0.535414
1	-0.524243	1.155774	-0.811712
1	-0.719948	-0.579451	-1.244009
6	-0.649218	-0.171872	0.853172
1	-0.424259	0.608133	1.587619
6	-0.873059	-1.528961	1.383677
1	0.057652	-1.856011	1.880127
1	-1.642889	-1.482487	2.167786
1	-1.161819	-2.243536	0.605077
15	-3.857386	0.126235	-0.123762
9	-2.992495	-1.156255	-0.663062
9	-2.539079	0.516780	0.913245
9	-4.448636	-0.795671	1.075133
9	-4.623216	1.422158	0.473865
9	-5.091165	-0.239197	-1.099710
9	-3.155952	1.054287	-1.264444

Structure S99. PF_5

15	-0.000318	-0.000558	0.000003
9	-1.603006	-0.003228	-0.000692
9	0.001620	-1.574386	0.077700
9	1.603366	-0.000794	0.001760
9	-0.002237	0.857485	1.321166
9	0.000786	0.721853	-1.399940

Structure S100. Co^{II}(salen)(diox)$_2$

8	-0.539386	-1.458814	-0.338894
8	1.501585	0.193033	0.198013
7	-2.194858	0.731844	-0.648594
7	-0.259741	2.323746	0.114635
6	-1.603143	-2.179002	-0.461647
6	-1.526170	-3.615714	-0.280030
6	-2.676751	-4.367877	-0.487850

1	-2.636991	-5.450633	-0.364917	1	-1.067292	-6.059000	1.095021
6	-3.919393	-3.802777	-0.850946	1	0.645134	-6.202100	0.653127
6	-4.016494	-2.434699	-0.988528	6	4.153316	-0.863485	0.575285
1	-4.972806	-1.970536	-1.250605	6	5.658050	-1.109005	0.786355
6	-2.887155	-1.603034	-0.784299	1	6.023015	-0.683771	1.735302
6	-3.077845	-0.180194	-0.903052	1	6.267067	-0.694334	-0.033000
1	-4.079791	0.128313	-1.231165	1	5.851609	-2.193225	0.818506
6	-2.450485	2.160712	-0.869348	6	3.398371	-1.526005	1.750713
1	-2.016193	2.395797	-1.858530	1	2.314624	-1.441936	1.614695
6	-1.602688	2.912933	0.173851	1	3.672792	-1.055075	2.709424
1	-2.006549	2.634352	1.165637	1	3.655157	-2.596593	1.815485
6	-1.707985	4.429078	0.002895	6	3.745304	-1.552573	-0.745258
1	-1.244191	4.717124	-0.957574	1	4.291694	-1.128559	-1.603070
1	-1.149620	4.946224	0.798927	1	2.671717	-1.437236	-0.922056
6	-3.174323	4.878164	0.030802	1	3.972766	-2.630482	-0.701900
1	-3.593064	4.686127	1.035269	1	5.335771	3.719115	0.766872
1	-3.234323	5.966857	-0.129747	1	-4.787811	-4.446585	-1.007533
6	-4.010280	4.136099	-1.014702	27	-0.367072	0.441141	-0.166561
1	-3.655456	4.408916	-2.025029	6	-1.905769	-0.608549	2.557677
1	-5.065155	4.450403	-0.958592	6	-2.412607	-0.175844	3.923910
6	-3.910995	2.615568	-0.841576	6	-0.349260	0.827178	4.385945
1	-4.485528	2.117902	-1.638100	6	0.173417	0.404648	3.022815
1	-4.363939	2.313560	0.119832	1	-2.943312	0.795448	3.827309
6	0.818223	3.010472	0.318236	1	-3.123545	-0.917164	4.322026
1	0.736335	4.096119	0.464191	1	-1.479931	-1.625734	2.610203
6	2.158998	2.487824	0.391891	1	-2.712146	-0.607554	1.812863
6	3.213431	3.423191	0.540744	1	-0.755098	1.859120	4.319230
1	2.971870	4.490851	0.559825	1	0.465772	0.826335	5.126927
6	4.519805	3.000919	0.659390	1	0.877432	1.142006	2.616379
6	4.793017	1.615413	0.658273	1	0.690422	-0.569108	3.093836
1	5.834052	1.312438	0.773160	8	-0.911634	0.306771	2.100802
6	3.810573	0.640122	0.526791	8	-1.347225	-0.066224	4.851551
6	2.434395	1.070085	0.358394	6	-0.303210	-0.299445	-3.362701
6	-0.195919	-4.264753	0.151712	6	0.976364	-1.105971	-3.494402
6	0.253834	-3.668845	1.506340	6	2.255450	0.833859	-3.225381
1	-0.475908	-3.904955	2.298579	6	0.986881	1.657465	-3.073407
1	0.363503	-2.580130	1.438366	1	1.253686	-1.488403	-2.497322
1	1.225013	-4.093605	1.809667	1	0.827001	-1.963120	-4.169547
6	0.893095	-4.002604	-0.911448	1	-0.662695	0.017148	-4.361821
1	1.079032	-2.929719	-1.015022	1	-1.089210	-0.883882	-2.867085
1	0.590898	-4.403972	-1.893030	1	2.610435	0.534932	-2.224905
1	1.838434	-4.491264	-0.622407	1	3.044612	1.429632	-3.710469
6	-0.323085	-5.788140	0.328740	1	1.137985	2.485742	-2.367074
1	-0.596299	-6.295747	-0.610525	1	0.682649	2.074415	-4.054131

8	-0.072648	0.855562	-2.555961
8	2.022524	-0.309784	-4.033981

Structure S101. (diox)Co^{III}(salen)-F

27	0.511041	-0.015132	-0.347697
8	-1.081476	1.030694	-0.345433
8	-0.559784	-1.516066	0.085096
7	1.612283	1.457928	-0.880088
7	2.128151	-1.015893	-0.190895
6	-1.248323	2.273557	-0.648290
6	-2.555379	2.877830	-0.478531
6	-2.708302	4.212370	-0.834980
1	-3.685182	4.683590	-0.724996
6	-1.660104	5.010904	-1.344908
6	-0.408539	4.456148	-1.487051
1	0.424599	5.053116	-1.870550
6	-0.172712	3.103715	-1.129679
6	1.168728	2.612551	-1.258506
1	1.881710	3.319965	-1.703711
6	2.976455	0.998779	-1.170657
1	2.936439	0.519352	-2.165676
6	3.279727	-0.115958	-0.152861
1	3.264828	0.356630	0.846953
6	4.654810	-0.739330	-0.387068
1	4.657207	-1.255958	-1.362942
1	4.867494	-1.498105	0.382522
6	5.742581	0.341848	-0.367890
1	5.802776	0.779376	0.645024
1	6.724588	-0.115215	-0.569941
6	5.449509	1.449669	-1.383035
1	5.494980	1.029406	-2.403589
1	6.222964	2.233155	-1.332195
6	4.066071	2.073659	-1.160026
1	3.874656	2.825444	-1.940749
1	4.037222	2.600474	-0.189290
6	2.206360	-2.304689	-0.186935
1	3.201586	-2.768283	-0.163308
6	1.099751	-3.218234	-0.204127
6	1.385630	-4.603528	-0.294937
1	2.430471	-4.928122	-0.322769
6	0.363551	-5.525537	-0.355727
6	-0.972571	-5.067536	-0.375085
1	-1.757548	-5.817824	-0.475729
6	-1.321747	-3.723774	-0.297673
6	-0.261073	-2.754614	-0.140782
6	-3.733435	2.041481	0.060310
6	-3.390793	1.459834	1.451877
1	-3.189310	2.266609	2.176568
1	-2.515069	0.802845	1.399908
1	-4.238199	0.868827	1.836865
6	-4.029138	0.888700	-0.922919
1	-3.152732	0.245215	-1.045253
1	-4.312712	1.281900	-1.912999
1	-4.864239	0.271757	-0.551579
6	-5.016329	2.878408	0.212654
1	-5.365101	3.287051	-0.749140
1	-4.888344	3.716493	0.917298
1	-5.824477	2.241121	0.605766
6	-2.773395	-3.241575	-0.473615
6	-3.757738	-4.414365	-0.632820
1	-3.785259	-5.059434	0.260982
1	-3.523909	-5.044711	-1.505407
1	-4.775302	-4.019377	-0.782766
6	-3.242899	-2.405991	0.739512
1	-2.645593	-1.495458	0.849697
1	-3.163160	-2.992622	1.670772
1	-4.299709	-2.116874	0.616029
6	-2.827170	-2.395860	-1.769755
1	-2.593584	-3.025674	-2.643870
1	-2.103742	-1.569835	-1.749457
1	-3.835962	-1.976968	-1.916938
9	0.384313	-0.448197	-2.088798
1	-1.849068	6.051842	-1.615933
1	0.575112	-6.595191	-0.419565
6	1.067918	1.988970	3.475560
6	0.401717	1.738631	2.134601
6	0.422061	-0.595913	2.602335
6	1.083297	-0.292177	3.934979
1	-0.693341	1.794986	2.222017
1	0.738754	2.464316	1.387274
1	2.169290	2.035367	3.341334
1	0.730703	2.957311	3.877124
1	-0.674820	-0.640198	2.697400
1	0.776714	-1.547538	2.192338
1	0.759196	-1.032881	4.682414
1	2.185639	-0.370991	3.826463
8	0.725343	0.989477	4.415052

8	0.766960	0.431563	1.650744

Optimized geometries calculated by M06 functional.

Structure S102. Co^{II}(salen)

27	-0.000010	0.896016	-0.000104
8	-1.289624	-0.458411	0.116772
8	1.289623	-0.458402	-0.116890
7	-1.263420	2.268346	-0.190468
7	1.263376	2.268376	0.190198
6	-2.575056	-0.381509	0.058164
6	-3.375438	-1.574617	0.182492
6	-4.752161	-1.449029	0.103550
1	-5.363767	-2.352449	0.191678
6	-5.435869	-0.224383	-0.085763
6	-4.668609	0.911739	-0.195020
1	-5.150750	1.887439	-0.338829
6	-3.255719	0.862178	-0.126833
6	-2.547169	2.098065	-0.240384
1	-3.188707	2.981179	-0.389063
6	2.547117	2.098089	0.240327
1	3.188636	2.981209	0.389045
6	3.255681	0.862198	0.126930
6	4.668562	0.911768	0.195306
1	5.150676	1.887470	0.339191
6	5.435846	-0.224344	0.086123
6	4.752173	-1.448990	-0.103319
1	5.363801	-2.352400	-0.191395
6	3.375462	-1.574592	-0.182437
6	2.575049	-0.381494	-0.058161
6	-2.702736	-2.931873	0.402283
6	-1.943118	-2.918174	1.734131
1	-2.638951	-2.754220	2.575394
1	-1.180010	-2.127476	1.752512
1	-1.438620	-3.887088	1.896961
6	-1.740193	-3.240458	-0.751153
1	-0.920194	-2.509536	-0.799379
1	-2.276442	-3.234465	-1.716464
1	-1.302224	-4.245953	-0.618767
6	-3.719515	-4.069757	0.465625
1	-4.294248	-4.167341	-0.471348
1	-4.434485	-3.948115	1.296998
1	-3.189732	-5.023293	0.627455
6	2.702815	-2.931858	-0.402352
6	3.719629	-4.069712	-0.465649
1	4.294150	-4.167441	0.471438
1	4.434786	-3.947913	-1.296839
1	3.189903	-5.023232	-0.627755
6	1.740177	-3.240528	0.750978
1	0.920191	-2.509595	0.799197
1	2.276348	-3.234625	1.716334
1	1.302204	-4.246005	0.618472
6	1.943320	-2.918126	-1.734270
1	2.639221	-2.754088	-2.575460
1	1.180173	-2.127467	-1.752677
1	1.438893	-3.887060	-1.897201
6	0.652936	3.600357	0.427073
6	-0.652980	3.600285	-0.427560
6	1.580348	4.747443	0.047078
1	1.033857	5.702195	0.050565
1	2.396496	4.858729	0.777623
1	2.029303	4.613119	-0.948937
6	0.334336	3.689554	1.919737
1	1.252645	3.511247	2.501875
1	-0.042158	4.688871	2.187904
1	-0.413276	2.939663	2.223621
6	-1.580384	4.747443	-0.047774
1	-2.029311	4.613331	0.948282
1	-1.033894	5.702194	-0.051475
1	-2.396554	4.858572	-0.778320
6	-0.334378	3.689215	-1.920241
1	-1.252686	3.510800	-2.502346
1	0.042117	4.688486	-2.188585
1	0.413238	2.939272	-2.223988
6	6.944909	-0.183786	0.165054
6	7.594926	-0.674534	-1.124140
6	7.469472	-0.959811	1.368596
1	7.226006	0.878662	0.300911
1	7.242924	-0.101905	-1.997497
1	8.692904	-0.583126	-1.075269
1	7.363724	-1.738401	-1.308530
1	7.028133	-0.592568	2.309285
1	7.229534	-2.034451	1.285872
1	8.566145	-0.875062	1.449209
6	-6.944944	-0.183830	-0.164471
6	-7.594762	-0.674553	1.124834

6	-7.469696	-0.959875	-1.367917
1	-7.226063	0.878616	-0.300304
1	-7.242633	-0.101899	1.998123
1	-8.692749	-0.583157	1.076128
1	-7.363519	-1.738413	1.309214
1	-7.028495	-0.592658	-2.308681
1	-7.229762	-2.034517	-1.285208
1	-8.566380	-0.875115	-1.448367

Structure S103. $[Me_3NFPy]^+$

6	0.375158	-1.216215	-0.001768
6	-1.008347	-1.203158	-0.010857
6	-1.726896	-0.000448	-0.012455
6	-1.008816	1.202600	-0.010841
6	0.374624	1.216285	-0.001743
1	-1.528786	-2.163950	-0.018967
1	-1.529738	2.163128	-0.018966
6	-3.212744	-0.000389	0.008970
1	-3.564200	0.006021	1.055002
1	-3.624003	0.894513	-0.477820
1	-3.624372	-0.900577	-0.467509
6	1.230480	2.423981	-0.000383
1	1.886258	2.438171	-0.884623
1	0.603627	3.322540	-0.003392
1	1.880846	2.440131	0.887731
6	1.231483	-2.423572	-0.000372
1	1.887501	-2.437397	-0.884436
1	1.881625	-2.439565	0.887915
1	0.604975	-3.322370	-0.003634
7	0.971885	0.000139	0.003631
9	2.310380	0.000431	0.008886

Structure S104. ^{2}**TS1**

27	0.249146	1.210968	-0.451598
8	-0.977155	0.095339	-1.321182
8	1.523871	-0.075167	-0.851113
7	-0.974815	2.631213	-0.274103
7	1.465719	2.337953	0.433266
6	-2.261217	0.165212	-1.262043
6	-3.056438	-1.015540	-1.481301
6	-4.433643	-0.874644	-1.508438
1	-5.045075	-1.766093	-1.679703
6	-5.118756	0.349636	-1.311524
6	-4.356870	1.461731	-1.039927
1	-4.841652	2.425723	-0.840915
6	-2.943954	1.389400	-0.978024
6	-2.234209	2.558835	-0.580582
1	-2.845868	3.471703	-0.501712
6	2.730297	2.097082	0.572601
1	3.340042	2.816634	1.140517
6	3.456027	0.978653	0.055772
6	4.849627	0.934880	0.290250
1	5.310651	1.746520	0.866651
6	5.624456	-0.095810	-0.191361
6	4.972878	-1.098759	-0.945264
1	5.594367	-1.906731	-1.342752
6	3.612957	-1.120620	-1.213550
6	2.808945	-0.058153	-0.677609
6	-2.376664	-2.381833	-1.598656
6	-1.614062	-2.664574	-0.295646
1	-2.314377	-2.714577	0.559781
1	-0.862461	-1.884138	-0.097988
1	-1.094513	-3.637133	-0.356819
6	-1.412687	-2.414486	-2.790068
1	-0.597575	-1.686742	-2.670932
1	-1.949114	-2.193449	-3.729069
1	-0.966667	-3.420263	-2.887100
6	-3.389921	-3.507042	-1.791103
1	-3.967519	-3.390350	-2.723680
1	-4.101720	-3.578265	-0.951179
1	-2.857908	-4.470728	-1.852150
6	2.976531	-2.220453	-2.067994
6	4.013835	-3.228440	-2.557752
1	4.507887	-3.756966	-1.724745
1	4.794339	-2.757040	-3.178467
1	3.516099	-3.990234	-3.179987
6	1.930418	-2.992104	-1.256092
1	1.086406	-2.347066	-0.972614
1	2.378511	-3.420319	-0.341586
1	1.527944	-3.828347	-1.854768
6	2.317364	-1.595141	-3.303896
1	3.066663	-1.069538	-3.920661
1	1.529065	-0.880716	-3.024134
1	1.859997	-2.383047	-3.927864
6	0.829246	3.528913	1.058539
6	-0.326151	3.918974	0.083224

6	1.814522	4.674692	1.251512
1	1.278664	5.595328	1.526083
1	2.509938	4.466829	2.079356
1	2.407176	4.879728	0.347260
6	0.289892	3.108622	2.426695
1	1.094973	2.626392	3.005705
1	-0.051091	3.984639	2.999461
1	-0.542349	2.395285	2.342555
6	-1.302300	4.896318	0.723593
1	-1.898748	4.430356	1.523048
1	-0.761611	5.752411	1.153283
1	-1.995121	5.313914	-0.023069
6	0.221649	4.523666	-1.208996
1	-0.594107	4.621143	-1.942835
1	0.636336	5.528437	-1.035952
1	1.006858	3.891784	-1.654332
6	7.113681	-0.160068	0.058062
6	7.909264	-0.092300	-1.240987
6	7.496182	-1.392859	0.870187
1	7.372288	0.733101	0.658792
1	7.657085	0.808759	-1.822983
1	8.993092	-0.076683	-1.039420
1	7.708790	-0.969657	-1.880468
1	6.945167	-1.436162	1.823637
1	7.277142	-2.321871	0.315234
1	8.574741	-1.396248	1.098933
6	-6.628620	0.401608	-1.340843
6	-7.232206	-0.388129	-0.183624
6	-7.192567	-0.067248	-2.676991
1	-6.911249	1.463589	-1.207675
1	-6.852934	-0.031405	0.788260
1	-8.331430	-0.302046	-0.173243
1	-6.987880	-1.462053	-0.263699
1	-6.773622	0.508812	-3.517675
1	-6.966633	-1.132838	-2.856859
1	-8.289421	0.040881	-2.701753
6	-2.177370	-0.922995	2.810732
6	-2.471590	-1.962603	3.685797
6	-1.475239	-2.849877	4.112359
6	-0.166230	-2.654452	3.653830
6	0.137410	-1.614129	2.784219
1	-3.504923	-2.074296	4.026020
1	0.643558	-3.316920	3.971047
6	-1.804779	-3.990793	5.009699
1	-2.097195	-4.864936	4.403388
1	-0.940417	-4.290302	5.618403
1	-2.651200	-3.755219	5.669622
6	1.477793	-1.328947	2.220992
1	1.778738	-0.291655	2.442268
1	2.221712	-2.022352	2.630971
1	1.447194	-1.424510	1.123282
6	-3.171944	0.030910	2.263609
1	-2.826042	1.071183	2.363233
1	-3.318305	-0.159926	1.186080
1	-4.132459	-0.089682	2.778572
7	-0.893432	-0.830696	2.447445
9	-0.565617	0.237528	1.354017

Structure S105. ^{2}INT1

27	0.222679	1.290083	-0.232715
8	-1.003293	0.313209	-1.258427
8	1.508641	0.166180	-0.916190
7	-0.920046	2.786249	-0.114683
7	1.479919	2.374439	0.676412
6	-2.285033	0.382203	-1.149436
6	-3.093062	-0.759112	-1.485613
6	-4.467820	-0.618872	-1.406887
1	-5.092836	-1.483570	-1.650087
6	-5.134790	0.567017	-1.010448
6	-4.356994	1.649308	-0.675128
1	-4.825296	2.584518	-0.345440
6	-2.943518	1.575882	-0.717224
6	-2.202230	2.719152	-0.314430
1	-2.800441	3.626570	-0.140864
6	2.730310	2.085204	0.812321
1	3.352234	2.757008	1.423604
6	3.432383	0.985801	0.223978
6	4.805056	0.844039	0.519894
1	5.268852	1.548097	1.221135
6	5.557584	-0.156370	-0.056706
6	4.909323	-1.008178	-0.976975
1	5.514827	-1.789282	-1.445931
6	3.567838	-0.917597	-1.322807
6	2.788622	0.095827	-0.678617
6	-2.428807	-2.090703	-1.839480
6	-1.625537	-2.571685	-0.623400
1	-2.307108	-2.796561	0.217366

1	-0.897491	-1.814450	-0.289755
1	-1.077709	-3.499680	-0.865140
6	-1.514753	-1.941475	-3.061309
1	-0.674248	-1.261573	-2.864971
1	-2.082187	-1.559125	-3.927396
1	-1.099875	-2.925908	-3.340769
6	-3.458810	-3.168915	-2.166969
1	-4.069850	-2.905634	-3.047077
1	-4.138421	-3.371013	-1.322016
1	-2.936905	-4.112065	-2.397698
6	2.929101	-1.867274	-2.339252
6	3.953582	-2.830468	-2.934506
1	4.403922	-3.486789	-2.170842
1	4.767189	-2.302054	-3.459702
1	3.454882	-3.481501	-3.670951
6	1.841037	-2.705834	-1.660315
1	1.031916	-2.073758	-1.266546
1	2.262345	-3.301783	-0.831072
1	1.396627	-3.408797	-2.386881
6	2.322140	-1.063490	-3.496183
1	3.097420	-0.465744	-4.005814
1	1.528550	-0.385574	-3.149511
1	1.883427	-1.750309	-4.240856
6	0.859654	3.569614	1.310654
6	-0.219128	4.035940	0.281459
6	1.884112	4.660182	1.590920
1	1.374792	5.588167	1.889358
1	2.535005	4.383244	2.434462
1	2.520256	4.882094	0.720702
6	0.227795	3.123993	2.629064
1	0.992561	2.624317	3.245536
1	-0.141394	3.992802	3.194791
1	-0.590421	2.407456	2.472061
6	-1.168938	5.063979	0.875646
1	-1.791998	4.649169	1.682425
1	-0.600355	5.911736	1.284510
1	-1.832549	5.481376	0.102692
6	0.419734	4.609443	-0.982421
1	-0.357770	4.763957	-1.746929
1	0.888758	5.584375	-0.781624
1	1.182055	3.934411	-1.404161
6	7.020641	-0.342464	0.271126
6	7.903954	-0.189528	-0.961893
6	7.269278	-1.679291	0.961801
1	7.290190	0.461261	0.982678
1	7.742636	0.780883	-1.458251
1	8.970256	-0.261983	-0.692030
1	7.700628	-0.982460	-1.702525
1	6.653601	-1.786454	1.869485
1	7.029203	-2.524414	0.293205
1	8.327652	-1.782193	1.252473
6	-6.640997	0.601623	-0.903865
6	-7.125482	-0.302361	0.225810
6	-7.321905	0.249798	-2.220925
1	-6.916764	1.641985	-0.645899
1	-6.656241	-0.031862	1.186169
1	-8.219114	-0.235295	0.347978
1	-6.881229	-1.359651	0.021067
1	-6.985534	0.906159	-3.039491
1	-7.110321	-0.791936	-2.518389
1	-8.416515	0.345998	-2.134315
6	-2.116736	-1.544547	2.663873
6	-2.424753	-2.813419	3.164986
6	-1.421095	-3.776946	3.309405
6	-0.106079	-3.441343	2.953671
6	0.187706	-2.167852	2.469031
1	-3.463794	-3.039709	3.422769
1	0.704692	-4.170194	3.049303
6	-1.732716	-5.146904	3.810624
1	-1.076545	-5.413535	4.653607
1	-2.777747	-5.238032	4.135594
1	-1.551318	-5.893341	3.020362
6	1.527540	-1.700527	2.030485
1	1.830853	-0.812347	2.606957
1	2.280210	-2.491068	2.145372
1	1.469101	-1.389771	0.975567
6	-3.114841	-0.481655	2.376499
1	-2.735149	0.506638	2.671686
1	-3.296576	-0.446917	1.287584
1	-4.066064	-0.691859	2.882213
7	-0.840301	-1.334284	2.398089
9	-0.386357	0.390069	1.359223

Structure S106. Co^{III}(salen)-F

27	-0.024208	0.827914	0.151690
8	-1.262263	-0.531245	-0.219064
8	1.286375	-0.426210	-0.285905

7	-1.214663	2.198138	-0.468163
7	1.235968	2.240628	0.300558
6	-2.541988	-0.422522	-0.126229
6	-3.336466	-1.594881	0.127178
6	-4.713539	-1.457022	0.122180
1	-5.324882	-2.344886	0.312316
6	-5.397771	-0.236861	-0.100982
6	-4.632336	0.885661	-0.310642
1	-5.114322	1.857623	-0.473945
6	-3.217773	0.823438	-0.313167
6	-2.497508	2.030939	-0.544081
1	-3.122535	2.900729	-0.801406
6	2.513400	2.073372	0.365202
1	3.146208	2.963636	0.503889
6	3.233201	0.842687	0.236142
6	4.636161	0.877307	0.398102
1	5.110017	1.827684	0.673574
6	5.405045	-0.251042	0.217810
6	4.735020	-1.438794	-0.152784
1	5.347634	-2.333751	-0.299469
6	3.364434	-1.541356	-0.339155
6	2.572004	-0.364003	-0.129468
6	-2.648533	-2.927681	0.425877
6	-1.790382	-2.774152	1.689608
1	-2.432776	-2.572053	2.564290
1	-1.067509	-1.949325	1.601878
1	-1.235930	-3.708360	1.888647
6	-1.783613	-3.364514	-0.763088
1	-0.971256	-2.650925	-0.960909
1	-2.398125	-3.460833	-1.675449
1	-1.331489	-4.351268	-0.557949
6	-3.659457	-4.041766	0.687435
1	-4.298037	-4.239832	-0.190574
1	-4.313950	-3.820175	1.547397
1	-3.120417	-4.975415	0.918989
6	2.692252	-2.861232	-0.724988
6	3.713542	-3.978500	-0.925433
1	4.283381	-4.194086	-0.005722
1	4.432271	-3.747208	-1.730158
1	3.188828	-4.905710	-1.209247
6	1.738337	-3.296315	0.394193
1	0.930663	-2.565274	0.548073
1	2.285067	-3.422387	1.344897
1	1.275713	-4.266900	0.140716
6	1.918220	-2.701070	-2.039910
1	2.596712	-2.404935	-2.859012
1	1.123368	-1.946053	-1.951596
1	1.452194	-3.662057	-2.321030
6	0.583578	3.573986	0.349716
6	-0.538027	3.488217	-0.739912
6	1.561468	4.705312	0.069998
1	1.019903	5.658735	-0.014889
1	2.270341	4.826198	0.903861
1	2.139119	4.556300	-0.855024
6	-0.002152	3.751956	1.749630
1	0.808864	3.664243	2.490201
1	-0.451226	4.750749	1.860983
1	-0.742181	2.974485	1.984019
6	-1.491754	4.670660	-0.675645
1	-2.074254	4.693645	0.257900
1	-0.933288	5.614741	-0.755087
1	-2.195548	4.654984	-1.522461
6	0.053147	3.392546	-2.145865
1	-0.750877	3.168180	-2.864496
1	0.517811	4.342871	-2.449946
1	0.806042	2.591289	-2.221070
6	6.905147	-0.232565	0.402710
6	7.640353	-0.581532	-0.886710
6	7.343304	-1.142570	1.545272
1	7.176865	0.805432	0.675509
1	7.347976	0.086724	-1.712769
1	8.731988	-0.502157	-0.752996
1	7.424944	-1.617095	-1.203216
1	6.836814	-0.880104	2.488066
1	7.111708	-2.199529	1.325703
1	8.431327	-1.073933	1.710805
6	-6.908221	-0.185568	-0.091791
6	-7.480386	-0.579672	1.265665
6	-7.508282	-1.037002	-1.205556
1	-7.189635	0.867895	-0.283358
1	-7.070817	0.047025	2.074225
1	-8.578321	-0.477997	1.276596
1	-7.247457	-1.631271	1.508484
1	-7.121635	-0.740771	-2.194061
1	-7.273165	-2.106283	-1.062459
1	-8.606884	-0.944383	-1.226354
9	-0.364467	0.715956	1.964789

Structure S107. $[Me_3MPy]^{+\cdot}$

6	0.705408	-1.213092	0.001142
6	-0.695182	-1.208752	-0.008732
6	-1.406664	-0.001985	-0.011133
6	-0.698439	1.206729	-0.008542
6	0.702083	1.214930	0.001378
1	-1.206024	-2.176767	-0.017752
1	-1.212042	2.173278	-0.017105
6	-2.896759	-0.003665	0.005018
1	-3.254108	-0.000157	1.048484
1	-3.306310	0.890543	-0.484255
1	-3.304545	-0.902046	-0.477962
6	1.561361	2.429329	-0.000474
1	2.208672	2.438375	-0.889776
1	0.934628	3.328371	-0.001162
1	2.210326	2.439882	0.887480
6	1.567945	-2.425191	-0.000661
1	2.221715	-2.428464	-0.885211
1	2.210448	-2.438204	0.892001
1	0.943503	-3.325787	-0.009647
7	1.216460	0.001594	0.012417

Structure S108. $[Co^{IV}(salen)\text{-}F]^+$

27	0.018844	0.824622	-0.081091
8	1.268746	-0.580513	0.282279
8	-1.286980	-0.395789	0.325717
7	1.239984	2.191674	0.571376
7	-1.186757	2.243330	-0.287657
6	2.519298	-0.493003	0.202751
6	3.305550	-1.704030	-0.030385
6	4.685089	-1.585602	-0.038146
1	5.290244	-2.477302	-0.210290
6	5.357495	-0.364827	0.151625
6	4.587915	0.807047	0.347606
1	5.106457	1.760326	0.501915
6	3.210613	0.776334	0.360441
6	2.509129	2.022123	0.599314
1	3.164348	2.880460	0.815741
6	-2.467143	2.090745	-0.385545
1	-3.075903	2.991780	-0.550364
6	-3.208000	0.877138	-0.266213
6	-4.604754	0.925898	-0.469155
1	-5.062372	1.877510	-0.763613
6	-5.384409	-0.197377	-0.303524
6	-4.734727	-1.389085	0.089636
1	-5.358769	-2.277843	0.221829
6	-3.370568	-1.505633	0.314881
6	-2.572480	-0.333621	0.125651
6	2.596143	-3.017131	-0.317800
6	1.761051	-2.852008	-1.599475
1	2.416970	-2.650096	-2.462974
1	1.029089	-2.033984	-1.528725
1	1.216868	-3.789683	-1.802538
6	1.706061	-3.417405	0.869460
1	0.872955	-2.719192	1.027567
1	2.297636	-3.481406	1.798450
1	1.278493	-4.415881	0.677010
6	3.591802	-4.150351	-0.552756
1	4.215341	-4.347856	0.335245
1	4.255418	-3.954634	-1.411040
1	3.036391	-5.074810	-0.775781
6	-2.722386	-2.832111	0.716625
6	-3.761345	-3.937008	0.893564
1	-4.311931	-4.146582	-0.038796
1	-4.494283	-3.697631	1.682565
1	-3.253250	-4.869612	1.188403
6	-1.754164	-3.275927	-0.386247
1	-0.943547	-2.547728	-0.536979
1	-2.287028	-3.406195	-1.343711
1	-1.296888	-4.245356	-0.120688
6	-1.976381	-2.682869	2.048813
1	-2.669287	-2.380306	2.852799
1	-1.168676	-1.938732	1.987700
1	-1.529899	-3.650413	2.337452
6	-0.512055	3.573396	-0.319723
6	0.562204	3.488138	0.818296
6	-1.491512	4.711678	-0.079182
1	-0.942751	5.659420	0.018691
1	-2.166502	4.834746	-0.939897
1	-2.101637	4.573110	0.825921
6	0.127830	3.743629	-1.695577
1	-0.652828	3.650540	-2.466813
1	0.575123	4.744133	-1.792705
1	0.882635	2.972480	-1.901552
6	1.526579	4.659979	0.801707
1	2.124964	4.707941	-0.120667

1	0.973012	5.604655	0.899213
1	2.212291	4.613813	1.662333
6	-0.082364	3.373730	2.199211
1	0.693311	3.152318	2.948277
1	-0.561079	4.321909	2.485023
1	-0.835483	2.570820	2.242028
6	-6.877004	-0.172503	-0.535435
6	-7.652706	-0.550432	0.721399
6	-7.271948	-1.058452	-1.712332
1	-7.139239	0.870946	-0.794591
1	-7.384656	0.095055	1.573232
1	-8.738255	-0.460341	0.553075
1	-7.455012	-1.595394	1.017309
1	-6.737020	-0.771965	-2.631984
1	-7.042747	-2.118994	-1.508767
1	-8.354106	-0.989280	-1.910421
6	6.851236	-0.245812	0.080802
6	7.237946	0.260722	-1.314004
6	7.600486	-1.521241	0.424015
1	7.134779	0.539622	0.808425
1	6.750817	1.217622	-1.559042
1	8.327920	0.406363	-1.373212
1	6.947327	-0.475246	-2.082647
1	7.285825	-1.939856	1.392988
1	7.460074	-2.296800	-0.347693
1	8.680514	-1.316788	0.477509
9	0.538216	0.708908	-1.841951

Structure S109. Me_3MPy

6	0.702809	-1.151447	0.000777
6	-0.694030	-1.192345	-0.009534
6	-1.422452	-0.000923	-0.011461
6	-0.695463	1.191428	-0.009402
6	0.701379	1.152237	0.000889
1	-1.213908	-2.156777	-0.018715
1	-1.216527	2.155227	-0.018500
6	-2.917338	-0.001594	0.008399
1	-3.290542	0.004478	1.046703
1	-3.329094	0.889778	-0.488281
1	-3.328360	-0.898939	-0.477953
6	1.514413	2.409244	0.001784
1	2.168298	2.442336	-0.884647
1	0.886511	3.311552	0.008209
1	2.177237	2.434805	0.881634
6	1.517326	-2.407493	0.001852
1	2.173381	-2.438560	-0.883027
1	2.178051	-2.433529	0.883282
1	0.890468	-3.310542	0.005643
7	1.380661	0.000791	0.006547

Structure S110. $[Co^{III}(salen)]^+$

27	0.000013	0.916161	0.000005
8	-1.273729	-0.423541	0.029060
8	1.273744	-0.423554	-0.029058
7	-1.263682	2.275855	-0.193747
7	1.263719	2.275846	0.193754
6	-2.559014	-0.369670	0.023560
6	-3.330159	-1.575099	0.198510
6	-4.706033	-1.465120	0.121296
1	-5.308364	-2.370151	0.240072
6	-5.403198	-0.250929	-0.098958
6	-4.659406	0.903450	-0.227292
1	-5.159352	1.866881	-0.379531
6	-3.252501	0.871719	-0.160521
6	-2.547290	2.104095	-0.277596
1	-3.179835	2.986311	-0.455292
6	2.547325	2.104077	0.277601
1	3.179877	2.986289	0.455294
6	3.252527	0.871696	0.160520
6	4.659434	0.903415	0.227280
1	5.159389	1.866842	0.379515
6	5.403213	-0.250970	0.098937
6	4.706035	-1.465155	-0.121312
1	5.308356	-2.370190	-0.240088
6	3.330157	-1.575120	-0.198513
6	2.559030	-0.369686	-0.023557
6	-2.636618	-2.908036	0.475755
6	-1.838135	-2.801355	1.781846
1	-2.508391	-2.575767	2.628947
1	-1.066355	-2.019179	1.730749
1	-1.337234	-3.761237	1.995838
6	-1.711553	-3.276274	-0.690058
1	-0.901214	-2.544926	-0.817809
1	-2.280119	-3.341365	-1.633702
1	-1.252973	-4.263547	-0.506180
6	-3.643217	-4.043794	0.642744

1	-4.239954	-4.209738	-0.269973
1	-4.335442	-3.869710	1.483555
1	-3.100992	-4.979694	0.853711
6	2.636561	-2.908034	-0.475740
6	3.643077	-4.043856	-0.642811
1	4.239874	-4.209846	0.269858
1	4.335248	-3.869816	-1.483676
1	3.100775	-4.979721	-0.853739
6	1.711541	-3.276230	0.690118
1	0.901272	-2.544816	0.817946
1	2.280166	-3.341397	1.633721
1	1.252864	-4.263458	0.506239
6	1.837997	-2.801282	-1.781775
1	2.508213	-2.575733	-2.628917
1	1.066279	-2.019047	-1.730619
1	1.337008	-3.761123	-1.995744
6	0.646130	3.610106	0.435497
6	-0.646083	3.610112	-0.435483
6	1.582396	4.752076	0.067437
1	1.036050	5.706300	0.067487
1	2.387798	4.862237	0.809276
1	2.040436	4.619258	-0.924223
6	0.314550	3.686066	1.926096
1	1.228318	3.512874	2.516120
1	-0.068061	4.683141	2.191395
1	-0.433051	2.933597	2.225754
6	-1.582340	4.752090	-0.067424
1	-2.040386	4.619275	0.924233
1	-1.035984	5.706310	-0.067469
1	-2.387737	4.862261	-0.809267
6	-0.314498	3.686074	-1.926080
1	-1.228265	3.512893	-2.516108
1	0.068124	4.683147	-2.191373
1	0.433098	2.933600	-2.225737
6	6.909296	-0.237357	0.184404
6	7.552577	-0.742427	-1.102753
6	7.401768	-1.027534	1.393047
1	7.209920	0.818212	0.323617
1	7.213753	-0.167021	-1.979062
1	8.650199	-0.662628	-1.045416
1	7.311792	-1.804236	-1.283859
1	6.958837	-0.653412	2.329861
1	7.145415	-2.097408	1.304075
1	8.498134	-0.959597	1.482312
6	-6.909279	-0.237301	-0.184436
6	-7.552576	-0.742365	1.102715
6	-7.401752	-1.027470	-1.393084
1	-7.209892	0.818272	-0.323650
1	-7.213752	-0.166962	1.979028
1	-8.650197	-0.662554	1.045370
1	-7.311803	-1.804177	1.283823
1	-6.958808	-0.653353	-2.329894
1	-7.145414	-2.097348	-1.304111
1	-8.498117	-0.959519	-1.482358

Structure S111. HF

9	0.000000	0.000000	0.092128
1	0.000000	0.000000	-0.829150

Structure S112. ^{1}INT2

6	-0.195418	1.162773	0.048096
6	1.197499	1.194697	0.005752
6	1.921857	-0.000003	-0.018727
6	1.197477	-1.194699	0.005754
6	-0.195432	-1.162755	0.048093
1	1.717882	2.158084	-0.012211
1	1.717848	-2.158092	-0.012205
6	3.413100	-0.000039	-0.101088
1	3.845144	-0.894558	0.371376
1	3.739157	-0.000647	-1.155147
1	3.845155	0.894992	0.370387
6	-1.017075	-2.409863	0.095799
1	-1.999663	-2.235491	-0.365385
1	-0.515563	-3.249926	-0.405530
1	-1.198513	-2.710374	1.141881
6	-1.017024	2.409906	0.095794
1	-1.999717	2.235483	-0.365143
1	-1.198205	2.710593	1.141870
1	-0.515604	3.249877	-0.405783
7	-0.861321	0.000018	0.066044
1	-2.462480	0.000008	-0.055320
9	-3.419567	-0.000019	-0.198660

Structure S113. $R_3Si^{\bullet}$

8	0.104659	-0.731652	0.343662

14	1.457735	-0.114852	-0.421497
14	-1.549552	-0.543217	0.211299
1	-2.160533	-1.833099	0.645267
6	1.397047	1.766961	-0.350933
1	2.303859	2.204409	-0.799028
1	0.524394	2.175343	-0.886438
1	1.339194	2.096192	0.702987
6	2.956617	-0.758067	0.506162
1	2.999088	-1.858179	0.499853
1	3.886992	-0.373457	0.058804
1	2.911710	-0.420982	1.557408
6	-1.986411	-0.181720	-1.570835
1	-1.552439	0.781288	-1.891666
1	-1.600473	-0.968027	-2.240511
1	-3.077974	-0.119793	-1.712485
6	-2.107970	0.837909	1.338307
1	-3.206905	0.927832	1.334730
1	-1.785287	0.659619	2.376634
1	-1.689149	1.804537	1.011709

Structure S114. ^{2}TS6

6	1.890484	-1.290188	-0.128175
6	3.197330	-1.526055	0.272433
6	4.170339	-0.528615	0.128908
6	3.776475	0.703078	-0.406092
6	2.458978	0.906215	-0.792543
1	3.457059	-2.496021	0.706248
1	4.498308	1.517535	-0.515685
6	5.586979	-0.780424	0.520742
1	6.131641	-1.255087	-0.313299
1	6.113710	0.153037	0.765333
1	5.652813	-1.465453	1.378668
6	1.920352	2.194389	-1.300578
1	1.325138	2.043358	-2.213207
1	1.226363	2.613157	-0.546894
1	2.719179	2.921903	-1.493050
6	0.777085	-2.262604	0.019899
1	-0.013604	-1.830306	0.661972
1	0.302357	-2.467908	-0.952993
1	1.121205	-3.207924	0.458539
7	1.570186	-0.094070	-0.655507
1	0.488814	0.113609	-0.985923
9	-0.720110	0.449868	-1.283821
8	-2.272169	-0.253633	0.805343
14	-1.137078	0.983065	0.938504
14	-3.068410	-0.985445	-0.459481
1	-2.183726	-1.980470	-1.142292
6	-1.894554	2.622123	0.398917
1	-1.279303	3.464389	0.760210
1	-1.971459	2.691407	-0.696567
1	-2.905304	2.735054	0.833094
6	-0.905718	1.097786	2.826179
1	-0.500222	0.160184	3.241669
1	-0.211079	1.913739	3.088512
1	-1.875293	1.296728	3.321559
6	-3.748723	0.243659	-1.693386
1	-4.381795	0.993729	-1.189358
1	-2.914466	0.760342	-2.190928
1	-4.364871	-0.263784	-2.454647
6	-4.484769	-1.935484	0.322295
1	-5.052776	-2.496939	-0.438701
1	-4.119885	-2.656655	1.071991
1	-5.184477	-1.248846	0.828041

Structure S115. R_3Si-F

9	1.688985	-0.921634	-1.348060
8	-0.166882	-0.345401	0.420943
14	1.399495	-0.046731	0.006819
14	-1.657214	0.003297	-0.262832
1	-1.440581	0.203146	-1.731425
6	1.634182	1.731913	-0.459403
1	2.668618	1.930026	-0.782209
1	0.963115	2.007502	-1.290415
1	1.411881	2.394340	0.393004
6	2.516913	-0.675448	1.337330
1	2.328599	-1.742885	1.531962
1	3.574784	-0.556089	1.055454
1	2.349115	-0.122830	2.275342
6	-2.313875	1.572505	0.503625
1	-2.437779	1.448666	1.592088
1	-1.627885	2.418051	0.332066
1	-3.294875	1.840216	0.078079
6	-2.784476	-1.446415	0.044672
1	-3.780606	-1.268879	-0.392308
1	-2.376310	-2.369216	-0.396891
1	-2.912282	-1.611381	1.127083

Structure S116. Me_3NHPy

6	-0.623102	1.232249	-0.000117
6	0.742269	1.195633	-0.011519
6	1.471570	-0.033408	-0.019522
6	0.695318	-1.225965	-0.010275
6	-0.673527	-1.209690	0.000396
1	1.280873	2.150521	-0.019205
1	1.195283	-2.201816	-0.016222
6	2.963691	-0.051941	0.015921
1	3.375727	0.161064	1.023020
1	3.362491	-1.034182	-0.286117
1	3.401876	0.705702	-0.658396
6	-1.550870	-2.408086	0.002182
1	-2.212350	-2.428619	-0.884035
1	-0.956258	-3.332159	0.006474
1	-2.214702	-2.423296	0.886909
6	-1.451670	2.465577	0.002846
1	-2.112789	2.509632	-0.882304
1	-2.112595	2.504742	0.888556
1	-0.821666	3.365706	0.006029
7	-1.327114	0.026902	-0.002087
1	-2.338173	0.048169	0.070430

Structure S117. ^{1}**TS8**

27	0.105361	1.103309	-0.271428
8	-1.191038	-0.208598	-0.706319
8	1.390498	-0.252157	-0.592377
7	-1.123245	2.511122	-0.285539
7	1.385961	2.410319	0.100698
6	-2.466448	-0.088604	-0.811485
6	-3.301193	-1.253762	-1.004267
6	-4.672474	-1.076797	-1.081965
1	-5.305825	-1.960061	-1.213099
6	-5.322791	0.178020	-1.013272
6	-4.523307	1.289201	-0.869441
1	-4.978751	2.287486	-0.822537
6	-3.117873	1.186613	-0.757629
6	-2.384930	2.400775	-0.569346
1	-2.989692	3.318069	-0.661714
6	2.668930	2.262410	-0.011210
1	3.325313	3.120051	0.205267
6	3.364326	1.060035	-0.362850
6	4.777005	1.114193	-0.386340
1	5.265121	2.073869	-0.169483
6	5.543524	0.003738	-0.659044
6	4.854014	-1.201903	-0.927077
1	5.460656	-2.086464	-1.146539
6	3.475096	-1.330186	-0.929767
6	2.672838	-0.165342	-0.632005
6	-2.669136	-2.642287	-1.127081
6	-1.930847	-2.997596	0.166846
1	-2.641807	-3.054499	1.010678
1	-1.163630	-2.247749	0.411957
1	-1.440213	-3.983735	0.073616
6	-1.695023	-2.658993	-2.309274
1	-0.898690	-1.913386	-2.174868
1	-2.225630	-2.441529	-3.253005
1	-1.228528	-3.655834	-2.407049
6	-3.709099	-3.732835	-1.373567
1	-4.273484	-3.567803	-2.307261
1	-4.432851	-3.817183	-0.544936
1	-3.200279	-4.707344	-1.463905
6	2.797025	-2.663172	-1.251617
6	3.806173	-3.777445	-1.519984
1	4.452576	-3.974161	-0.647469
1	4.454137	-3.556760	-2.385250
1	3.265355	-4.711943	-1.745814
6	1.922624	-3.114721	-0.075527
1	1.164515	-2.359007	0.179205
1	2.545804	-3.299882	0.818591
1	1.408249	-4.060878	-0.323071
6	1.946726	-2.498723	-2.515549
1	2.584352	-2.231239	-3.376269
1	1.189610	-1.713002	-2.383330
1	1.428683	-3.443572	-2.758869
6	0.806827	3.679022	0.601141
6	-0.513528	3.863993	-0.208934
6	1.738591	4.874071	0.436140
1	1.200545	5.810143	0.649422
1	2.573852	4.827311	1.152418
1	2.162097	4.949085	-0.576861
6	0.531514	3.493393	2.095172
1	1.458647	3.167335	2.595816
1	0.214232	4.438208	2.563484
1	-0.235768	2.728710	2.284806

6	-1.440559	4.876103	0.456976
1	-1.891924	4.476395	1.378721
1	-0.894792	5.797742	0.710725
1	-2.256965	5.178840	-0.216371
6	-0.217051	4.312067	-1.639959
1	-1.141137	4.274096	-2.238543
1	0.155879	5.347596	-1.670620
1	0.524930	3.654055	-2.120183
6	7.054350	0.055323	-0.672844
6	7.624307	-0.283692	-2.046191
6	7.662733	-0.838717	0.402674
1	7.337246	1.100622	-0.440372
1	7.212189	0.375043	-2.827742
1	8.722717	-0.183084	-2.058127
1	7.388395	-1.324288	-2.330434
1	7.281895	-0.580694	1.404281
1	7.423873	-1.901229	0.219855
1	8.762054	-0.749575	0.421357
6	-6.828793	0.278869	-1.094539
6	-7.502769	-0.405978	0.090100
6	-7.371284	-0.259945	-2.413878
1	-7.076567	1.357216	-1.044580
1	-7.139493	-0.001046	1.048931
1	-8.597887	-0.277505	0.057166
1	-7.299814	-1.491478	0.089743
1	-6.907690	0.244631	-3.277072
1	-7.174168	-1.341578	-2.515725
1	-8.463288	-0.120137	-2.482064
6	-1.509011	-0.383921	2.722740
6	-1.793523	-1.633658	3.258447
6	-0.765401	-2.548418	3.501794
6	0.541500	-2.128357	3.247026
6	0.782761	-0.858251	2.731356
1	-2.834148	-1.898238	3.475015
1	1.388998	-2.788493	3.460009
6	-1.061718	-3.927581	3.986429
1	-1.304656	-4.582479	3.131164
1	-0.200697	-4.373819	4.504997
1	-1.932577	-3.942804	4.658919
6	2.162030	-0.329218	2.549590
1	2.160266	0.503660	1.837228
1	2.544600	0.050294	3.512394
1	2.858144	-1.104980	2.195143
6	-2.569670	0.636090	2.492522
1	-2.266400	1.328812	1.696977
1	-3.530502	0.172415	2.220763
1	-2.726296	1.230666	3.409118
7	-0.239298	-0.031343	2.442284
1	-0.063936	0.718225	1.275548

Structure S118. 1

6	1.307803	0.572633	-0.062735
6	0.271933	1.457538	0.246031
6	-1.038407	0.995102	0.371716
6	-1.352790	-0.353236	0.200253
6	-0.308731	-1.233808	-0.103148
6	1.003457	-0.793822	-0.236535
1	0.477894	2.521681	0.383033
1	-1.836609	1.708142	0.606107
1	-0.499812	-2.302509	-0.251178
8	1.975795	-1.685802	-0.572715
8	2.600339	0.927035	-0.226882
6	2.884678	-2.006777	0.457428
1	2.357618	-2.422128	1.336375
1	3.572239	-2.769792	0.067233
1	3.471782	-1.129156	0.776532
6	2.950638	2.277350	-0.075311
1	2.726665	2.648209	0.941097
1	4.032054	2.351346	-0.246990
1	2.430552	2.919784	-0.808325
6	-2.773181	-0.840729	0.350281
1	-2.805522	-1.916465	0.099415
1	-3.094303	-0.759215	1.405917
6	-3.738457	-0.091488	-0.513853
6	-4.781468	0.606749	-0.064672
1	-3.535466	-0.124553	-1.594169
1	-5.453374	1.141792	-0.742665
1	-5.005638	0.665927	1.007675

Structure S119. ^{3}TS9

27	1.428242	1.235976	-0.029690
8	2.193768	-0.484411	-0.321431
8	-0.133349	1.013394	1.110036
7	3.268064	2.118063	-0.127283
7	0.873232	3.141577	-0.356599
6	3.401085	-0.893596	-0.109362

6	3.682651	-2.306376	-0.094341	1	-1.375154	-0.226863	4.623235
6	4.982120	-2.716311	0.161023	6	1.945953	4.009274	-0.875699
1	5.196416	-3.789459	0.186935	6	3.241001	3.590702	-0.085406
6	6.062905	-1.836384	0.388906	6	1.617842	5.485952	-0.686069
6	5.791975	-0.486296	0.345317	1	2.496704	6.115255	-0.891698
1	6.603744	0.235685	0.505016	1	0.834863	5.809855	-1.389366
6	4.491645	0.011815	0.102521	1	1.267233	5.704449	0.334407
6	4.350863	1.446981	0.068360	6	2.108750	3.720526	-2.367836
1	5.302771	1.988072	0.232037	1	1.141235	3.857361	-2.878644
6	-0.372531	3.466885	-0.406846	1	2.828791	4.413670	-2.829862
1	-0.664770	4.436258	-0.852576	1	2.451525	2.688944	-2.547043
6	-1.481061	2.692391	0.096750	6	4.497076	4.202715	-0.695490
6	-2.775791	3.178324	-0.179758	1	4.741517	3.754500	-1.671009
1	-2.876380	4.059102	-0.828694	1	4.385778	5.288965	-0.831156
6	-3.905986	2.577457	0.336703	1	5.365649	4.062739	-0.033302
6	-3.707643	1.504757	1.230894	6	3.132681	4.007702	1.381304
1	-4.596748	1.067478	1.693157	1	3.974340	3.580761	1.950144
6	-2.464972	0.987237	1.573091	1	3.175891	5.102227	1.493771
6	-1.302319	1.534472	0.925912	1	2.195964	3.643388	1.833552
6	2.565734	-3.314247	-0.387297	6	-5.284152	3.047493	-0.074582
6	2.080217	-3.113825	-1.828321	6	-6.326410	2.937016	1.028393
1	2.890259	-3.330105	-2.545920	6	-5.748732	2.305137	-1.325771
1	1.740719	-2.080692	-1.992903	1	-5.184315	4.118790	-0.339307
1	1.240321	-3.796818	-2.051922	1	-5.992996	3.418597	1.962168
6	1.395580	-3.140108	0.589235	1	-7.272109	3.410257	0.718244
1	0.940154	-2.144421	0.500494	1	-6.559911	1.882644	1.258756
1	1.731233	-3.275672	1.632442	1	-5.023282	2.415211	-2.149701
1	0.616482	-3.898079	0.388460	1	-5.856910	1.223937	-1.123822
6	3.048568	-4.757820	-0.262992	1	-6.724642	2.680981	-1.677725
1	3.401284	-4.990874	0.756258	6	7.452682	-2.365393	0.661896
1	3.861561	-4.991882	-0.970701	6	7.994328	-3.175454	-0.511106
1	2.213607	-5.442362	-0.487822	6	7.506954	-3.175081	1.953136
6	-2.317036	-0.082514	2.663446	1	8.107525	-1.481760	0.791216
6	-3.667923	-0.509004	3.234551	1	7.984006	-2.590365	-1.445002
1	-4.304625	-0.987981	2.469903	1	9.030950	-3.502127	-0.323726
1	-4.227580	0.333253	3.675537	1	7.391302	-4.084648	-0.681328
1	-3.507759	-1.250788	4.034583	1	7.146729	-2.587819	2.813326
6	-1.631829	-1.352315	2.148452	1	6.879219	-4.080818	1.882715
1	-0.631208	-1.137511	1.749927	1	8.535823	-3.506650	2.172132
1	-2.233967	-1.831919	1.356944	1	0.722061	1.089458	-1.378103
1	-1.525875	-2.079980	2.972311	6	-4.882011	-3.298799	-0.750696
6	-1.494078	0.513688	3.812853	6	-3.658406	-3.959896	-0.863971
1	-1.999516	1.399340	4.235575	6	-2.490179	-3.240039	-1.120978
1	-0.492444	0.814843	3.473007	6	-2.500443	-1.852344	-1.251296

6	-3.731163	-1.194317	-1.130193
6	-4.908201	-1.894856	-0.895732
1	-3.605090	-5.046769	-0.768815
1	-1.541288	-3.780982	-1.210604
1	-3.807829	-0.103185	-1.199494
8	-6.094347	-1.223037	-0.859562
8	-6.069523	-3.903791	-0.533017
6	-6.692965	-1.102180	0.410502
1	-6.039265	-0.536485	1.101743
1	-7.632464	-0.545314	0.283768
1	-6.916322	-2.086066	0.855991
6	-6.093472	-5.298661	-0.382535
1	-5.485305	-5.629057	0.478706
1	-7.137975	-5.586361	-0.207454
1	-5.731289	-5.814562	-1.289809
6	-1.204502	-1.112137	-1.419771
1	-0.841260	-0.797214	-0.413170
1	-0.418787	-1.799904	-1.778250
6	-1.207131	0.127679	-2.238999
6	-0.086842	0.591183	-2.839474
1	-2.101708	0.766402	-2.217373
1	-0.085572	1.539024	-3.387419
1	0.785720	-0.060622	-2.974493

Structure S120. 3

6	-1.431334	-0.557436	-0.066505
6	-0.425775	-1.484915	0.214128
6	0.906389	-1.077444	0.303971
6	1.274689	0.255258	0.120506
6	0.259058	1.178565	-0.154142
6	-1.073350	0.794939	-0.250184
1	-0.671451	-2.539702	0.357987
1	1.682231	-1.821605	0.518398
1	0.491270	2.237708	-0.312936
8	-2.016200	1.727121	-0.562323
8	-2.742525	-0.856269	-0.195917
6	-2.878356	2.090087	0.493423
1	-2.307403	2.484095	1.354680
1	-3.543755	2.881476	0.121611
1	-3.493136	1.239524	0.833384
6	-3.144939	-2.190633	-0.035930
1	-2.911043	-2.572254	0.974336
1	-4.232543	-2.219426	-0.180172
1	-2.670699	-2.853489	-0.781903
6	2.713092	0.685966	0.243689
1	2.813952	1.711368	-0.177115
1	2.975596	0.809779	1.315676
6	3.687728	-0.244736	-0.385539
1	3.393078	-0.721575	-1.330574
6	5.113304	-0.258115	0.015076
1	5.635197	-1.165859	-0.326832
1	5.678286	0.602098	-0.403517
1	5.227177	-0.188167	1.111945

Structure S121. Co^{II}(salen)

27	-0.654199	0.000204	-0.000030
8	0.685129	-1.303075	0.066638
8	0.686010	1.302574	-0.066680
7	-2.024603	-1.259186	-0.259620
7	-2.023751	1.260522	0.259602
6	0.605711	-2.585372	-0.015836
6	1.800169	-3.384361	0.105059
6	1.677389	-4.759928	-0.000714
1	2.572675	-5.381410	0.082148
6	0.449627	-5.418712	-0.211994
6	-0.695028	-4.670263	-0.316962
1	-1.667705	-5.149906	-0.476026
6	-0.642902	-3.259968	-0.221595
6	-1.872963	-2.544226	-0.330668
1	-2.764752	-3.170456	-0.495749
6	-3.318844	-0.607460	-0.459817
1	-3.321990	-0.212268	-1.500266
6	-3.318444	0.609676	0.459759
1	-3.321894	0.214482	1.500206
6	-4.561144	1.457198	0.264315
1	-4.546590	1.890004	-0.755673
1	-4.571528	2.304053	0.970764
6	-5.810411	0.608191	0.458240
1	-5.856336	0.269736	1.511369
1	-6.712286	1.220336	0.293140
6	-5.810807	-0.604278	-0.458372
1	-5.856469	-0.265788	-1.511501
1	-6.713104	-1.215806	-0.293301
6	-4.562127	-1.454137	-0.264412
1	-4.573069	-2.300979	-0.970866
1	-4.547900	-1.886960	0.755574

6	-1.871225	2.545453	0.330722
1	-2.762576	3.172294	0.495855
6	-0.640670	3.260352	0.221714
6	-0.691833	4.670667	0.317246
1	-1.664183	5.150952	0.476372
6	0.453332	5.418349	0.212357
6	1.680642	4.758747	0.000995
1	2.576355	5.379620	-0.081826
6	1.802480	3.383111	-0.104943
6	0.607475	2.584922	0.015863
6	3.152180	-2.709809	0.350596
6	3.121134	-1.969515	1.692421
1	2.947950	-2.674429	2.524536
1	2.329241	-1.207642	1.717030
1	4.086409	-1.465297	1.876993
6	3.472314	-1.730642	-0.784884
1	2.745180	-0.907200	-0.829154
1	3.471743	-2.247839	-1.760603
1	4.478540	-1.297988	-0.641115
6	4.290719	-3.724620	0.412521
1	4.407115	-4.283095	-0.532417
1	4.163423	-4.454751	1.230268
1	5.242031	-3.197727	0.596974
6	3.154041	2.707731	-0.350677
6	4.293190	3.721865	-0.412378
1	4.409820	4.280175	0.532630
1	4.166413	4.452157	-1.230062
1	5.244205	3.194424	-0.596796
6	3.473629	1.728062	0.784532
1	2.746163	0.904893	0.828456
1	3.473169	2.244946	1.760418
1	4.479698	1.295050	0.640735
6	3.122501	1.967844	-1.692713
1	2.949998	2.673142	-2.524645
1	2.329959	1.206660	-1.717610
1	4.087366	1.462861	-1.877334
1	0.424661	6.508512	0.287935
1	0.420210	-6.508864	-0.287451

Structure S122. 11

6	3.372760	-1.344521	-0.472791
6	3.980011	-0.096090	-0.368276
6	2.019273	-1.464872	-0.184790
6	1.257950	-0.347526	0.173513
6	1.864822	0.918078	0.302291
6	3.233402	1.009869	0.026619
1	3.953024	-2.223147	-0.767940
1	5.046913	0.017490	-0.582688
1	1.524985	-2.439442	-0.239088
6	-0.171864	-0.631768	0.505217
6	1.122044	2.141011	0.745260
1	3.724465	1.983021	0.135362
8	-0.496333	-1.558507	1.220367
7	-1.120246	0.235979	-0.015433
9	-0.667369	0.842453	-1.177487
6	-2.577199	-0.029086	-0.116638
1	0.392904	1.922510	1.540966
1	0.556413	2.594134	-0.085458
1	1.819036	2.902305	1.126342
6	-3.119874	-0.251672	1.290027
6	-2.828597	-1.231500	-1.016290
6	-3.228629	1.222082	-0.694290
1	-2.733392	-1.171278	1.745801
1	-4.218653	-0.319535	1.237928
1	-2.863415	0.597062	1.945384
1	-2.964555	2.115156	-0.104425
1	-4.322882	1.102377	-0.660421
1	-2.943112	1.400320	-1.741009
1	-2.404846	-2.150672	-0.582677
1	-2.381513	-1.073287	-2.011582
1	-3.911264	-1.386912	-1.153141

Structure S123. ^{2}INT5

9	0.753202	-0.032000	1.174192
7	0.939194	-0.377642	2.513158
6	-0.278923	-1.043642	3.051504
6	-0.242720	-0.941145	4.571389
1	0.565386	-1.536722	5.013683
1	-0.120840	0.107655	4.887629
1	-1.205092	-1.303521	4.968010
6	-0.324637	-2.491729	2.583765
1	0.505996	-3.079344	3.004296
1	-1.272472	-2.963435	2.891323
1	-0.273428	-2.535151	1.484351
6	-1.488444	-0.274404	2.540014
1	-2.400823	-0.737403	2.949371

1	-1.456638	0.777646	2.869556
1	-1.565964	-0.289596	1.442933
6	2.241247	-0.796272	2.743288
8	2.503098	-1.512013	3.689448
6	3.301103	-0.312922	1.805457
6	3.464139	1.028867	1.405263
6	4.230278	-1.286679	1.419684
6	4.558265	1.328144	0.583299
6	5.300733	-0.966903	0.593702
6	5.459538	0.351243	0.170461
1	4.706013	2.369371	0.275580
1	6.011721	-1.740683	0.288803
1	6.301857	0.626072	-0.471833
27	-0.434645	-0.271113	-1.151927
8	-2.278158	-0.338720	-0.797188
8	-0.528478	1.592283	-0.964906
7	-0.237428	-2.140355	-1.076912
7	1.321677	-0.231180	-1.839055
6	-3.040345	-1.348244	-0.553722
6	-4.431987	-1.129912	-0.251021
6	-5.218152	-2.235988	0.030414
1	-6.274465	-2.090078	0.270873
6	-4.731222	-3.557826	0.026146
6	-3.410207	-3.778237	-0.274522
1	-2.999167	-4.794302	-0.290101
6	-2.548866	-2.695311	-0.563984
6	-1.178566	-2.997844	-0.839825
1	-0.921100	-4.069502	-0.807392
6	1.169630	-2.516497	-1.202698
1	1.655081	-2.251188	-0.234230
6	1.763757	-1.566018	-2.239534
1	1.260454	-1.802269	-3.203904
6	3.255692	-1.773040	-2.403995
1	3.759939	-1.466320	-1.467424
1	3.651754	-1.128034	-3.206567
6	3.563830	-3.231777	-2.710012
1	3.140136	-3.496865	-3.698192
1	4.653964	-3.374599	-2.795365
6	2.985177	-4.157379	-1.652320
1	3.470359	-3.946944	-0.679194
1	3.212415	-5.209984	-1.888291
6	1.481180	-3.967047	-1.509506
1	1.092685	-4.623376	-0.712026
1	0.968012	-4.260922	-2.446755
6	2.056820	0.824168	-1.980433
1	3.072066	0.710259	-2.395081
6	1.687478	2.162364	-1.637296
6	2.657338	3.175468	-1.814343
1	3.627183	2.901663	-2.246669
6	2.392284	4.471408	-1.446212
6	1.142791	4.772411	-0.867029
1	0.967407	5.806208	-0.557701
6	0.146820	3.830831	-0.669145
6	0.396078	2.474792	-1.096179
6	-5.001542	0.291652	-0.248744
6	-4.845072	0.916586	-1.639784
1	-5.396986	0.331707	-2.396618
1	-3.790731	0.969222	-1.946665
1	-5.254486	1.942569	-1.647477
6	-4.280522	1.154242	0.793760
1	-3.206916	1.248704	0.573766
1	-4.397410	0.728069	1.806321
1	-4.717693	2.168702	0.811474
6	-6.488407	0.306053	0.096344
1	-6.689087	-0.094396	1.105139
1	-7.095699	-0.264148	-0.627593
1	-6.858767	1.344898	0.081073
6	-1.168189	4.172133	0.035378
6	-1.245205	5.648231	0.414377
1	-1.215998	6.310214	-0.468568
1	-0.434340	5.951818	1.098609
1	-2.197573	5.844878	0.935232
6	-2.367505	3.867458	-0.870205
1	-2.435547	2.797773	-1.113510
1	-2.296270	4.433235	-1.815917
1	-3.306449	4.170428	-0.372855
6	-1.258289	3.355027	1.331491
1	-0.452972	3.643814	2.031177
1	-1.171360	2.275952	1.132946
1	-2.221401	3.536196	1.842224
1	-5.402674	-4.388609	0.258245
1	3.135199	5.261200	-1.585659
6	2.546843	2.128732	1.836706
1	1.649670	2.164848	1.196452
1	2.190560	1.999505	2.870558
1	3.042750	3.107861	1.761342
1	4.099196	-2.309155	1.788154

Structure S124. ^{2}TS16

9	0.352246	-0.326901	1.036592
7	0.623102	-0.531681	2.722565
6	-0.572932	-1.232478	3.184947
6	-0.517696	-1.212499	4.716873
1	0.331412	-1.792603	5.102605
1	-0.441989	-0.178782	5.091771
1	-1.452150	-1.648691	5.108105
6	-0.657608	-2.657182	2.652300
1	0.128944	-3.298885	3.075840
1	-1.638921	-3.098861	2.893871
1	-0.555391	-2.649645	1.555626
6	-1.785638	-0.423929	2.737948
1	-2.697780	-0.847664	3.189742
1	-1.695179	0.629430	3.054792
1	-1.895653	-0.438473	1.644274
6	1.895520	-1.050141	2.792977
8	2.177396	-1.949737	3.571425
6	2.951251	-0.413243	1.945972
6	3.017218	0.960433	1.624555
6	3.980320	-1.276740	1.547952
6	4.126027	1.398046	0.887626
6	5.062457	-0.821015	0.805686
6	5.131648	0.530160	0.472585
1	4.197712	2.464541	0.646114
1	5.851122	-1.514289	0.496998
1	5.980257	0.915794	-0.101512
27	-0.205868	-0.205133	-0.985630
8	-2.057269	-0.348047	-0.834377
8	-0.414762	1.643722	-0.842088
7	0.032763	-2.067802	-1.108199
7	1.490640	-0.058980	-1.811588
6	-2.812906	-1.393684	-0.724710
6	-4.226698	-1.222998	-0.535140
6	-4.999390	-2.363807	-0.370332
1	-6.075106	-2.258253	-0.208625
6	-4.474365	-3.668347	-0.402481
6	-3.128973	-3.839777	-0.621389
1	-2.688759	-4.842167	-0.666216
6	-2.284644	-2.720475	-0.784040
6	-0.889916	-2.963951	-1.002440
1	-0.601492	-4.025913	-1.066478
6	1.450247	-2.378061	-1.269394
1	1.934888	-2.134235	-0.297404
6	1.982549	-1.358474	-2.275733
1	1.474555	-1.574261	-3.241889
6	3.479701	-1.492700	-2.469538
1	3.985288	-1.212372	-1.525149
1	3.836174	-0.796222	-3.247183
6	3.839690	-2.922304	-2.849984
1	3.407534	-3.157444	-3.842086
1	4.932555	-3.015749	-2.961579
6	3.319267	-3.919603	-1.827708
1	3.812917	-3.737004	-0.853655
1	3.583391	-4.949552	-2.118376
6	1.811687	-3.798320	-1.652273
1	1.460910	-4.506585	-0.882515
1	1.297779	-4.065754	-2.597063
6	2.172913	1.040036	-1.922563
1	3.181287	0.987032	-2.365001
6	1.757201	2.341304	-1.521622
6	2.677614	3.406846	-1.669385
1	3.662142	3.192508	-2.101561
6	2.343335	4.674638	-1.268908
6	1.069998	4.902578	-0.701186
1	0.840210	5.920964	-0.376984
6	0.120503	3.911429	-0.532837
6	0.454985	2.576985	-0.968193
6	-4.840512	0.180381	-0.534353
6	-4.571314	0.858413	-1.883101
1	-5.028079	0.284960	-2.708733
1	-3.494228	0.953472	-2.084659
1	-5.011483	1.871347	-1.896536
6	-4.255681	1.028763	0.600743
1	-3.169303	1.165319	0.494235
1	-4.456324	0.566557	1.583398
1	-4.728128	2.027249	0.603551
6	-6.353607	0.135182	-0.337841
1	-6.638916	-0.308310	0.631726
1	-6.866489	-0.426115	-1.137860
1	-6.756004	1.161929	-0.354949
6	-1.236542	4.175121	0.124281
6	-1.388921	5.637461	0.533340
1	-1.343830	6.322720	-0.330907
1	-0.623028	5.952552	1.262856
1	-2.371565	5.785297	1.011988
6	-2.369671	3.849206	-0.856013

1	-2.384149	2.783363	-1.125361
1	-2.267562	4.439871	-1.783427
1	-3.346348	4.103199	-0.406599
6	-1.375430	3.324782	1.395515
1	-0.617378	3.614513	2.144984
1	-1.264291	2.248361	1.189918
1	-2.368260	3.483166	1.853924
1	-5.135966	-4.527221	-0.263776
1	3.047279	5.503688	-1.377954
6	1.990068	1.964257	2.041256
1	1.063787	1.839103	1.458147
1	1.696787	1.850722	3.096478
1	2.361294	2.989607	1.888664
1	3.914740	-2.327508	1.847636

Structure S125. ^{4}INT6

9	0.271594	0.074474	0.683053
7	0.760507	-0.759579	3.372070
6	-0.662481	-0.990788	3.552861
6	-0.789065	-1.716025	4.895422
1	-0.282308	-2.694310	4.855490
1	-0.335561	-1.125476	5.707589
1	-1.852954	-1.887000	5.132499
6	-1.365944	-1.778756	2.453736
1	-0.998945	-2.813590	2.390660
1	-2.451404	-1.804102	2.657239
1	-1.204971	-1.286134	1.485442
6	-1.308868	0.394215	3.658291
1	-2.360649	0.283181	3.970033
1	-0.793735	1.026836	4.399453
1	-1.291462	0.900148	2.679553
6	1.569663	-1.340858	2.441623
8	1.440617	-2.530985	2.159881
6	2.758565	-0.560248	1.963519
6	2.880509	0.846722	2.006087
6	3.796297	-1.327795	1.421977
6	4.035044	1.416694	1.453519
6	4.944833	-0.742934	0.901187
6	5.055931	0.645395	0.905375
1	4.129149	2.508370	1.462117
1	5.747257	-1.367872	0.495440
1	5.945052	1.132592	0.492131
27	-0.179419	-0.168679	-1.102206
8	-2.030130	-0.367017	-1.170064
8	-0.419234	1.681612	-1.300013
7	0.106180	-2.046466	-1.052847
7	1.539341	-0.101907	-1.960516
6	-2.761075	-1.399146	-0.868317
6	-4.166040	-1.224349	-0.644745
6	-4.917081	-2.352037	-0.336740
1	-5.988908	-2.240540	-0.155404
6	-4.373160	-3.642812	-0.230561
6	-3.023978	-3.813904	-0.429128
1	-2.560321	-4.802062	-0.337803
6	-2.206918	-2.707563	-0.738256
6	-0.803339	-2.941977	-0.885650
1	-0.490254	-3.996758	-0.834048
6	1.529611	-2.339767	-1.184644
1	2.003477	-1.984265	-0.246176
6	2.029184	-1.434413	-2.310998
1	1.499929	-1.748986	-3.236793
6	3.521763	-1.573614	-2.526505
1	4.047817	-1.199568	-1.626906
1	3.849346	-0.952884	-3.378154
6	3.880986	-3.034074	-2.763321
1	3.414066	-3.378257	-3.706598
1	4.969573	-3.133466	-2.905593
6	3.408383	-3.912474	-1.615989
1	3.931877	-3.614207	-0.687630
1	3.676651	-4.966302	-1.795703
6	1.905863	-3.790292	-1.400971
1	1.596555	-4.390863	-0.528322
1	1.366010	-4.185493	-2.284997
6	2.275946	0.962981	-1.958785
1	3.320139	0.876231	-2.301097
6	1.881584	2.261547	-1.525643
6	2.877595	3.262053	-1.456115
1	3.901242	3.006058	-1.752021
6	2.564188	4.520625	-1.008468
6	1.242777	4.790519	-0.601136
1	1.030107	5.791089	-0.215785
6	0.220163	3.856220	-0.645303
6	0.525946	2.547896	-1.158976
6	-4.784601	0.174511	-0.674151
6	-4.581300	0.832884	-2.042761
1	-5.078350	0.249174	-2.837434
1	-3.516489	0.927084	-2.299075

1	-5.024193	1.844666	-2.046555
6	-4.135154	1.025805	0.423087
1	-3.060616	1.175077	0.241400
1	-4.254756	0.550099	1.413155
1	-4.616970	2.018666	0.470538
6	-6.286029	0.136842	-0.401892
1	-6.523251	-0.266865	0.597374
1	-6.835656	-0.455830	-1.153495
1	-6.690159	1.162239	-0.439987
6	-1.171143	4.145285	-0.079601
6	-1.299701	5.585969	0.406566
1	-1.176973	6.317122	-0.411678
1	-0.574720	5.830590	1.201246
1	-2.305391	5.739558	0.832739
6	-2.264057	3.916163	-1.129897
1	-2.334947	2.860719	-1.428141
1	-2.072686	4.518268	-2.035722
1	-3.244150	4.229452	-0.728569
6	-1.383914	3.222148	1.127137
1	-0.671300	3.471939	1.933452
1	-1.233811	2.164112	0.858370
1	-2.403219	3.339060	1.537069
1	-5.017767	-4.489859	0.016998
1	3.325143	5.302782	-0.947573
6	1.838927	1.747677	2.583217
1	0.873828	1.576857	2.081830
1	1.691303	1.554259	3.659046
1	2.121988	2.805080	2.457879
1	3.674633	-2.415707	1.424933

Structure S126. Co^{III}(salen)-F

27	-0.584271	-0.041840	0.176199
8	0.606150	1.337667	-0.223904
8	0.821628	-1.213418	-0.201745
7	-2.036889	1.160051	0.352207
7	-1.898180	-1.254549	-0.561684
6	0.478728	2.619350	-0.089773
6	1.634192	3.456039	-0.244427
6	1.458924	4.826963	-0.117116
1	2.324946	5.484446	-0.226055
6	0.217054	5.430292	0.151443
6	-0.891340	4.633734	0.307589
1	-1.873669	5.068722	0.522386
6	-0.778359	3.231145	0.200320
6	-1.964151	2.446522	0.355620
1	-2.897327	3.018780	0.482044
6	-3.276155	0.400023	0.460561
1	-3.208317	-0.160952	1.415990
6	-3.220372	-0.637790	-0.666018
1	-3.251704	-0.069385	-1.621146
6	-4.412937	-1.573373	-0.609942
1	-4.352155	-2.171011	0.320795
1	-4.390966	-2.285455	-1.452282
6	-5.711335	-0.778042	-0.632431
1	-5.801922	-0.257504	-1.605291
1	-6.571499	-1.464333	-0.570320
6	-5.758005	0.244571	0.491520
1	-5.750487	-0.280424	1.465621
1	-6.698385	0.818480	0.457048
6	-4.567663	1.191447	0.427302
1	-4.601120	1.908817	1.265003
1	-4.611043	1.782570	-0.509278
6	-1.684905	-2.524832	-0.698472
1	-2.535409	-3.169990	-0.973892
6	-0.448491	-3.205919	-0.509095
6	-0.447468	-4.616703	-0.617169
1	-1.388193	-5.127042	-0.852134
6	0.708818	-5.326673	-0.419238
6	1.890963	-4.632776	-0.089175
1	2.789770	-5.228172	0.091773
6	1.961641	-3.255064	0.030344
6	0.763036	-2.497634	-0.216450
6	3.005343	2.830693	-0.513765
6	2.986610	2.065605	-1.841987
1	2.757996	2.743772	-2.682964
1	2.241860	1.257233	-1.838028
1	3.976730	1.616177	-2.036270
6	3.380181	1.885533	0.634886
1	2.679071	1.042346	0.723631
1	3.394354	2.424492	1.598307
1	4.391334	1.472225	0.471245
6	4.097850	3.892329	-0.612356
1	4.206480	4.472817	0.319935
1	3.923239	4.600394	-1.440834
1	5.067689	3.403930	-0.804830
6	3.243273	-2.530765	0.446363
6	4.389578	-3.509078	0.689767

1	4.670130	-4.065215	-0.221784
1	4.157916	-4.239868	1.483424
1	5.283586	-2.951727	1.016642
6	3.694999	-1.561831	-0.652839
1	2.958732	-0.764594	-0.826837
1	3.855867	-2.096845	-1.605588
1	4.653630	-1.090197	-0.371729
6	2.993888	-1.777299	1.760285
1	2.792797	-2.488540	2.580287
1	2.136400	-1.090708	1.701048
1	3.887377	-1.191230	2.040514
9	-0.627534	-0.509356	1.944584
1	0.145425	6.517435	0.237865
1	0.719868	-6.416879	-0.495875

Structure S127. 12

6	3.479962	-1.054772	0.153478
6	3.853079	0.287297	0.170712
6	2.140855	-1.380459	-0.001343
6	1.161439	-0.388643	-0.145964
6	1.529486	0.975039	-0.120094
6	2.887132	1.279033	0.037882
1	4.231094	-1.842554	0.258873
1	4.904116	0.566713	0.291383
1	1.812464	-2.423216	-0.019086
6	-0.236562	-0.890464	-0.299207
6	0.551302	2.101947	-0.238907
1	3.188620	2.331718	0.058715
8	-0.510156	-2.081857	-0.228728
7	-1.212255	0.015132	-0.633390
6	-2.468392	0.122515	0.091971
1	-0.204422	2.074631	0.564838
1	-0.001530	2.071774	-1.192277
1	1.065521	3.072629	-0.170348
6	-2.301094	-0.100423	1.591315
6	-3.406663	-0.934586	-0.508885
6	-3.043401	1.507532	-0.186018
1	-1.938309	-1.116392	1.811481
1	-3.264482	0.034388	2.109773
1	-1.585361	0.621953	2.021287
1	-2.422885	2.301496	0.260552
1	-4.056147	1.591875	0.240933
1	-3.106636	1.692418	-1.270497
1	-3.021383	-1.948420	-0.332666
1	-3.513967	-0.786648	-1.595322
1	-4.402504	-0.837538	-0.043731

Structure S128. $[Co^{IV}(salen)\text{-}F]^{+}$

27	-0.587444	-0.110994	0.203734
8	0.375582	1.393303	-0.198515
8	1.008789	-1.090678	-0.131210
7	-2.186026	0.827337	0.395228
7	-1.706680	-1.518067	-0.602430
6	0.077344	2.650956	-0.039715
6	1.097331	3.636406	-0.226306
6	0.731900	4.965511	-0.056204
1	1.488741	5.742526	-0.184899
6	-0.569743	5.378202	0.278516
6	-1.552778	4.434693	0.453156
1	-2.576084	4.725222	0.711295
6	-1.245098	3.065662	0.303836
6	-2.296638	2.114519	0.447091
1	-3.303611	2.532527	0.598196
6	-3.309194	-0.108562	0.454531
1	-3.184787	-0.687936	1.392447
6	-3.099716	-1.085306	-0.711838
1	-3.168117	-0.484372	-1.643418
6	-4.154042	-2.170997	-0.728398
1	-4.045270	-2.789381	0.184179
1	-4.009103	-2.837580	-1.595681
6	-5.543455	-1.548251	-0.764188
1	-5.673569	-1.002754	-1.718162
1	-6.307321	-2.341824	-0.757359
6	-5.750005	-0.592863	0.399480
1	-5.701457	-1.153783	1.351801
1	-6.754016	-0.141984	0.358376
6	-4.694916	0.504576	0.410538
1	-4.843551	1.172680	1.275061
1	-4.790183	1.123455	-0.503524
6	-1.329817	-2.741836	-0.644039
1	-2.068869	-3.530992	-0.858849
6	0.017964	-3.226775	-0.425225
6	0.233283	-4.589489	-0.506834
1	-0.605811	-5.256073	-0.726990
6	1.518122	-5.121717	-0.315503
6	2.604206	-4.286719	-0.037877

1	3.580344	-4.749974	0.115340
6	2.475756	-2.907108	0.053665
6	1.143312	-2.339852	-0.160216
6	2.527544	3.222809	-0.578913
6	2.544597	2.463022	-1.910311
1	2.161384	3.095702	-2.729587
1	1.939369	1.545163	-1.875121
1	3.579702	2.179384	-2.169121
6	3.102801	2.349042	0.542432
1	2.540053	1.412644	0.674266
1	3.099125	2.890916	1.503788
1	4.151150	2.087893	0.314935
6	3.441136	4.435577	-0.731710
1	3.522090	5.021139	0.199714
1	3.112274	5.112301	-1.538734
1	4.458339	4.097401	-0.988912
6	3.638573	-1.995269	0.404410
6	4.927541	-2.787795	0.600576
1	5.241817	-3.312708	-0.317625
1	4.851891	-3.525338	1.417201
1	5.739697	-2.094166	0.869887
6	3.878547	-0.989835	-0.733253
1	3.053445	-0.274332	-0.851460
1	4.034553	-1.508579	-1.694800
1	4.795003	-0.414451	-0.519235
6	3.330697	-1.267168	1.724039
1	3.263842	-1.984874	2.558855
1	2.390709	-0.696880	1.697011
1	4.150515	-0.565719	1.953279
9	-0.604475	-0.775876	1.895481
1	-0.788918	6.441960	0.396030
1	1.670368	-6.201983	-0.380549

Structure S129. 15

6	3.413034	-1.251786	-0.177306
6	3.965253	0.026129	-0.162536
6	2.035124	-1.394893	-0.060940
6	1.167852	-0.300658	0.051738
6	1.728233	0.999756	0.072671
6	3.121914	1.126049	-0.031435
1	4.054698	-2.134686	-0.274565
1	5.048026	0.170824	-0.245985
1	1.559501	-2.380106	-0.042535
6	-0.318901	-0.649960	0.149676
6	0.921466	2.253903	0.216084
1	3.556767	2.133284	-0.006572
8	-0.586957	-1.843957	0.438590
7	-1.132356	0.350388	-0.121609
6	-2.564052	0.102602	-0.096515
1	0.255703	2.208101	1.091812
1	0.232479	2.385914	-0.631588
1	1.580516	3.134830	0.306075
6	-3.043165	-0.338162	1.290192
6	-2.982157	-0.939858	-1.138712
6	-3.238524	1.429635	-0.441440
1	-2.561693	-1.288354	1.566964
1	-4.142456	-0.463787	1.325722
1	-2.762340	0.420516	2.042971
1	-2.948877	2.205867	0.289537
1	-4.342372	1.351273	-0.447146
1	-2.908484	1.779915	-1.435664
1	-2.514388	-1.909178	-0.908031
1	-2.640288	-0.624567	-2.141074
1	-4.081112	-1.067458	-1.176235

Structure S130. ^{2}TS17

6	3.572333	-0.990796	-0.061064
6	3.905236	0.364660	-0.064142
6	2.236424	-1.371774	-0.032791
6	1.228414	-0.406136	-0.004151
6	1.558998	0.961578	0.030044
6	2.907059	1.332893	-0.023340
1	4.359235	-1.749832	-0.091586
1	4.955595	0.669739	-0.095200
1	1.942839	-2.425414	-0.046205
6	-0.197686	-0.864562	-0.038543
6	0.467581	1.954677	0.133280
1	3.169137	2.396171	-0.014558
8	-0.508592	-2.026774	0.185005
7	-1.096703	0.089320	-0.427869
6	-2.508067	0.116362	-0.036819
1	0.138456	2.177509	1.161709
1	-0.492669	1.264276	-0.342981
1	0.589149	2.872725	-0.460848
6	-2.686290	-0.118897	1.458670
6	-3.239399	-0.957443	-0.845300

6	-3.050966	1.488037	-0.420551
1	-2.305840	-1.106975	1.757989
1	-3.753318	-0.067304	1.732269
1	-2.152376	0.650283	2.043513
1	-2.563069	2.291293	0.158415
1	-4.133001	1.541328	-0.219618
1	-2.887515	1.689499	-1.492186
1	-2.867973	-1.960329	-0.592118
1	-3.094202	-0.794577	-1.925555
1	-4.320606	-0.911032	-0.629760

Structure S131. 13

6	3.397107	-1.234706	-0.375034
6	3.943948	0.054885	-0.383709
6	2.039129	-1.401261	-0.107675
6	1.203680	-0.314751	0.132888
6	1.754087	1.011071	0.182048
6	3.145228	1.146208	-0.107154
1	4.026861	-2.105027	-0.579579
1	5.007261	0.198924	-0.597181
1	1.595778	-2.401328	-0.095409
6	-0.247351	-0.641660	0.347319
6	1.030170	2.156126	0.552691
1	3.578602	2.151730	-0.081548
8	-0.582041	-1.621819	0.994597
7	-1.125399	0.192888	-0.268625
6	-2.593577	0.095573	-0.210535
1	-0.009282	2.116473	0.887721
1	-0.735888	0.909663	-0.873847
1	1.534897	3.127155	0.578525
6	-3.063661	0.197246	1.236256
6	-3.064729	-1.209835	-0.842415
6	-3.130011	1.277379	-1.004624
1	-2.670584	-0.632973	1.840759
1	-4.165144	0.170115	1.282941
1	-2.726954	1.145454	1.689864
1	-2.790475	2.235660	-0.573809
1	-4.231561	1.277539	-0.997881
1	-2.801241	1.235623	-2.057654
1	-2.677098	-2.077536	-0.288881
1	-2.718661	-1.283399	-1.887249
1	-4.166514	-1.261392	-0.843512

Structure S132. ^{2}TS18

6	3.936052	-2.368855	-0.225796
6	3.058344	-3.219650	-0.904069
6	3.680482	-1.000951	-0.185483
6	2.562107	-0.448633	-0.805446
6	1.689335	-1.297282	-1.550968
6	1.957392	-2.690092	-1.552848
1	4.817762	-2.775104	0.278161
1	3.246228	-4.296623	-0.934684
1	4.351320	-0.322135	0.348517
6	2.395110	1.040013	-0.637809
6	0.597067	-0.835713	-2.332416
1	1.281860	-3.346051	-2.112049
8	3.380052	1.755508	-0.520352
7	1.118462	1.488398	-0.615387
6	0.709903	2.900447	-0.558184
1	0.028361	-1.568475	-2.912638
1	0.518967	0.207026	-2.645545
6	1.410262	3.706310	-1.646933
6	1.012496	3.483534	0.817054
6	-0.789267	2.908790	-0.823080
1	2.495429	3.753633	-1.482186
1	1.012836	4.734893	-1.663977
1	1.231267	3.257800	-2.639571
1	-1.008442	2.526162	-1.835845
1	-1.190444	3.932576	-0.749823
1	-1.334257	2.272921	-0.103531
1	2.085686	3.399058	1.048526
1	0.445990	2.950565	1.598473
1	0.731633	4.549481	0.858883
1	0.367803	0.799525	-0.541084
6	1.250946	-1.787588	2.102111
6	1.624525	-0.699779	2.888699
6	-0.002872	-1.800325	1.500747
6	-0.889152	-0.742797	1.703556
6	-0.544063	0.342056	2.525473
6	0.734253	0.350057	3.094455
1	1.943540	-2.618955	1.940526
1	2.617756	-0.669241	3.347068
1	-0.303018	-2.635443	0.857627
6	-2.262947	-0.806504	1.112532
6	-1.532198	1.427967	2.820218
1	1.027885	1.197761	3.723479

8	-3.209245	-1.247409	1.739448
7	-2.426168	-0.213105	-0.120382
6	-3.485839	-0.538925	-1.076467
1	-1.059083	2.281227	3.329883
1	-2.337747	1.057080	3.477070
6	-4.799722	-0.045375	-0.458275
6	-3.536523	-2.031200	-1.371907
6	-3.239629	0.258119	-2.352210
1	-5.073879	-0.620512	0.435131
1	-5.601698	-0.142782	-1.208965
1	-4.720869	1.018585	-0.179433
1	-3.134455	1.331942	-2.126808
1	-4.096105	0.133634	-3.034181
1	-2.332943	-0.076716	-2.877139
1	-3.752352	-2.615637	-0.464081
1	-2.575423	-2.373996	-1.789382
1	-4.325696	-2.248734	-2.110177
1	-2.027345	1.805367	1.909406
9	-0.973272	-0.501379	-0.982416

Structure S134. 14

6	3.413019	-1.404673	-0.400065
6	3.942361	-0.128618	-0.227640
6	2.047878	-1.611575	-0.240476
6	1.187053	-0.553765	0.064208
6	1.720453	0.737104	0.258577
6	3.098484	0.924665	0.107818
1	4.066903	-2.244442	-0.652212
1	5.015754	0.046092	-0.343514
1	1.617490	-2.611153	-0.347681
6	-0.267355	-0.916094	0.227052
6	0.888999	1.920944	0.651200
1	3.514446	1.925059	0.268709
8	-0.585692	-1.977967	0.740529
7	-1.148759	-0.003748	-0.247110
6	-2.614237	-0.076885	-0.131173
1	1.529103	2.714677	1.069206
1	0.124099	1.660481	1.402768
6	-3.017869	-0.179940	1.335683
6	-3.151214	-1.264544	-0.920872
6	-3.140290	1.225854	-0.716671
1	-2.628137	-1.101071	1.793144
1	-4.116643	-0.184064	1.429588
1	-2.632417	0.682239	1.907155
1	-2.724899	2.096308	-0.179358
1	-4.238648	1.269128	-0.645106
1	-2.868157	1.323312	-1.782016
1	-2.756338	-2.211243	-0.522814
1	-2.863948	-1.189287	-1.983169
1	-4.252455	-1.296791	-0.866956
1	-0.775233	0.798674	-0.747261
9	0.230247	2.459690	-0.448978