Dehydration of alcohols catalyzed by copper (II) sulfate: type II dyotropic reactions and stepwise mechanisms

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Comparative study of DFT funcitonals

We observed that the computed activation free energy barriers when using M06(PCM) resulted in an overestimation of the reaction time associated with respect to the processes reported in literature. Therefore, we decided to perform a functional benchmarking using the dehydration of **1a** as model reaction. We performed single-point energy calculations using optimized geometries and thermochemistries computed at the M06(PCM)/6-31G(d,p)&LanL2dz level.

To this end, we selected different functionals, including Grimme's dispersion with Becke–Jonson damping (D3BJ)[1] and 6-31G(d,p)&LanL2dz basis set:denoted as B3LYP-D3BJ(PCM);[2] pure and hybrid Perdew, Burke and Ernzerhof functionals PBE-D3BJ(PCM) and PBE0-D3BJ(PCM);[3] non-local correlated B3PW91-D3BJ(PCM) and meta-GGA TPSS-D3BJ(PCM).[4] Additionally we also used Head–Gordon functional (including dispersion) wB97XD(PCM).

Our results show the suitability of TPSSTPSS-D3BJ meta–GGA functional, with an improved correlation term, in which the empirical gradient coefficient parameter D is set as 0 (compared to the D value of 0.113 assigned to other functionals). The obtained activation barriers by using the TPSS/(PCM)/6-31G(d,p)&LanL2dz//M06(PCM)/6-31G(d,p)&LanL2dz procedure provided more realistic reaction times, in line with the experimental evidences (see main manuscript).

Supplementary Table1. Relative Gibbs energies associated with the dehydration reaction of **1a** (see Fig. 1) using different functionals. Thermal corrections at 298.15K and 423.15K (in brackets) were computed at M06(PCM) level. 6-31G(d,p)&LanL2dz basis set was used in all cases.

Functional	**RCa**	**TSa**	**PCa**	**2a** + $CuSO_4 \cdot MeOH \cdot H_2O$
M06(PCM)	–5.1 (-6.5)	44.8 (43.6)	25.2 (22.7)	–0.4 (1.7)
B3LYP-D3BJ(PCM)	–8.2 (–9.7)	37.9 (36.6)	20.6 (18.1)	–2.6 (–0.5)
PBE-D3BJ(PCM)	–6.8 (–8.3)	33.9 (32.6)	23.1 (20.7)	0.2 (2.3)
PBE0-D3BJ(PCM)	–7.4 (–8.9)	42.7 (41.4)	26.2 (23.7)	0.8 (2.9)
B3PW91-D3BJ(PCM)	–7.0 (–8.5)	40.5 (39.3)	24.4 (21.9)	–0.1 (2.0)
TPSS-GD3BJ(PCM)	–7.3 (–8.8)	35.5 (34.2)	24.2 (21.7)	0-4 (2.6)
wB97XD(PCM)	–6.4 (–7.9)	45.8 (44.5)	25.1 (22.6)	–0.2 (1.9)

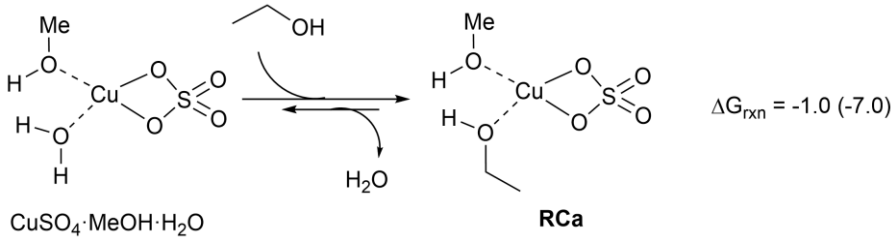
Supplementary Table2. Total electronic energies (E, in a.u.) of stationary points associated with the dehydration reaction of **1a** computed using different functionals. (Values obtained with M06(PCM) and TPSSTPSS(PCM) are collected in Supplementary Table 4)

Structure	B3LYP-D3BJ(PCM)	PBE-D3BJ(PCM)	PBE0-D3BJ(PCM)
$CuSO_4$·MeOH	-1010.994055	-1010.36481	-1010.334315
$CuSO_4$·MeOH·H_2O	-1087.458959	-1086.741623	-1086.716242
1a	-155.0617862	-154.854775	-154.8744132
RCa	-1166.09098	-1165.252497	-1165.242541
TS_{con}a	-1166.006299	-1165.176321	-1165.151484
PCa	-1166.037681	-1165.197323	-1165.181583
2a	-78.5997241	-78.4762578	-78.48987

Structure	B3PW91-D3BJ(PCM)	wB97XD(PCM)
$CuSO_4$·MeOH	-1010.829077	-1010.828027
$CuSO_4$·MeOH·H_2O	-1087.265064	-1087.268835
1a	-155.0046688	-155.0058321
RCa	-1165.866887	-1165.866159
TS_{con}a	-1165.779933	-1165.771723
PCa	-1165.809448	-1165.808532
2a	-78.5674977	-78.5640228

Regeneration of the catalyst

In order to complete the catalytic cycle, we analyzed the recovery of the reactive complex **RCa** by water-ethanol exchange. Our calculations showed that this latter step is thermodynamically favored, ensuring that, after the dehydration of the first ethanol molecule, Cu(II) sulphate complex would continue reacting (Supplementary Scheme 1). Note that, since ethanol is used as solvent, the exchange equilibrium will be displaced to the right, further favoring **RCa** regeneration.

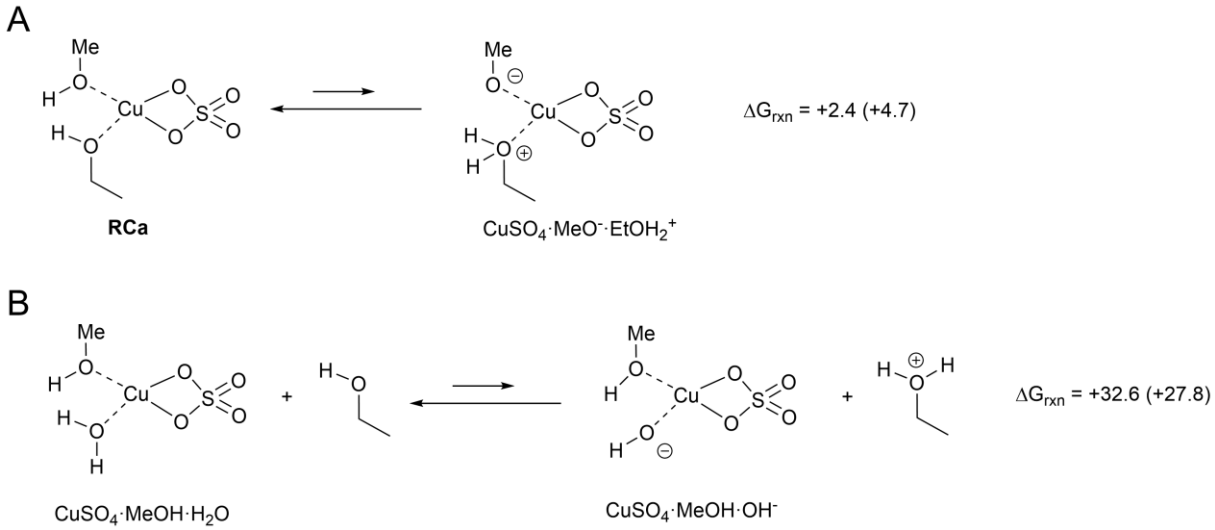


Supplementary Scheme 1. Reaction Gibbs energies (in kcal mol^{-1}, computed at 298 K and 423 K (values between brackets)) associated with the water-alcohol exchange to close the catalytic cycle of ethane dehydration catalyzed by Cu(II) sulphate computed at UTPSS/(PCM)/6-31G(d,p)&LanL2dz//UM06(PCM)/6-31G(d,p)&LanL2dz level of theory.

Exploration of additional mechanisms

The role of Cu(II) salts as Brønsted acids was explored. Within this framework, two different possibilities were considered: (A) Intramolecular protonation of ethanol (Supplementary Scheme 2A); and (B) protonation of a non coordinated ethanol molecule by $CuSO_4 \cdot MeOH \cdot H_2O$ (Supplementary Scheme 2B). Our calculations showed that both processes are endergonic, especially at high temperatures. According the reaction Gibbs energy of the reaction, these equilibria should be displaced towards neutral complex **RCa**, and $CuSO_4 \cdot MeOH \cdot H_2O$ + ethanol, respectively.

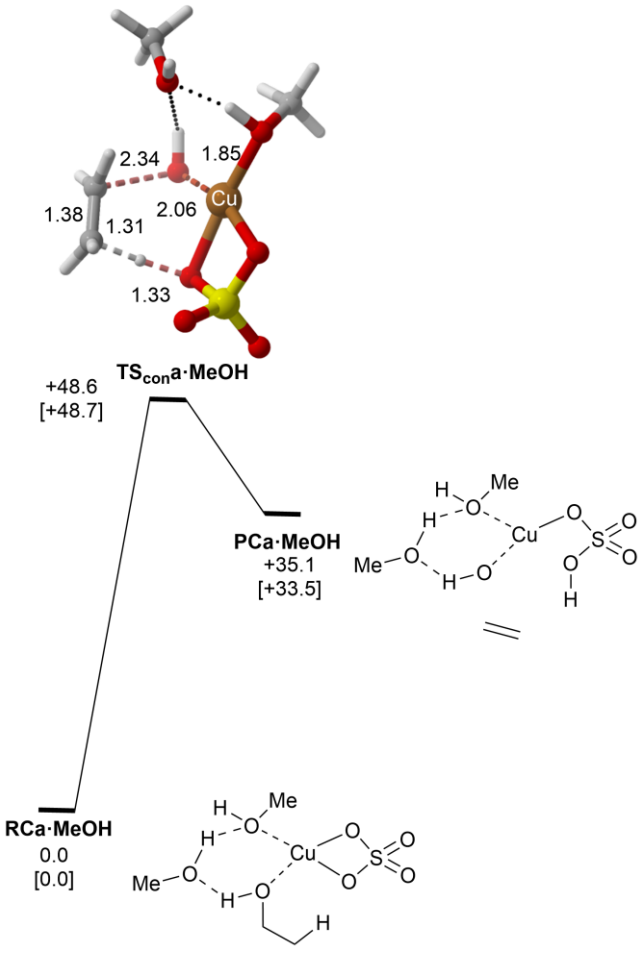
All our attempts to minimize a complex in which Cu(II) sulphate anion and protonated ethanol are stabilized by hydrogen bonding evolved towards neutral Cu(II) sulphate interacting with ethanol.



Supplementary Scheme 2. Reaction Gibbs energies (in kcal mol^{-1}, computed at 298 K and 423 K (values between brackets)) associated with the (A) intramolecular, or (B) intermolecular protonation of ethanol (**1a**) by Cu(II) sulphate complexes computed at UTPSS/(PCM)/6-31G(d,p)&LanL2dz//UM06(PCM)/6-31G(d,p)&LanL2dz level of theory.

Additional explicit solvent molecules

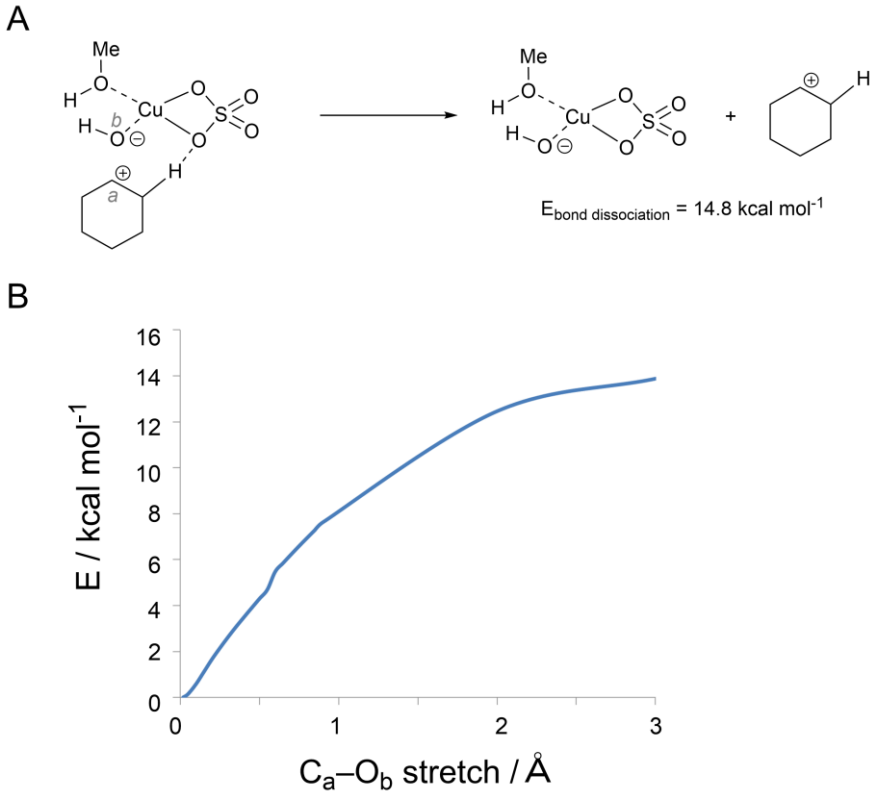
The effect of an additional solvent molecule on the energetic profile associated with the dehydration of **1a** was also explored. Our calculations show that the additional molecule of MeOH interacts with the OH moiety of the two alcohols (namely 1a and MeOH) directly connected to Cu atom via hydrogen bonding interaction. Geometrical inspection of the computed transition structure **TS_{con}a·MeOH** show that no significant modifications arises due to the presence of the additional explicit methanol molecules. In addition, the computed activation barrier associated with this step increases. Therefore, only one explicit model solvent molecule (i.e. the one directly coordinated to the copper atom) was considered.



Supplementary Figure 1. Energy profile and main geometrical features of transition structure associated with the dehydration reaction of alcohol **1a** catalyzed by $CuSO_4$ considering two explicit molecules of solvent (one additional MeOH compared to the profile collected in Fig.1) computed at the UTPSS/(PCM)/6-31G(d,p)&LanL2dz//UM06(PCM)/6-31G(d,p)&LanL2dz level of theory. Relative Gibbs energies, in kcal mol^{-1}, were computed at 298.15 K and 423.15 K (values between brackets). Distances are in Å.

Evaluation of INTb ion pair dissociation energy

The ion pair dissociation energy of **INTb** has been computed by using two different approaches: (A) electronic energy difference between the complete molecule and the sum of the cationic and anionic fragments; (B) relaxed energy profile scan, in which the C-O bond was constantly stretched. Our calculations indicate that the attractive Coulombic interaction between the two opposite charged moieties is a strong interaction, even at long distances which avoids **INTb** dissociation.



Supplementary Figure 2. (A) Ion pair dissociation energy of **INTb** and (B) **INTb** relaxed energy profile scan computed at the UTPSS/(PCM)/6-31G(d,p)&LanL2dz//UM06(PCM)/6-31G(d,p)&LanL2dz level of theory.

Supplementary Table3. Calculated kinetic constants[a] (k_i, in s^{-1}) associated with the dehydration reaction of alcohols **1c**, **1e** and **1f** catalyzed by $CuSO_4$.

Reaction	k_i	k_{-i}
RCc –-> **PCc** (dyotropic)	$1.4\ 10^{-6}$	–
RCc –-> **INTc** (stepwise)	$1.3\ 10^{-5}$	$1.7\ 10^{11}$
INTc –-> **PCc**	$9.0\ 10^{9}$	–
RCe(Sz) –-> **INTe(Sz)**	$7.4\ 10^{-3}$	$3.9\ 10^{11}$
INTe(Sz) –-> **PCe(Sz)**	$1.9\ 10^{12}$	–
RCe(aS) –-> **INTe(aS)**	$2.7\ 10^{-4}$	$3.4\ 10^{12}$
INTe(aS) –-> **PCe(aS)**	$1.4\ 10^{12}$	–
(Z)-**RCf(Sz)** –-> (Z)-**INTf(Sz)**	$2.8\ 10^{-3}$	$9.6\ 10^{10}$
(Z)-**INTf(Sz)** –-> (Z)-**PCf(Sz)**	$1.2\ 10^{12}$	–
(E)-**RCf(Sz)** –-> (E)-**INTf(Sz)**	$4.9\ 10^{-3}$	$1.7\ 10^{11}$
(E)-**INTf(Sz)** –-> **(E)-PCf(Sz)**	$4.3\ 10^{12}$	–
RCf(aS) –-> **INTf(aS)**	$2.1\ 10^{-3}$	$6.4\ 10^{12}$
INTf(aS) –-> **PCf(aS)**	$6.5\ 10^{11}$	–

[a] Values computed using Eyring equation from Gibbs energy barriers computed at 423.15K at TPSS/(PCM)/6-31G(d,p)&LanL2dz // M06(PCM)/6-31G(d,p)&LanL2dz level.

Supplementary Table4. Total electronic energies (E, in a.u.), zero point correction of the energy[a,b] (ZPE, in a.u.), thermal corrections to Gibbs energies[c] (TCGE, in a.u.), and number of imaginary frequencies[d] (NIMAG) of all stationary points discussed in the main text.

Structure	E	ZPE	TCGE	NIMAG(ν)
$CuSO_4$·MeOH	-1010.787124[a] (-1010.974378)[b]	0.071628 (0.063953)	0.034075 (0.012580)	0
$CuSO_4$·MeOH·H_2O	-1087.216180[a] (-1087.437910)[b]	0.097975 (0.087478)	0.058549 (0.034920)	0
H_2O	-76.398661[a] (-76.4329934)[b]	0.021564 (0.021564)	0.003911 (0.005360)	0
$CuSO_4$·MeO^-·$EtOH2^+$	-1165.709033[a] (-1166.026017)[b]	0.154294 (0.154294)	0.110249 (0.083166)	0
$CuSO_4$·MeOH·OH^-	-1086.745825[a] (-1166.026017)[b]	0.084762 (0.084762)	0.044880 (0.021184)	0
$EtOH2^+$	-155.3715289[a] (-155.502967)[b]	0.093705 (0.093705)	0.068226 (0.054667)	0
1a	-154.950318[a] (-155.074838)[b]	0.079595 (0.071067)	0.054208 (0.031795)	0
RCa	-1165.76756[a] (-1166.082813)[b]	0.154414 (0.137869)	0.110302 (0.064012)	0
TS_{con}a	-1165.676765[a] (-1166.003504)[b]	0.144033 (0.128601)	0.099086 (0.053163)	1 (-1580.1703)
PCa	-1165.711958[a] (-1166.025272)[b]	0.149388 (0.133382)	0.102915 (0.055028)	0
2a	-78.520539[a] (-78.609210)[b]	0.050566 (0.045148)	0.028379 (0.011457)	0
RCa·MeOH	-1281.449033[a] (-1281.852786)[b]	0.208861 (0.208861)	0.159918 (0.128683)	0
TS_{con}a·MeOH	-1281.352578[a] (-1281.766584)[b]	0.199244 (0.199244)	0.151140 (0.120088)	1 (-1561.5781)
PCa·MeOH	-1281.385693[a] (-1281.787260)[b]	0.202905 (0.202905)	0.150352 (0.116496)	0
1b	-310.893873[a] (-311.179497)[b]	0.173446 (0.154862)	0.143011 (0.105949)	0
RCb	-1321.706973[a] (-1322.188340)[b]	0.248623 (0.221985)	0.201971 (0.142090)	0
TS1b	-1321.636293[a] (-1322.118429)[b]	0.240349 (0.214597)	0.192004 (0.131548	1 (-573.6477)
INTb	-1321.636592[a] (-1322.118299)[b]	0.241067 (0.215239)	0.192057 (0.13080)	0
TS2b	-1321.632629[a] (-1322.113700)[b]	0.237227 (0.21181)	0.188367 (0.127811)	1 (-941.8871)
PCb	-1321.655483[a] (-1322.138485)[b]	0.242959 (0.216928)	0.192646 (0.130462)	0
2b	-234.4659392[a] (-234.717190)[b]	0.145126 (0.129577)	0.116529 (0.084434)	0
1c	-385.835600[a] (-386.199464)[b]	0.160635 (0.143424)	0.127348 (0.089425)	0

RCc	-1396.650813 [a] (-1397.213505)[b]	0.234902 (0.209734)	0.184656 (0.123534)	0
TS$_{con}$c	-1396.579274 [a] (-1397.148929)[b]	0.225724 (0.201539)	0.1769 (0.116982)	1 (-1659.6776)
PCc	-1396.604129 [a] (-1397.165272)[b]	0.230723 (0.206003)	0.180495 (0.116982)	0
TS1c	-1396.589750 [a] (-1397.153602+)[b]	0.230682 (0.205966)	0.17989 (0.118835)	1 (-62.6801)
INTc	-1396.594716 [a] (-1397.156875)[b]	0.230197 (0.205533)	0.178808 (0.118558)	0
TS2c	-1396.576098 [a] (-1397.146558)[b]	0.22552 (0.201357)	0.175826 (0.115515)	1 (-1700.87)
2c	-309.409597 [a] (-309.738849)[b]	0.132544 (0.118343)	0.100721 (0.067615)	0
$CuSO_4$-anion	-1086.966033[b]	-	-	-
Cyclohexane-cation	-235.1286425[b]	-	-	-
1d	-425.123859 [a] (-425.529288)[b]	0.188573 (0.168369)	0.154322 (0.111985)	0
RCd	-1435.937146 [a] (-1436.541848)[b]	0.262534 (0.234406)	0.21233 (0.147165)	0
TS1d	-1435.890215 [a] (-1436.495587)[b]	0.258125 (0.230469)	0.205681 (0.139433)	1 (-70.4167)
INTd	-1435.891918 [a] (-1436.497372)[b]	0.258542 (0.230841)	0.207375 (0.141376)	0
TS2d	-1435.87332 [a] (-1436.486200)[b]	0.253926 (0.22672)	0.203633 (0.139076)	1 (-1635.0868)
PCd	-1435.888553 [a] (-1436.494895)[b]	0.258585 (0.23088)	0.206041 (0.139274)	0
2d	-348.696783 [a] (-349.067870)[b]	0.160731 (0.14351)	0.127991 (0.090482)	0
1e	-351.3796377 [a] (-351.712521)[b]	0.219885 (0.196326)	0.184696 (0.163465)	0
RCe–*aS*	-1362.193722 [a] (-1362.72221)[b]	0.294386 (0.262845)	0.24238 (0.208149)	0
TS1e–*aS*	-1362.137258 [a] (-1362.664579)[b]	0.288411 (0.257510)	0.236153 (0.201446)	1 (-74.9467)
INTe–*aS*	-1362.138036 [a] (-1362.665617)[b]	0.287199 (0.256427)	0.231869 (0.201126)	0
TS2e–*aS*	-1362.125613 [a] (1362.661275)[b]	0.285206 (0.254648)	0.233623 (0.19926)	1 (-1529.0935)
PCe–*aS*	-1362.136051 [a] (-1362.668177)[b]	0.290688 (0.259543)	0.236342 (0.200431)	0
2e–*aS*	-274.9479679 [a] (-275.247489)[b]	0.191837 (0.171283)	0.157676 (0.137667)	0
RCe–*Sz*	-1362.193947 [a] (-1362.722700	0.295351 (0.263706)	0.246615 (0.213996)	0

TS1e–*Sz*	-1362.134549 [a] (-1362.661716)[b]	0.287638 (0.256819)	0.234644 (0.199514)	1 (-39.7485)
INTe–*Sz*	-1362.134786 [a] (-1362.664140)[b]	0.287824 (0.256986)	0.233658 (0.19769)	0
TS2e–*Sz*	-1362.123118 [a] (-1362.659580)[b]	0.284068 (0.253632)	0.230704 (0.195326)	1 (-1489.8149)
PCe–*Sz*	-1362.142223 [a] (-1362.674481)[b]	0.290766 (0.259613)	0.238429 (0.203392)	0
2e–*Sz*	-274.951225 [a] (-275.251736)[b]	0.191463 (0.170949)	0.156836 (0.136498)	0
1f	-465.520227 [a] (-465.965297)[b]	0.23374 (0.208697)	0.193886 (0.16896)	0
RCf–*aS*	-1476.326387 [a] (-1476.970478)[b]	0.308147 (0.275131)	0.251513 (0.21354)	0
TS1f–*aS*	-1476.269303 [a] (-1476.919222)[b]	0.303003 (0.250538)	0.245869 (0.207407)	1 (-104.4025)
INTf–*aS*	-1476.269665 [a] (-1476.918667)[b]	0.303542 (0.271020)	0.245687 (0.206544)	0
TS2f–*aS*	-1476.25508 [a] (-1476.910377)[b]	0.298818 (0.266802)	0.240735 (0.201395)	1 (-1635.1228)
PCf–*aS*	-1476.289667 [a] (-1476.936253)[b]	0.304739 (0.272088)	0.304739 (0.210181)	0
2f–*aS*	-389.095955 [a] (-389.508221)[b]	0.206218 (0.184123)	0.16744 (0.143879)	0
(E)-**RCf**–*Sz*	-1476.326606 [a] (-1476.971287)[b]	0.309646 (0.276470)	0.256576 (0.220541)	0
(E)-**TS1e**–*Sz*	-1476.265299 [a] (-1476.913589)[b]	0.302644 (0.270217)	0.245382 (0.206849)	1 (-42.1017)
(E)-**INTe**–*Sz*	-1476.26467 [a] (-1476.914225)[b]	0.302737 (0.270301)	0.242708 (0.202495)	0
(E)-**TS2e**– *Sz*	-1476.257411 [a] (-1476.912985)[b]	0.298309 (0.266347)	0.24097 (0.202206)	1 (-1131.0359)
(E)-**PCe**– *Sz*	-1476.295513 [a] (-1476.943065)[b]	0.304107 (0.271524)	0.246291 (0.207081)	0
(E)-**2e**– *Sz*	-389.098885 [a] (-389.511970)[b]	0.205817 (0.183765)	0.166609 (0.14271)	0
(Z)-**RCf**–*Sz*	-1476.32576 [a] (-1476.970526)[b]	0.308632 (0.275564)	0.25253 (0.220541)	0
(Z)-**TS1e**–*Sz*	-1476.268776 [a] (-1476.915700)[b]	0.302606 (0.270184)	0.245561 (0.206849)	1 (-63.0919)
(Z)-**INTe**–*Sz*	-1476.268981 [a] (-1476.918204)[b]	0.302096 (0.269729)	0.243156 (0.202495)	0
(Z)-**TS2e**– *Sz*	-1476.256051 [a] (-1476.910799)[b]	0.297831 (0.265920)	0.240571 (0.202206)	1 (-1432.8115)
(Z)-**PCe**– *Sz*	-1476.295067 [a] (-1476.942609)[b]	0.303606 (0.271077)	0.245148 (0.207081)	0
(Z)-**2e**– *Sz*	-389.1008906 [a] (-389.514013)[b]	0.205676 (0.183640)	0.166336 (0.14271)	0

[a] Computed at M06(PCM)/6-31G(d,p)&LanL2dz level. [b] Computed at TPSSTPSS/(PCM)/6-31G(d,p)//M06(PCM)/6-31G(d,p)&LanL2dz level. [c] Thermal corrections computed at 298.15 K (and 423.15K between brackets) at M06(PCM)/6-31G(d,p)&LanL2dz level. [d] If NIMAG=1, the imaginary frequency ν (in parentheses) is given in cm^{-1}.

Cartesian coordinates of all the stationary points discussed in the main text and in the ESI

$CuSO_4$·MeOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.805487	-0.631615	-0.107425
2	8	0	-0.318373	0.902055	0.464473
3	16	0	-1.635219	0.207995	0.032867
4	8	0	-2.286615	0.940302	-1.055344
5	8	0	2.668443	-0.197536	0.170149
6	6	0	2.998620	1.189541	-0.044712
7	8	0	-0.994568	-1.111458	-0.499010
8	8	0	-2.492749	-0.065912	1.188103
9	1	0	2.974436	-0.465674	1.048875
10	1	0	4.083878	1.307009	-0.022990
11	1	0	2.614592	1.451636	-1.031432
12	1	0	2.530661	1.819092	0.716313

$CuSO_4$·MeOH·H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.366645	-2.079022	-0.047725
2	8	0	-2.435725	-0.645262	-0.013534
3	29	0	-0.730531	0.384390	0.016800
4	8	0	1.054003	1.189239	-0.003568
5	16	0	1.801754	-0.169226	-0.003367
6	8	0	2.596735	-0.327481	1.219578
7	8	0	0.560636	-1.097515	0.021482
8	8	0	2.561943	-0.346624	-1.245744
9	1	0	-2.985059	-0.372726	0.735556
10	1	0	-3.375998	-2.486255	-0.141258
11	1	0	-1.779079	-2.346822	-0.926116
12	1	0	-1.882656	-2.470837	0.851223
13	8	0	-1.818688	2.069824	0.032995
14	1	0	-1.235270	2.842470	0.027121
15	1	0	-2.335968	2.131148	-0.783159

H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.119662
2	1	0	-0.000000	0.754844	-0.478649
3	1	0	-0.000000	-0.754844	-0.478649

$CuSO_4$·MeO^-·$EtOH2^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.219258	-2.196085	1.368277
2	6	0	-1.220255	-2.678983	-0.045409
3	8	0	-1.851389	-1.603485	-0.903577
4	29	0	-0.541245	0.669495	-0.445043

5	8	0	1.032827	-0.232961	-1.168586
6	16	0	1.930249	0.021767	0.067597
7	8	0	3.111104	0.815595	-0.307654
8	8	0	0.959775	0.850295	0.931084
9	8	0	-2.079371	1.445285	0.078062
10	6	0	-1.978364	2.680854	0.715305
11	8	0	2.259633	-1.252296	0.729865
12	1	0	-2.232021	-1.985620	1.727211
13	1	0	-0.590506	-1.307610	1.491892
14	1	0	-1.806668	-3.582359	-0.214518
15	1	0	-0.223010	-2.777235	-0.475567
16	1	0	-0.802887	-2.994780	1.989962
17	1	0	-2.983223	3.043598	0.988198
18	1	0	-1.401993	2.617156	1.656052
19	1	0	-1.509161	3.458040	0.087442
20	1	0	-1.804407	-1.813105	-1.857431
21	1	0	-2.787376	-1.435883	-0.671158

$CuSO_4 \cdot MeOH \cdot OH^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.415377	-2.021446	-0.057189
2	8	0	2.489639	-0.605004	0.143693
3	29	0	0.762210	0.487215	0.017405
4	8	0	1.652279	2.096625	-0.107267
5	8	0	-1.157563	1.213144	-0.046804
6	16	0	-1.776090	-0.192290	-0.002374
7	8	0	-2.562254	-0.385047	1.229535
8	8	0	-0.491359	-1.046447	0.039150
9	8	0	-2.542799	-0.470146	-1.230138
10	1	0	3.098646	-0.226394	-0.505593
11	1	0	3.415079	-2.456846	0.018738
12	1	0	1.782408	-2.422857	0.734995
13	1	0	1.974973	-2.261804	-1.029815
14	1	0	2.446443	2.019007	0.432691

$EtOH2^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.263177	-0.259416	-0.026643
2	6	0	-0.044054	0.601716	0.054950
3	8	0	1.159065	-0.290848	-0.098015
4	1	0	-1.305721	-0.796803	-0.977400
5	1	0	1.998442	0.208939	-0.083098
6	1	0	-2.139535	0.391001	0.041608
7	1	0	0.072838	1.119194	1.007327
8	1	0	0.057370	1.296949	-0.776948
9	1	0	-1.312708	-0.974336	0.800702
10	1	0	1.200181	-0.971954	0.602084

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.084039	0.544050	0.000053
2	8	0	1.147154	-0.397763	0.000126
3	6	0	-1.215773	-0.220115	-0.000086
4	1	0	-1.287781	-0.857934	-0.888069
5	1	0	1.975775	0.095186	-0.000892
6	1	0	-2.067970	0.466437	0.000792

7	1	0	0.140045	1.196912	0.885287
8	1	0	0.140416	1.197285	-0.884874
9	1	0	-1.287314	-0.859394	0.886946

RCa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.441994	1.793807	0.469375
2	6	0	-2.470517	2.222136	-0.972563
3	8	0	-2.229104	0.368424	0.602014
4	29	0	-0.444853	-0.389139	0.157924
5	8	0	-1.332537	-2.176197	-0.070253
6	6	0	-0.521351	-3.307163	-0.427021
7	16	0	1.987775	0.513681	-0.015155
8	8	0	2.893584	0.610260	1.135246
9	8	0	0.653560	1.247075	0.268563
10	8	0	1.419925	-0.922194	-0.151651
11	8	0	2.573076	0.964945	-1.283069
12	1	0	-3.288029	1.732505	-1.514183
13	1	0	-2.919087	-0.099152	0.107069
14	1	0	-1.524510	1.981099	-1.469760
15	1	0	-3.376760	2.034755	0.987193
16	1	0	-1.616534	2.255313	1.016930
17	1	0	-2.625049	3.303789	-1.037872
18	1	0	-1.820192	-2.384926	0.739937
19	1	0	-1.165715	-4.171871	-0.602171
20	1	0	0.000819	-3.044733	-1.347328
21	1	0	0.206517	-3.531821	0.357322

TS_{con}a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.494800	2.963846	0.594496
2	6	0	0.859071	2.723911	0.717551
3	8	0	-1.632891	1.489413	-0.864117
4	29	0	-0.794613	-0.105499	-0.410497
5	16	0	1.756653	-0.726619	0.027209
6	8	0	2.619317	-1.437142	-0.915574
7	8	0	1.133762	0.537617	-0.722164
8	8	0	0.459224	-1.486913	0.304826
9	8	0	2.405226	-0.277250	1.259935
10	1	0	1.011350	1.654446	-0.004029
11	1	0	-1.184068	1.814585	-1.656062
12	1	0	1.205774	2.300312	1.662098
13	1	0	-0.889317	3.676188	-0.122793
14	1	0	-1.210388	2.549126	1.297524
15	1	0	1.540949	3.406153	0.209330
16	8	0	-2.541394	-1.062602	-0.128129
17	1	0	-3.223109	-0.375690	-0.173603
18	6	0	-2.664396	-1.777526	1.110740
19	1	0	-3.656550	-2.230601	1.175327
20	1	0	-1.905255	-2.560223	1.100380
21	1	0	-2.497271	-1.115293	1.965951

PCa

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.182635	2.497501	0.437952
2	6	0	0.967611	3.151586	0.272160
3	8	0	-1.926560	0.456487	-1.868021
4	29	0	-0.992334	-0.316503	-0.541391
5	8	0	-2.483373	-1.015377	0.659396
6	6	0	-2.616084	-0.237152	1.860016
7	16	0	1.830689	-0.667755	0.166863
8	8	0	2.528971	0.107824	1.187025
9	8	0	1.585879	0.304185	-1.111096
10	8	0	0.421625	-1.013084	0.604475
11	8	0	2.528859	-1.814318	-0.395625
12	1	0	1.339486	1.201493	-0.787421
13	1	0	-2.449831	-0.221562	-2.312971
14	1	0	1.820844	2.976989	0.925109
15	1	0	-1.043149	2.676687	-0.205038
16	1	0	-0.312076	1.766453	1.236895
17	1	0	1.094859	3.893886	-0.512825
18	1	0	-3.311115	-0.956365	0.160047
19	1	0	-3.450614	-0.617725	2.453962
20	1	0	-1.685373	-0.355867	2.417016
21	1	0	-2.772921	0.821335	1.625747

RCa·MeOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.453340	-2.244221	-0.362919
2	6	0	-1.566137	-2.200546	1.140492
3	8	0	-1.271289	-0.929927	-0.933574
4	29	0	0.144788	0.168002	-0.076676
5	8	0	1.650017	-0.973349	-0.653849
6	16	0	2.733800	-0.067340	-0.020564
7	8	0	3.619338	0.486604	-1.052718
8	8	0	-1.114198	1.472445	0.760336
9	6	0	-1.027929	2.779673	0.169592
10	8	0	1.802191	1.029076	0.552229
11	8	0	3.437660	-0.770929	1.059233
12	8	0	-3.425922	0.620185	-0.398139
13	6	0	-4.647427	-0.002043	-0.000279
14	1	0	-0.629169	-1.863649	1.603082
15	1	0	-2.125674	-0.439478	-0.874389
16	1	0	-1.790314	-3.198370	1.531279
17	1	0	-2.349496	-2.677944	-0.821743
18	1	0	-0.588351	-2.832428	-0.683501
19	1	0	-2.370920	-1.523401	1.454323
20	1	0	-3.619858	1.317721	-1.038342
21	1	0	-5.290477	0.702276	0.536427
22	1	0	-5.183874	-0.401459	-0.866489
23	1	0	-4.386368	-0.826523	0.667558
24	1	0	-1.650990	3.479027	0.733348
25	1	0	0.015782	3.093897	0.222696
26	1	0	-1.350496	2.752362	-0.877253
27	1	0	-2.032824	1.153340	0.616172

TS_{con}a·MeOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.772490	2.576849	-0.425485
2	6	0	-0.552455	2.804075	-0.108703
3	8	0	1.059503	0.545067	-1.549355
4	29	0	0.103334	-0.508748	-0.362153
5	8	0	1.569368	-1.611967	0.421243
6	6	0	2.304654	-2.399357	-0.521286
7	8	0	-1.379295	-1.183305	0.814849
8	16	0	-2.468252	-0.236126	0.314416
9	8	0	-2.865649	0.734103	1.336865

10	8	0	-1.635676	0.514489	-0.819508
11	8	0	-3.567280	-0.955430	-0.329751
12	8	0	2.941900	0.508420	1.312074
13	6	0	4.113641	0.767590	0.544703
14	1	0	-1.117009	1.688057	-0.488678
15	1	0	2.005215	0.423053	-1.398420
16	1	0	-1.100507	3.528866	-0.710845
17	1	0	1.457195	2.124584	0.289747
18	1	0	1.213072	2.949820	-1.344283
19	1	0	-0.831159	2.737895	0.944978
20	1	0	3.200686	0.396994	2.235813
21	1	0	4.727218	1.546092	1.008448
22	1	0	4.718715	-0.136837	0.409664
23	1	0	3.790166	1.129773	-0.436120
24	1	0	3.019915	-3.034909	0.008966
25	1	0	1.589403	-3.026753	-1.056404
26	1	0	2.838445	-1.767816	-1.240051
27	1	0	2.171036	-0.933060	0.822264

PCa·MeOH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.281981	2.375271	0.213089
2	6	0	0.783663	3.157461	0.037737
3	8	0	-1.263310	-0.490458	2.026690
4	29	0	-0.290395	-0.670404	0.523453
5	8	0	2.237661	0.446450	1.079737
6	16	0	2.526462	-0.265109	-0.350164
7	8	0	3.479763	-1.316790	-0.024542
8	8	0	-1.671088	-1.143199	-0.863209
9	6	0	-2.576667	-2.190337	-0.502475
10	8	0	1.176925	-0.819358	-0.751448
11	8	0	2.968182	0.772401	-1.277316
12	8	0	-3.256571	0.967527	-1.246571
13	6	0	-3.854761	1.184702	0.026562
14	1	0	1.752219	1.286240	0.918875
15	1	0	-1.994719	0.119873	1.872120
16	1	0	1.222233	3.717106	0.861913
17	1	0	-0.741669	1.837408	-0.618557
18	1	0	-0.749409	2.258413	1.190135
19	1	0	1.250139	3.278271	-0.937515
20	1	0	-3.940343	0.657985	-1.854621
21	1	0	-4.747042	1.813320	-0.054713
22	1	0	-4.126168	0.239950	0.517057
23	1	0	-3.119525	1.710523	0.643763
24	1	0	-3.305692	-2.334979	-1.306170
25	1	0	-1.992861	-3.103975	-0.373994
26	1	0	-3.098972	-1.962314	0.432900
27	1	0	-2.204170	-0.329512	-1.064905

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.664278	-0.000035	0.000202
2	6	0	0.664317	-0.000008	0.000043
3	1	0	-1.237760	0.924769	-0.000892
4	1	0	1.237919	-0.924759	-0.000636
5	1	0	1.237142	0.925215	0.000156
6	1	0	-1.237537	-0.924972	-0.000100

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.752552	0.053512	-0.089333
2	6	0	0.958525	-1.228631	-0.314212
3	6	0	-0.272209	-1.276023	0.585887
4	6	0	-1.152778	-0.046768	0.422827
5	6	0	-0.349484	1.234831	0.612263
6	6	0	0.874835	1.283418	-0.294956
7	8	0	-1.726367	-0.113407	-0.883132
8	1	0	-0.999998	2.105300	0.444554
9	1	0	-2.234918	0.695919	-1.017547
10	1	0	-1.957799	-0.079794	1.177052
11	1	0	-0.029742	1.281557	1.664769
12	1	0	0.547634	1.324638	-1.344702
13	1	0	1.445212	2.202274	-0.108957
14	1	0	0.044406	-1.325225	1.638403
15	1	0	-0.869998	-2.175687	0.388704
16	1	0	2.625397	0.087161	-0.754280
17	1	0	2.141334	0.059005	0.942431
18	1	0	1.587526	-2.109630	-0.133452
19	1	0	0.643238	-1.280298	-1.366778

RCb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.577502	0.112415	-1.008146
2	6	0	2.543400	-1.406359	-1.067442
3	6	0	1.824424	-2.066605	0.105377
4	6	0	2.365885	-1.557781	1.434492
5	6	0	2.223375	-0.044336	1.519278
6	6	0	2.947104	0.640962	0.364366
7	8	0	1.302426	0.705015	-1.408496
8	29	0	-0.335547	0.685642	-0.290337
9	8	0	-1.209435	-0.916739	-1.055081
10	16	0	-2.287204	-0.988793	0.054365
11	8	0	-3.633611	-0.889727	-0.520617
12	8	0	-1.914719	0.312450	0.811736
13	8	0	-2.078236	-2.164397	0.908442
14	1	0	2.115966	-1.725512	-2.028206
15	1	0	1.075227	0.368858	-2.288498
16	1	0	3.299519	0.488100	-1.745081
17	1	0	3.593179	-1.736614	-1.072444
18	1	0	0.744291	-1.866568	0.052696
19	1	0	1.939516	-3.155164	0.030122
20	1	0	4.025939	0.461431	0.480585
21	1	0	2.811553	1.729692	0.386522
22	1	0	1.845689	-2.039093	2.272116
23	1	0	3.431362	-1.825548	1.523479
24	1	0	2.622265	0.335718	2.468130
25	1	0	1.149612	0.209671	1.531896
26	8	0	0.071188	2.506041	0.461566
27	1	0	0.774562	2.892006	-0.080879
28	6	0	-1.048979	3.406656	0.477922
29	1	0	-0.740152	4.365619	0.900334
30	1	0	-1.449958	3.550684	-0.529849
31	1	0	-1.809619	2.952948	1.113514

TS1b

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.900645	-1.515668	-0.862788
2	6	0	-2.502681	-0.280901	-1.211738
3	6	0	-3.330170	0.479566	-0.175278
4	6	0	-3.393639	-0.228308	1.175602
5	6	0	-2.055306	-0.857884	1.540785
6	6	0	-1.696352	-1.919507	0.516535
7	8	0	0.909376	-1.742130	-1.762458
8	29	0	1.091924	-0.510041	-0.401021
9	8	0	0.272004	1.180494	-1.205321
10	16	0	0.572468	2.024510	0.059212
11	8	0	1.523789	3.100914	-0.256313
12	8	0	1.234060	0.948270	0.941104
13	8	0	-0.678204	2.502579	0.672600
14	1	0	-1.462330	0.200666	-1.269562
15	1	0	0.653585	-1.247215	-2.549409
16	1	0	-1.494602	-2.149986	-1.651009
17	1	0	-2.848499	-0.229630	-2.246914
18	1	0	-2.903729	1.481946	-0.056691
19	1	0	-4.338076	0.614215	-0.582135
20	1	0	-2.369933	-2.799359	0.595744
21	1	0	-0.697469	-2.360425	0.628471
22	1	0	-3.713706	0.478222	1.948592
23	1	0	-4.152262	-1.024239	1.137984
24	1	0	-2.085121	-1.306485	2.538390
25	1	0	-1.267782	-0.089638	1.553115
26	8	0	2.017565	-1.916773	0.763536
27	1	0	2.125082	-2.666902	0.159756
28	6	0	3.313443	-1.499448	1.219659
29	1	0	3.809185	-2.325143	1.736607
30	1	0	3.930408	-1.156287	0.382617
31	1	0	3.153363	-0.674635	1.914799

INT1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.411582	-0.879008	-1.560505
2	6	0	1.617811	-1.827857	-0.678009
3	6	0	1.645393	-1.505646	0.738635
4	6	0	2.385671	-0.423133	1.266557
5	6	0	3.485491	0.223060	0.431080
6	6	0	3.726327	-0.514775	-0.882115
7	8	0	-0.335631	1.212154	1.210422
8	16	0	-0.421930	2.004089	-0.118184
9	8	0	-1.275485	3.190809	0.042298
10	29	0	-1.257231	-0.427280	0.420469
11	8	0	-1.104756	0.947913	-1.007391
12	8	0	-1.241458	-1.625512	1.825959
13	8	0	-2.162950	-1.808617	-0.784381
14	6	0	-3.433906	-1.366268	-1.284094
15	8	0	0.929038	2.313095	-0.618537
16	1	0	1.410185	0.192199	1.196910
17	1	0	-0.929717	-1.139189	2.597925
18	1	0	0.956417	-2.040165	1.399475
19	1	0	2.538113	-0.465296	2.348187
20	1	0	3.215369	1.267331	0.233681
21	1	0	4.400900	0.245691	1.031518
22	1	0	2.045051	-2.852384	-0.688028
23	1	0	0.576778	-1.995235	-0.994553
24	1	0	4.346458	0.098878	-1.543849
25	1	0	4.289004	-1.439288	-0.683257
26	1	0	2.581158	-1.342978	-2.537004
27	1	0	1.817596	0.029842	-1.730807
28	1	0	-2.302791	-2.575671	-0.209674
29	1	0	-3.895679	-2.157802	-1.879947
30	1	0	-4.098626	-1.078351	-0.463209
31	1	0	-3.239896	-0.498865	-1.916297

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.434818	-2.047240	0.412999
2	6	0	-1.628792	-1.490133	-0.951884
3	6	0	-2.531467	-0.498382	-1.225872
4	6	0	-3.483744	0.041524	-0.198399
5	6	0	-3.497914	-0.796067	1.077483
6	6	0	-2.087970	-1.197627	1.494369
7	8	0	1.563016	-1.529612	-1.775498
8	29	0	1.345744	-0.335050	-0.400010
9	8	0	2.462107	-1.504228	0.853277
10	6	0	3.674870	-0.867519	1.280189
11	8	0	-0.135891	0.944954	-1.086645
12	16	0	0.092863	1.955835	0.101121
13	8	0	-1.153115	2.133184	0.856190
14	8	0	1.127136	1.160495	0.902944
15	8	0	0.661297	3.196055	-0.436664
16	1	0	-1.273169	0.003657	-1.021988
17	1	0	1.162948	-1.122986	-2.552764
18	1	0	-0.994374	-1.869080	-1.753761
19	1	0	-2.657284	-0.186005	-2.262785
20	1	0	-3.207776	1.082651	0.016737
21	1	0	-4.478707	0.080212	-0.657026
22	1	0	-1.885950	-3.052668	0.379999
23	1	0	-0.367218	-2.220041	0.602003
24	1	0	-3.997329	-0.241445	1.879280
25	1	0	-4.088982	-1.707399	0.904010
26	1	0	-2.100409	-1.749593	2.440039
27	1	0	-1.480875	-0.294165	1.654304
28	1	0	2.688777	-2.281322	0.321275
29	1	0	4.251787	-1.548820	1.910810
30	1	0	4.275611	-0.553412	0.420364
31	1	0	3.383175	0.009377	1.859718

PCb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.223790	-1.166091	1.465323
2	6	0	-1.571611	-1.981397	0.355363
3	6	0	-1.795961	-1.364054	-0.993563
4	6	0	-2.734432	-0.432690	-1.226578
5	6	0	-3.673982	0.073422	-0.172386
6	6	0	-3.651563	-0.796734	1.080783
7	8	0	1.641273	-1.589466	-1.789216
8	29	0	1.403698	-0.415341	-0.422589
9	8	0	1.114691	1.056198	0.905502
10	16	0	0.217098	2.016065	0.161574
11	8	0	0.907422	3.211803	-0.291441
12	8	0	2.424967	-1.610802	0.870673
13	6	0	3.629538	-1.005987	1.365995
14	8	0	-0.004947	1.110009	-1.211193
15	8	0	-1.089726	2.187771	0.780292
16	1	0	-0.864168	0.610178	-1.151102
17	1	0	1.245562	-1.180305	-2.568815
18	1	0	-1.161916	-1.706427	-1.813566
19	1	0	-2.845939	-0.029511	-2.234424
20	1	0	-3.404267	1.111288	0.079420
21	1	0	-4.689636	0.128257	-0.586964
22	1	0	-1.981783	-3.004601	0.346900
23	1	0	-0.494650	-2.110125	0.543049
24	1	0	-4.159963	-0.283425	1.905828
25	1	0	-4.215381	-1.722525	0.888072

26	1	0	-2.205036	-1.726005	2.408087
27	1	0	-1.641546	-0.245247	1.628584
28	1	0	2.656386	-2.401148	0.360389
29	1	0	4.128578	-1.689700	2.057436
30	1	0	4.303296	-0.744959	0.543897
31	1	0	3.331008	-0.100843	1.896556

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.687553	-1.179002	0.327639
2	6	0	0.687330	-1.179128	-0.327620
3	6	0	1.488559	0.042056	0.110753
4	6	0	0.665404	1.295683	0.059479
5	6	0	-0.665184	1.295808	-0.059377
6	6	0	-1.488547	0.042306	-0.110827
7	1	0	-2.384176	0.161335	0.514440
8	1	0	-1.197639	2.245837	-0.117637
9	1	0	-1.867971	-0.104691	-1.135581
10	1	0	-0.560719	-1.155638	1.421113
11	1	0	-1.235958	-2.099389	0.092251
12	1	0	1.198000	2.245682	0.117498
13	1	0	1.235518	-2.099605	-0.092083
14	1	0	0.560589	-1.155866	-1.421115
15	1	0	2.384201	0.161092	-0.514609
16	1	0	1.868105	-0.105094	1.135439

1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.258610	-0.712752	1.022808
2	6	0	-1.653248	-0.278700	-0.298138
3	8	0	-2.307668	0.926997	-0.664052
4	1	0	-2.054570	0.044402	1.789920
5	1	0	-1.918983	1.232937	-1.493542
6	1	0	-1.825859	-1.663314	1.350552
7	1	0	-1.851101	-1.059543	-1.053024
8	6	0	-0.156332	-0.112295	-0.177142
9	1	0	-3.342902	-0.834053	0.927226
10	6	0	0.682985	-1.208983	-0.379232
11	6	0	2.059762	-1.086156	-0.221965
12	6	0	2.613816	0.141172	0.135964
13	6	0	1.782571	1.239651	0.338308
14	6	0	0.404534	1.112508	0.185067
15	1	0	0.248256	-2.166630	-0.666237
16	1	0	2.703114	-1.947545	-0.386123
17	1	0	3.690144	0.241353	0.253307
18	1	0	2.209091	2.200766	0.616515
19	1	0	-0.248721	1.968974	0.339811

RCc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.511740	-0.889084	2.045857

2	6	0	-2.616025	-1.640093	1.649318
3	6	0	-3.446393	-1.168792	0.634273
4	6	0	-3.166053	0.045631	0.011758
5	6	0	-2.056264	0.803018	0.397443
6	6	0	-1.236672	0.328895	1.428872
7	6	0	-1.694533	2.036509	-0.387080
8	6	0	-1.100961	3.170284	0.412641
9	8	0	-0.749017	1.587498	-1.416438
10	29	0	0.472355	0.059949	-0.877773
11	8	0	-0.738261	-1.237433	-1.809124
12	6	0	-0.628939	-2.627061	-1.462630
13	16	0	2.648914	-0.128490	0.525414
14	8	0	2.582092	-0.156544	1.992278
15	8	0	1.903789	1.111283	-0.033149
16	8	0	1.741335	-1.225331	-0.083757
17	8	0	4.008301	-0.208471	-0.021416
18	1	0	-0.151345	2.884539	0.876908
19	1	0	-0.258287	2.351508	-1.756582
20	1	0	-1.796954	3.469647	1.202369
21	1	0	-2.583819	2.385685	-0.928661
22	1	0	-0.923159	4.040742	-0.227924
23	1	0	-3.810729	0.413648	-0.785663
24	1	0	-0.367924	0.902948	1.748035
25	1	0	-4.313741	-1.747072	0.325966
26	1	0	-0.860697	-1.247577	2.839687
27	1	0	-2.831743	-2.589590	2.132731
28	1	0	-1.649382	-0.950434	-1.632722
29	1	0	-0.795922	-2.773494	-0.390111
30	1	0	-1.357759	-3.201663	-2.039434
31	1	0	0.380099	-2.945414	-1.725681

$TS_{con}c$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.326620	0.016479	1.469938
2	6	0	3.681848	-0.339780	0.170017
3	6	0	2.802579	-1.085879	-0.598381
4	6	0	1.570524	-1.509160	-0.064483
5	6	0	1.226633	-1.145856	1.253387
6	6	0	2.097610	-0.377429	2.006582
7	6	0	0.702488	-2.284531	-0.903428
8	6	0	-0.539386	-2.804605	-0.574703
9	8	0	0.263532	0.528693	-2.559085
10	29	0	-0.343202	0.751773	-0.840585
11	16	0	-2.415038	-0.044341	0.651807
12	8	0	-3.737899	0.563465	0.500448
13	8	0	-1.943897	-0.570270	-0.776784
14	8	0	-1.329275	0.999241	0.895937
15	8	0	-2.341212	-1.146323	1.616042
16	1	0	-1.223070	-1.710294	-0.735813
17	1	0	-0.390054	-0.023934	-3.003415
18	1	0	-0.787532	-2.961832	0.476514
19	1	0	1.037812	-2.394602	-1.936973
20	1	0	-0.982744	-3.509072	-1.275665
21	1	0	3.054491	-1.356285	-1.621598
22	1	0	0.268901	-1.449664	1.671625
23	1	0	4.636605	-0.026212	-0.242090
24	1	0	1.828768	-0.086078	3.018254
25	1	0	4.009638	0.610769	2.071667
26	8	0	1.208862	2.014875	-0.442817
27	1	0	1.401079	2.476769	-1.270810
28	6	0	1.073028	2.969278	0.614991
29	1	0	1.997079	3.546073	0.711303
30	1	0	0.227527	3.641839	0.439710
31	1	0	0.902397	2.402008	1.531900

PCc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.492200	-2.249226	-1.934618
2	6	0	-0.814023	-2.425927	-1.483514
3	6	0	-1.088932	-2.334372	-0.120058
4	6	0	-0.058095	-2.050331	0.779394
5	6	0	1.255073	-1.834435	0.327690
6	6	0	1.517290	-1.955762	-1.041005
7	6	0	2.280990	-1.472577	1.311970
8	6	0	3.478002	-0.931966	1.047039
9	8	0	-1.715054	-0.062541	2.406181
10	29	0	-1.143716	0.333183	0.734347
11	8	0	-2.961132	0.858093	-0.099443
12	6	0	-3.244462	0.241725	-1.362336
13	16	0	1.097235	1.817681	-0.575086
14	8	0	2.231216	1.326864	-1.354106
15	8	0	1.448279	1.590231	0.988723
16	8	0	-0.131556	0.969921	-0.812464
17	8	0	0.800334	3.242604	-0.656658
18	1	0	1.965808	0.759128	1.091630
19	1	0	-2.318210	0.638455	2.684151
20	1	0	3.807395	-0.714573	0.032397
21	1	0	2.000234	-1.640036	2.353854
22	1	0	4.170598	-0.692841	1.848815
23	1	0	-0.263214	-2.017574	1.847842
24	1	0	2.531250	-1.824996	-1.412964
25	1	0	-2.098265	-2.499461	0.253578
26	1	0	0.715350	-2.340896	-2.994649
27	1	0	-1.611180	-2.650754	-2.187878
28	1	0	-3.663185	0.626285	0.524978
29	1	0	-3.331082	-0.845242	-1.261727
30	1	0	-4.168825	0.654343	-1.775764
31	1	0	-2.409636	0.478817	-2.024169

TS1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.257867	0.735306	0.508861
2	6	0	2.746556	-0.588591	0.441545
3	6	0	3.590880	-1.643469	0.005999
4	6	0	4.894804	-1.372989	-0.348410
5	6	0	5.374843	-0.059870	-0.279867
6	6	0	4.562488	0.994844	0.149080
7	6	0	1.409804	-0.793635	0.790997
8	6	0	0.657427	-2.038064	0.786194
9	8	0	0.427713	0.499593	-1.623319
10	29	0	-1.093049	0.691089	-0.594018
11	8	0	-2.693133	0.613574	0.575470
12	16	0	-3.119650	-0.799106	0.123930
13	8	0	-4.457963	-0.771280	-0.487371
14	8	0	-0.511097	2.586823	-0.098523
15	6	0	-0.527887	2.898252	1.299225
16	8	0	-2.037224	-1.070268	-0.943908
17	8	0	-2.998315	-1.756381	1.236652
18	1	0	0.871183	0.086346	1.151092
19	1	0	-0.223185	-1.899245	0.135846
20	1	0	0.409753	-0.401341	-1.966694
21	1	0	0.226650	-2.187846	1.786553
22	1	0	1.219775	-2.918621	0.476464
23	1	0	0.392573	2.670856	-0.436489
24	1	0	0.116231	2.217527	1.867921
25	1	0	-0.202111	3.930038	1.455244
26	1	0	-1.558739	2.785559	1.636789
27	1	0	3.209690	-2.658588	-0.043432

28	1	0	5.549629	-2.171604	-0.681741
29	1	0	6.403360	0.143994	-0.565736
30	1	0	4.958299	2.004260	0.193539
31	1	0	2.599162	1.535600	0.840526

INT1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.683244	-0.296345	-1.337264
2	6	0	-1.759057	-1.355143	-0.388163
3	6	0	-2.835367	-1.384851	0.540224
4	6	0	-3.794426	-0.397438	0.506318
5	6	0	-3.698888	0.633653	-0.437858
6	6	0	-2.648359	0.688650	-1.358828
7	6	0	-0.755792	-2.321004	-0.415926
8	6	0	-0.624180	-3.507544	0.415526
9	8	0	1.472737	-0.756650	1.034064
10	16	0	2.409081	-0.699824	-0.189092
11	8	0	3.781752	-0.357469	0.219686
12	29	0	0.408031	0.882711	0.437850
13	8	0	1.762835	0.461032	-0.969512
14	8	0	-0.702073	1.180472	1.872343
15	8	0	-0.197588	2.627542	-0.479201
16	6	0	0.734729	3.680070	-0.194244
17	8	0	2.328623	-1.953074	-0.964289
18	1	0	0.040083	-2.175949	-1.151422
19	1	0	0.356032	-3.457871	0.912789
20	1	0	-0.461283	0.531344	2.542461
21	1	0	-0.547030	-4.382114	-0.247160
22	1	0	-1.415271	-3.660421	1.149433
23	1	0	-1.049214	2.849131	-0.074135
24	1	0	0.406898	4.611550	-0.663735
25	1	0	0.845575	3.823124	0.886376
26	1	0	1.692832	3.373436	-0.619360
27	1	0	-2.899991	-2.182312	1.273902
28	1	0	-4.621547	-0.411092	1.208528
29	1	0	-4.460714	1.408355	-0.454161
30	1	0	-2.595479	1.497878	-2.079911
31	1	0	-0.851859	-0.281620	-2.039209

TS2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.089381	-1.840625	1.787985
2	6	0	0.580916	-2.069136	0.838967
3	6	0	-0.095997	-2.902457	-0.035123
4	8	0	0.852322	0.909157	-1.834526
5	29	0	-0.300985	0.731019	-0.419011
6	8	0	0.502507	2.433636	0.418852
7	6	0	-0.406936	3.542866	0.444305
8	16	0	-2.644693	-0.452073	0.114417
9	8	0	-2.909117	-1.587152	1.003540
10	8	0	-1.572751	-0.880570	-0.969968
11	8	0	-1.851878	0.645543	0.827253
12	8	0	-3.818830	0.086505	-0.575520
13	1	0	-0.814835	-1.909846	-0.468225
14	1	0	1.170793	0.028476	-2.064666
15	1	0	-0.871154	-3.546931	0.376687
16	6	0	1.777976	-1.331370	0.563593
17	1	0	0.401525	-3.259127	-0.937225
18	1	0	1.201719	2.611444	-0.230215
19	1	0	0.123405	4.451483	0.741275

20	1	0	-0.878434	3.687533	-0.533486
21	1	0	-1.172483	3.309700	1.185389
22	6	0	2.611375	-1.646248	-0.528484
23	6	0	3.736071	-0.883269	-0.782597
24	6	0	4.043683	0.202499	0.043337
25	6	0	3.234038	0.520740	1.131500
26	6	0	2.108814	-0.246834	1.397337
27	1	0	2.378152	-2.499081	-1.160510
28	1	0	4.383140	-1.129651	-1.619600
29	1	0	4.929343	0.798335	-0.162018
30	1	0	3.482207	1.364298	1.769414
31	1	0	1.463225	-0.010103	2.241803

1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.798626	-1.200017	-0.018480
2	6	0	-0.065067	-0.013006	-0.019268
3	6	0	-0.764100	1.199002	0.002072
4	6	0	-2.154258	1.221732	0.010486
5	6	0	-2.876076	0.030101	-0.000829
6	6	0	-2.191784	-1.180244	-0.012795
7	6	0	1.459057	-0.030787	-0.001100
8	8	0	1.955896	-1.351307	-0.224570
9	6	0	1.960381	0.348688	1.385184
10	1	0	1.575521	-0.356323	2.130935
11	1	0	1.694736	-1.614172	-1.117614
12	1	0	1.628350	1.356208	1.655976
13	6	0	2.042924	0.896204	-1.061467
14	1	0	3.056302	0.322424	1.407504
15	1	0	-0.218879	2.141321	0.017584
16	1	0	-2.676602	2.175536	0.024888
17	1	0	-3.963191	0.047203	0.002414
18	1	0	-2.741892	-2.118566	-0.016398
19	1	0	-0.271018	-2.150071	-0.019135
20	1	0	3.135585	0.812184	-1.050929
21	1	0	1.679317	0.621005	-2.059273
22	1	0	1.779889	1.943677	-0.882214

$CuSO_4$-anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.123695	1.160838	0.320351
2	16	0	-1.792590	-0.200945	0.007414
3	8	0	-2.449263	-0.741701	1.206988
4	29	0	0.752122	0.447919	-0.045949
5	8	0	-0.544827	-1.026129	-0.359473
6	8	0	1.814254	1.938978	0.199056
7	8	0	2.389681	-0.672940	-0.538046
8	6	0	2.582715	-1.794229	0.337261
9	8	0	-2.693806	-0.074244	-1.151340
10	1	0	1.242761	2.627080	0.558967
11	1	0	3.137322	-0.065397	-0.437342
12	1	0	3.495081	-2.329254	0.061331
13	1	0	2.638933	-1.470505	1.381600
14	1	0	1.720765	-2.449505	0.205501

Cyclohexane-cation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.852514	-1.108857	0.341337
2	6	0	1.470098	0.213475	-0.082000
3	6	0	0.534211	1.322018	-0.163931
4	6	0	-0.849945	1.179619	0.085829
5	6	0	-1.482961	-0.207632	0.081351
6	6	0	-0.498024	-1.293833	-0.339299
7	1	0	-0.622502	1.517142	1.167219
8	1	0	0.942403	2.329363	-0.289407
9	1	0	-1.461750	2.010158	-0.275887
10	1	0	-1.877315	-0.422074	1.081818
11	1	0	-2.343461	-0.187459	-0.595515
12	1	0	1.864104	0.169516	-1.118877
13	1	0	2.351876	0.521894	0.500503
14	1	0	-0.914574	-2.280514	-0.111325
15	1	0	-0.352711	-1.252307	-1.429269
16	1	0	1.537487	-1.927054	0.098558
17	1	0	0.721093	-1.107410	1.432463

RCd

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.154562	-0.269108	1.478891
2	6	0	-1.360321	-1.582205	1.894709
3	6	0	-2.438081	-2.311754	1.400944
4	6	0	-3.300516	-1.720117	0.482512
5	6	0	-3.090849	-0.407853	0.064352
6	6	0	-2.017609	0.341282	0.558523
7	6	0	-1.731024	1.743853	0.039761
8	6	0	-1.040712	2.636140	1.056704
9	8	0	-0.813166	1.527262	-1.098798
10	29	0	0.621698	0.143523	-0.839130
11	8	0	2.088186	-1.068697	-0.324460
12	16	0	2.863037	0.013727	0.467365
13	8	0	4.204847	0.212438	-0.091856
14	8	0	-0.426801	-1.151116	-1.966608
15	6	0	-0.276192	-2.549487	-1.672005
16	8	0	1.947082	1.222137	0.146695
17	8	0	2.842674	-0.283621	1.905375
18	1	0	-0.068627	2.241437	1.363980
19	1	0	-0.433853	2.381156	-1.362705
20	1	0	-1.673917	2.750434	1.942861
21	6	0	-2.954156	2.449057	-0.518736
22	1	0	-0.880284	3.631110	0.625318
23	1	0	-3.783224	0.029504	-0.649972
24	1	0	-0.303212	0.276412	1.880385
25	1	0	-4.146574	-2.278745	0.089989
26	1	0	-0.675619	-2.029508	2.611377
27	1	0	-2.603923	-3.334768	1.729006
28	1	0	-1.362955	-0.918816	-1.862232
29	1	0	-0.507345	-2.750122	-0.619895
30	1	0	-0.939108	-3.128290	-2.319745
31	1	0	0.761475	-2.811009	-1.879635
32	1	0	-2.677758	3.452407	-0.861688
33	1	0	-3.383794	1.908940	-1.366929
34	1	0	-3.717559	2.551991	0.260084

TS1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.927040	-1.848528	-0.303174
2	6	0	0.883245	-2.870444	-0.086799
3	8	0	0.491441	-0.201073	-2.298633

4	29	0	-0.558189	0.415478	-0.906384
5	8	0	-1.868790	-1.118828	-0.669084
6	16	0	-2.537101	-0.474958	0.564841
7	8	0	-3.978229	-0.284233	0.335535
8	8	0	-1.800324	0.877262	0.592081
9	8	0	-2.234943	-1.256190	1.779459
10	1	0	-0.113628	-2.418672	-0.213063
11	1	0	0.083971	-1.021266	-2.600755
12	1	0	0.989485	-3.703854	-0.782797
13	8	0	0.451989	2.201847	-0.882859
14	1	0	1.137939	2.091866	-1.557624
15	6	0	-0.390690	3.298555	-1.263542
16	1	0	0.197911	4.217316	-1.329281
17	1	0	-0.884180	3.101324	-2.221214
18	1	0	-1.145060	3.404810	-0.482552
19	1	0	0.920595	-3.249308	0.940993
20	6	0	2.876104	-2.134005	-1.388818
21	1	0	3.465060	-3.007944	-1.068270
22	1	0	2.322937	-2.469283	-2.273266
23	1	0	3.554638	-1.326832	-1.656742
24	6	0	2.025243	-0.708560	0.542838
25	6	0	3.042130	0.261110	0.360414
26	6	0	1.080987	-0.512213	1.581517
27	6	0	3.108508	1.369006	1.182199
28	1	0	3.780315	0.142072	-0.425427
29	6	0	1.149452	0.602082	2.393931
30	1	0	0.278688	-1.228509	1.734443
31	6	0	2.162475	1.542215	2.195156
32	1	0	3.892053	2.106531	1.038257
33	1	0	0.410105	0.746897	3.176325
34	1	0	2.214175	2.419733	2.834315

INTd

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.929940	0.198310	-2.254361
2	6	0	2.988359	-0.356468	-1.531515
3	6	0	3.219863	0.011032	-0.202686
4	6	0	2.384977	0.925728	0.409270
5	6	0	1.319309	1.522463	-0.311396
6	6	0	1.113013	1.140725	-1.660478
7	6	0	0.477728	2.481378	0.318241
8	6	0	-0.518126	3.261343	-0.423078
9	8	0	0.359669	-0.523664	2.601954
10	29	0	-0.253757	-0.897186	0.893943
11	8	0	1.147824	-2.388217	0.677758
12	6	0	1.158947	-3.148846	-0.535153
13	16	0	-2.322286	-0.211684	-0.572066
14	8	0	-2.346121	0.860634	-1.584854
15	8	0	-1.878107	0.335011	0.798497
16	8	0	-1.168968	-1.195960	-0.853116
17	8	0	-3.604937	-0.926971	-0.457319
18	1	0	-1.466430	2.704213	-0.318334
19	1	0	-0.371678	-0.075461	3.042239
20	1	0	-0.315390	3.371696	-1.488209
21	6	0	0.546999	2.702397	1.773019
22	1	0	-0.672580	4.235624	0.048685
23	1	0	2.568358	1.210643	1.440361
24	1	0	0.286958	1.562831	-2.223885
25	1	0	4.055741	-0.414781	0.345044
26	1	0	1.754046	-0.104950	-3.281734
27	1	0	3.641447	-1.083314	-2.008113
28	1	0	2.010001	-1.958948	0.787051
29	1	0	1.276937	-2.499811	-1.410034
30	1	0	1.967770	-3.883735	-0.503899
31	1	0	0.199613	-3.664482	-0.596999
32	1	0	-0.276119	3.328128	2.121871
33	1	0	0.565997	1.744819	2.312950
34	1	0	1.489929	3.217836	2.007177

TS2d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.728416	0.721891	2.091784
2	6	0	2.940109	1.098425	1.512974
3	6	0	3.487172	0.334587	0.482389
4	6	0	2.822167	-0.797174	0.029273
5	6	0	1.599850	-1.192886	0.601802
6	6	0	1.067810	-0.413310	1.647683
7	6	0	0.886294	-2.360036	0.086160
8	6	0	-0.337000	-2.767440	0.605671
9	8	0	0.417933	-0.140397	-2.510286
10	29	0	-0.354844	0.576026	-1.002935
11	8	0	0.977984	2.138156	-1.034720
12	6	0	0.673771	3.293587	-0.246372
13	16	0	-2.491355	0.058339	0.540813
14	8	0	-2.412384	-0.585449	1.855707
15	8	0	-1.793631	-0.878221	-0.541456
16	8	0	-1.568607	1.269425	0.442041
17	8	0	-3.846503	0.362275	0.078514
18	1	0	-1.039485	-1.852757	-0.027510
19	1	0	-0.112093	-0.911773	-2.744274
20	1	0	-0.621104	-2.482889	1.617813
21	6	0	1.405783	-3.045969	-1.125522
22	1	0	-0.732605	-3.720748	0.259376
23	1	0	3.260445	-1.376597	-0.777502
24	1	0	0.117073	-0.674415	2.105170
25	1	0	4.433203	0.621018	0.031582
26	1	0	1.296750	1.318232	2.891249
27	1	0	3.457105	1.988590	1.862562
28	1	0	1.829443	1.775383	-0.738100
29	1	0	0.585735	3.037292	0.814951
30	1	0	1.453109	4.048455	-0.383222
31	1	0	-0.279172	3.684812	-0.606258
32	1	0	0.746995	-3.859738	-1.433382
33	1	0	1.510963	-2.329216	-1.948783
34	1	0	2.401214	-3.460176	-0.925024

PCd

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.994867	0.584802	-1.544544
2	6	0	1.650580	-0.522471	-2.071562
3	6	0	2.883529	-0.918916	-1.558021
4	6	0	3.450613	-0.199862	-0.509559
5	6	0	2.793076	0.905720	0.020355
6	6	0	1.557844	1.327096	-0.493702
7	6	0	0.863059	2.507398	0.074942
8	6	0	1.237734	2.930009	1.464244
9	6	0	-0.080993	3.180014	-0.609000
10	8	0	-1.707737	0.845173	0.716654
11	16	0	-2.505075	0.038783	-0.506925
12	8	0	-3.817341	-0.262192	0.041322
13	29	0	-0.242257	-0.760582	0.883625
14	8	0	-1.600768	-1.162484	-0.585829
15	8	0	0.562308	-0.365628	2.482258
16	8	0	0.942318	-2.398678	0.705691
17	6	0	0.520305	-3.463657	-0.154038
18	8	0	-2.454232	0.897870	-1.682053
19	1	0	-1.210793	1.622072	0.346547
20	1	0	-0.012981	0.280376	2.912301

21	1	0	-0.346539	2.935224	-1.634558
22	1	0	-0.580103	4.037826	-0.163497
23	1	0	3.253454	1.451123	0.840419
24	1	0	0.019162	0.862111	-1.938644
25	1	0	4.410145	-0.502019	-0.096619
26	1	0	1.187191	-1.085694	-2.879098
27	1	0	3.392046	-1.790383	-1.963987
28	1	0	1.085958	-2.735465	1.602097
29	1	0	1.306439	-4.221879	-0.210206
30	1	0	-0.412761	-3.914456	0.198688
31	1	0	0.365623	-3.027534	-1.143509
32	1	0	0.576387	3.723830	1.822634
33	1	0	1.186574	2.078725	2.154809
34	1	0	2.266764	3.309175	1.499277

2d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.571878	1.209769	-0.177955
2	6	0	-0.206711	0.057559	0.007925
3	6	0	0.460959	-1.163551	0.171571
4	6	0	1.851045	-1.227759	0.175950
5	6	0	2.607372	-0.072990	0.004625
6	6	0	1.959009	1.147274	-0.176242
7	6	0	-1.687449	0.122388	0.020737
8	6	0	-2.343823	1.249002	0.328909
9	1	0	-3.431072	1.281003	0.317484
10	6	0	-2.441190	-1.133229	-0.307179
11	1	0	-1.831313	2.163701	0.617204
12	1	0	-0.109892	-2.078762	0.308669
13	1	0	2.343707	-2.187522	0.312366
14	1	0	3.693348	-0.122871	0.001698
15	1	0	2.537886	2.055250	-0.328152
16	1	0	0.081796	2.165775	-0.349208
17	1	0	-3.514497	-0.935911	-0.380947
18	1	0	-2.099238	-1.570850	-1.253181
19	1	0	-2.297265	-1.900583	0.464021

1e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.210836	1.265700	-0.367987
2	6	0	1.359105	0.056809	-0.008504
3	6	0	1.651855	-0.389377	1.412862
4	6	0	-0.121501	0.386244	-0.213573
5	6	0	-1.091119	-0.737365	0.123721
6	6	0	-2.509808	-0.481614	-0.371479
7	6	0	-3.155286	0.749573	0.245836
8	8	0	1.739793	-1.049788	-0.840791
9	1	0	3.275411	1.020995	-0.274874
10	1	0	1.582684	-0.784358	-1.756801
11	1	0	1.990746	2.112519	0.292928
12	1	0	2.017159	1.583317	-1.400887
13	1	0	1.334588	0.379056	2.127153
14	1	0	1.127962	-1.321638	1.650288
15	1	0	2.727220	-0.559766	1.541443
16	1	0	-0.354566	1.283593	0.379447
17	1	0	-0.257752	0.677502	-1.270304
18	1	0	-0.714440	-1.673060	-0.313130
19	1	0	-1.117240	-0.892173	1.213840
20	1	0	-3.128200	-1.363876	-0.155491
21	1	0	-2.496399	-0.380464	-1.467690

22	1	0	-4.202751	0.851421	-0.058571
23	1	0	-3.129976	0.695177	1.342424
24	1	0	-2.637287	1.670243	-0.048705

RCe–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.210836	1.265700	-0.367987
2	6	0	1.359105	0.056809	-0.008504
3	6	0	1.651855	-0.389377	1.412862
4	6	0	-0.121501	0.386244	-0.213573
5	6	0	-1.091119	-0.737365	0.123721
6	6	0	-2.509808	-0.481614	-0.371479
7	6	0	-3.155286	0.749573	0.245836
8	8	0	1.739793	-1.049788	-0.840791
9	1	0	3.275411	1.020995	-0.274874
10	1	0	1.582684	-0.784358	-1.756801
11	1	0	1.990746	2.112519	0.292928
12	1	0	2.017159	1.583317	-1.400887
13	1	0	1.334588	0.379056	2.127153
14	1	0	1.127962	-1.321638	1.650288
15	1	0	2.727220	-0.559766	1.541443
16	1	0	-0.354566	1.283593	0.379447
17	1	0	-0.257752	0.677502	-1.270304
18	1	0	-0.714440	-1.673060	-0.313130
19	1	0	-1.117240	-0.892173	1.213840
20	1	0	-3.128200	-1.363876	-0.155491
21	1	0	-2.496399	-0.380464	-1.467690
22	1	0	-4.202751	0.851421	-0.058571
23	1	0	-3.129976	0.695177	1.342424
24	1	0	-2.637287	1.670243	-0.048705

TS1e–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.693542	-2.512991	-0.472300
2	6	0	1.398210	-1.494824	0.288151
3	6	0	2.715309	-1.047767	-0.151459
4	6	0	3.307971	0.213907	0.450294
5	6	0	4.668257	0.553780	-0.146430
6	6	0	5.736535	-0.487022	0.149470
7	6	0	0.821179	-1.018168	1.540942
8	8	0	0.565998	0.747504	-1.725999
9	29	0	-0.791653	0.751701	-0.478563
10	8	0	0.077553	2.388199	0.409451
11	6	0	-0.834317	3.452085	0.716036
12	8	0	-2.255877	0.500830	0.845599
13	16	0	-2.845312	-0.740854	0.148704
14	8	0	-2.613368	-1.949268	0.962013
15	8	0	-1.968736	-0.773807	-1.123247
16	8	0	-4.258378	-0.526562	-0.199273
17	1	0	-0.218385	-2.013280	-0.857130
18	1	0	0.357990	0.049127	-2.357453
19	1	0	0.302878	-3.285724	0.201090
20	1	0	1.272245	-2.933010	-1.296040
21	1	0	1.454140	-1.447174	2.337339
22	1	0	0.929141	0.067955	1.648160
23	1	0	-0.210719	-1.343983	1.689534
24	1	0	3.322006	-1.940972	0.114203
25	1	0	2.744359	-1.052484	-1.251209
26	1	0	2.610311	1.045657	0.279198
27	1	0	3.405479	0.098134	1.539077

28	1	0	4.985468	1.527351	0.249118
29	1	0	4.563465	0.685572	-1.233710
30	1	0	6.716767	-0.169717	-0.221882
31	1	0	5.827032	-0.658026	1.230076
32	1	0	5.509175	-1.452388	-0.319757
33	1	0	0.699851	2.692620	-0.267941
34	1	0	-0.280391	4.333988	1.047937
35	1	0	-1.450937	3.702574	-0.153459
36	1	0	-1.474617	3.098952	1.525327

INTe–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.145253	-2.124208	1.574123
2	6	0	-2.492604	-1.390770	0.371812
3	6	0	-2.913110	-2.103900	-0.821677
4	6	0	-2.328361	0.058001	0.368560
5	6	0	-1.960229	0.747888	-0.940461
6	6	0	-1.906769	2.263020	-0.778326
7	6	0	-3.271828	2.895869	-0.560675
8	8	0	0.920375	-1.321950	0.971907
9	29	0	1.033394	0.655324	0.502339
10	8	0	1.623235	-0.400720	-1.086839
11	16	0	1.372766	-1.772408	-0.432541
12	8	0	0.278501	-2.482194	-1.122493
13	8	0	2.615975	-2.556098	-0.355082
14	8	0	1.492490	2.485764	-0.303272
15	6	0	2.900135	2.641557	-0.534667
16	8	0	0.389120	1.441823	2.041972
17	1	0	-1.047068	-2.249024	1.447197
18	1	0	0.219486	0.718441	2.656866
19	1	0	-2.605571	-3.109622	1.648954
20	1	0	-2.259897	-1.522906	2.481222
21	1	0	-3.528594	-1.501584	-1.493519
22	1	0	-1.948967	-2.273143	-1.343532
23	1	0	-3.349423	-3.080522	-0.607636
24	1	0	-3.347661	0.364918	0.693512
25	1	0	-1.665305	0.373878	1.189580
26	1	0	-0.978877	0.366562	-1.263020
27	1	0	-2.674235	0.491163	-1.734832
28	1	0	-1.439108	2.691906	-1.674732
29	1	0	-1.242248	2.509529	0.063319
30	1	0	-3.200027	3.987320	-0.502405
31	1	0	-3.955250	2.648274	-1.383382
32	1	0	-3.738829	2.552989	0.371714
33	1	0	1.220852	3.115580	0.380887
34	1	0	3.112062	3.658629	-0.874935
35	1	0	3.473569	2.422533	0.372742
36	1	0	3.172951	1.931456	-1.316846

TS2e–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.698226	-2.429447	-1.628530
2	6	0	1.545903	-2.193492	-0.562152
3	6	0	2.297865	-0.915528	-0.479055
4	6	0	2.158212	-0.179759	0.856462
5	6	0	2.818157	1.193232	0.828176
6	6	0	4.330438	1.131842	0.685030
7	6	0	1.662599	-3.157962	0.553007
8	8	0	-1.330631	-0.908651	-0.895844
9	16	0	-2.028890	-1.067139	0.521438

10	8	0	-3.459472	-1.307110	0.324696
11	29	0	-0.665893	1.006235	-0.466916
12	8	0	-0.234430	2.813551	0.384016
13	6	0	-1.386439	3.671141	0.369029
14	8	0	0.265607	1.456121	-1.983975
15	8	0	-1.755836	0.330560	1.072698
16	8	0	-1.321419	-2.105703	1.276998
17	1	0	-0.274728	-1.733320	-1.106474
18	1	0	0.182892	0.707275	-2.586809
19	1	0	0.285625	-3.428774	-1.762679
20	1	0	0.824686	-1.824353	-2.529009
21	1	0	2.725765	-3.369717	0.726090
22	1	0	1.284762	-2.711661	1.480791
23	1	0	1.125240	-4.087813	0.356448
24	1	0	3.355211	-1.180287	-0.646333
25	1	0	1.992047	-0.252536	-1.300721
26	1	0	1.087413	-0.075340	1.097151
27	1	0	2.597253	-0.778466	1.667577
28	1	0	2.555924	1.725827	1.752369
29	1	0	2.390225	1.780823	0.001202
30	1	0	4.778318	2.129439	0.747040
31	1	0	4.773148	0.515996	1.478687
32	1	0	4.631696	0.698715	-0.276662
33	1	0	0.441975	3.199199	-0.192431
34	1	0	-1.129064	4.648365	0.785174
35	1	0	-1.773326	3.785996	-0.649121
36	1	0	-2.142266	3.193764	0.994761

PCe–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.749055	-3.028084	-0.127644
2	6	0	1.377382	-2.043989	0.536461
3	6	0	2.713869	-1.525664	0.090790
4	6	0	2.784737	-0.006982	-0.052828
5	6	0	4.077028	0.477250	-0.699085
6	6	0	5.323207	0.144944	0.107223
7	6	0	0.799545	-1.431055	1.774890
8	8	0	-1.254681	-0.948470	-1.120067
9	16	0	-2.531555	-0.938596	-0.062136
10	8	0	-3.707642	-0.842219	-0.911206
11	29	0	-0.720133	1.113142	-0.434648
12	8	0	-0.069226	2.485396	0.931277
13	6	0	-1.108988	3.326195	1.453701
14	8	0	0.331839	1.825121	-1.739398
15	8	0	-2.208726	0.353138	0.652508
16	8	0	-2.411641	-2.114465	0.786755
17	1	0	-0.538360	-1.553773	-0.788062
18	1	0	0.606318	1.096065	-2.310089
19	1	0	-0.185325	-3.454308	0.237651
20	1	0	1.183639	-3.472514	-1.021775
21	1	0	1.545107	-1.412220	2.580712
22	1	0	0.511507	-0.383956	1.596926
23	1	0	-0.087679	-1.969892	2.120257
24	1	0	3.459110	-1.849809	0.835540
25	1	0	2.995747	-2.000563	-0.860742
26	1	0	1.931423	0.341064	-0.654589
27	1	0	2.679326	0.465667	0.936649
28	1	0	4.012201	1.565001	-0.841967
29	1	0	4.161068	0.042412	-1.706904
30	1	0	6.220560	0.586496	-0.340093
31	1	0	5.238119	0.527155	1.133252
32	1	0	5.488713	-0.937310	0.172143
33	1	0	0.552568	3.028723	0.423494
34	1	0	-0.674356	4.088994	2.104453
35	1	0	-1.674227	3.800393	0.645287
36	1	0	-1.771114	2.685111	2.036832

2e–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.505007	-1.108338	-0.059751
2	6	0	1.622378	-0.109576	-0.149472
3	6	0	2.032931	1.324533	-0.009017
4	6	0	0.162094	-0.365847	-0.393226
5	6	0	-0.741312	0.137791	0.733409
6	6	0	-2.189480	-0.314350	0.591827
7	6	0	-2.867230	0.203308	-0.667350
8	1	0	3.563431	-0.919607	0.114666
9	1	0	2.198123	-2.148564	-0.159307
10	1	0	1.676660	1.917505	-0.862475
11	1	0	1.590335	1.778353	0.887512
12	1	0	3.120168	1.430881	0.060009
13	1	0	-0.130925	0.125510	-1.335086
14	1	0	-0.004434	-1.444453	-0.534663
15	1	0	-0.337814	-0.215452	1.694144
16	1	0	-0.709382	1.237749	0.770225
17	1	0	-2.753617	0.019789	1.473427
18	1	0	-2.226270	-1.414408	0.605858
19	1	0	-3.929352	-0.063912	-0.690681
20	1	0	-2.796503	1.297491	-0.727676
21	1	0	-2.406758	-0.206009	-1.574467

RCe–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.836544	0.102138	0.216415
2	6	0	2.517355	0.193993	0.961034
3	6	0	1.770478	-1.133382	1.000195
4	6	0	1.358229	-1.741248	-0.334091
5	6	0	0.382751	-2.897939	-0.159914
6	6	0	-0.293138	-3.277987	-1.466252
7	6	0	2.705734	0.729703	2.367097
8	8	0	1.675382	1.146556	0.224868
9	29	0	-0.247273	0.984513	-0.264531
10	8	0	0.163879	1.805651	-2.072667
11	6	0	0.748449	0.887327	-3.011253
12	8	0	-2.088551	0.519767	-0.738364
13	16	0	-2.478939	0.057274	0.691336
14	8	0	-2.779731	-1.379903	0.701510
15	8	0	-1.130238	0.349953	1.392964
16	8	0	-3.546985	0.901858	1.237794
17	1	0	0.871558	-0.992079	1.615965
18	1	0	1.974727	2.051459	0.390847
19	1	0	2.410880	-1.843219	1.544151
20	1	0	3.317797	0.036524	2.954766
21	1	0	3.216396	1.700682	2.352480
22	1	0	1.736511	0.846570	2.866721
23	1	0	4.490823	-0.626839	0.708797
24	1	0	3.683996	-0.214800	-0.821394
25	1	0	4.348621	1.071854	0.212377
26	1	0	0.874278	-0.990146	-0.981137
27	1	0	2.238239	-2.075547	-0.904420
28	1	0	0.907555	-3.761535	0.274131
29	1	0	-0.385515	-2.605548	0.572354
30	1	0	-0.947256	-4.149503	-1.354479
31	1	0	-0.910129	-2.443202	-1.828725
32	1	0	0.444404	-3.508557	-2.246216
33	1	0	-0.672497	2.128400	-2.440840
34	1	0	0.128661	-0.011095	-3.117187
35	1	0	0.866914	1.378212	-3.979891

36	1	0	1.729520	0.614431	-2.616486

TS1e–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.222391	1.796365	1.614150
2	6	0	-0.888013	2.486866	0.516216
3	6	0	-0.415444	3.810303	0.132966
4	6	0	-1.944614	1.848987	-0.249722
5	6	0	-2.797688	0.773892	0.407810
6	6	0	-3.724423	0.110020	-0.599728
7	6	0	-4.529072	-1.011577	0.033878
8	8	0	1.042989	1.489765	-1.582877
9	29	0	1.422628	0.003943	-0.550930
10	8	0	1.427077	-1.650048	0.537868
11	16	0	-0.002383	-2.091040	0.150145
12	8	0	0.016477	-3.405014	-0.516212
13	8	0	-0.360821	-0.975813	-0.845141
14	8	0	-0.883086	-2.050332	1.335311
15	1	0	-1.288280	1.369064	-1.017993
16	1	0	1.851153	2.015465	-1.611986
17	1	0	-2.537218	2.589706	-0.799507
18	1	0	0.109983	4.324357	0.941616
19	1	0	0.342458	3.556433	-0.636189
20	1	0	-1.180410	4.430635	-0.339220
21	1	0	-0.808008	2.097559	2.503762
22	1	0	-0.284392	0.706034	1.558398
23	1	0	0.798589	2.156120	1.774090
24	1	0	-2.160149	0.002893	0.857471
25	1	0	-3.384998	1.224157	1.221161
26	1	0	-4.395206	0.862873	-1.039807
27	1	0	-3.119741	-0.286272	-1.429397
28	1	0	-5.195530	-1.494220	-0.688945
29	1	0	-3.860777	-1.781216	0.442281
30	1	0	-5.145951	-0.637141	0.861074
31	8	0	3.372902	0.544257	-0.197873
32	1	0	3.929651	0.132170	-0.874606
33	6	0	3.884882	0.198563	1.096557
34	1	0	3.947774	-0.886620	1.223606
35	1	0	4.871451	0.649683	1.235587
36	1	0	3.187787	0.607575	1.831888

INTe–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.223437	2.265909	1.422653
2	6	0	-1.557196	2.275782	0.000933
3	6	0	-0.777331	3.090627	-0.898314
4	6	0	-2.650409	1.459546	-0.523517
5	6	0	-3.299240	0.427484	0.379738
6	6	0	-4.087929	-0.601674	-0.416178
7	6	0	-4.745933	-1.630609	0.486272
8	8	0	2.056331	2.009719	-0.430689
9	29	0	1.861525	0.209327	0.010674
10	8	0	1.462987	-1.713619	0.270201
11	16	0	-0.015883	-1.612315	-0.157948
12	8	0	-0.285275	-2.453885	-1.335462
13	8	0	-0.072068	-0.117775	-0.533565
14	8	0	-0.900059	-1.905783	0.985281
15	1	0	-2.293099	1.021672	-1.470083
16	1	0	2.069042	2.484582	0.410003
17	1	0	-3.383876	2.212559	-0.874401

18	1	0	-0.648632	4.101263	-0.492003
19	1	0	0.261109	2.660116	-0.842860
20	1	0	-1.137647	3.096219	-1.928050
21	1	0	-2.130708	2.368632	2.030287
22	1	0	-0.841645	1.255691	1.644767
23	1	0	-0.473908	3.010081	1.695523
24	1	0	-2.529458	-0.103946	0.954861
25	1	0	-3.956704	0.922571	1.108978
26	1	0	-4.842204	-0.096031	-1.037349
27	1	0	-3.399727	-1.104535	-1.114169
28	1	0	-5.309012	-2.375629	-0.085843
29	1	0	-3.989785	-2.163004	1.077428
30	1	0	-5.439690	-1.152664	1.189624
31	8	0	3.794593	0.129607	0.676560
32	1	0	4.103373	1.001681	0.385146
33	6	0	4.581442	-0.880709	0.028439
34	1	0	4.452255	-0.841683	-1.058444
35	1	0	5.635976	-0.750837	0.284302
36	1	0	4.232387	-1.844450	0.401144

TS2e–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.208087	2.462157	1.376713
2	6	0	-1.550749	2.333751	-0.064117
3	6	0	-0.838684	3.210619	-1.016756
4	6	0	-2.390633	1.331481	-0.509261
5	6	0	-3.274955	0.498777	0.384457
6	6	0	-3.858169	-0.701322	-0.348908
7	6	0	-4.665323	-1.595930	0.574150
8	8	0	2.161270	1.977949	-0.358642
9	29	0	1.851105	0.198283	0.018670
10	8	0	1.352797	-1.710823	0.238079
11	16	0	-0.113778	-1.616686	-0.183959
12	8	0	-0.412284	-2.479522	-1.331103
13	8	0	-0.118075	-0.107438	-0.643151
14	8	0	-1.015445	-1.789475	0.961318
15	1	0	-1.243826	0.672731	-0.577974
16	1	0	1.976936	2.459109	0.457355
17	1	0	-2.678163	1.379359	-1.564076
18	1	0	-0.978541	4.255557	-0.714312
19	1	0	0.241576	3.002552	-0.935127
20	1	0	-1.169168	3.075917	-2.049472
21	1	0	-2.106327	2.716196	1.952573
22	1	0	-0.849519	1.499224	1.765392
23	1	0	-0.441157	3.221393	1.547250
24	1	0	-2.713703	0.153510	1.264831
25	1	0	-4.091654	1.128468	0.771662
26	1	0	-4.483865	-0.345764	-1.180787
27	1	0	-3.040737	-1.277641	-0.807642
28	1	0	-5.112125	-2.439118	0.036769
29	1	0	-4.029431	-2.004843	1.369871
30	1	0	-5.477668	-1.035894	1.054998
31	8	0	3.734901	-0.012073	0.768127
32	1	0	4.075411	0.877904	0.583967
33	6	0	4.530597	-0.970408	0.053628
34	1	0	4.472042	-0.800359	-1.026439
35	1	0	5.569741	-0.908696	0.386618
36	1	0	4.129291	-1.956527	0.290015

PCe–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.605571	1.761920	1.689208
2	6	0	-1.119807	2.172627	0.342671
3	6	0	-2.308490	1.804889	-0.173116
4	6	0	-3.379473	0.964188	0.446554
5	6	0	-3.953924	-0.064743	-0.524325
6	6	0	-5.011451	-0.936117	0.129642
7	6	0	-0.204950	3.084265	-0.419161
8	8	0	2.470554	1.227480	-1.621360
9	29	0	1.833872	0.029334	-0.408122
10	8	0	3.352949	0.490730	0.882179
11	6	0	4.297119	-0.582302	1.030717
12	8	0	1.123212	-1.526465	0.620719
13	16	0	-0.242909	-1.750173	0.017260
14	8	0	-1.333187	-1.539325	0.958745
15	8	0	-0.242868	-0.465658	-1.035383
16	8	0	-0.308443	-2.929193	-0.830391
17	1	0	-0.837815	0.257774	-0.699081
18	1	0	1.750517	1.406235	-2.239649
19	1	0	-2.556908	2.200273	-1.163939
20	1	0	-0.001695	3.994046	0.162397
21	1	0	0.770044	2.610306	-0.606152
22	1	0	-0.632487	3.381491	-1.382832
23	1	0	-0.460769	2.647045	2.323052
24	1	0	-1.263499	1.066768	2.216839
25	1	0	0.384758	1.289823	1.595584
26	1	0	-3.016312	0.451719	1.347395
27	1	0	-4.202479	1.618384	0.780457
28	1	0	-4.374256	0.458139	-1.396318
29	1	0	-3.139858	-0.696677	-0.910616
30	1	0	-5.444606	-1.653921	-0.575265
31	1	0	-4.581061	-1.504746	0.964439
32	1	0	-5.829924	-0.326265	0.533612
33	1	0	3.794237	1.235859	0.446931
34	1	0	4.676234	-0.906994	0.056318
35	1	0	5.125221	-0.260252	1.666686
36	1	0	3.766456	-1.405848	1.510306

2e–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.787641	1.454422	-0.112643
2	6	0	-1.566187	-0.020015	0.036522
3	6	0	-2.796298	-0.848378	-0.185913
4	6	0	-0.394845	-0.594551	0.343584
5	6	0	0.930889	0.055859	0.578992
6	6	0	1.991452	-0.412087	-0.416600
7	6	0	3.356237	0.191316	-0.134685
8	1	0	-0.381451	-1.687406	0.413814
9	1	0	-3.593186	-0.564216	0.515554
10	1	0	-3.203694	-0.683037	-1.193177
11	1	0	-2.599756	-1.919065	-0.066468
12	1	0	-2.540169	1.803728	0.607805
13	1	0	-0.882135	2.050379	0.028756
14	1	0	-2.191994	1.681017	-1.108768
15	1	0	0.856123	1.151423	0.538932
16	1	0	1.284482	-0.185862	1.595258
17	1	0	2.051678	-1.510416	-0.387430
18	1	0	1.664603	-0.154514	-1.434616
19	1	0	4.110365	-0.147197	-0.853403
20	1	0	3.318332	1.287134	-0.181314
21	1	0	3.705165	-0.081353	0.869523

1f–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.115937	-0.401030	0.301541
2	6	0	2.710504	0.003277	-0.024420
3	6	0	2.415700	1.457730	0.184399
4	6	0	1.810442	-0.889174	-0.458896
5	6	0	0.374723	-0.608124	-0.793076
6	6	0	-0.528382	-0.714387	0.433184
7	6	0	-1.979762	-0.287161	0.206466
8	8	0	-2.620875	-0.485846	1.466489
9	6	0	-2.032731	1.144840	-0.151096
10	6	0	-2.075002	2.318678	-0.440253
11	6	0	-2.668061	-1.122049	-0.865799
12	1	0	-2.577962	-2.184086	-0.610367
13	1	0	-0.121894	-0.093093	1.244243
14	1	0	-0.549794	-1.749726	0.802840
15	1	0	0.034976	-1.316429	-1.560343
16	1	0	0.265615	0.393962	-1.232049
17	1	0	2.131338	-1.930056	-0.548079
18	1	0	4.285233	-1.470384	0.137076
19	1	0	4.836608	0.159993	-0.309669
20	1	0	4.358195	-0.170322	1.348220
21	1	0	1.383161	1.731823	-0.053955
22	1	0	2.603579	1.735411	1.230797
23	1	0	3.087099	2.081370	-0.421797
24	1	0	-2.120854	3.357274	-0.691098
25	1	0	-3.554304	-0.258480	1.358406
26	1	0	-3.730686	-0.861537	-0.926410
27	1	0	-2.223523	-0.954555	-1.852020

RCf–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.230715	-2.503141	-1.087937
2	6	0	4.588236	-1.197269	-0.731303
3	6	0	3.626056	-0.661605	-1.495766
4	6	0	2.898453	0.623286	-1.225672
5	6	0	1.694331	0.404030	-0.309683
6	6	0	0.998661	1.690831	0.129258
7	6	0	1.926270	2.546345	0.881318
8	6	0	2.697859	3.248264	1.492464
9	6	0	5.104963	-0.571890	0.529072
10	6	0	0.367155	2.448353	-1.025583
11	8	0	-0.042878	1.276703	1.068504
12	29	0	-1.380859	-0.154986	0.551380
13	8	0	-0.290375	-1.494262	1.549894
14	6	0	-0.968896	-2.624328	2.119538
15	8	0	-2.645379	0.966726	-0.449379
16	16	0	-3.624857	-0.194928	-0.758304
17	8	0	-3.688324	-0.455144	-2.200714
18	8	0	-2.854664	-1.323724	-0.026891
19	8	0	-4.928534	0.040721	-0.127693
20	1	0	-0.299549	1.781294	-1.583028
21	1	0	2.015435	-0.132699	0.594024
22	1	0	0.956520	-0.229998	-0.824664
23	1	0	2.561765	1.058944	-2.175319
24	1	0	3.569887	1.362606	-0.767570
25	1	0	3.310666	-1.218565	-2.381336
26	1	0	4.822145	-2.924181	-2.012719
27	1	0	6.315994	-2.383598	-1.212835
28	1	0	5.094803	-3.239492	-0.283697
29	1	0	4.630190	0.385110	0.768558
30	1	0	4.945364	-1.248630	1.380128
31	1	0	6.190181	-0.412257	0.465681
32	1	0	3.375254	3.873905	2.034193
33	1	0	-0.536166	2.064324	1.350030
34	1	0	-0.209094	3.302947	-0.655396

35	1	0	1.138892	2.829631	-1.701308
36	1	0	0.192129	-1.023624	2.245333
37	1	0	-0.242465	-3.268602	2.620010
38	1	0	-1.740434	-2.304305	2.825693
39	1	0	-1.430474	-3.164785	1.293069

TS1f–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.117069	-2.655798	-0.709847
2	6	0	3.703189	-1.219329	-0.632247
3	6	0	4.212585	-0.478935	0.564926
4	6	0	2.912039	-0.674747	-1.570434
5	6	0	2.407682	0.732154	-1.567522
6	6	0	1.140566	0.808998	-0.644746
7	6	0	0.579356	2.163234	-0.669740
8	6	0	-0.545996	2.473161	-1.544980
9	6	0	1.185244	3.160596	0.084245
10	6	0	1.745011	4.031271	0.723197
11	8	0	-0.900729	1.543312	1.999940
12	29	0	-1.214995	-0.050738	1.130522
13	8	0	-2.759789	0.523537	-0.062478
14	16	0	-2.752956	-0.803060	-0.854408
15	8	0	-4.060912	-1.470900	-0.759818
16	8	0	-1.681105	-1.578607	-0.063894
17	8	0	-2.305273	-0.573348	-2.239593
18	1	0	-1.421032	1.936163	-1.125273
19	1	0	1.458887	0.546687	0.370827
20	1	0	0.400974	0.088787	-1.015814
21	1	0	2.123773	1.048253	-2.576813
22	1	0	3.155394	1.441118	-1.193905
23	1	0	2.553489	-1.312257	-2.380726
24	1	0	3.701363	-3.157802	-1.589427
25	1	0	5.211246	-2.746749	-0.740595
26	1	0	3.789171	-3.200642	0.187039
27	1	0	4.005946	0.595558	0.538015
28	1	0	3.753736	-0.884513	1.478890
29	1	0	5.295522	-0.621106	0.675398
30	1	0	2.233109	4.802203	1.284404
31	1	0	-1.612507	2.133797	1.726723
32	1	0	-0.758412	3.537241	-1.636067
33	1	0	-0.383755	1.999182	-2.523231
34	8	0	0.312952	-0.976586	2.149522
35	1	0	-0.001041	-1.152299	3.047596
36	6	0	0.860502	-2.181322	1.602599
37	1	0	1.675544	-2.538323	2.239220
38	1	0	0.098046	-2.959368	1.503213
39	1	0	1.258040	-1.930548	0.613759

INTf–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.237243	-2.492534	-0.649363
2	6	0	3.723020	-1.087936	-0.596776
3	6	0	2.948327	-0.595971	-1.577103
4	6	0	2.366208	0.779625	-1.607465
5	6	0	1.057097	0.800870	-0.736819
6	6	0	0.471529	2.142041	-0.759936
7	6	0	1.024412	3.124944	0.050952
8	6	0	1.528424	3.973977	0.761786
9	6	0	4.116031	-0.316863	0.624550
10	6	0	-0.649126	2.447481	-1.638764

11	8	0	-1.152194	1.397026	2.259595
12	29	0	-1.226286	-0.077210	1.166305
13	8	0	0.424875	-0.887981	2.101945
14	6	0	0.953537	-2.125355	1.614190
15	8	0	-2.759519	0.439772	-0.078416
16	16	0	-2.641912	-0.862773	-0.899612
17	8	0	-2.206960	-0.568791	-2.277160
18	8	0	-1.516477	-1.569993	-0.120279
19	8	0	-3.893759	-1.634166	-0.831282
20	1	0	-1.518820	1.927985	-1.182124
21	1	0	1.349017	0.535845	0.286820
22	1	0	0.350539	0.065480	-1.140816
23	1	0	2.106800	1.074642	-2.629396
24	1	0	3.059171	1.530000	-1.209921
25	1	0	2.674676	-1.254206	-2.403543
26	1	0	3.899733	-3.021684	-1.546295
27	1	0	5.335360	-2.507330	-0.628276
28	1	0	3.906080	-3.058775	0.232765
29	1	0	3.838351	0.741236	0.584660
30	1	0	3.635356	-0.755535	1.511864
31	1	0	5.198317	-0.385285	0.794754
32	1	0	1.965027	4.727545	1.385867
33	1	0	-1.930244	1.923104	2.043199
34	1	0	-0.859515	3.511055	-1.740740
35	1	0	-0.515140	1.948709	-2.607230
36	1	0	0.215305	-0.980237	3.041754
37	1	0	1.805747	-2.430852	2.228707
38	1	0	0.193603	-2.912418	1.612222
39	1	0	1.295569	-1.944436	0.589937

TS2f–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.249631	-0.227053	0.243239
2	6	0	1.084557	0.456225	0.857831
3	6	0	0.771188	1.777574	0.556309
4	6	0	0.264628	-0.275627	1.744892
5	6	0	-0.464736	-0.922159	2.467839
6	8	0	-1.368278	1.262465	-0.937071
7	16	0	-2.682258	1.670459	-0.156182
8	8	0	-2.333462	2.540963	0.971367
9	29	0	-1.655722	-0.797405	-0.462650
10	8	0	-0.293854	-1.491600	-1.473001
11	8	0	-3.131046	0.288511	0.320096
12	8	0	-3.632124	2.247406	-1.111152
13	1	0	-0.209676	1.504274	-0.224935
14	1	0	2.071604	-1.301940	0.135931
15	1	0	2.444923	0.207199	-0.744840
16	1	0	-1.110760	-1.484043	3.110641
17	1	0	0.069136	-2.263296	-1.022979
18	1	0	0.178388	2.340127	1.279552
19	8	0	-2.433161	-2.535552	0.319933
20	1	0	-1.824635	-3.269850	0.156332
21	6	0	-3.702002	-2.859301	-0.268986
22	1	0	-3.608516	-2.994301	-1.351520
23	1	0	-4.102623	-3.767683	0.188182
24	1	0	-4.367877	-2.020451	-0.062442
25	6	0	3.488513	0.009828	1.145809
26	1	0	3.616993	1.091227	1.281695
27	1	0	3.286739	-0.412586	2.138142
28	6	0	4.709221	-0.619490	0.548972
29	6	0	5.545000	-0.039700	-0.324801
30	1	0	4.901996	-1.656211	0.833796
31	6	0	6.731485	-0.775697	-0.867560
32	1	0	6.804934	-1.792039	-0.466801
33	1	0	6.683913	-0.838120	-1.963510
34	1	0	7.662526	-0.242185	-0.631235
35	6	0	5.386341	1.356745	-0.842914
36	1	0	5.273228	1.342300	-1.935669

37	1	0	4.523840	1.884292	-0.424083
38	1	0	6.287479	1.950126	-0.636588
39	1	0	1.502864	2.334961	-0.029031

PCf–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.240503	-2.026014	1.458504
2	6	0	-0.652659	-1.850286	0.190955
3	6	0	-2.070014	-1.578000	-0.241954
4	6	0	-3.024468	-1.210912	0.889225
5	6	0	-4.407986	-0.955469	0.373637
6	6	0	-4.942717	0.231751	0.054411
7	6	0	-4.231431	1.543931	0.183320
8	6	0	0.313134	-1.918384	-0.867435
9	29	0	2.331647	-0.619943	-0.313104
10	8	0	3.095006	-2.024588	0.580915
11	6	0	1.104902	-1.966054	-1.794733
12	6	0	-6.338133	0.333548	-0.483459
13	8	0	4.126572	0.393254	-0.029382
14	6	0	4.037730	1.441250	0.943380
15	8	0	1.534792	1.062097	-0.994474
16	16	0	0.470039	1.777541	-0.203793
17	8	0	-0.870914	1.500597	-0.718577
18	8	0	0.548265	1.127228	1.280234
19	8	0	0.818706	3.175280	0.019981
20	1	0	0.098873	0.255821	1.277327
21	1	0	0.805560	-2.228530	1.675895
22	1	0	1.748096	-2.066456	-2.646095
23	1	0	2.637951	-2.832382	0.316599
24	1	0	-2.055229	-0.763052	-0.979674
25	1	0	-3.056537	-2.027053	1.624482
26	1	0	-2.622659	-0.332259	1.415106
27	1	0	-5.019655	-1.846377	0.207089
28	1	0	-6.342273	0.817479	-1.470019
29	1	0	-6.816164	-0.647318	-0.578857
30	1	0	-6.963392	0.960627	0.167326
31	1	0	-4.821830	2.246211	0.787636
32	1	0	-3.234865	1.460190	0.625282
33	1	0	-4.117267	2.011160	-0.805226
34	1	0	-0.935276	-1.978615	2.292057
35	1	0	4.669762	-0.321614	0.335909
36	1	0	3.588712	1.077210	1.874430
37	1	0	5.031923	1.849439	1.144456
38	1	0	3.402388	2.219796	0.517269
39	1	0	-2.443052	-2.459693	-0.784957

2f–*aS*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.836223	-0.324730	-0.222137
2	6	0	-2.407636	0.042506	0.040523
3	6	0	-2.066951	1.471599	-0.257024
4	6	0	-1.527571	-0.858520	0.498674
5	6	0	-0.074813	-0.610403	0.772081
6	6	0	0.798263	-0.830410	-0.470688
7	6	0	2.237710	-0.458715	-0.232636
8	6	0	3.237681	-1.349925	-0.219668
9	6	0	2.487958	0.931489	0.007509
10	6	0	2.639448	2.118134	0.201992
11	1	0	0.397130	-0.217204	-1.291438
12	1	0	0.740375	-1.878411	-0.791613

13	1	0	0.279392	-1.276911	1.570042
14	1	0	0.083827	0.413577	1.137627
15	1	0	-1.881952	-1.880568	0.654396
16	1	0	-4.040456	-1.375394	0.009355
17	1	0	-4.516641	0.298469	0.374813
18	1	0	-4.100764	-0.145135	-1.273425
19	1	0	-1.015493	1.717010	-0.076377
20	1	0	-2.289544	1.702423	-1.307928
21	1	0	-2.687887	2.151579	0.342382
22	1	0	2.797158	3.161557	0.374119
23	1	0	4.265820	-1.053283	-0.030839
24	1	0	3.041839	-2.403864	-0.402873

(E)-**RCf**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.117564	-2.419866	-1.839627
2	6	0	1.271182	-1.451824	-1.030977
3	6	0	1.516854	-1.611745	0.409491
4	6	0	1.697692	-1.762317	1.596235
5	6	0	1.428299	-0.002128	-1.498177
6	6	0	2.861743	0.530988	-1.564362
7	6	0	3.565670	0.570097	-0.239366
8	6	0	3.415032	1.507100	0.706969
9	6	0	4.102040	1.386420	2.032509
10	6	0	2.527809	2.706176	0.565487
11	8	0	-1.722013	0.778790	-1.327529
12	29	0	-1.468978	-0.771865	-0.131597
13	8	0	-1.719235	-2.326239	1.119126
14	6	0	-1.738962	-2.009087	2.520753
15	16	0	-2.354377	1.667118	-0.230000
16	8	0	-3.700695	2.102144	-0.617925
17	8	0	-1.446303	2.760389	0.140646
18	8	0	-2.419151	0.606345	0.900173
19	8	0	-0.137259	-1.778363	-1.283951
20	1	0	0.975587	0.045220	-2.498361
21	1	0	1.887960	-3.455247	-1.566898
22	1	0	1.923412	-2.275100	-2.907952
23	1	0	1.871698	-1.887901	2.644375
24	1	0	-0.265441	-2.726565	-1.117344
25	1	0	0.831847	0.648163	-0.842161
26	1	0	3.443253	-0.064796	-2.279696
27	1	0	2.799906	1.538498	-1.996679
28	1	0	4.215464	-0.278521	-0.009594
29	1	0	3.363956	1.353400	2.847263
30	1	0	4.718902	0.482981	2.094280
31	1	0	4.740389	2.258167	2.233046
32	1	0	3.061365	3.621258	0.855719
33	1	0	2.139392	2.840730	-0.448910
34	1	0	1.665015	2.624172	1.242529
35	1	0	3.180656	-2.249271	-1.644843
36	1	0	-2.537680	-2.790448	0.890949
37	1	0	-2.608967	-1.397208	2.772955
38	1	0	-1.745012	-2.934214	3.102420
39	1	0	-0.823591	-1.450555	2.727300

(E)-**TS1f**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.257305	-2.722770	-1.592664
2	6	0	0.969423	-1.792116	-0.497549
3	6	0	1.422991	-0.408867	-0.512829
4	6	0	2.723164	-0.058164	-1.243402

5	6	0	3.938791	-0.451100	-0.457591
6	6	0	4.513698	0.277953	0.509986
7	6	0	4.020635	1.618779	0.961250
8	6	0	0.202947	-2.223870	0.578672
9	6	0	-0.472829	-2.590157	1.522446
10	6	0	5.728233	-0.216006	1.234464
11	8	0	-1.144636	1.245699	-1.398384
12	16	0	-1.122944	2.200714	-0.188979
13	8	0	0.261061	2.568890	0.162090
14	29	0	-2.020138	-0.278160	-0.312665
15	8	0	-2.017922	-1.527077	-1.670334
16	8	0	-1.730604	1.278248	0.888919
17	8	0	-1.992374	3.364976	-0.426799
18	1	0	0.574501	0.070958	-1.062612
19	1	0	0.622594	-3.608347	-1.573347
20	1	0	1.205298	-2.208428	-2.558171
21	1	0	-1.058608	-2.920586	2.356984
22	1	0	-2.118760	-2.389536	-1.250990
23	1	0	1.376829	0.027490	0.492126
24	1	0	2.737238	-0.526190	-2.234297
25	1	0	2.697168	1.023384	-1.418933
26	1	0	4.367095	-1.430222	-0.685187
27	1	0	5.536416	-0.290307	2.313734
28	1	0	6.054128	-1.196888	0.872776
29	1	0	6.562593	0.489799	1.119981
30	1	0	4.801948	2.380357	0.831620
31	1	0	3.119173	1.956332	0.440740
32	1	0	3.796033	1.592903	2.036564
33	1	0	2.308405	-3.033553	-1.470828
34	8	0	-3.095255	-1.437750	0.998907
35	1	0	-3.939591	-1.661957	0.582785
36	6	0	-3.336870	-0.927259	2.315398
37	1	0	-3.967049	-0.033641	2.286448
38	1	0	-3.807860	-1.699361	2.930022
39	1	0	-2.363547	-0.669421	2.737245

(E)*-INTf–*Sz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.347547	-2.663364	-1.463182
2	6	0	1.050989	-1.738609	-0.365561
3	6	0	1.499565	-0.354548	-0.371008
4	6	0	2.761517	0.023545	-1.150801
5	6	0	4.018476	-0.413485	-0.460268
6	6	0	4.700716	0.291073	0.454328
7	6	0	4.302806	1.649459	0.944103
8	6	0	0.292193	-2.180353	0.714810
9	6	0	-0.369883	-2.552793	1.664895
10	6	0	5.952932	-0.249666	1.073025
11	8	0	-1.106148	1.172814	-1.346873
12	16	0	-1.187611	2.170021	-0.173529
13	8	0	0.160961	2.586313	0.251040
14	29	0	-1.995093	-0.343630	-0.261103
15	8	0	-1.832041	-1.653922	-1.551658
16	8	0	-1.841783	1.266890	0.893720
17	8	0	-2.069762	3.299475	-0.509859
18	1	0	0.623690	0.129217	-0.874395
19	1	0	0.738461	-3.566065	-1.435361
20	1	0	1.267172	-2.151636	-2.428194
21	1	0	-0.949693	-2.881170	2.503890
22	1	0	-1.751423	-2.501790	-1.100409
23	1	0	1.491454	0.062330	0.643796
24	1	0	2.717693	-0.393532	-2.163520
25	1	0	2.731878	1.112533	-1.270461
26	1	0	4.390485	-1.407223	-0.721328
27	1	0	5.853790	-0.313935	2.165098
28	1	0	6.207473	-1.243066	0.689383
29	1	0	6.801082	0.422434	0.882168
30	1	0	5.098307	2.380264	0.744551

31	1	0	3.374694	2.021891	0.501576
32	1	0	4.171380	1.632112	2.034356
33	1	0	2.409176	-2.940403	-1.356197
34	8	0	-3.132629	-1.406126	1.087281
35	1	0	-3.403687	-2.229192	0.656623
36	6	0	-4.313627	-0.714401	1.521631
37	1	0	-4.955132	-0.463766	0.671214
38	1	0	-4.863728	-1.331698	2.236230
39	1	0	-3.981779	0.202933	2.008375

(E)-**TS2f**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.918660	2.753734	1.328001
2	6	0	0.863672	1.855585	0.147002
3	6	0	1.538558	0.635683	0.095002
4	6	0	2.673805	0.259650	1.025734
5	6	0	3.997724	0.643630	0.429925
6	6	0	4.756782	-0.125000	-0.364213
7	6	0	4.397508	-1.516481	-0.786999
8	6	0	-0.021331	2.178263	-0.906476
9	6	0	-0.803464	2.445296	-1.794531
10	6	0	6.061149	0.373503	-0.906428
11	8	0	-0.470542	-0.791111	1.153073
12	16	0	-0.691788	-2.045658	0.227018
13	8	0	0.536119	-2.326067	-0.526783
14	29	0	-2.107391	0.239730	0.231259
15	8	0	-2.292261	1.669484	1.371283
16	8	0	-1.795224	-1.496770	-0.683486
17	8	0	-1.175790	-3.159190	1.048705
18	1	0	0.531734	0.060093	0.591154
19	1	0	0.236355	3.599137	1.234652
20	1	0	0.664787	2.182988	2.229767
21	1	0	-1.486623	2.680693	-2.584344
22	1	0	-2.157763	2.467053	0.845234
23	1	0	1.563814	0.156398	-0.889167
24	1	0	2.537548	0.739280	2.001686
25	1	0	2.616918	-0.821509	1.201758
26	1	0	4.336472	1.660896	0.641734
27	1	0	6.055377	0.366866	-2.005149
28	1	0	6.287819	1.389782	-0.567706
29	1	0	6.885856	-0.285095	-0.600701
30	1	0	5.152202	-2.234001	-0.436742
31	1	0	3.416606	-1.845735	-0.431541
32	1	0	4.396862	-1.585737	-1.883295
33	1	0	1.944945	3.118232	1.459458
34	8	0	-3.621797	0.826108	-1.015309
35	1	0	-4.008139	1.581308	-0.547239
36	6	0	-4.643756	-0.165396	-1.201077
37	1	0	-5.017016	-0.528365	-0.238052
38	1	0	-5.464878	0.256462	-1.785948
39	1	0	-4.189828	-0.990841	-1.749880

(E)-**PCf**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.518326	-2.560501	-1.482698
2	6	0	0.846390	-1.729508	-0.274635
3	6	0	-0.030165	-1.878235	0.838526
4	6	0	-0.851364	-1.987002	1.740752
5	6	0	1.864287	-0.847526	-0.143421
6	6	0	2.901262	-0.490396	-1.153750

7	6	0	4.282040	-0.714291	-0.592615
8	6	0	4.998342	0.160894	0.126497
9	6	0	6.353806	-0.200233	0.653171
10	6	0	4.540533	1.542118	0.479774
11	8	0	-0.651596	0.948896	-1.346751
12	29	0	-2.216083	-0.666517	0.499040
13	8	0	-4.076605	0.293780	0.341374
14	6	0	-4.214567	1.008201	-0.894054
15	16	0	-0.655776	1.888089	-0.020195
16	8	0	-1.446258	3.041813	-0.435824
17	8	0	0.739159	2.146771	0.333620
18	8	0	-1.346903	1.056292	1.027411
19	8	0	-2.986298	-2.113943	-0.323809
20	1	0	-0.016180	0.216866	-1.209003
21	1	0	0.556511	-3.627778	-1.236798
22	1	0	-0.503506	-2.345621	-1.821457
23	1	0	-1.413531	-2.205303	2.627296
24	1	0	-2.403667	-2.872751	-0.197600
25	1	0	1.950024	-0.320966	0.809532
26	1	0	2.769368	-1.061738	-2.078577
27	1	0	2.755080	0.569157	-1.414549
28	1	0	4.701877	-1.708014	-0.760230
29	1	0	6.380369	-0.117906	1.748531
30	1	0	6.646073	-1.218503	0.376327
31	1	0	7.116640	0.494368	0.275170
32	1	0	5.262113	2.289975	0.123677
33	1	0	3.554954	1.795307	0.078938
34	1	0	4.496676	1.656073	1.571654
35	1	0	1.206143	-2.370643	-2.309496
36	1	0	-4.683282	-0.460626	0.315837
37	1	0	-3.973470	0.364192	-1.747897
38	1	0	-5.234772	1.388939	-0.995412
39	1	0	-3.513940	1.844563	-0.858442

(E)-**2f**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.598454	-1.607247	-0.155028
2	6	0	2.036683	-0.231334	0.065902
3	6	0	0.784647	0.058089	0.467674
4	6	0	-0.331070	-0.897129	0.754687
5	6	0	-1.437267	-0.719513	-0.251540
6	6	0	-2.513279	0.070276	-0.134450
7	6	0	-2.819476	0.915270	1.063560
8	6	0	2.945159	0.846927	-0.186716
9	6	0	3.739320	1.734784	-0.412558
10	6	0	-3.519882	0.173337	-1.239759
11	1	0	3.453616	-1.786100	0.507514
12	1	0	1.858389	-2.391155	0.021898
13	1	0	4.431107	2.526459	-0.606459
14	1	0	0.518709	1.112903	0.569184
15	1	0	0.022351	-1.934172	0.737745
16	1	0	-0.702617	-0.711391	1.771792
17	1	0	-1.301516	-1.260648	-1.190940
18	1	0	-3.612003	1.210941	-1.589326
19	1	0	-3.257874	-0.456482	-2.096230
20	1	0	-4.518302	-0.120477	-0.887398
21	1	0	-3.806094	0.661347	1.474413
22	1	0	-2.080116	0.823632	1.864328
23	1	0	-2.872542	1.974055	0.775284
24	1	0	2.967163	-1.709674	-1.182418

(Z)-**RCf**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.987052	3.223512	-2.066953
2	6	0	-0.636268	2.278358	-0.927042
3	6	0	-0.525456	3.013933	0.337900
4	6	0	-0.437323	3.630080	1.374469
5	6	0	-1.641438	1.129782	-0.846341
6	6	0	-1.695241	0.333041	0.456747
7	6	0	-2.490889	-0.922533	0.265992
8	6	0	-3.794046	-1.099354	0.524625
9	6	0	-4.470141	-2.405527	0.235090
10	6	0	-4.695493	-0.048832	1.098191
11	8	0	0.659459	1.686551	-1.254943
12	29	0	1.513918	0.236094	-0.152646
13	8	0	2.477794	1.557899	0.997897
14	6	0	3.183896	1.078616	2.154275
15	8	0	2.147329	-1.424063	0.680035
16	16	0	1.390191	-2.358072	-0.299897
17	8	0	2.329495	-3.186313	-1.064928
18	8	0	0.761900	-1.265364	-1.197911
19	8	0	0.354604	-3.119131	0.409733
20	1	0	-1.423319	0.466854	-1.695631
21	1	0	-0.216090	3.992174	-2.187929
22	1	0	-1.076505	2.653772	-2.997962
23	1	0	-0.363950	4.178271	2.289908
24	1	0	1.296109	2.405487	-1.395577
25	1	0	-1.939448	3.720984	-1.860588
26	1	0	-2.640295	1.549226	-1.029105
27	1	0	-0.684420	0.065655	0.805037
28	1	0	-2.119092	0.965065	1.247562
29	1	0	-1.941358	-1.752789	-0.186689
30	1	0	-5.299051	-2.268104	-0.473354
31	1	0	-3.777954	-3.143713	-0.183620
32	1	0	-4.914374	-2.827324	1.147606
33	1	0	-4.187533	0.898061	1.303493
34	1	0	-5.524633	0.156150	0.406799
35	1	0	-5.156503	-0.400867	2.031362
36	1	0	3.080366	2.085603	0.453690
37	1	0	4.015931	0.429974	1.867194
38	1	0	3.551217	1.930686	2.731336
39	1	0	2.466277	0.514172	2.750769

(Z)-**TS1f**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.150887	3.624460	-0.173436
2	6	0	-0.474159	2.286294	0.321924
3	6	0	0.319354	1.713132	1.311195
4	6	0	1.008182	1.184351	2.163825
5	6	0	-1.628943	1.553073	-0.197279
6	6	0	-2.301125	0.532717	0.721506
7	6	0	-3.238610	-0.340332	-0.051727
8	6	0	-4.573440	-0.243144	-0.120161
9	6	0	-5.373783	-1.200820	-0.949925
10	6	0	-5.389772	0.789535	0.594339
11	8	0	1.252639	1.342386	-1.880402
12	29	0	1.817702	0.063413	-0.667317
13	8	0	3.615216	0.977253	-0.307507
14	6	0	4.448612	0.446558	0.730889
15	8	0	2.065582	-1.487531	0.548952
16	16	0	0.714226	-2.156767	0.213924
17	8	0	0.928584	-3.480794	-0.395450
18	8	0	0.171281	-1.158653	-0.822325
19	8	0	-0.147163	-2.199345	1.410274
20	1	0	-1.149575	1.020252	-1.047525
21	1	0	-0.493648	3.759746	-1.202479
22	1	0	-0.749941	4.310018	0.451040
23	1	0	1.607841	0.716028	2.919399

24	1	0	1.847057	2.097101	-1.798056
25	1	0	0.900873	3.885349	-0.044371
26	1	0	-2.338602	2.251098	-0.659839
27	1	0	-1.528811	-0.093247	1.186126
28	1	0	-2.809380	1.069741	1.530905
29	1	0	-2.750695	-1.122836	-0.640688
30	1	0	-5.956150	-0.665480	-1.712597
31	1	0	-4.740362	-1.938284	-1.453815
32	1	0	-6.103610	-1.739065	-0.329298
33	1	0	-4.789635	1.503680	1.165376
34	1	0	-5.996093	1.356206	-0.125322
35	1	0	-6.100409	0.310774	1.281964
36	1	0	4.106690	0.967293	-1.140944
37	1	0	4.742802	-0.584695	0.516033
38	1	0	5.336397	1.073926	0.846695
39	1	0	3.862613	0.470224	1.651577

(Z)-**INTf**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.212787	-2.333750	1.860593
2	6	0	-0.714996	-1.771095	0.620627
3	6	0	-0.045127	-2.077419	-0.562496
4	6	0	0.569243	-2.323460	-1.583431
5	6	0	-1.833130	-0.828827	0.604453
6	6	0	-2.460542	-0.491644	-0.744024
7	6	0	-3.604216	0.463192	-0.579234
8	6	0	-4.890156	0.134897	-0.391087
9	6	0	-5.940744	1.187935	-0.213949
10	6	0	-5.403691	-1.270838	-0.327218
11	8	0	2.663329	-1.341168	1.613310
12	29	0	2.141192	-0.198433	0.245431
13	8	0	3.268448	-0.958590	-1.303301
14	6	0	4.300080	-0.047702	-1.716731
15	8	0	1.387461	1.235514	-0.905738
16	16	0	0.758193	2.037529	0.253828
17	8	0	1.441424	3.331645	0.420059
18	8	0	1.073109	1.093380	1.426764
19	8	0	-0.698315	2.170722	0.064920
20	1	0	-1.391352	0.089413	1.051491
21	1	0	0.829770	-1.930325	1.970559
22	1	0	-0.833787	-2.088697	2.722396
23	1	0	1.105839	-2.538855	-2.485628
24	1	0	2.900113	-2.192542	1.225728
25	1	0	-0.057491	-3.415091	1.759964
26	1	0	-2.571727	-1.157202	1.351054
27	1	0	-1.691196	-0.047146	-1.389533
28	1	0	-2.782945	-1.421813	-1.229218
29	1	0	-3.340062	1.523090	-0.572623
30	1	0	-6.452256	1.070667	0.751427
31	1	0	-5.523105	2.198888	-0.262853
32	1	0	-6.718005	1.096764	-0.985339
33	1	0	-4.626390	-2.027055	-0.470083
34	1	0	-5.877773	-1.454842	0.646711
35	1	0	-6.185159	-1.432072	-1.082222
36	1	0	3.684706	-1.789898	-1.035302
37	1	0	4.989490	0.163624	-0.892875
38	1	0	4.846706	-0.466389	-2.565443
39	1	0	3.801711	0.873810	-2.020091

(Z)-**TS2f**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.437252	2.567782	1.942457
2	6	0	0.739357	1.951036	0.630603
3	6	0	-0.033215	2.352654	-0.485580
4	6	0	-0.694970	2.687460	-1.445261
5	6	0	1.632165	0.892465	0.493525
6	6	0	2.118577	0.407601	-0.865212
7	6	0	3.294595	-0.520175	-0.755931
8	6	0	4.558798	-0.147386	-0.511887
9	6	0	5.657169	-1.158921	-0.391892
10	6	0	4.993452	1.273686	-0.322840
11	8	0	-2.600452	1.485189	1.314447
12	29	0	-2.048081	0.136700	0.187438
13	8	0	-3.341855	0.687742	-1.312721
14	6	0	-4.303529	-0.318506	-1.661962
15	8	0	-1.508290	-1.563488	-0.676551
16	16	0	-0.524062	-2.062053	0.388389
17	8	0	-1.124032	-3.109276	1.221827
18	8	0	-0.392919	-0.749312	1.249907
19	8	0	0.771895	-2.412355	-0.197898
20	1	0	0.659703	0.123958	0.866683
21	1	0	-0.607597	2.339734	2.197735
22	1	0	1.109611	2.204949	2.722112
23	1	0	-1.277723	2.986612	-2.292090
24	1	0	-2.376884	2.318345	0.881271
25	1	0	0.514652	3.657679	1.858509
26	1	0	2.314589	0.753873	1.337924
27	1	0	1.293593	-0.089949	-1.392552
28	1	0	2.374357	1.289598	-1.470196
29	1	0	3.082084	-1.585403	-0.853768
30	1	0	6.144037	-1.090428	0.590846
31	1	0	5.290342	-2.182202	-0.523694
32	1	0	6.443530	-0.973740	-1.136680
33	1	0	4.190794	1.999645	-0.483839
34	1	0	5.380811	1.420234	0.695112
35	1	0	5.820660	1.517801	-1.002998
36	1	0	-3.809763	1.438992	-0.918103
37	1	0	-4.850416	-0.663015	-0.778432
38	1	0	-5.001947	0.079305	-2.402628
39	1	0	-3.747758	-1.151632	-2.093344

(Z)*-PCf–*Sz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.282091	-2.554072	1.774708
2	6	0	-0.807471	-1.880421	0.538334
3	6	0	0.023135	-1.935196	-0.619158
4	6	0	0.781070	-1.989038	-1.577449
5	6	0	-2.014929	-1.278195	0.466536
6	6	0	-2.614540	-0.636351	-0.746061
7	6	0	-3.582499	0.463145	-0.410710
8	6	0	-4.892810	0.317419	-0.170451
9	6	0	-5.752548	1.497299	0.167276
10	6	0	-5.619931	-0.991670	-0.203658
11	8	0	0.472109	0.888340	1.387513
12	29	0	2.166367	-0.617924	-0.369215
13	8	0	4.075571	0.212762	-0.583717
14	6	0	4.319215	1.238598	0.386982
15	16	0	0.589239	1.889866	0.114113
16	8	0	1.413435	2.979754	0.622556
17	8	0	-0.770880	2.229493	-0.298646
18	8	0	1.288115	1.070513	-0.940604
19	8	0	2.995156	-1.980316	0.535170
20	1	0	-0.228289	0.226437	1.204268
21	1	0	0.703838	-2.154945	2.044538
22	1	0	-0.968491	-2.406392	2.613231
23	1	0	1.322990	-2.137790	-2.490513
24	1	0	2.451546	-2.774111	0.459292
25	1	0	-0.157662	-3.630660	1.608108

26	1	0	-2.634849	-1.297022	1.365813
27	1	0	-1.812768	-0.253677	-1.393973
28	1	0	-3.115029	-1.424757	-1.329559
29	1	0	-3.152885	1.463128	-0.331272
30	1	0	-6.232836	1.364523	1.146532
31	1	0	-5.180735	2.430897	0.187058
32	1	0	-6.567854	1.606462	-0.561435
33	1	0	-4.982094	-1.841233	-0.464156
34	1	0	-6.070689	-1.198497	0.776779
35	1	0	-6.452289	-0.952976	-0.919707
36	1	0	4.581947	-0.573613	-0.326837
37	1	0	3.979257	0.925788	1.382455
38	1	0	5.385049	1.480411	0.419250
39	1	0	3.751733	2.116476	0.075275

(Z)-**2f**–*Sz*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.848876	1.675819	-0.636341
2	6	0	2.049054	0.527828	-0.087946
3	6	0	0.757204	0.644395	0.266646
4	6	0	-0.126622	-0.439125	0.797960
5	6	0	-1.272089	-0.699278	-0.143014
6	6	0	-2.496839	-0.158493	-0.090117
7	6	0	-2.951427	0.811759	0.956349
8	6	0	2.748142	-0.714548	0.040809
9	6	0	3.382687	-1.743417	0.134563
10	6	0	-3.534263	-0.492080	-1.118918
11	1	0	3.227800	1.447492	-1.639775
12	1	0	2.239586	2.582918	-0.693198
13	1	0	3.933991	-2.655560	0.218872
14	1	0	3.722222	1.882431	-0.006383
15	1	0	0.281978	1.619314	0.132883
16	1	0	0.455884	-1.358028	0.941801
17	1	0	-0.501058	-0.143726	1.787905
18	1	0	-1.045403	-1.366872	-0.977717
19	1	0	-3.875389	0.413704	-1.639044
20	1	0	-3.160441	-1.198762	-1.867046
21	1	0	-4.425950	-0.927964	-0.647339
22	1	0	-2.183170	1.046334	1.698554
23	1	0	-3.263671	1.754466	0.486403
24	1	0	-3.834721	0.427099	1.484126

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