Supporting Information

Tunneling Assisted Hydrogen Elimination Mechanisms of $FeCl_3$/TEMPO

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In the supplementary information we provide more computational details of the simulations reported in the manuscript and additional discussions in support of the conclusions reached. The contents are organised in the following order:

I. Computation of the translation partition function in solution and dispersion

II. Spin density data for the reactants and the transition states

III. The reaction mechanisms and electronic energy profile along the intrinsic reaction coordinates for first step

IV. Results for AlCl3/TEMPO

V. Summary of the energy and free energy raw data

VI. Coordinate data for all the optimized structures

I. The translational partition in solution and dispersion.

The translational partition function is given by:

$$Q_t = \left(\frac{2\pi MkT}{h^2}\right)^{\frac{3}{2}} V = \left(\frac{M}{2\pi\beta\hbar^2}\right)^{\frac{3}{2}} V \qquad (1)$$

Here *V* is calculated based on the ideal-gas equation, *V=RT/P*, assuming *P* with 1 atm in general. Such assumption is valid in the gas-phase, however, *V* needs to be redefined for molecules in solution. In order to estimate the translational partition function in solution, one can calculate the free volume that one solute molecule translates along three coordinate axes within a cavity formed by solvent molecules. The cavity volume (*V1*) and molecule volume (*V2*) can be estimated by the overlapping spheres(1) with our IDSCRF radii(2) and Bader radii,(3) respectively, as shown in Figure S1. Herein, each atom has its own individual sphere, including hydrogen atoms. In general, the molecule volume is defined as one inside a contour of 0.001 electron/bohr^3 density, however, a simple way to deal with molecule volume is via the overlapping spheres with Bader atomic radii, a distance from nuclear to a contour of 0.001 electron/bohr^3 electron density for each atom. According to the calculated entropies in solution for 141 common solvent molecules, the average overestimation of the molecular volume by simple method is *ca.* 12%, therefore, a scaling factor of 0.88 has been applied for calculating molecule volume *V2*. If one can approximate the cavity and solute molecule with a respective square cube, then free volume can be counted as $V_f = (\sqrt[3]{V1} - \sqrt[3]{V2})^3$. The solution translational entropy correction has been coded into our *THERMO*

program,(4) quite different from that generated directly from *Gaussian* 09 output. Such method has successfully been applied to calculate the activation entropies for typical chemical reactions in solution.(5-9)

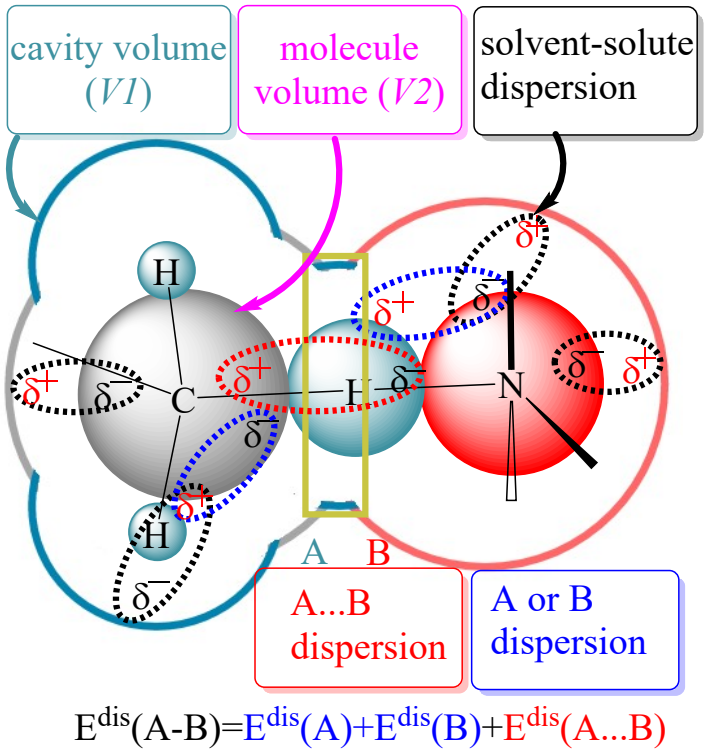


Figure S1 The definition of cavity volume(*V1*) and molecular volume(*V2*), along with the description of intra-solute dispersion and solvent-solute dispersion.

In order to apply the present dispersion method into solutional systems, one need to consider the solvent-solute dispersion as well, which is not counted in default PCM calculation and is denoted as B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) in this paper. The detailed information is described in **Figure S1**.

(1) J. Busa, J. Dzurina, E. Hayryan, S. Hayryan, C.-K. Hu, J. Plavka, I. Pokorny, J. Skrivanek and M.-C. Wu, *Computer Physics Communications,* 2005,**165**,59-96.

(2) J.-Y. Tao, W.-H. Mu, G.A. Chass, T.-H. Tang and D.-C. Fang, *Int. J. Quantum Chem.* 2013, **113**, 975-984.

(3) W.-H. Mu, G.A. Chass and D.-C. Fang, *Int. J. Quantum Chem.,* 2008, **108**, 1422-1434.

(4) D.-C. Fang, *THERMO program*, Beijing Normal University, 2013.

(5) Y. Li and D.-C. Fang, *Phys. Chem. Chem. Phys.,* 2014, **16**, 15224-15230.

(6) L. Zhao, S.-J. Li and D.-C. Fang, *ChemPhysChem,* 2015, **16**, 3711-3718.

(7) L.-L. Han, S.-J. Li and D.-C. Fang, *Phys. Chem. Chem. Phys.,* 2016, **18**, 6182-6190.

(8) S.-J. Li and D.-C. Fang, *Phys. Chem. Chem. Phys.,* 2016, **18**, 30815-30823.

(9) Y. Li and D.-C. Fang, *Chem. J. Chin. Univ.,* 2015, **36**, 1954-1960.

II. Spin state of the reactants and transition states

We optimized transition states (TSs) for both mechanisms in both the quintet and septet states. For the four TSs, the spin densities of $FeCl_3$ part in **TS1a**(quintet), **TS1a**(septet), **TS1a-O**(quintet) and **TS1a-O**(septet) are 4.734, 4.787, 4.733 and 4.856,

respectively, which are quite close to those in **R2**(quintet) and **R2**(septet) at the calculation level of B3LYP-IDSCRF-D3a/TZP-DKH(-dfg). As the H transfers from C to N or to O, the redistribution of spin densities takes place mainly on fragments of TEMPO and **R1a**. For the N-pathway, the bond lengths of C…H and N…H in **TS1a** are 1.385 and 1.377 (quintet state) and 1.358 and 1.405 Å (septet state), respectively (Figure S2c and S2d), and the O-Fe bond lengths are decreased from **R2** to **TS1a** for both spin states. However, for the O-pathway, the O-Fe bond lengths are increased for both spin state (Figure S2e and S2f), since the oxygen atom is going to accept a hydrogen atom.

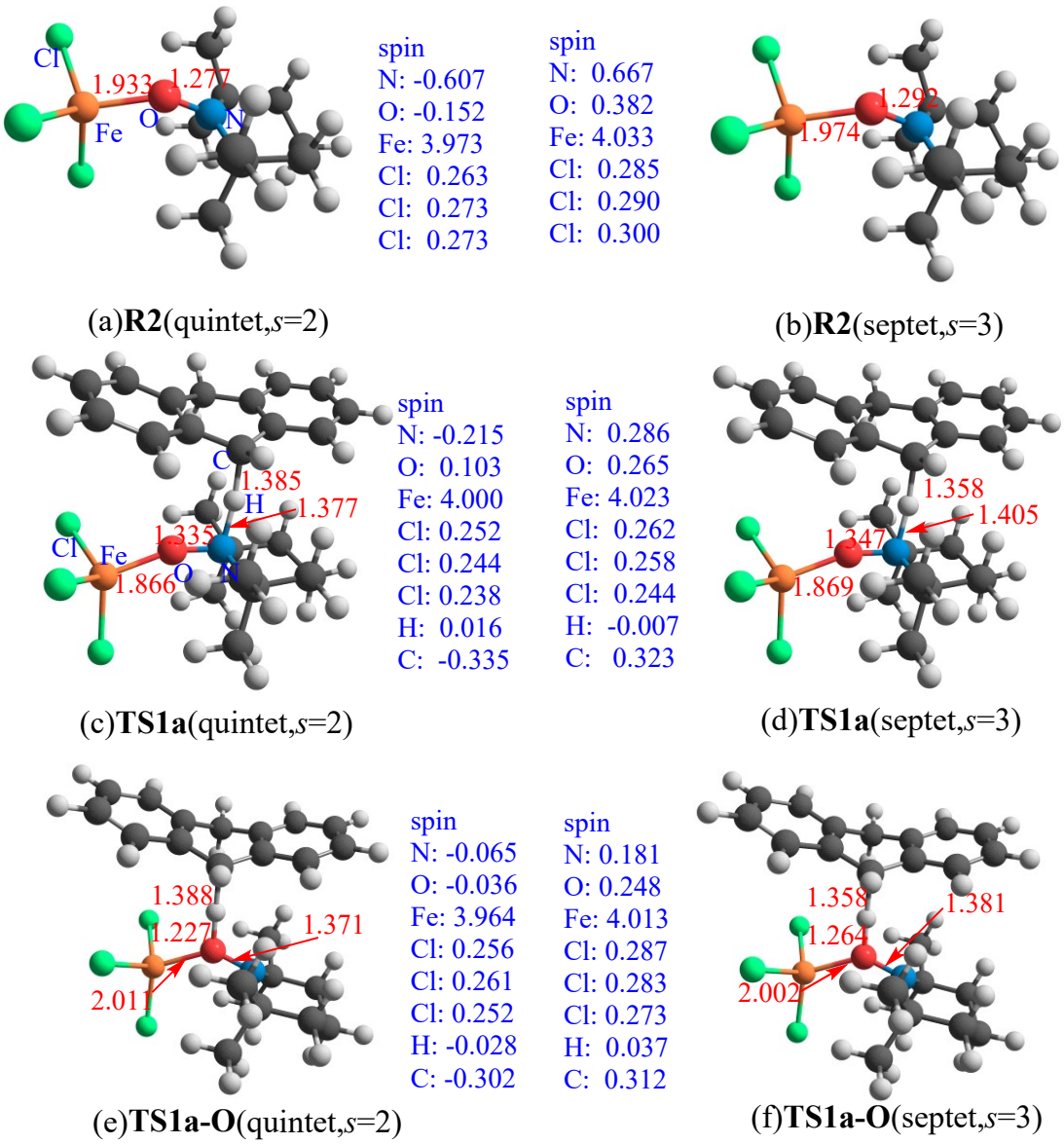


Figure S2. Geometries of $FeCl_3$/TEMPO(**R2**) and transition states for hydrogen elimination reactions with nitrogen atom in N-O (**TS1a**) and oxygen atom in N-O (**TS1a-O**) on quintet and septet state PESs with the calculation of B3LYP-IDSCRF-D3a/TZP-DKH(-dfg). The length of important bonds (red arrows) are given in Å. The atomic spin densities (in blue) for those structures are also given.

III. The reaction mechanisms and electronic energy profile along the intrinsic reaction coordinates for first step

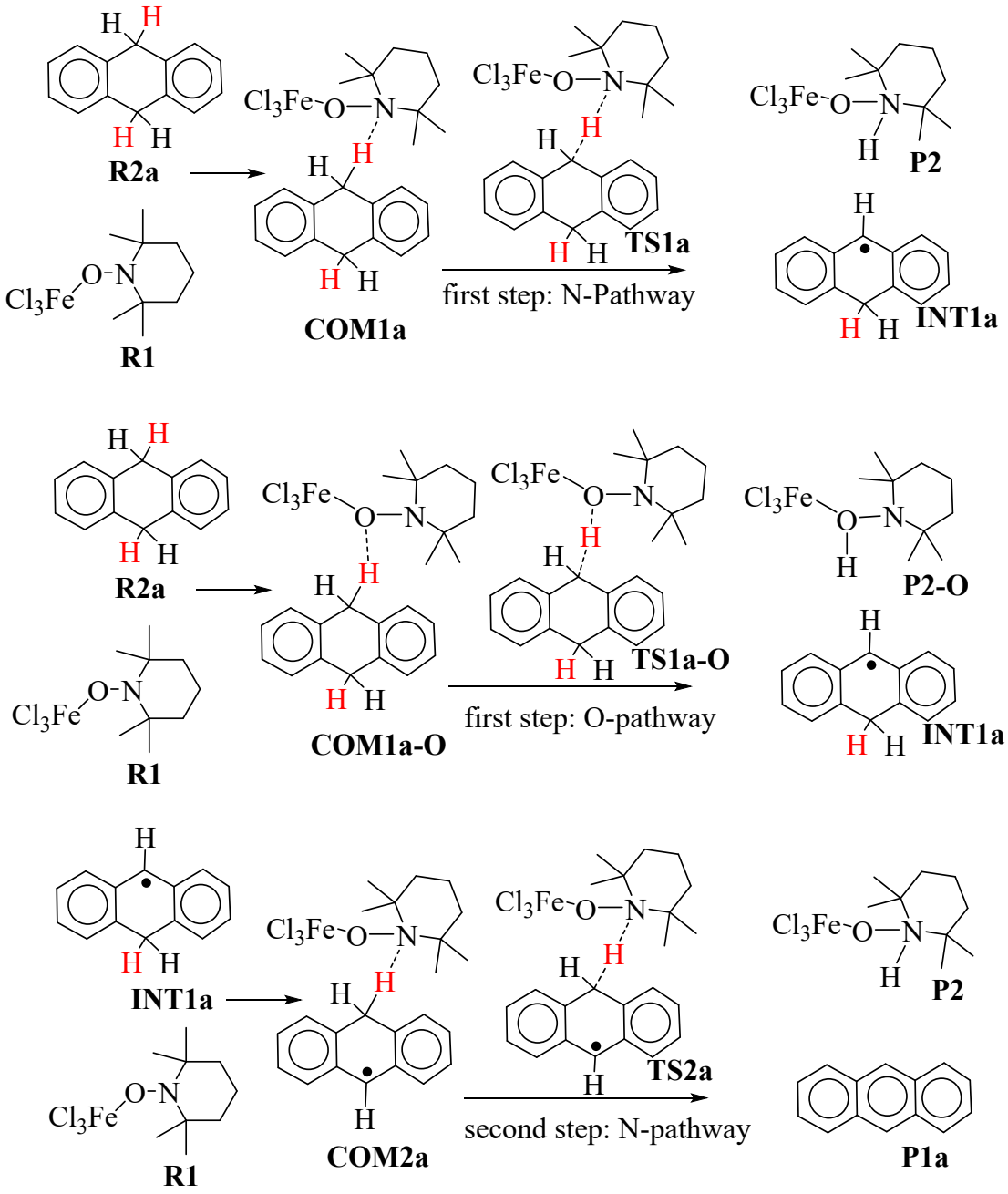


Figure S3 The possible reaction mechanisms for reaction (1)

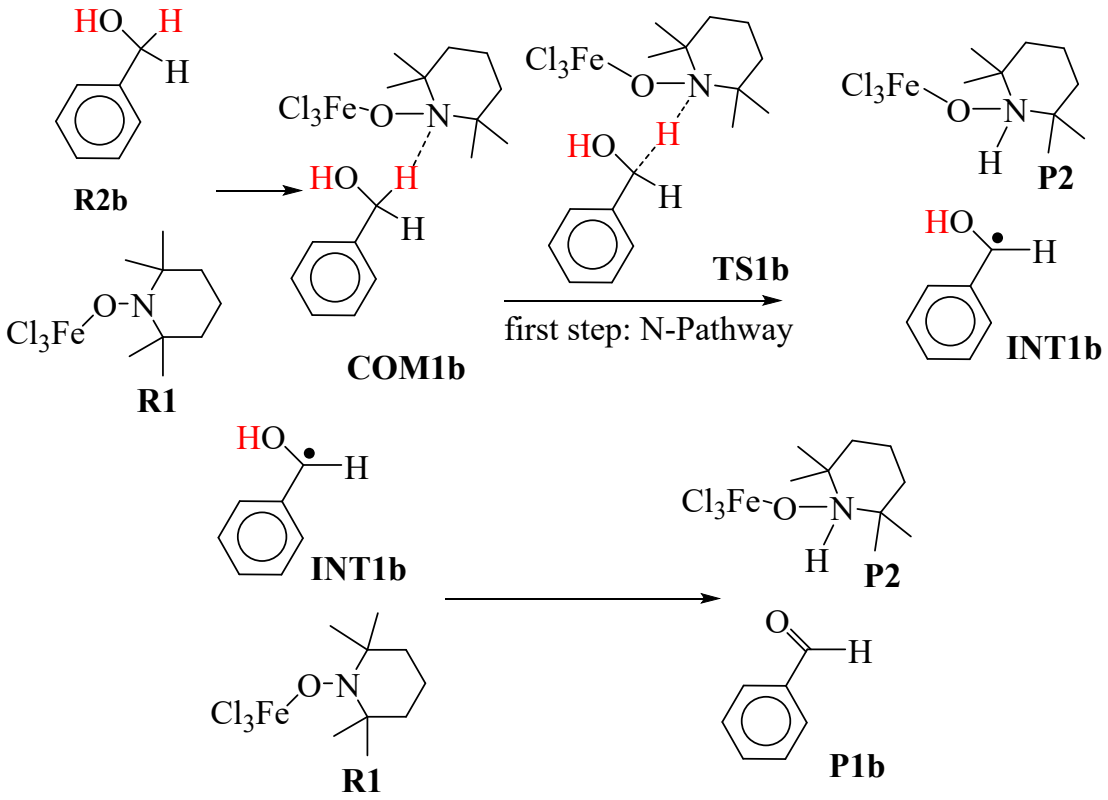


Figure S4 The possible reaction mechanisms for reaction (2)

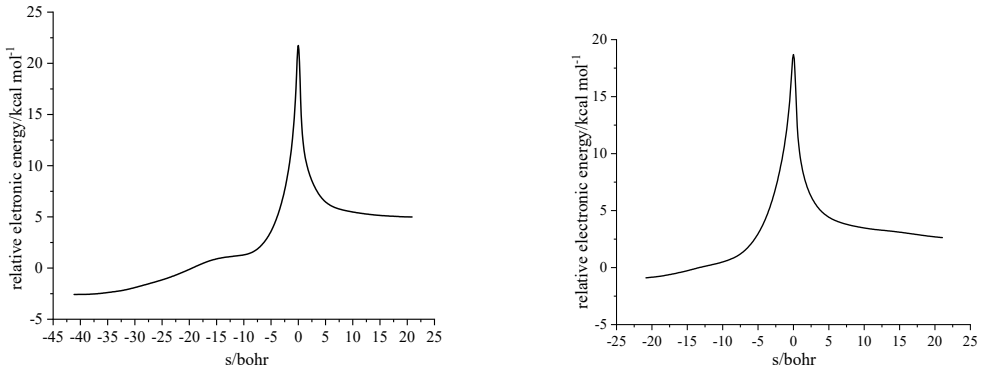
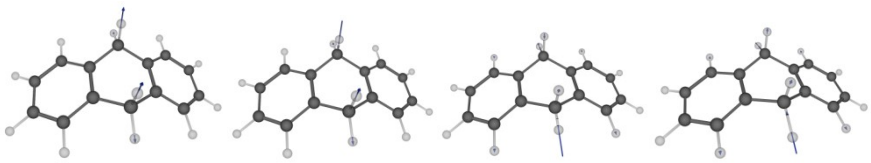


Figure S5 IRC for the first step of reactions (1) and (2)



2965(2164) 2971(2168) 3065(2263) 3067(2264)

C-H: 1.100 1.092

2994(2184) 3049(2256)

C-H: 1.097 1.094

Figure S6 The frequencies (cm^{-1}) and modes for **R1a** and **R1b** (the data for C-D bonds are given in parentheses), along with the relevant C-H bond length (in Å)

IV. Al center vs Fe center

Table S1 The activation electronic energies, activation enthalpies and activation free-energies(298K, kcal mol^{-1}), imaginary frequencies for transition states(cm^{-1}) and the ratio of k_{inst} over k_{tst} for reaction (1) with $FeCl_3$/TEMPO or $AlCl_3$/TEMPO

	$\Delta E^{\ddagger}_{e}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}_{g}$	$\Delta G^{\ddagger}_{l}$	$\omega^{\ddagger}$	T_c	k_{inst}/k_{ts}	$\Delta G^{\ddagger}_{l+inst}$	$\Delta G^{\ddagger}_{exp}$
$FeCl_3$ /TEMPO	31.1[a] 21.7[b] 24.6[c]	29.2 20.0	43.5 34.7	36.7 27.9	-1772i -1746i	406 400	160.5 67.3	33.9 25.4 28.3[d]	24.2[e]
$AlCl_3$ /TEMPO	30.5[a] 21.8[b] 24.0[c]	28.6 20.1	42.6 34.2	35.8 27.5	-1765i -1740i	404 398	317.3 58.6	32.4 25.1 27.3[d]	24.2[e]

a) B3LYP+IDSCRF/TZP-DKH(-dfg); b) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg);

c) B2GP-PLYP+IDSCRF/TZP-DKH(-dfg);

d) estimated using the free energies computed with the B3LYP+IDSCRF-D3a/TZP-DKH(-dfg) method

e) estimated from experimental reaction time

V. Raw energy and free energy data

Table S2 The calculated total electronic energies (E_0, in Hartree), total enthalpies (H, in Hartree), total entropies with gas-phase translational entropy (S_g, in cal mol^{-1} K^{-1}) and with translational entropy in solution (S_l, Hartree), and their corresponding Gibbs free energies (G_g and G_l, in Hartree) for reaction (1) at 298.15K

	E_0	H	S_g	S_l	G_g	$\boldsymbol{G_l}$
R1a(singlet)	-540.90572[a]	-540.67828	98.2	76.0	-540.72493	-540.71438
	-540.92352[b]	-540.69585	98.2	76.0	-540.74252	-540.73196
	-540.94694[c]	-540.71942	98.0	75.8	-540.76600	-540.75544

	-540.33380[d]					
R2(quintet)	-3126.12142[a] - 3126.16897[b] -3126.18992[c] - 3124.86656[d]	-3125.83447 -3125.88099 -3125.90210	151.7 144.1 146.7	129.9 122.3 124.8	-3125.90657 -3125.94947 -3125.97179	-3125.89620 -3125.93909 -3125.96140
R2(septet)	-3126.11537[a] - 3126.15600[b] -3126.17990[c] - 3124.85951[d]	-3125.82870 -3125.86831 -3125.89228	152.8 149.9 149.2	131.0 128.1 127.4	-3125.90128 -3125.93953 -3125.96318	-3125.89093 -3125.92917 -3125.95281
TS1a(quintet)	-3666.97756[a] - 3667.06760[b] -3667.10223[c] - 3665.16127[d]	-3666.46626 -3666.55470 -3666.58957	202.0 197.0 195.7	180.7 175.6 174.3	-3666.56223 -3666.64829 -3666.68254	-3666.55213 -3666.63814 -3666.67240
TS1a(septet)	-3666.97417[a] - 3667.06140[b] -3667.09844[c] - 3665.15925[d]	-3666.46305 -3666.54882 -3666.58600	202.2 198.0 197.2	181.0 176.6 175.9	-3666.55912 -3666.64288 -3666.67971	-3666.54902 -3666.63273 -3666.66957
TS1a-O(quintet)	-3666.97398[a] -	-3666.46418	202.0	180.7	-3666.56015	-3666.55005

	3667.06007[b] -3667.09733[c] -3665.14994[d]	-3666.54880 -3666.58616	196.9 196.9	175.5 175.5	-3666.64233 -3666.67970	-3666.63218 -3666.66955
TS1a-O(septet)	-3666.96835[a] -3667.05419[b] -3667.09146[c]	-3666.45873 -3666.54314 -3666.58054	202.5 197.2 197.6	181.3 175.9 176.2	-3666.55495 -3666.63686 -3666.67443	-3666.54485 -3666.62671 -3666.66428
INT1a(doublet)	-540.27489[a] -540.29124[b] -540.31487[c] -539.69331[d]	-540.06075 -540.07696 -540.10067	101.6 101.7 100.6	79.4 79.5 78.4	-540.10903 -540.12529 -540.14846	-540.09847 -540.11474 -540.13791
P2(sextet)	-3126.73054[a] -3126.78041[b] -3126.80470[c] -3125.47844[d]	-3126.42989 -3126.47874 -3126.50310	149.5 144.2 143.7	127.7 122.4 121.8	-3126.50092 -3126.54727 -3126.57136	-3126.49054 -3126.53688 -3126.56097
P2-O(sextet)	-3126.70944[a] -3126.76033[b] -3126.78354[c] -3125.46020[d]	-3126.41084 -3126.46035 -3126.48404	149.6 143.8 145.8	127.7 121.9 123.9	-3126.48191 -3126.52866 -3126.55329	-3126.47153 -3126.51827 -3126.54290
TS2a(sextet)	-3666.38511[a] -	-3665.88544 -3665.96954	200.5 194.0	179.2 172.7	-3665.98071 -3666.06173	-3665.97061 -3666.05159

	3666.47114[b] -3666.50817[c] - 3664.57585[d]	-3666.00673	193.9	172.6	-3666.09886	-3666.08872
P1a(singlet)	-539.69929[a] -539.71453[b] -539.73806[c] -539.13242[d]	-539.49534 -539.51043 -539.53403	93.8 93.7 93.7	71.5 71.5 71.5	-539.53990 -539.55497 -539.57854	-539.52934 -539.54441 -539.56798

a) B3LYP+IDSCRF/TZP-DKH(-dfg); b) B3LYP+IDSCRF-D3/TZP-DKH(-dfg);

c) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg); d) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)

Table S3 Same as **Table S2** for reaction (2).

R1b(singlet)	-346.89783[a] -346.90587[b] -346.92308[c] -346.53790[d]	-346.75696 -346.76477 -346.78225	83.6 84.0 83.6	60.7 61.1 60.6	-346.79669 -346.80470 -346.82196	-346.78579 -346.79380 -346.81106
TS1b(quintet)	-3472.98025[a] - 3473.05302[b] -3473.08322[c] - 3471.37385[d]	-3472.55569 -3472.62711 -3472.65741	185.5 181.0 180.8	164.1 159.5 159.3	-3472.64383 -3472.71311 -3472.74331	-3472.63364 -3472.70290 -3472.73310
TS1b(septet)	-3472.97681[a] - 3473.04721[b]	-3472.55239 -3472.62144 -3472.65374	186.9 182.0 182.2	165.5 160.5 160.7	-3472.64119 -3472.70790 -3472.74031	-3472.63100 -3472.69769 -3472.73010

	-3473.07941[c]					
TS1b-O(quintet)	-3472.96967[a] -3473.04062[b] -3473.07284[c] -3471.35465[d]	-3472.54670 -3472.61642 -3472.64876	187.0 182.1 182.8	165.5 160.5 161.2	-3472.63555 -3472.70294 -3472.73560	-3472.62534 -3472.69269 -3472.72536
TS1b-O(septet)	-3472.96305[a] -3473.03370[b]	-3472.54026 -3472.60972	188.2 183.7	166.7 162.2	-3472.62966 -3472.69702	-3472.61946 -3472.68678
INT1b(doublet)	-346.25916[a] -346.26554[b] -346.28334[c]	-346.13196 -346.13805 -346.15616	82.7 82.8 82.6	59.7 59.8 59.6	-346.17127 -346.17738 -346.19541	-346.16034 -346.16645 -346.18448
INT1b′(doublet)	-346.22509[a] -346.23280[b] -346.24869[c]	-346.09939 -346.10717 -346.12309	85.5 85.2 84.8	62.6 62.3 61.9	-346.14000 -346.14766 -346.16340	-346.12911 -346.13677 -346.15251
P1b(singlet)	-345.69176[a] -345.69890[b] -345.71472[c]	-345.57485 -345.58196 -345.59790	79.7 79.6 79.5	56.7 56.7 56.5	-345.61272 -345.61980 -345.63567	-345.60181 -345.60888 -345.62475

VI. Geometry data

Table S4. The optimized Cartesian Coordinates (in Å) of species studied with B3LYP+IDSCRF/TZP-DKH(-dfg).

Species	Cartesian coordinates			Species	Cartesian coordinates		
R2 (quintet)	C	4.04824	0.00010	0.15985	**R2** (septet)	C	-4.10718	-0.02407	0.18931
	C	3.38787	-1.24235	-0.42338		C	-3.47023	1.22348	-0.40942
	C	1.87986	-1.34899	-0.13332		C	-1.96169	1.35146	-0.13591
	N	1.23706	-0.00003	-0.36667		N	-1.30237	0.01098	-0.33165
	C	1.87972	1.34898	-0.13334		C	-1.92444	-1.34353	-0.10954
	C	3.38774	1.24244	-0.42347		C	-3.43410	-1.25997	-0.39380
	H	5.11106	0.00015	-0.09086		H	-5.17251	-0.04080	-0.04954
	H	3.99202	0.00014	1.25133		H	-4.03833	-0.01656	1.28008
	H	3.85344	-2.15297	-0.04081		H	-3.94542	2.13015	-0.02977
	H	3.53626	-1.24492	-1.50750		H	-3.63009	1.21465	-1.49163
	H	3.85325	2.15314	-0.04103		H	-3.88609	-2.17522	-0.00650
	H	3.53605	1.24491	-1.50760		H	-3.58818	-1.26718	-1.47692
	O	-0.00586	-0.00013	-0.66273		O	-0.02237	0.03440	-0.48079
	Fe	-1.83849	-0.00003	-0.00063		Fe	1.89595	-0.00119	0.00863
	Cl	-2.74848	-1.84679	-0.78603		Cl	2.73852	1.92305	-0.65144
	Cl	-1.69977	0.00008	2.20016		Cl	1.91522	-0.22232	2.20543
	Cl	-2.74838	1.84675	-0.78613		Cl	2.75148	-1.71874	-1.07101
	C	1.61443	1.77031	1.32356		C	-1.64818	-1.77032	1.34402
	H	1.96744	2.79468	1.45221		H	-1.98928	-2.79857	1.47314
	H	0.55098	1.74374	1.55643		H	-0.58334	-1.73214	1.56897
	H	2.13843	1.13989	2.04027		H	-2.17491	-1.14615	2.06474
	C	1.23992	2.35642	-1.09359		C	-1.27129	-2.33366	-1.07940
	H	1.31489	2.01635	-2.12724		H	-1.36185	-1.98927	-2.11037
	H	0.19272	2.54014	-0.86369		H	-0.21850	-2.49232	-0.85719
	H	1.78209	3.29887	-1.00422		H	-1.78896	-3.28991	-0.99161
	C	1.61451	-1.77029	1.32359		C	-1.68538	1.81334	1.30712
	H	2.13859	-1.13991	2.04028		H	-2.18733	1.18794	2.04416
	H	0.55107	-1.74361	1.55646		H	-0.61712	1.80944	1.52031
	H	1.96741	-2.79470	1.45225		H	-2.05290	2.83414	1.42122
	C	1.24015	-2.35647	-1.09359		C	-1.33968	2.33896	-1.12920
	H	0.19297	-2.54033	-0.86367		H	-0.29027	2.52851	-0.91490

	H 1.31506 -2.01636 -2.12723 H 1.78245 -3.29886 -1.00426		H -1.42712 1.97118 -2.15239 H -1.88229 3.28274 -1.05804
R1a(singlet)	C -0.00000 1.42572 0.69010 C 1.25445 -0.69951 0.26292 C 1.25444 0.69956 0.26278 C -1.25444 0.69956 0.26278 C -1.25445 -0.69951 0.26291 C -0.00000 -1.42562 0.69032 H 0.00000 -2.44687 0.30492 H -0.00000 -1.51541 1.78636 H -0.00000 2.44694 0.30463 C 3.55016 0.69521 -0.50179 H 4.43662 1.24092 -0.80219 C 2.40370 1.38527 -0.12457 H 2.39941 2.46998 -0.13460 C 3.55017 -0.69530 -0.50163 H 4.43664 -1.24106 -0.80190 C 2.40372 -1.38529 -0.12427 H 2.39944 -2.47000 -0.13407 C -3.55015 0.69522 -0.50180 H -4.43661 1.24092 -0.80220 C -2.40370 1.38527 -0.12457 H -2.39941 2.46998 -0.13460 C -3.55017 -0.69530 -0.50164 H -4.43664 -1.24105 -0.80191 C -2.40372 -1.38529 -0.12428 H -2.39944 -2.47000 -0.13408 H -0.00000 1.51558 1.78613	**TS1a**(quintet)	C 1.33161 -3.81242 0.03597 C 1.54954 -2.74550 -1.03439 C 0.33908 -1.82576 -1.26435 N -0.09156 -1.27076 0.11944 C -0.33395 -2.28944 1.26520 C 0.91890 -3.17383 1.36019 H 2.25625 -4.37648 0.17788 H 0.58298 -4.53856 -0.28817 H 1.78721 -3.20944 -1.99466 H 2.41528 -2.13711 -0.76413 H 0.71810 -3.94079 2.11199 H 1.74897 -2.57666 1.74658 O -1.08115 -0.37209 0.01976 Fe -2.79784 0.35205 -0.26727 Cl -2.55142 1.94871 -1.79115 Cl -4.22056 -1.19018 -1.01604 Cl -3.51013 1.10688 1.70450 C 1.89348 0.44985 1.04692 H 0.98188 -0.48900 0.51958 C -1.59850 -3.12665 1.02067 H -1.85186 -3.62282 1.95852 H -2.44696 -2.50911 0.73458 H -1.46785 -3.89952 0.27037 C -0.54285 -1.51432 2.56966 H 0.32851 -0.93112 2.85645 H -1.40700 -0.85480 2.51065 H -0.72302 -2.23732 3.36599 C -0.80562 -2.56149 -1.97480 H -0.97039 -3.56770 -1.60141

			H -1.74341 -2.01376 -1.91791 H -0.53624 -2.64677 -3.02857 C 0.74087 -0.62919 -2.12713 H -0.09599 0.04681 -2.29379 H 1.56256 -0.07643 -1.68238 H 1.08006 -1.00218 -3.09432 C 3.71039 1.09779 -0.53833 C 3.23692 0.25539 0.48434 C 1.25442 1.74875 0.84535 C 1.71588 2.61992 -0.16438 C 2.84558 2.20999 -1.07214 H 3.46865 3.07927 -1.29858 H 2.42540 1.90456 -2.04067 H 1.80736 0.07732 2.06492 C 5.35793 -0.92787 0.47950 H 5.99930 -1.70070 0.88488 C 4.08506 -0.74483 0.98859 H 3.73766 -1.37215 1.80162 C 5.81442 -0.10386 -0.54866 H 6.81114 -0.23636 -0.95128 C 4.99515 0.90252 -1.04163 H 5.36257 1.55917 -1.82270 C -0.37796 3.41152 1.52422 H -1.19469 3.71144 2.16753 C 0.20254 2.16878 1.68096 H -0.15791 1.50498 2.45553 C 0.08266 4.26696 0.52467 H -0.36991 5.24201 0.39316 C 1.12369 3.86956 -0.30518 H 1.48563 4.54482 -1.07264

TS1a(septet)				**TS1a-O**(quintet)			
	C	1.36443	-3.83354 -0.00812		C	3.98042	2.47828 0.23127
	C	1.58215	-2.75463 -1.06609		C	2.89031	2.64444 -0.82009
	C	0.36688	-1.83934 -1.29034		C	2.11728	1.34472 -1.12119
	N	-0.06951	-1.30166 0.09251		N	1.68659	0.77898 0.20011
	C	-0.31264	-2.32647 1.22573		C	2.60193	0.63494 1.37773
	C	0.94275	-3.20834 1.31938		C	3.36187	1.96916 1.52696
	H	2.29071	-4.39524 0.13281		H	4.47042	3.43856 0.41060
	H	0.62018	-4.55937 -0.34306		H	4.76122	1.79921 -0.12096
	H	1.82799	-3.20635 -2.03013		H	3.30748	3.00770 -1.76211
	H	2.44245	-2.14359 -0.78360		H	2.17650	3.39801 -0.47459
	H	0.74157	-3.98216 2.06404		H	4.12355	1.83231 2.29803
	H	1.76883	-2.61076 1.71384		H	2.66267	2.72340 1.90070
	O	-1.07993	-0.41164 -0.01483		O	0.72469	-0.20255 0.10956
	Fe	-2.79699	0.34495 -0.23823		Fe	0.66972	-2.19542 -0.37838
	Cl	-2.58628	2.01149 -1.68521		Cl	-0.92861	-2.18129 -1.90105
	Cl	-4.21706	-1.16885 -1.04480		Cl	2.49937	-3.12060 -1.18966
	Cl	-3.50339	1.01997 1.76312		Cl	0.17022	-3.12414 1.56732
	C	1.85926	0.47703 1.03641		C	-1.54365	0.74106 1.09137
	H	0.99073	-0.46731 0.50947		H	-0.35808	0.22746 0.49139
	C	-1.57399	-3.16757 0.97346		C	3.58784	-0.54202 1.25758
	H	-1.82738	-3.67254 1.90661		H	4.15136	-0.62508 2.18901
	H	-2.42369	-2.55040 0.69024		H	3.07137	-1.48832 1.10617
	H	-1.43881	-3.93370 0.21691		H	4.30198	-0.41652 0.44734
	C	-0.52502	-1.56466 2.53800		C	1.75693	0.42204 2.64033
	H	0.34624	-0.98499 2.83250		H	1.04024	1.23259 2.77342
	H	-1.38866	-0.90419 2.48437		H	1.22472	-0.52792 2.62025
	H	-0.70724	-2.29532 3.32688		H	2.41864	0.41580 3.50787
	C	-0.77107	-2.57373 -2.01466		C	2.98207	0.38444 -1.95861
	H	-0.93435	-3.58365 -1.65060		H	3.93572	0.14969 -1.49190
	H	-1.71020	-2.02829 -1.95604		H	2.46747	-0.55343 -2.15631
	H	-0.49645	-2.64935 -3.06788		H	3.19014	0.85387 -2.92213
	C	0.76743	-0.63384 -2.14229		C	0.87197	1.69899 -1.94012
	H	-0.07174	0.04012 -2.30493		H	0.30172	0.81171 -2.21316

	H 1.58534 -0.08141 -1.68994		H 0.22593 2.38446 -1.39548
	H 1.11116 -0.99659 -3.11179		H 1.18869 2.18824 -2.86266
	C 3.70968 1.12215 -0.51304		C -2.46829 2.32516 -0.57379
	C 3.21697 0.28492 0.50476		C -1.65271 2.09184 0.55507
	C 1.22238 1.77420 0.81285		C -2.63568 -0.18667 0.82096
	C 1.70506 2.64178 -0.18977		C -3.47464 0.03239 -0.29121
	C 2.85223 2.22706 -1.07301		C -3.15532 1.15986 -1.23457
	H 3.47696 3.09574 -1.29697		H -4.05501 1.49275 -1.75587
	H 2.44994 1.91046 -2.04567		H -2.48729 0.76262 -2.01456
	H 1.75792 0.12083 2.05935		H -1.13624 0.67853 2.09896
	C 5.34126 -0.89118 0.55354		C -1.12557 4.45826 0.65322
	H 5.97614 -1.65927 0.97770		H -0.61564 5.28567 1.13107
	C 4.05692 -0.70937 1.03337		C -0.98637 3.17543 1.15389
	H 3.69380 -1.33261 1.84261		H -0.37483 3.00086 2.03037
	C 5.81747 -0.07192 -0.46953		C -1.93461 4.68237 -0.45937
	H 6.82324 -0.20344 -0.84930		H -2.05433 5.68510 -0.85110
	C 5.00579 0.92844 -0.98683		C -2.60080 3.61897 -1.06151
	H 5.38804 1.58145 -1.76383		H -3.23767 3.80127 -1.91998
	C -0.42605 3.43715 1.45008		C -3.97820 -2.10245 1.44891
	H -1.25722 3.73851 2.07403		H -4.17340 -2.93101 2.11809
	C 0.15079 2.19509 1.62289		C -2.90103 -1.26672 1.67906
	H -0.22745 1.53167 2.38952		H -2.25082 -1.44044 2.52707
	C 0.05680 4.29013 0.45864		C -4.80995 -1.87471 0.35359
	H -0.39298 5.26469 0.31455		H -5.65676 -2.52497 0.17079
	C 1.11595 3.89072 -0.34730		C -4.55494 -0.81182 -0.50706
	H 1.49445 4.56406 -1.10844		H -5.20610 -0.63887 -1.35660
TS1a-O(septet)	C 4.08727 2.35271 0.16203	**INT1a**(doublet)	C 0.00000 1.39331 0.07002
	C 2.99434 2.55847 -0.87919		C 1.27952 -0.70665 0.02995
	C 2.16106 1.29177 -1.16036		C 1.24493 0.71082 0.03903
	N 1.71706 0.76130 0.16983		C -1.24493 0.71082 0.03903
	C 2.64331 0.57615 1.33144		C -1.27952 -0.70665 0.02995
	C 3.46038 1.87807 1.46669		C 0.00000 -1.50372 0.11449
	H 4.61969 3.29231 0.33007		H 0.00000 -2.27544 -0.66359

	H 4.83479 1.63861 -0.19335		H 0.00000 -2.06138 1.06140
	H 3.41656 2.89574 -1.82869		H 0.00000 2.47729 0.08137
	H 2.31842 3.34548 -0.53197		C 3.67646 0.75283 -0.05559
	H 4.22298 1.71338 2.23147		H 4.60338 1.31292 -0.08725
	H 2.79701 2.66310 1.84218		C 2.46838 1.41856 -0.00086
	O 0.73390 -0.21133 0.07509		H 2.44334 2.50253 0.00756
	Fe 0.59351 -2.20275 -0.33177		C 3.70143 -0.64359 -0.07388
	Cl -1.06351 -2.26772 -1.77913		H 4.64572 -1.17194 -0.12092
	Cl 2.35583 -3.20549 -1.19405		C 2.50652 -1.35564 -0.03044
	Cl 0.12270 -3.12675 1.61916		H 2.53128 -2.44054 -0.04177
	C -1.51528 0.76903 1.07812		C -3.67646 0.75283 -0.05559
	H -0.37042 0.24423 0.48191		H -4.60338 1.31293 -0.08725
	C 3.57955 -0.64005 1.20647		C -2.46838 1.41856 -0.00085
	H 4.15248 -0.74113 2.13041		H -2.44334 2.50253 0.00756
	H 3.02349 -1.56600 1.06976		C -3.70143 -0.64359 -0.07388
	H 4.28691 -0.54999 0.38560		H -4.64572 -1.17194 -0.12092
	C 1.80661 0.40459 2.60607		C -2.50652 -1.35564 -0.03044
	H 1.12251 1.24247 2.73975		H -2.53128 -2.44054 -0.04177
	H 1.23747 -0.52388 2.59937		
	H 2.47659 0.37821 3.46701		
	C 2.97051 0.28914 -2.00299		
	H 3.92227 0.01974 -1.55104		
	H 2.41335 -0.62838 -2.18067		
	H 3.18081 0.73824 -2.97577		
	C 0.92207 1.69849 -1.96549		
	H 0.31245 0.83542 -2.23131		
	H 0.31061 2.40784 -1.41112		
	H 1.24588 2.17571 -2.89201		
	C -2.39618 2.42679 -0.54402		
	C -1.58519 2.13844 0.57500		
	C -2.64166 -0.11313 0.78796		
	C -3.47207 0.15748 -0.31978		
	C -3.12417 1.30253 -1.23260		

	H -4.01846 1.67875 -1.73362 H -2.47733 0.91186 -2.03262 H -1.12548 0.67755 2.09142 C -0.98282 4.48430 0.72978 H -0.44479 5.28244 1.22632 C -0.88303 3.18550 1.19719 H -0.27360 2.96994 2.06579 C -1.78777 4.76267 -0.37363 H -1.87629 5.77813 -0.74003 C -2.48952 3.73608 -0.99869 H -3.12359 3.95969 -1.84950 C -4.04121 -2.00440 1.36605 H -4.26268 -2.84233 2.01515 C -2.94231 -1.20505 1.61958 H -2.30176 -1.41609 2.46651 C -4.86302 -1.72695 0.27422 H -5.72751 -2.34803 0.07363 C -4.57575 -0.65000 -0.55823 H -5.22045 -0.43635 -1.40350		
P2(sextet)	Fe 1.71937 -0.00006 -0.01415 Cl 2.75476 1.83147 -0.71293 Cl 1.56286 0.00004 2.20418 O 0.01738 -0.00016 -0.85563 N -1.36283 -0.00012 -0.86649 C -1.93818 -1.34602 -0.28979 C -1.88203 -1.26330 1.23788 H -2.37813 -2.15537 1.62792 H -0.84086 -1.31966 1.55897 C -2.51890 0.00035 1.81916 H -2.37598 0.00053 2.90128 H -3.60033 0.00033 1.65879 C -3.36138 -1.56242 -0.82223 H -4.11745 -0.96621 -0.32306	**P2-O**(sextet)	Fe -1.79737 -0.00967 0.04785 Cl -2.77641 -1.59462 -1.11070 Cl -1.66909 -0.41195 2.19117 O 0.03925 -0.02101 -0.94568 N 1.53896 -0.00179 -0.93243 C 1.96271 1.30832 -0.31172 C 1.79870 1.29107 1.21875 H 2.23681 2.20585 1.62660 H 0.73394 1.32839 1.46629 C 2.42378 0.05799 1.87463 H 2.20409 0.06555 2.94454 H 3.51348 0.09476 1.79119 C 3.42851 1.57374 -0.71452 H 4.15242 0.99328 -0.15238

	H -3.61666 -2.60953 -0.65999		H 3.64402 2.62581 -0.52472
	H -3.42657 -1.38192 -1.89809		H 3.57847 1.38384 -1.77747
	C -1.06171 -2.47892 -0.82530		C 1.14076 2.44292 -0.93687
	H -1.06465 -2.50434 -1.91778		H 1.22140 2.42284 -2.02615
	H -1.48200 -3.42079 -0.47023		H 1.54097 3.39620 -0.58944
	H -0.03227 -2.41504 -0.48894		H 0.08966 2.40836 -0.66612
	C -1.93812 1.34600 -0.29024		C 2.00484 -1.28367 -0.27678
	C -1.88200 1.26379 1.23745		C 1.88094 -1.23304 1.25753
	H -2.37809 2.15600 1.62719		H 2.39921 -2.10118 1.67364
	H -0.84084 1.32024 1.55854		H 0.83099 -1.34326 1.53445
	C -3.36127 1.56231 -0.82281		C 3.46469 -1.52936 -0.71269
	H -4.11737 0.96615 -0.32363		H 4.18908 -0.92311 -0.17855
	H -3.61657 2.60944 -0.66070		H 3.70723 -2.57284 -0.50821
	H -3.42636 1.38169 -1.89865		H 3.58567 -1.35628 -1.78225
	C -1.06158 2.47868 -0.82608		C 1.18869 -2.45513 -0.84039
	H -1.06448 2.50375 -1.91857		H 1.24201 -2.47863 -1.93136
	H -1.48181 3.42070 -0.47134		H 1.61268 -3.38726 -0.46531
	H -0.03215 2.41484 -0.48967		H 0.14319 -2.42683 -0.54468
	Cl 2.75462 -1.83149 -0.71351		Cl -2.64845 1.95763 -0.40368
	H -1.60735 -0.00027 -1.86355		H -0.14491 -0.10829 -1.89473
TS2a(sextet)	C 1.37849 -3.77946 -0.36289	**P1a**(singlet)	C 0.00000 1.39963 -0.00026
	C 1.54722 -2.58859 -1.30238		C -1.21929 -0.72013 -0.00024
	C 0.31647 -1.66623 -1.37096		C -1.21929 0.72013 -0.00024
	N -0.04953 -1.28696 0.06485		C 1.21929 0.72013 -0.00024
	C -0.25225 -2.41777 1.07977		C 1.21929 -0.72013 -0.00024
	C 1.00658 -3.30077 1.03760		C 0.00000 -1.39963 -0.00026
	H 2.31090 -4.34791 -0.32081		H 0.00000 -2.48471 -0.00038
	H 0.62232 -4.46859 -0.74557		H 0.00000 2.48471 -0.00038
	H 1.76117 -2.92663 -2.31929		C -3.64756 0.71109 0.00030
	H 2.41334 -2.00318 -0.98244		H -4.59154 1.24270 0.00058
	H 0.83730 -4.14928 1.70510		C -2.47169 1.40266 -0.00000
	H 1.84692 -2.74121 1.45726		H -2.47087 2.48691 0.00006
	O -1.09625 -0.40393 0.09446		C -3.64756 -0.71109 0.00030

	Fe -2.79704 0.30588 -0.12190		H -4.59154 -1.24270 0.00058
	Cl -2.66019 1.90478 -1.68101		C -2.47169 -1.40266 -0.00000
	Cl -4.30888 -1.21101 -0.76554		H -2.47087 -2.48691 0.00006
	Cl -3.37939 1.12731 1.88609		C 3.64756 0.71109 0.00030
	C 1.85955 0.56021 1.12928		H 4.59154 1.24270 0.00058
	H 1.09194 -0.32569 0.58059		C 2.47169 1.40266 -0.00000
	C -1.51831 -3.24981 0.81574		H 2.47087 2.48691 0.00006
	H -1.71379 -3.85800 1.70062		C 3.64756 -0.71109 0.00030
	H -2.38877 -2.61998 0.64752		H 4.59154 -1.24270 0.00058
	H -1.42112 -3.92755 -0.02702		C 2.47169 -1.40266 -0.00000
	C -0.39820 -1.79138 2.47238		H 2.47087 -2.48691 0.00006
	H 0.49462 -1.24889 2.77730		
	H -1.25254 -1.11797 2.52007		
	H -0.55430 -2.59030 3.19839		
	C -0.83663 -2.33397 -2.13989		
	H -0.98608 -3.37588 -1.87172		
	H -1.77758 -1.80688 -1.99820		
	H -0.59720 -2.30300 -3.20408		
	C 0.68352 -0.37710 -2.11472		
	H -0.16437 0.30238 -2.18269		
	H 1.51283 0.14236 -1.64007		
	H 0.99621 -0.63700 -3.12725		
	C 3.77348 1.12973 -0.35720		
	C 3.21435 0.30516 0.66387		
	C 1.25950 1.84492 0.80563		
	C 1.85321 2.66324 -0.21031		
	C 3.06379 2.26631 -0.77862		
	H 3.50563 2.89375 -1.54675		
	H 1.68667 0.25090 2.15880		
	C 5.24997 -1.00330 0.66085		
	H 5.83866 -1.81504 1.07103		
	C 3.99388 -0.75082 1.16611		
	H 3.60436 -1.36194 1.97116		

	C 5.78485 -0.21736 -0.38074 H 6.76966 -0.43941 -0.77154 C 5.06045 0.83212 -0.87877 H 5.46250 1.45878 -1.66629 C -0.45208 3.52110 1.09442 H -1.35061 3.85695 1.59617 C 0.10291 2.31403 1.44768 H -0.36762 1.71150 2.21293 C 0.11200 4.31627 0.07136 H -0.35911 5.25231 -0.19956 C 1.23943 3.89570 -0.57277 H 1.68847 4.49100 -1.35897		
R1b(singlet)	C -1.44244 -1.30319 0.03937 C -0.08007 -1.09794 0.21169 C -2.29741 -0.21778 -0.13844 H 0.58506 -1.94309 0.34504 H -3.36041 -0.37886 -0.27190 C 0.45030 0.19500 0.20669 C -1.77987 1.07146 -0.14638 H -2.43751 1.92075 -0.28894 C -0.41256 1.27368 0.02178 H -0.01197 2.28172 0.00898 H -1.84106 -2.31086 0.04630 C 1.93184 0.41483 0.40203 H 2.23019 0.11933 1.41065 H 2.16365 1.48033 0.29174 O 2.74611 -0.37459 -0.46771 H 2.48444 -0.18887 -1.38063	**TS1b**(quintet)	C 2.07164 3.05126 -0.19861 C 1.65666 2.40480 1.11902 C 0.23277 1.82540 1.12462 N 0.08525 0.91097 -0.12266 C 0.53606 1.46399 -1.50476 C 1.94690 2.04612 -1.33934 H 3.10704 3.39032 -0.12397 H 1.47410 3.94308 -0.39955 H 1.71090 3.12470 1.93894 H 2.36641 1.60953 1.35963 H 2.21787 2.50587 -2.29245 H 2.65507 1.22871 -1.17891 O -1.14866 0.40081 -0.22025 Fe -2.67513 -0.62815 0.05291 Cl -3.72173 -0.70118 -1.90344 Cl -1.95542 -2.68861 0.68937 Cl -3.89244 0.28758 1.67656 C 4.98491 -1.59482 -0.93229 C 3.60294 -1.70195 -0.87782 C 5.69890 -1.12543 0.16752 H 3.05391 -2.08686 -1.72624

			H 6.77767 -1.04554 0.12157 C 2.91016 -1.33949 0.28557 C 5.02124 -0.77269 1.33172 H 5.57188 -0.42563 2.19707 C 3.63981 -0.87838 1.39098 H 3.12358 -0.62358 2.30891 H 5.50974 -1.88592 -1.83365 C 1.44433 -1.43690 0.36728 H 1.04357 -1.56006 1.37487 H 0.91290 -0.17895 0.12396 O 0.87246 -2.26416 -0.55336 H -0.04426 -2.47682 -0.27103 C -0.46170 2.50678 -2.02956 H -0.25342 2.65682 -3.08971 H -1.48526 2.14862 -1.93884 H -0.37949 3.47345 -1.54218 C 0.55495 0.29513 -2.49230 H 1.21907 -0.50498 -2.17910 H -0.44205 -0.11658 -2.63946 H 0.91045 0.67191 -3.45217 C -0.83771 2.92583 1.12255 H -0.65528 3.70410 0.38838 H -1.82999 2.50998 0.96077 H -0.83071 3.39580 2.10675 C 0.02775 0.96743 2.37670 H -0.95340 0.49739 2.39523 H 0.79323 0.20247 2.48464 H 0.09786 1.61899 3.24820
TS1b(septet)	C -2.09206 3.06084 0.11413 C -1.57606 2.42726 -1.17385 C -0.14931 1.86054 -1.07726 N -0.09475 0.93536 0.16018 C -0.63179 1.47705 1.50742	**TS1b-O**(quintet)	C -0.70222 4.07646 0.29032 C -0.68638 3.46045 -1.10309 C 0.22036 2.21902 -1.21945 N -0.13582 1.30899 -0.08483 C -0.32095 1.75577 1.33173

C	-2.03384	2.05222	1.25741
H	-3.12397	3.38784	-0.03163
H	-1.52145	3.95939	0.35957
H	-1.57808	3.15246	-1.99106
H	-2.25784	1.62632	-1.47093
H	-2.36732	2.50749	2.19291
H	-2.72572	1.23165	1.04972
O	1.14520	0.42043	0.35967
Fe	2.65052	-0.63512	-0.03403
Cl	3.98785	0.45348	-1.42187
Cl	3.61716	-1.03710	1.91047
Cl	1.94441	-2.55610	-0.98442
C	-4.94316	-1.69659	0.89695
C	-3.56033	-1.78152	0.82615
C	-5.67284	-1.17943	-0.17064
H	-2.99868	-2.20360	1.64868
H	-6.75244	-1.11651	-0.11163
C	-2.88291	-1.34899	-0.32195
C	-5.01019	-0.75662	-1.32017
H	-5.57322	-0.37222	-2.16184
C	-3.62821	-0.84056	-1.39571
H	-3.12196	-0.53199	-2.30332
H	-5.45643	-2.04218	1.78608
C	-1.41579	-1.41841	-0.42439
H	-1.03793	-1.51445	-1.44396
H	-0.90247	-0.18079	-0.14699
O	-0.81868	-2.27287	0.45996
H	0.08930	-2.47105	0.14806
C	0.32053	2.52323	2.10717
H	0.04678	2.65757	3.15460
H	1.35132	2.17612	2.07254
H	0.25755	3.49560	1.62802
C	-0.70656	0.30115	2.48529

C	-1.17800	3.03736	1.29780
H	-1.37469	4.93767	0.30482
H	0.28653	4.45751	0.55865
H	-0.35352	4.18537	-1.84938
H	-1.70726	3.17157	-1.37156
H	-1.19463	3.45050	2.30885
H	-2.20632	2.75551	1.05237
O	0.36410	0.03796	-0.20988
Fe	2.11159	-0.98346	0.12927
Cl	3.94809	0.20735	0.31632
Cl	1.67933	-2.15969	1.94356
Cl	2.09932	-2.21566	-1.75593
C	-4.42310	-1.80589	1.06105
C	-3.16865	-2.10259	0.55640
C	-5.20922	-0.82052	0.46381
H	-2.55578	-2.86472	1.01845
H	-6.18952	-0.59259	0.86399
C	-2.68093	-1.41889	-0.57091
C	-4.73436	-0.13399	-0.65117
H	-5.34683	0.62388	-1.12396
C	-3.48177	-0.42815	-1.16529
H	-3.12453	0.09248	-2.04536
H	-4.79469	-2.34294	1.92517
C	-1.36355	-1.70611	-1.11643
H	-1.19817	-1.42851	-2.16112
H	-0.51639	-0.71750	-0.58855
O	-0.81493	-2.89456	-0.73824
H	0.06202	-2.99489	-1.15822
C	1.01152	2.00725	2.06165
H	0.80399	2.23562	3.10874
H	1.65284	1.12672	2.04531
H	1.57239	2.84016	1.64295
C	-1.10205	0.67434	2.08828

	H -1.33831 -0.50367 2.12108 H 0.28263 -0.10181 2.69496 H -1.13306 0.66562 3.42088 C 0.90524 2.97415 -0.98951 H 0.64533 3.75891 -0.28595 H 1.88235 2.57235 -0.72990 H 0.98690 3.43310 -1.97580 C 0.15401 1.02380 -2.32417 H 1.15847 0.60604 -2.30435 H -0.56444 0.22058 -2.47147 H 0.08996 1.67870 -3.19399		H -2.03786 0.44313 1.58032 H -0.52507 -0.24192 2.20304 H -1.33862 1.04694 3.08644 C 1.70298 2.63093 -1.24161 H 1.98710 3.23163 -0.38036 H 2.36090 1.76523 -1.27679 H 1.88984 3.22530 -2.13828 C -0.10131 1.50314 -2.53750 H 0.54468 0.64129 -2.70213 H -1.14208 1.17877 -2.56191 H 0.05295 2.19793 -3.36430
TS1b-O(septet)	C -0.65041 4.12411 0.29203 C -0.63312 3.51702 -1.10530 C 0.24086 2.25139 -1.21768 N -0.17369 1.34206 -0.10364 C -0.32854 1.78779 1.31601 C -1.15789 3.08836 1.28755 H -1.30401 4.99989 0.30585 H 0.34367 4.48169 0.57301 H -0.27169 4.23757 -1.84269 H -1.65765 3.25678 -1.38838 H -1.17371 3.49376 2.30188 H -2.18981 2.83061 1.03138 O 0.37087 0.06794 -0.21811 Fe 2.05882 -0.97987 0.13574 Cl 3.92018 0.14521 0.40866 Cl 1.62198 -2.23204 1.88722 Cl 2.15949 -2.21300 -1.73014 C -4.40621 -1.85878 1.03914 C -3.15546 -2.14513 0.51913 C -5.18832 -0.84761 0.48109 H -2.54677 -2.92819 0.95058 H -6.16585 -0.62805 0.89259	**INT1b**(doublet)	C 1.34308 -1.34086 0.00000 C -0.01454 -1.08112 -0.00031 C 2.27352 -0.29932 0.00035 H -0.72720 -1.89504 -0.00099 H 3.33485 -0.51332 0.00094 C -0.49257 0.25667 0.00004 C 1.81963 1.02378 -0.00005 H 2.53426 1.83869 -0.00027 C 0.46853 1.30329 -0.00034 H 0.12733 2.33262 -0.00104 H 1.68799 -2.36862 -0.00018 C -1.86058 0.56435 0.00057 H -2.22330 1.58445 0.00039 O -2.78506 -0.43518 -0.00001 H -3.67597 -0.05806 -0.00026

	C -2.66557 -1.42382 -0.58348 C -4.71158 -0.12391 -0.60975 H -5.32012 0.65517 -1.05231 C -3.46213 -0.40618 -1.13719 H -3.10155 0.14752 -1.99532 H -4.77829 -2.42463 1.88453 C -1.34687 -1.69515 -1.14019 H -1.19883 -1.39921 -2.18432 H -0.51326 -0.73777 -0.60728 O -0.82130 -2.91862 -0.81451 H 0.05644 -3.01319 -1.22833 C 1.00455 2.00790 2.05369 H 0.79773 2.23580 3.10110 H 1.62636 1.11326 2.03835 H 1.58808 2.82939 1.64390 C -1.13552 0.72244 2.06913 H -2.07409 0.51314 1.55682 H -0.58009 -0.20780 2.17965 H -1.36583 1.09346 3.06952 C 1.73418 2.62262 -1.21837 H 2.02575 3.21177 -0.35180 H 2.36798 1.73863 -1.25082 H 1.95159 3.21447 -2.10986 C -0.08238 1.55822 -2.54796 H 0.54160 0.67985 -2.71089 H -1.13083 1.26106 -2.58649 H 0.10149 2.25396 -3.36817		
INT1b′(doublet)	C -1.35521 -1.33137 0.00006 C 0.01300 -1.08071 0.00013 C -2.26191 -0.27605 -0.00007 H 0.72345 -1.89714 0.00020 H -3.32681 -0.47327 -0.00013 C 0.48564 0.22846 0.00009	**P1b**(singlet)	C -1.33223 -1.32249 0.00002 C 0.03568 -1.10473 0.00010 C -2.21181 -0.23923 -0.00009 H 0.73529 -1.93074 0.00011 H -3.28077 -0.41393 -0.00022 C 0.53291 0.20305 0.00010

	C -1.79424 1.03460 -0.00011 H -2.49400 1.86140 -0.00022 C -0.42714 1.28400 -0.00003 H -0.06711 2.30771 -0.00005 H -1.71434 -2.35341 0.00009 C 1.96885 0.52760 0.00025 H 2.23475 1.18033 0.85883 H 2.23477 1.18153 -0.85742 O 2.82942 -0.51579 -0.00040		C -1.72352 1.06327 -0.00006 H -2.40939 1.90096 -0.00019 C -0.35204 1.28324 0.00007 H 0.03997 2.29431 0.00021 H -1.72081 -2.33321 0.00009 C 1.98550 0.46262 0.00003 H 2.26087 1.53673 0.00006 O 2.84600 -0.39105 -0.00014

Table S2. The optimized Cartesian Coordinates(in Å) of some selected species studied with B3LYP+IDSCRF-D3, B3LYP+IDSCRF-D3a and B2GP-PLYP-IDSCRF with basis set of TZP-DKH(-dfg) .

Species	Cartesian coordinates	Species	Cartesian coordinates
R2 (quintet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 3.98067 0.00031 0.28409 C 3.36292 -1.24323 -0.34424 C 1.84128 -1.34589 -0.15237 N 1.22251 -0.00004 -0.42182 C 1.84095 1.34594 -0.15236 C 3.36259 1.24364 -0.34433 H 5.05850 0.00046 0.11105 H 3.84291 0.00034 1.36781 H 3.80161 -2.15417 0.06695 H 3.58040 -1.24267 -1.41642 H 3.80109 2.15472 0.06676 H 3.58002 1.24303 -1.41653 O -0.01195 -0.00021 -0.74578 Fe -1.79792 -0.00002 -0.00628 Cl -2.68643 -1.87542 -0.75807 Cl -1.64287 -0.00005 2.19566	**R2** (septet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C -3.98538 0.25815 0.38839 C -3.26637 1.41990 -0.28497 C -1.73318 1.35133 -0.18399 N -1.27798 -0.05802 -0.42565 C -2.04766 -1.32034 -0.15981 C -3.55340 -1.04255 -0.27722 H -5.06483 0.38483 0.28519 H -3.77808 0.23707 1.46110 H -3.57394 2.37758 0.13917 H -3.54682 1.43929 -1.34227 H -4.07489 -1.90096 0.15058 H -3.82475 -1.00373 -1.33653 O -0.01942 -0.23720 -0.65569 Fe 1.82905 -0.04244 0.01053 Cl 2.55097 1.99774 -0.36924 Cl 1.72551 -0.47944 2.16502

	Cl -2.68640 1.87536 -0.75809 C 1.47086 1.75995 1.28162 H 1.82153 2.77996 1.44391 H 0.39216 1.73868 1.42571 H 1.92978 1.11682 2.02988 C 1.24533 2.34313 -1.15023 H 1.39443 2.00433 -2.17615 H 0.18056 2.49408 -0.98403 H 1.75779 3.29748 -1.02381 C 1.47117 -1.76007 1.28155 H 1.92989 -1.11691 2.02989 H 0.39246 -1.73903 1.42554 H 1.82203 -2.78003 1.44382 C 1.24598 -2.34320 -1.15031 H 0.18124 -2.49442 -0.98420 H 1.39508 -2.00432 -2.17620 H 1.75869 -3.29742 -1.02389		Cl 2.91546 -1.55687 -1.13883 C -1.66897 -1.80217 1.25166 H -2.12836 -2.77720 1.42046 H -0.58951 -1.90245 1.34775 H -2.01952 -1.12053 2.02521 C -1.61844 -2.36091 -1.19910 H -1.77697 -1.98761 -2.21172 H -0.57025 -2.62986 -1.08696 H -2.22734 -3.25542 -1.06143 C -1.23891 1.77321 1.21041 H -1.71056 1.19538 2.00381 H -0.15981 1.65689 1.29591 H -1.48010 2.82636 1.36016 C -1.10490 2.24108 -1.26101 H -0.02289 2.28407 -1.17045 H -1.36361 1.88209 -2.25810 H -1.50155 3.25071 -1.14491
R1a (singlet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C -0.00000 1.41879 0.71773 C 1.25166 -0.69944 0.27349 C 1.25166 0.69950 0.27335 C -1.25166 0.69950 0.27335 C -1.25166 -0.69944 0.27348 C 0.00000 -1.41868 0.71794 H 0.00000 -2.44940 0.35956 H -0.00000 -1.47532 1.81565 H -0.00000 2.44948 0.35928 C 3.53556 0.69533 -0.52243 H 4.41776 1.24051 -0.83502 C 2.39423 1.38614 -0.12916 H 2.38933 2.47050 -0.13865 C 3.53557 -0.69541 -0.52227 H 4.41779 -1.24065 -0.83472 C 2.39425 -1.38616 -0.12886	**TS1a** (quintet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 1.48186 -3.70047 -0.14564 C 1.67011 -2.55698 -1.14108 C 0.42648 -1.67360 -1.31738 N -0.02557 -1.24400 0.09457 C -0.24600 -2.33051 1.16658 C 1.03912 -3.16733 1.21615 H 2.42385 -4.24158 -0.03420 H 0.75825 -4.42531 -0.52394 H 1.93354 -2.94437 -2.12763 H 2.50649 -1.93397 -0.81725 H 0.86917 -3.98722 1.91713 H 1.84034 -2.55667 1.63962 O -1.02499 -0.35938 0.05758 Fe -2.75306 0.28427 -0.22897 Cl -2.49529 1.94390 -1.68734 Cl -4.11465 -1.26939 -1.06331

	H 2.38937 -2.47052 -0.13811		Cl -3.47251 0.89861 1.79354
	C -3.53555 0.69533 -0.52245		C 1.85104 0.47632 1.11792
	H -4.41776 1.24051 -0.83504		H 1.01992 -0.47612 0.55409
	C -2.39423 1.38614 -0.12916		C -1.48247 -3.18290 0.85416
	H -2.38933 2.47050 -0.13864		H -1.72429 -3.75830 1.74835
	C -3.53557 -0.69542 -0.52228		H -2.34269 -2.56206 0.61437
	H -4.41779 -1.24065 -0.83474		H -1.32924 -3.88749 0.04442
	C -2.39425 -1.38616 -0.12887		C -0.49850 -1.63288 2.50615
	H -2.38937 -2.47052 -0.13813		H 0.34802 -1.03617 2.83431
	H -0.00000 1.47549 1.81543		H -1.38231 -0.99867 2.45747
			H -0.66744 -2.39964 3.26247
			C -0.69279 -2.39145 -2.07951
			H -0.82834 -3.42434 -1.77581
			H -1.64258 -1.87230 -1.97741
			H -0.42472 -2.39402 -3.13657
			C 0.77544 -0.39505 -2.07879
			H -0.08975 0.25912 -2.17347
			H 1.57865 0.14681 -1.59299
			H 1.11821 -0.67036 -3.07646
			C 3.66955 1.22197 -0.41662
			C 3.20663 0.34142 0.57621
			C 1.12164 1.71503 0.87583
			C 1.56645 2.62513 -0.10484
			C 2.80132 2.34544 -0.92025
			H 3.40196 3.25709 -0.99294
			H 2.49834 2.12643 -1.95264
			H 1.75319 0.09378 2.13034
			C 5.33589 -0.82341 0.53072
			H 5.98342 -1.60543 0.90666
			C 4.06324 -0.66721 1.04790
			H 3.71875 -1.32715 1.83520
			C 5.78310 0.03789 -0.47182
			H 6.77834 -0.07549 -0.88289

			C 4.95512 1.05346 -0.92878 H 5.31317 1.73675 -1.69071 C -0.74048 3.18126 1.39131 H -1.64724 3.37733 1.94642 C -0.03899 2.01437 1.61419 H -0.39880 1.30739 2.34848 C -0.29345 4.07974 0.42383 H -0.84444 4.99229 0.23588 C 0.85255 3.80020 -0.30983 H 1.19718 4.50589 -1.05722
TS1a (septet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 1.52940 -3.71361 -0.17356 C 1.70819 -2.56203 -1.16152 C 0.45527 -1.68996 -1.33262 N 0.00337 -1.27502 0.07590 C -0.21530 -2.36408 1.13603 C 1.07530 -3.19292 1.18943 H 2.47656 -4.24587 -0.06187 H 0.81478 -4.44380 -0.55910 H 1.97926 -2.94032 -2.14979 H 2.53641 -1.93154 -0.83008 H 0.90764 -4.01879 1.88438 H 1.86961 -2.57854 1.62098 O -1.01909 -0.40011 0.03492 Fe -2.74734 0.27004 -0.20478 Cl -2.55073 1.96105 -1.61948 Cl -4.10597 -1.27286 -1.04918 Cl -3.46573 0.86051 1.81753 C 1.81958 0.50832 1.11098 H 1.03429 -0.44861 0.55426 C -1.44472 -3.22482 0.81357 H -1.70939 -3.78342 1.71202 H -2.29749 -2.60824 0.53835 H -1.27072 -3.94533 0.02157	**TS1a-O** (quintet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 4.38234 1.58924 0.17464 C 3.32733 2.03242 -0.83215 C 2.26115 0.95874 -1.11499 N 1.76234 0.48164 0.21210 C 2.65060 0.11348 1.35501 C 3.70198 1.23023 1.49054 H 5.10080 2.39595 0.33843 H 4.95446 0.74139 -0.21021 H 3.78314 2.30871 -1.78543 H 2.82349 2.92358 -0.44601 H 4.43130 0.91291 2.23903 H 3.20762 2.12404 1.88360 O 0.64830 -0.31184 0.12084 Fe 0.19113 -2.20069 -0.39553 Cl -1.39912 -1.77122 -1.86407 Cl 1.76692 -3.47678 -1.25372 Cl -0.44234 -2.99944 1.56758 C -1.35975 0.97463 1.18211 H -0.32751 0.28637 0.56185 C 3.32097 -1.26054 1.18873 H 3.89376 -1.48630 2.09008 H 2.58225 -2.05062 1.06779 H 3.99904 -1.30166 0.34080

	C	-0.47801	-1.67635	2.47936		C	1.79802	0.07655	2.62908
	H	0.35967	-1.06741	2.80856		H	1.29452	1.02982	2.78771
	H	-1.37070	-1.05426	2.43444		H	1.05535	-0.71938	2.58748
	H	-0.63449	-2.44828	3.23333		H	2.44688	-0.11003	3.48603
	C	-0.65825	-2.41216	-2.10134		C	2.82855	-0.17057	-1.99001
	H	-0.78292	-3.44926	-1.80672		H	3.68436	-0.66972	-1.54424
	H	-1.61259	-1.90271	-1.98932		H	2.07220	-0.92493	-2.19531
	H	-0.39436	-2.40258	-3.15955		H	3.14337	0.24878	-2.94730
	C	0.79568	-0.40525	-2.08927		C	1.09387	1.60248	-1.86749
	H	-0.07496	0.24190	-2.18396		H	0.30314	0.87793	-2.06117
	H	1.59210	0.14238	-1.59837		H	0.68372	2.43899	-1.30799
	H	1.14485	-0.67317	-3.08696		H	1.45373	1.97414	-2.82814
	C	3.65914	1.25323	-0.40124		C	-1.89324	2.69003	-0.51566
	C	3.18585	0.37829	0.59145		C	-1.17200	2.30892	0.63613
	C	1.09063	1.74423	0.84988		C	-2.58797	0.26017	0.86860
	C	1.54550	2.64891	-0.13044		C	-3.33493	0.63149	-0.26699
	C	2.79132	2.36636	-0.92831		C	-2.78560	1.68342	-1.18833
	H	3.38819	3.28030	-1.00569		H	-3.58977	2.18366	-1.73178
	H	2.50122	2.13286	-1.96151		H	-2.18668	1.15940	-1.94967
	H	1.71440	0.14397	2.13038		H	-0.98145	0.82194	2.19072
	C	5.32116	-0.77551	0.58834		C	-0.10178	4.48354	0.68190
	H	5.96699	-1.55132	0.98058		H	0.58881	5.17931	1.14207
	C	4.03961	-0.62230	1.08387		C	-0.27318	3.21914	1.21797
	H	3.68595	-1.27724	1.87164		H	0.27696	2.92708	2.10311
	C	5.77963	0.08083	-0.41336		C	-0.82894	4.86081	-0.44621
	H	6.78222	-0.03016	-0.80769		H	-0.70513	5.85184	-0.86527
	C	4.95361	1.08834	-0.89139		C	-1.71878	3.96622	-1.03401
	H	5.32029	1.76787	-1.65304		H	-2.28049	4.26520	-1.91187
	C	-0.78272	3.20679	1.33275		C	-4.23430	-1.43252	1.39612
	H	-1.69803	3.40301	1.87425		H	-4.58048	-2.23787	2.03156
	C	-0.08083	2.04391	1.57139		C	-3.05014	-0.78186	1.68763
	H	-0.44911	1.33733	2.30257		H	-2.46287	-1.07847	2.54662
	C	-0.32661	4.09985	0.36393		C	-4.97770	-1.05077	0.27977

	H -0.87917 5.00878 0.16170 C 0.82978 3.81952 -0.35316 H 1.18156 4.52182 -1.10093		H -5.90705 -1.55689 0.04861 C -4.52620 -0.02373 -0.54263 H -5.10422 0.26359 -1.41366
TS1a-O (septet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 4.47298 1.40396 0.11211 C 3.43263 1.90400 -0.88322 C 2.30480 0.89117 -1.15244 N 1.79582 0.44205 0.17900 C 2.67989 0.01323 1.30216 C 3.78665 1.07641 1.43307 H 5.23403 2.17182 0.27073 H 4.99649 0.52849 -0.28018 H 3.89199 2.15460 -1.84201 H 2.98380 2.82184 -0.49177 H 4.50540 0.72149 2.17496 H 3.33996 1.99243 1.83198 O 0.65035 -0.32098 0.07379 Fe 0.09427 -2.19612 -0.35094 Cl -1.59004 -1.83056 -1.71562 Cl 1.57222 -3.53187 -1.28472 Cl -0.48804 -2.99971 1.62173 C -1.31514 1.01543 1.17174 H -0.33274 0.31386 0.55088 C 3.28438 -1.38924 1.12033 H 3.87051 -1.64094 2.00619 H 2.50901 -2.14671 1.02231 H 3.93650 -1.46221 0.25448 C 1.84363 0.00798 2.58764 H 1.38944 0.98353 2.75849 H 1.06120 -0.74880 2.54973 H 2.49160 -0.21840 3.43579 C 2.79442 -0.26245 -2.04197 H 3.64126 -0.79760 -1.62089	**INT1a** (doublet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 0.00000 1.39448 0.06985 C 1.27860 -0.70561 0.02935 C 1.24452 0.71168 0.03880 C -1.24452 0.71168 0.03880 C -1.27860 -0.70561 0.02935 C 0.00000 -1.50237 0.11367 H 0.00000 -2.27396 -0.66444 H 0.00000 -2.05880 1.06095 H 0.00000 2.47853 0.08160 C 3.67594 0.75170 -0.05522 H 4.60332 1.31096 -0.08657 C 2.46836 1.41869 -0.00077 H 2.44448 2.50269 0.00773 C 3.69989 -0.64502 -0.07338 H 4.64375 -1.17410 -0.11999 C 2.50426 -1.35607 -0.03034 H 2.52656 -2.44097 -0.04137 C -3.67594 0.75170 -0.05521 H -4.60332 1.31096 -0.08657 C -2.46836 1.41869 -0.00077 H -2.44448 2.50269 0.00773 C -3.69989 -0.64502 -0.07338 H -4.64375 -1.17410 -0.11999 C -2.50426 -1.35607 -0.03034 H -2.52656 -2.44097 -0.04137

	H 1.99868 -0.98290 -2.21928 H 3.09822 0.13878 -3.01062 C 1.16413 1.60667 -1.88259 H 0.33552 0.92676 -2.07977 H 0.79999 2.45066 -1.30197 H 1.53149 1.97876 -2.84042 C -1.78625 2.79771 -0.48093 C -1.07798 2.35807 0.65723 C -2.57291 0.35985 0.84185 C -3.30405 0.78500 -0.28573 C -2.72606 1.84992 -1.17571 H -3.52010 2.40158 -1.68366 H -2.16165 1.33879 -1.97018 H -0.95611 0.83469 2.18367 C 0.07963 4.48654 0.75231 H 0.79949 5.14158 1.22725 C -0.14195 3.21738 1.25721 H 0.39994 2.88085 2.13140 C -0.63360 4.92122 -0.36416 H -0.46981 5.91595 -0.76008 C -1.56111 4.07808 -0.96908 H -2.11342 4.42101 -1.83688 C -4.26845 -1.30178 1.31158 H -4.64011 -2.11547 1.92156 C -3.07022 -0.69131 1.62881 H -2.49706 -1.02756 2.48274 C -4.99549 -0.86752 0.20294 H -5.93654 -1.34156 -0.04790 C -4.51223 0.17174 -0.58487 H -5.07822 0.50124 -1.44893		

P2 (sixtet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	Fe 1.66257 -0.00009 -0.02362 Cl 2.69077 1.83431 -0.71773 Cl 1.55418 -0.00031 2.19407 O 0.00240 -0.00014 -0.93185 N -1.37778 -0.00009 -0.88965 C -1.91255 -1.34276 -0.28425 C -1.72613 -1.26515 1.23077 H -2.18869 -2.15681 1.65999 H -0.66184 -1.32348 1.45786 C -2.30597 0.00024 1.86613 H -2.06578 0.00033 2.93058 H -3.39708 0.00032 1.80058 C -3.37455 -1.55290 -0.69645 H -4.08144 -0.96451 -0.12237 H -3.61564 -2.60240 -0.52941 H -3.53169 -1.35111 -1.75866 C -1.07773 -2.46820 -0.89611 H -1.17742 -2.48829 -1.98427 H -1.45465 -3.41487 -0.50735 H -0.02368 -2.38955 -0.65065 C -1.91247 1.34272 -0.28453 C -1.72594 1.26540 1.23049 H -2.18827 2.15724 1.65958 H -0.66162 1.32358 1.45747 C -3.37448 1.55286 -0.69670 H -4.08138 0.96469 -0.12242 H -3.61546 2.60242 -0.52995 H -3.53169 1.35076 -1.75884 C -1.07764 2.46796 -0.89672 H -1.17748 2.48782 -1.98487 H -1.45446 3.41474 -0.50814 H -0.02359 2.38927 -0.65134 Cl 2.69122 -1.83380 -0.71870	**P2-O** (sixtet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	Fe -1.72517 -0.00928 0.03828 Cl -2.62199 -1.78232 -0.90188 Cl -1.67496 -0.08920 2.22683 O 0.06051 -0.02280 -1.00501 N 1.55308 -0.01190 -0.94819 C 1.93902 1.29857 -0.31168 C 1.63573 1.29803 1.19514 H 2.05303 2.20704 1.63526 H 0.55519 1.36076 1.34052 C 2.16690 0.05750 1.91726 H 1.83109 0.07398 2.95616 H 3.25938 0.07875 1.95044 C 3.43473 1.54742 -0.58572 H 4.09586 0.98238 0.06245 H 3.63887 2.60399 -0.41065 H 3.68239 1.31885 -1.62234 C 1.17208 2.42220 -1.02090 H 1.35339 2.38821 -2.09750 H 1.52775 3.38279 -0.64671 H 0.10100 2.37373 -0.84655 C 1.96420 -1.28895 -0.25782 C 1.68114 -1.23236 1.25157 H 2.14108 -2.10379 1.72416 H 0.60730 -1.33331 1.41126 C 3.45911 -1.53048 -0.54177 H 4.11998 -0.93274 0.07693 H 3.67862 -2.57692 -0.32816 H 3.69229 -1.33922 -1.58922 C 1.20095 -2.45320 -0.90350 H 1.37440 -2.47611 -1.98184 H 1.56635 -3.39022 -0.48195 H 0.12995 -2.40426 -0.72409 Cl -2.62825 1.85305 -0.69249

	H -1.66000 -0.00020 -1.87672		H -0.10387 -0.10545 -1.95337
TS2 (sixtet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 1.45584 -3.74898 -0.27821 C 1.64568 -2.56129 -1.21978 C 0.40459 -1.66075 -1.33352 N -0.00506 -1.29875 0.08073 C -0.24725 -2.40733 1.08890 C 1.02455 -3.26951 1.10648 H 2.39149 -4.30775 -0.19876 H 0.71988 -4.44595 -0.68486 H 1.90422 -2.90132 -2.22537 H 2.48671 -1.95862 -0.86600 H 0.84722 -4.11606 1.77395 H 1.83661 -2.68542 1.54943 O -1.02100 -0.39062 0.08460 Fe -2.71550 0.27619 -0.17279 Cl -2.48441 1.94003 -1.64679 Cl -4.16714 -1.22750 -0.95413 Cl -3.37616 0.98074 1.85518 C 1.84967 0.55098 1.19213 H 1.15719 -0.32561 0.65414 C -1.49857 -3.24220 0.77526 H -1.75340 -3.82917 1.65899 H -2.34681 -2.60317 0.54000 H -1.35672 -3.93617 -0.04725 C -0.46416 -1.75538 2.46010 H 0.39774 -1.17384 2.77982 H -1.34008 -1.10779 2.45179 H -0.62162 -2.54006 3.20109 C -0.72170 -2.33415 -2.13392 H -0.86818 -3.37766 -1.87192	**P1a** (singlet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 0.00000 1.39963 -0.00026 C -1.21929 -0.72013 -0.00024 C -1.21929 0.72013 -0.00024 C 1.21929 0.72013 -0.00024 C 1.21929 -0.72013 -0.00024 C 0.00000 -1.39963 -0.00026 H 0.00000 -2.48471 -0.00038 H 0.00000 2.48471 -0.00038 C -3.64756 0.71109 0.00030 H -4.59154 1.24270 0.00058 C -2.47169 1.40266 -0.00000 H -2.47087 2.48691 0.00006 C -3.64756 -0.71109 0.00030 H -4.59154 -1.24270 0.00058 C -2.47169 -1.40266 -0.00000 H -2.47087 -2.48691 0.00006 C 3.64756 0.71109 0.00030 H 4.59154 1.24270 0.00058 C 2.47169 1.40266 -0.00000 H 2.47087 2.48691 0.00006 C 3.64756 -0.71109 0.00030 H 4.59154 -1.24270 0.00058 C 2.47169 -1.40266 -0.00000 H 2.47087 -2.48691 0.00006

	H -1.66663 -1.81206 -1.99896 H -0.46424 -2.29497 -3.19333 C 0.76726 -0.35686 -2.05335 H -0.09395 0.30563 -2.12659 H 1.57165 0.17123 -1.54938 H 1.11121 -0.59582 -3.06067 C 3.68226 1.26333 -0.33335 C 3.20267 0.38369 0.67867 C 1.14426 1.78832 0.88702 C 1.66023 2.65892 -0.12642 C 2.88999 2.36181 -0.71289 H 3.27164 3.02915 -1.47974 H 1.73538 0.22927 2.22622 C 5.27778 -0.84688 0.54501 H 5.90884 -1.65548 0.89354 C 4.03382 -0.66099 1.10864 H 3.69154 -1.32155 1.89592 C 5.74255 0.00208 -0.47975 H 6.71869 -0.16620 -0.91636 C 4.96000 1.04142 -0.90955 H 5.30663 1.70989 -1.68898 C -0.72843 3.27867 1.16362 H -1.67157 3.50528 1.64292 C -0.05539 2.13433 1.52164 H -0.47950 1.47368 2.26505 C -0.23427 4.13281 0.15250 H -0.79842 5.01373 -0.12422 C 0.93482 3.83087 -0.48338 H 1.32489 4.46895 -1.26739		
R1b (singlet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 1.39230 -1.32788 -0.05429 C 0.03234 -1.06777 -0.17559 C 2.29552 -0.27894 0.09478 H -0.67340 -1.88137 -0.28800	**TS1b** (quintet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C -2.11601 2.97706 0.12177 C -1.51795 2.40470 -1.15958 C -0.09017 1.85905 -1.00893 N -0.08213 0.90169 0.20376

	H 3.35516 -0.48198 0.18946		C -0.70702 1.37756 1.53672
	C -0.44374 0.24394 -0.14556		C -2.10585 1.92218 1.22465
	C 1.82904 1.03068 0.12749		H -3.14288 3.29489 -0.06982
	H 2.52439 1.85209 0.25105		H -1.57317 3.87094 0.43571
	C 0.46639 1.28809 0.01284		H -1.48960 3.16003 -1.94788
	H 0.10709 2.31076 0.04983		H -2.16558 1.60267 -1.52027
	H 1.74915 -2.35053 -0.07793		H -2.50935 2.32758 2.15494
	C -1.92013 0.52752 -0.30493		H -2.75650 1.09242 0.93677
	H -2.19361 0.49543 -1.36262		O 1.13011 0.39267 0.44907
	H -2.14400 1.53824 0.05621		Fe 2.61627 -0.61683 -0.02315
	O -2.76317 -0.43772 0.32421		Cl 4.04269 0.70405 -1.09351
	H -2.52979 -0.47475 1.26001		Cl 3.36503 -1.41462 1.89882
			Cl 1.89973 -2.27591 -1.38379
			C -4.84073 -1.70542 0.83994
			C -3.46278 -1.83211 0.73886
			C -5.56850 -1.09700 -0.17987
			H -2.90097 -2.31945 1.52375
			H -6.64340 -0.99865 -0.09607
			C -2.79107 -1.34919 -0.39135
			C -4.91059 -0.62903 -1.31536
			H -5.47364 -0.17441 -2.12071
			C -3.53424 -0.75553 -1.42129
			H -3.02904 -0.40708 -2.31440
			H -5.35122 -2.08716 1.71525
			C -1.32896 -1.41646 -0.50882
			H -0.94282 -1.46516 -1.52782
			H -0.85673 -0.17933 -0.18456
			O -0.70678 -2.27400 0.35235
			H 0.19617 -2.44190 0.01318
			C 0.19060 2.42386 2.21193
			H -0.13418 2.52130 3.24833
			H 1.22869 2.09681 2.21086
			H 0.12835 3.40682 1.75660

			C -0.79022 0.16185 2.46174 H -1.40164 -0.63202 2.04685 H 0.20044 -0.23694 2.67250 H -1.24472 0.48032 3.40042 C 0.94915 2.97167 -0.82038 H 0.64443 3.72502 -0.10163 H 1.90888 2.55552 -0.52082 H 1.08487 3.46873 -1.78137 C 0.29152 1.06056 -2.25759 H 1.29595 0.64928 -2.18927 H -0.40774 0.25483 -2.46582 H 0.27103 1.73898 -3.11083
TS1b (septet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C -2.15193 2.96388 0.06500 C -1.53166 2.37091 -1.19590 C -0.10035 1.84109 -1.01465 N -0.10069 0.91020 0.21088 C -0.73774 1.40916 1.52271 C -2.14072 1.93220 1.18928 H -3.18030 3.26536 -0.14514 H -1.62353 3.87104 0.36592 H -1.50048 3.10959 -2.00000 H -2.16707 1.55478 -1.54679 H -2.55705 2.35183 2.10780 H -2.77967 1.08972 0.91230 O 1.13170 0.42113 0.49325 Fe 2.61472 -0.60263 -0.02468 Cl 4.01136 0.69162 -1.14611 Cl 3.46378 -1.34178 1.87024 Cl 1.91739 -2.31484 -1.30269 C -4.84858 -1.69435 0.84234 C -3.46938 -1.82518 0.76723 C -5.55927 -1.11523 -0.20630 H -2.92076 -2.28999 1.57527	**TS1b-O** (quintet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C -0.90044 3.98556 0.26443 C -0.78451 3.40042 -1.13879 C 0.15540 2.18426 -1.21591 N -0.24865 1.25016 -0.12431 C -0.53041 1.66037 1.28331 C -1.41972 2.91532 1.21811 H -1.58632 4.83586 0.25451 H 0.06373 4.37283 0.60292 H -0.42393 4.14696 -1.84974 H -1.77974 3.09215 -1.47413 H -1.51826 3.30621 2.23309 H -2.41919 2.61039 0.89359 O 0.35649 0.02935 -0.21837 Fe 2.10631 -0.86976 0.18533 Cl 3.83934 0.39233 0.64527 Cl 1.53766 -2.18713 1.85560 Cl 2.28785 -1.92939 -1.78831 C -4.15609 -1.96190 1.02790 C -2.94379 -2.26021 0.43123 C -4.93762 -0.90864 0.55115 H -2.32548 -3.06403 0.80692

	H -6.63554 -1.01320 -0.14252 C -2.77915 -1.37718 -0.36599 C -4.88270 -0.68158 -1.34430 H -5.43214 -0.25014 -2.17197 C -3.50507 -0.81307 -1.42438 H -2.98532 -0.49277 -2.32014 H -5.37379 -2.04981 1.72043 C -1.31414 -1.44749 -0.45959 H -0.92254 -1.52980 -1.47451 H -0.85494 -0.22123 -0.16106 O -0.70987 -2.29664 0.42761 H 0.19921 -2.47170 0.11265 C 0.13933 2.48084 2.18679 H -0.19460 2.59270 3.21897 H 1.18190 2.16897 2.19845 H 0.06616 3.45456 1.71315 C -0.81985 0.21422 2.47596 H -1.41048 -0.59945 2.06899 H 0.17292 -0.16375 2.71313 H -1.29679 0.54675 3.39875 C 0.92539 2.96956 -0.84251 H 0.60116 3.73971 -0.15025 H 1.88388 2.57211 -0.51508 H 1.07284 3.44129 -1.81467 C 0.29880 1.02400 -2.24667 H 1.31368 0.64053 -2.17369 H -0.37995 0.19599 -2.43485 H 0.25992 1.68205 -3.11539		H -5.88259 -0.67673 1.02670 C -2.49787 -1.51112 -0.67142 C -4.50237 -0.15709 -0.53791 H -5.11013 0.65655 -0.91405 C -3.29343 -0.45348 -1.14630 H -2.96299 0.12388 -2.00009 H -4.49604 -2.54588 1.87429 C -1.20029 -1.75795 -1.27143 H -1.05149 -1.40948 -2.29750 H -0.43352 -0.77640 -0.68190 O -0.61301 -2.94880 -0.96300 H 0.28679 -2.97088 -1.34117 C 0.75213 1.92636 2.08912 H 0.48301 2.14734 3.12337 H 1.40028 1.05112 2.10331 H 1.32760 2.76430 1.70400 C -1.31213 0.52968 1.96044 H -2.22447 0.30606 1.41033 H -0.71352 -0.37696 2.03805 H -1.58513 0.84252 2.96958 C 1.62808 2.61385 -1.12964 H 1.84686 3.19446 -0.23716 H 2.28996 1.75070 -1.13724 H 1.87169 3.22724 -1.99906 C -0.05750 1.46567 -2.55408 H 0.61512 0.61459 -2.66073 H -1.08658 1.11929 -2.64999 H 0.14363 2.16085 -3.37017
TS1b-O (septet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C -0.92667 4.01903 0.26773 C -0.79897 3.44175 -1.13784 C 0.13687 2.22161 -1.21221 N -0.29685 1.28059 -0.13953 C -0.55548 1.68880 1.27183	**INT1b** (doublet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C -1.34043 -1.34200 -0.00004 C 0.01699 -1.08030 0.00014 C -2.27228 -0.30131 -0.00020 H 0.73130 -1.89259 0.00035 H -3.33310 -0.51662 -0.00051

C	-1.44836	2.94229	1.21294
H	-1.61469	4.86776	0.25767
H	0.03412	4.40728	0.61486
H	-0.42899	4.19146	-1.84083
H	-1.79178	3.13855	-1.48455
H	-1.55170	3.32699	2.22994
H	-2.44563	2.63674	0.88243
O	0.36130	0.06748	-0.22337
Fe	2.07433	-0.84789	0.18524
Cl	3.80924	0.38107	0.70268
Cl	1.53295	-2.23387	1.79733
Cl	2.36590	-1.91503	-1.75627
C	-4.11540	-2.03064	1.02311
C	-2.89894	-2.30888	0.42473
C	-4.91300	-0.98785	0.55021
H	-2.26989	-3.10637	0.79602
H	-5.86156	-0.77198	1.02620
C	-2.46273	-1.54853	-0.67408
C	-4.48799	-0.22556	-0.53611
H	-5.10753	0.58068	-0.90910
C	-3.27410	-0.50022	-1.14363
H	-2.94843	0.08918	-1.99099
H	-4.44659	-2.62304	1.86720
C	-1.15824	-1.77129	-1.27304
H	-1.02629	-1.42542	-2.30402
H	-0.41793	-0.79761	-0.69404
O	-0.57355	-2.97758	-0.98631
H	0.32709	-2.99248	-1.35709
C	0.72494	1.95692	2.07956
H	0.45557	2.17305	3.11488
H	1.37535	1.08326	2.09200
H	1.30006	2.79751	1.70002
C	-1.33351	0.55580	1.95056
C	0.49248	0.25834	0.00018
C	-1.82030	1.02275	-0.00009
H	-2.53591	1.83642	-0.00008
C	-0.46943	1.30434	0.00010
H	-0.13011	2.33412	0.00028
H	-1.68395	-2.36990	-0.00003
C	1.85987	0.56647	0.00000
H	2.22174	1.58683	0.00005
O	2.78234	-0.43599	-0.00007
H	3.66989	-0.06012	-0.00010

	H -2.24271 0.32527 1.39787 H -0.73102 -0.34850 2.02823 H -1.61020 0.86573 2.95977 C 1.61018 2.64571 -1.10982 H 1.82137 3.23243 -0.21950 H 2.26798 1.77903 -1.10372 H 1.87005 3.25142 -1.97998 C -0.06600 1.51542 -2.55891 H 0.60678 0.66451 -2.66652 H -1.09408 1.16804 -2.66262 H 0.14083 2.21522 -3.36990		
INT1b′ (doublet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C 1.35444 1.33187 0.00004 C -0.01376 1.08115 0.00012 C 2.26126 0.27626 -0.00007 H -0.72543 1.89691 0.00018 H 3.32637 0.47363 -0.00013 C -0.48489 -0.22815 0.00008 C 1.79394 -1.03475 -0.00011 H 2.49394 -1.86164 -0.00021 C 0.42681 -1.28414 -0.00003 H 0.06544 -2.30773 -0.00006 H 1.71349 2.35417 0.00006 C -1.96737 -0.52771 0.00024 H -2.23056 -1.18203 0.85933 H -2.23057 -1.18315 -0.85798 O -2.82941 0.51532 -0.00035	**P1b** (singlet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C -1.32768 -1.32439 -0.00007 C 0.03954 -1.10197 0.00019 C -2.21058 -0.24354 -0.00021 H 0.74346 -1.92431 0.00032 H -3.27896 -0.42145 -0.00042 C 0.53237 0.20729 0.00032 C -1.72618 1.06070 -0.00010 H -2.41466 1.89619 -0.00021 C -0.35528 1.28536 0.00016 H 0.03242 2.29809 0.00026 H -1.71307 -2.33627 -0.00016 C 1.98550 0.46493 0.00066 H 2.26508 1.53849 -0.00062 O 2.84245 -0.39263 -0.00061
R2 (quintet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C -3.98900 -0.00011 0.24973 C -3.36058 1.24364 -0.36730 C -1.84198 1.34502 -0.15167 N -1.22060 0.00002 -0.41966 C -1.84185 -1.34504 -0.15168 C -3.36046 -1.24380 -0.36730 H -5.06419 -0.00017 0.05813	**R2** (septet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C -3.98966 0.23964 0.38321 C -3.27731 1.40759 -0.28617 C -1.74425 1.35006 -0.18052 N -1.27844 -0.05495 -0.42807 C -2.03799 -1.32338 -0.16155 C -3.54569 -1.05772 -0.28067 H -5.06999 0.35806 0.27564

	H -3.87150 -0.00010 1.33618 H -3.80624 2.15464 0.03754 H -3.56214 1.24470 -1.44300 H -3.80602 -2.15485 0.03755 H -3.56203 -1.24489 -1.44300 O 0.01519 0.00010 -0.74018 Fe 1.80034 0.00001 0.00201 Cl 2.69928 1.85843 -0.76021 Cl 1.62386 0.00017 2.19574 Cl 2.69916 -1.85857 -0.75995 C -1.49452 -1.75308 1.28936 H -1.84165 -2.77522 1.44860 H -0.41895 -1.72470 1.45387 H -1.97098 -1.11240 2.02892 C -1.23104 -2.34752 -1.13428 H -1.36349 -2.01501 -2.16483 H -0.16880 -2.49890 -0.95214 H -1.74591 -3.30144 -1.01130 C -1.49471 1.75309 1.28938 H -1.97111 1.11235 2.02893 H -0.41914 1.72481 1.45390 H -1.84194 2.77519 1.44862 C -1.23126 2.34757 -1.13424 H -0.16903 2.49903 -0.95210 H -1.36367 2.01507 -2.16480 H -1.74620 3.30145 -1.01125		H -3.78776 0.21982 1.45715 H -3.59399 2.36237 0.13852 H -3.55518 1.42700 -1.34443 H -4.06145 -1.92000 0.14701 H -3.81658 -1.02217 -1.34046 O -0.01869 -0.22286 -0.65911 Fe 1.82951 -0.03879 0.00966 Cl 2.56336 1.98767 -0.41755 Cl 1.72359 -0.42966 2.17300 Cl 2.90788 -1.58921 -1.10000 C -1.65602 -1.80065 1.25013 H -2.10550 -2.78055 1.41911 H -0.57571 -1.89060 1.34794 H -2.01444 -1.12324 2.02390 C -1.59929 -2.36144 -1.19869 H -1.75982 -1.99156 -2.21247 H -0.54918 -2.62271 -1.08551 H -2.20120 -3.26095 -1.06082 C -1.25738 1.76859 1.21704 H -1.72891 1.18646 2.00745 H -0.17807 1.65684 1.30633 H -1.50423 2.82023 1.37015 C -1.11769 2.24990 -1.24939 H -0.03617 2.29977 -1.15458 H -1.36942 1.89580 -2.25026 H -1.52155 3.25648 -1.12959
R1a (singlet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C -0.00000 1.42016 0.70482 C 1.25293 -0.69941 0.26705 C 1.25293 0.69946 0.26693 C -1.25294 0.69946 0.26693 C -1.25294 -0.69941 0.26705 C -0.00000 -1.42003 0.70508 H 0.00000 -2.44888 0.33968	**INT1a** (doublet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 0.00000 1.39443 0.05100 C 1.27924 -0.70551 0.02179 C 1.24473 0.71177 0.02876 C -1.24473 0.71177 0.02876 C -1.27924 -0.70551 0.02179 C 0.00000 -1.50336 0.08686 H 0.00000 -2.25377 -0.71251

	H -0.00000 -1.48624 1.80279 H -0.00000 2.44894 0.33923 C 3.54257 0.69519 -0.51200 H 4.42760 1.24080 -0.81811 C 2.39862 1.38584 -0.12711 H 2.39444 2.47084 -0.13638 C 3.54257 -0.69528 -0.51188 H 4.42760 -1.24095 -0.81790 C 2.39862 -1.38587 -0.12687 H 2.39444 -2.47087 -0.13595 C -3.54257 0.69519 -0.51202 H -4.42760 1.24080 -0.81813 C -2.39862 1.38584 -0.12712 H -2.39444 2.47084 -0.13639 C -3.54257 -0.69528 -0.51189 H -4.42760 -1.24095 -0.81791 C -2.39862 -1.38587 -0.12687 H -2.39444 -2.47087 -0.13596 H -0.00000 1.48657 1.80253		H 0.00000 -2.08642 1.01805 H 0.00000 2.47887 0.05882 C 3.67704 0.75186 -0.04100 H 4.60494 1.31150 -0.06415 C 2.46896 1.41860 -0.00011 H 2.44568 2.50302 0.00630 C 3.70163 -0.64472 -0.05530 H 4.64654 -1.17367 -0.09043 C 2.50583 -1.35574 -0.02342 H 2.52867 -2.44102 -0.03183 C -3.67704 0.75186 -0.04100 H -4.60494 1.31150 -0.06415 C -2.46896 1.41860 -0.00011 H -2.44568 2.50302 0.00630 C -3.70163 -0.64472 -0.05530 H -4.64654 -1.17367 -0.09043 C -2.50583 -1.35574 -0.02342 H -2.52867 -2.44102 -0.03183
TS1a (quintet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 1.47938 -3.71244 -0.12762 C 1.67660 -2.57485 -1.12773 C 0.43823 -1.68587 -1.31426 N -0.01947 -1.24776 0.09226 C -0.25156 -2.33032 1.16481 C 1.02976 -3.17186 1.22882 H 2.41914 -4.25660 -0.00825 H 0.75657 -4.43804 -0.50685 H 1.94393 -2.96897 -2.11111 H 2.51443 -1.95393 -0.80312 H 0.85129 -3.98873 1.93207 H 1.83074 -2.56317 1.65653 O -1.01872 -0.36327 0.04225 Fe -2.74741 0.28438 -0.23130	**TS1a** (septet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 1.50615 -3.73629 -0.14077 C 1.70357 -2.59593 -1.13741 C 0.46166 -1.71161 -1.32467 N 0.00343 -1.27913 0.07666 C -0.23206 -2.35715 1.14466 C 1.05023 -3.19754 1.21406 H 2.44667 -4.27866 -0.01873 H 0.78617 -4.46273 -0.52389 H 1.97755 -2.98594 -2.12062 H 2.53663 -1.97158 -0.80603 H 0.87115 -4.01475 1.91679 H 1.84846 -2.58657 1.64401 O -1.01133 -0.39607 0.01728 Fe -2.73974 0.27733 -0.21500

Cl	-2.50611	1.93844	-1.68710
Cl	-4.11535	-1.26500	-1.05220
Cl	-3.46554	0.90558	1.78375
C	1.85115	0.47934	1.11955
H	1.02280	-0.47681	0.55618
C	-1.48752	-3.17935	0.84200
H	-1.76025	-3.73030	1.74300
H	-2.33487	-2.55789	0.56154
H	-1.31897	-3.90673	0.05518
C	-0.51440	-1.62711	2.49883
H	0.32787	-1.02469	2.82855
H	-1.40071	-0.99678	2.44364
H	-0.68345	-2.39063	3.25900
C	-0.68301	-2.39898	-2.07776
H	-0.82511	-3.43092	-1.77307
H	-1.63073	-1.87498	-1.97857
H	-0.41388	-2.40548	-3.13489
C	0.79876	-0.41311	-2.07969
H	-0.06194	0.24617	-2.18234
H	1.60304	0.12582	-1.59249
H	1.14557	-0.69475	-3.07467
C	3.66584	1.22775	-0.41880
C	3.20659	0.34767	0.57622
C	1.11891	1.71649	0.87716
C	1.55828	2.62425	-0.10840
C	2.79152	2.34470	-0.92588
H	3.38853	3.25887	-1.00494
H	2.48726	2.12023	-1.95706
H	1.75668	0.09826	2.13353
C	5.34034	-0.80835	0.53221
H	5.99192	-1.58696	0.91037
C	4.06668	-0.65741	1.04825
H	3.72576	-1.31688	1.83823

Cl	-2.53743	1.97712	-1.61769
Cl	-4.10191	-1.25603	-1.07135
Cl	-3.46366	0.85566	1.80860
C	1.82221	0.50301	1.10920
H	1.03571	-0.45514	0.55482
C	-1.46666	-3.20965	0.82163
H	-1.74133	-3.75943	1.72282
H	-2.31331	-2.58897	0.53711
H	-1.29493	-3.93827	0.03647
C	-0.49703	-1.65615	2.47989
H	0.34418	-1.05252	2.81024
H	-1.38403	-1.02695	2.42542
H	-0.66514	-2.42042	3.23956
C	-0.65487	-2.42742	-2.09433
H	-0.79394	-3.46057	-1.79200
H	-1.60403	-1.90601	-1.99395
H	-0.38389	-2.43107	-3.15107
C	0.82201	-0.43790	-2.09021
H	-0.04034	0.21863	-2.19578
H	1.62287	0.10406	-1.60024
H	1.17319	-0.71847	-3.08398
C	3.65401	1.25378	-0.40985
C	3.18736	0.37723	0.58475
C	1.09028	1.73866	0.85326
C	1.53925	2.64452	-0.12890
C	2.77756	2.35975	-0.93688
H	3.37068	3.27519	-1.02794
H	2.47784	2.11754	-1.96552
H	1.72286	0.13768	2.12906
C	5.32871	-0.76503	0.57694
H	5.98023	-1.53690	0.96878
C	4.04691	-0.61968	1.07435
H	3.69910	-1.27657	1.86347

	C 5.78473 0.05388 -0.47034 H 6.78188 -0.05503 -0.87994 C 4.95233 1.06445 -0.92982 H 5.30865 1.74852 -1.69287 C -0.74287 3.18237 1.39538 H -1.64652 3.38122 1.95547 C -0.03850 2.01769 1.61985 H -0.39311 1.31455 2.36069 C -0.30203 4.07696 0.42161 H -0.85504 4.98907 0.23305 C 0.84145 3.79695 -0.31546 H 1.18235 4.50174 -1.06639		C 5.78110 0.09407 -0.42481 H 6.78456 -0.01062 -0.81987 C 4.94838 1.09613 -0.90236 H 5.31062 1.77765 -1.66488 C -0.77573 3.20512 1.35358 H -1.68507 3.40446 1.90443 C -0.07556 2.03942 1.58354 H -0.43895 1.33377 2.31804 C -0.32444 4.09947 0.38386 H -0.87486 5.01197 0.18977 C 0.82516 3.81762 -0.34325 H 1.17331 4.52187 -1.09138
TS1a-O (quintet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 4.37541 1.62660 0.17664 C 3.31755 2.06734 -0.82777 C 2.25342 0.99160 -1.10979 N 1.75979 0.50767 0.21683 C 2.65165 0.14427 1.35860 C 3.69807 1.26540 1.49313 H 5.09214 2.43554 0.33953 H 4.95018 0.78089 -0.20946 H 3.77104 2.34607 -1.78174 H 2.81312 2.95766 -0.44015 H 4.42972 0.95157 2.24119 H 3.20121 2.15768 1.88697 O 0.65407 -0.29785 0.12314 Fe 0.22453 -2.19222 -0.39813 Cl -1.36475 -1.78538 -1.87356 Cl 1.81995 -3.44634 -1.25269 Cl -0.40637 -3.00254 1.56069 C -1.37502 0.95910 1.18263 H -0.33008 0.28706 0.56485 C 3.32901 -1.22584 1.19242 H 3.91102 -1.44412 2.09005	**TS1a-O** (septet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 4.47639 1.40940 0.11660 C 3.43561 1.91518 -0.87501 C 2.30650 0.90515 -1.14811 N 1.79744 0.45033 0.18136 C 2.68183 0.01700 1.30260 C 3.79142 1.07669 1.43658 H 5.23863 2.17604 0.27804 H 4.99968 0.53571 -0.28038 H 3.89471 2.17026 -1.83308 H 2.98896 2.83225 -0.47900 H 4.51076 0.71676 2.17587 H 3.34838 1.99215 1.84123 O 0.65321 -0.31460 0.07178 Fe 0.10362 -2.19215 -0.35404 Cl -1.58713 -1.83227 -1.71184 Cl 1.58058 -3.52258 -1.29780 Cl -0.46905 -2.99892 1.62048 C -1.32034 1.01059 1.17190 H -0.33292 0.31488 0.55071 C 3.28331 -1.38571 1.11635 H 3.87296 -1.63970 1.99957

	H	2.59508	-2.02184	1.08222		H	2.50735	-2.14289	1.02125
	H	4.00059	-1.26726	0.33926		H	3.93233	-1.45886	0.24805
	C	1.79998	0.10326	2.63250		C	1.84612	0.01046	2.58780
	H	1.29099	1.05389	2.79103		H	1.39370	0.98656	2.76132
	H	1.06181	-0.69700	2.59204		H	1.06244	-0.74497	2.54924
	H	2.44967	-0.07918	3.49009		H	2.49362	-0.21873	3.43595
	C	2.82145	-0.13243	-1.99021		C	2.79485	-0.24460	-2.04298
	H	3.67710	-0.63438	-1.54705		H	3.64277	-0.78143	-1.62590
	H	2.06569	-0.88571	-2.20167		H	1.99926	-0.96467	-2.22280
	H	3.13732	0.29200	-2.94525		H	3.09751	0.16050	-3.01067
	C	1.08143	1.63391	-1.85575		C	1.16608	1.62530	-1.87368
	H	0.29335	0.90685	-2.05071		H	0.33697	0.94717	-2.07493
	H	0.66909	2.46631	-1.29148		H	0.80253	2.46638	-1.28850
	H	1.43656	2.01138	-2.81623		H	1.53317	2.00283	-2.82980
	C	-1.93775	2.65982	-0.52061		C	-1.80252	2.78958	-0.48148
	C	-1.21173	2.29578	0.63372		C	-1.09113	2.35446	0.65649
	C	-2.59130	0.22300	0.87059		C	-2.57525	0.34825	0.84376
	C	-3.34151	0.57645	-0.26869		C	-3.31041	0.76955	-0.28277
	C	-2.80712	1.63335	-1.19295		C	-2.74037	1.83796	-1.17333
	H	-3.61817	2.11594	-1.74271		H	-3.53917	2.38679	-1.67763
	H	-2.19546	1.11705	-1.94945		H	-2.17750	1.33063	-1.97146
	H	-0.99582	0.81689	2.19264		H	-0.96000	0.83295	2.18410
	C	-0.19007	4.49344	0.67994		C	0.05475	4.48925	0.74922
	H	0.48233	5.20593	1.14241		H	0.76961	5.14999	1.22474
	C	-0.33402	3.22578	1.21636		C	-0.15946	3.21937	1.25531
	H	0.21901	2.94771	2.10449		H	0.38336	2.88758	2.13094
	C	-0.92251	4.85364	-0.45013		C	-0.66044	4.91871	-0.36776
	H	-0.82075	5.84778	-0.86890		H	-0.50258	5.91463	-0.76433
	C	-1.79009	3.93891	-1.03986		C	-1.58306	4.07005	-0.97182
	H	-2.35667	4.22556	-1.91917		H	-2.13790	4.41014	-1.83959
	C	-4.21465	-1.48965	1.40521		C	-4.26117	-1.32277	1.31490
	H	-4.55221	-2.29471	2.04635		H	-4.62873	-2.13796	1.92611
	C	-3.04035	-0.82067	1.69497		C	-3.06607	-0.70583	1.63103

	H -2.45244 -1.10240 2.55878 C -4.96027 -1.12654 0.28438 H -5.88234 -1.64738 0.05469 C -4.52149 -0.09896 -0.54394 H -5.10238 0.17442 -1.41799		H -2.49163 -1.03817 2.48584 C -4.99157 -0.89294 0.20697 H -5.93073 -1.37224 -0.04283 C -4.51502 0.14897 -0.58104 H -5.08461 0.47545 -1.44437
P2 (sextet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	Fe 1.66240 -0.00007 -0.02427 Cl 2.69097 1.83475 -0.71730 Cl 1.55362 -0.00001 2.19342 O 0.00239 -0.00013 -0.93325 N -1.37787 -0.00004 -0.89046 C -1.91248 -1.34264 -0.28444 C -1.72522 -1.26504 1.23036 H -2.18789 -2.15670 1.66019 H -0.66094 -1.32421 1.45740 C -2.30432 0.00010 1.86607 H -2.06359 0.00014 2.93074 H -3.39574 0.00012 1.80241 C -3.37456 -1.55250 -0.69530 H -4.08159 -0.96446 -0.12085 H -3.61610 -2.60211 -0.52802 H -3.53315 -1.35138 -1.75763 C -1.07837 -2.46820 -0.89626 H -1.17876 -2.48940 -1.98457 H -1.45493 -3.41509 -0.50701 H -0.02403 -2.39007 -0.65177 C -1.91240 1.34263 -0.28456 C -1.72518 1.26516 1.23025 H -2.18781 2.15689 1.66000 H -0.66090 1.32432 1.45729 C -3.37445 1.55252 -0.69549 H -4.08154 0.96465 -0.12097 H -3.61590 2.60219 -0.52839 H -3.53302 1.35125 -1.75780	**P2-O** (sextet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	Fe -1.70545 0.00000 0.03520 Cl -2.61752 -1.81077 -0.79760 Cl -1.67885 0.00001 2.22032 O 0.06795 0.00019 -1.01961 N 1.55760 -0.00006 -0.95259 C 1.94765 1.29393 -0.28248 C 1.62620 1.26543 1.21993 H 2.05463 2.15665 1.68598 H 0.54522 1.34693 1.35209 C 2.12120 0.00005 1.92383 H 1.76587 0.00014 2.95668 H 3.21329 -0.00001 1.97918 C 3.44697 1.53798 -0.53552 H 4.09802 0.95801 0.11000 H 3.65691 2.59015 -0.33990 H 3.70545 1.32648 -1.57339 C 1.19519 2.43920 -0.97210 H 1.39033 2.43457 -2.04717 H 1.54951 3.38852 -0.56816 H 0.12117 2.39232 -0.81351 C 1.94744 -1.29397 -0.28235 C 1.62604 -1.26534 1.22008 H 2.05444 -2.15656 1.68617 H 0.54507 -1.34675 1.35227 C 3.44675 -1.53823 -0.53540 H 4.09788 -0.95821 0.11000 H 3.65656 -2.59039 -0.33963 H 3.70517 -1.32690 -1.57332

	C -1.07823 2.46807 -0.89648 H -1.17867 2.48921 -1.98479 H -1.45470 3.41501 -0.50728 H -0.02389 2.38986 -0.65201 Cl 2.69120 -1.83460 -0.71753 H -1.66040 -0.00008 -1.87761		C 1.19489 -2.43929 -0.97184 H 1.39019 -2.43495 -2.04689 H 1.54898 -3.38856 -0.56762 H 0.12085 -2.39220 -0.81342 Cl -2.61759 1.81084 -0.79735 H -0.10141 -0.00043 -1.97565
TS2 (sextet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 1.44649 -3.75567 -0.26700 C 1.64069 -2.57155 -1.21206 C 0.40307 -1.66657 -1.32849 N -0.00621 -1.29979 0.08482 C -0.25429 -2.40632 1.09412 C 1.01463 -3.27253 1.11614 H 2.38065 -4.31723 -0.18519 H 0.70986 -4.45268 -0.67290 H 1.89786 -2.91618 -2.21672 H 2.48446 -1.97129 -0.86073 H 0.83343 -4.11789 1.78452 H 1.82798 -2.69090 1.56025 O -1.01940 -0.38827 0.08623 Fe -2.71229 0.28125 -0.17810 Cl -2.47482 1.94039 -1.65610 Cl -4.16504 -1.22205 -0.95831 Cl -3.37971 0.99060 1.84561 C 1.85361 0.54491 1.19086 H 1.15641 -0.33317 0.65419 C -1.50693 -3.23769 0.77820 H -1.76728 -3.82126 1.66291 H -2.35268 -2.59729 0.53796 H -1.36481 -3.93562 -0.04104 C -0.47385 -1.75121 2.46280 H 0.38725 -1.16870 2.78349 H -1.34994 -1.10390 2.45195 H -0.63248 -2.53407 3.20586	**P1a** (singlet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 0.00000 1.39999 -0.00007 C -1.21877 -0.72020 -0.00004 C -1.21877 0.72020 -0.00004 C 1.21877 0.72020 -0.00004 C 1.21877 -0.72020 -0.00004 C 0.00000 -1.39999 -0.00007 H 0.00000 -2.48542 -0.00013 H 0.00000 2.48542 -0.00013 C -3.64660 0.71112 0.00007 H -4.59095 1.24285 0.00011 C -2.47088 1.40285 0.00000 H -2.47057 2.48750 -0.00002 C -3.64660 -0.71112 0.00007 H -4.59095 -1.24285 0.00011 C -2.47088 -1.40285 0.00000 H -2.47057 -2.48750 -0.00002 C 3.64660 0.71112 0.00007 H 4.59095 1.24285 0.00011 C 2.47088 1.40285 0.00000 H 2.47057 2.48750 -0.00002 C 3.64660 -0.71112 0.00007 H 4.59095 -1.24285 0.00011 C 2.47088 -1.40285 0.00000 H 2.47057 -2.48750 -0.00002

	C -0.72474 -2.33756 -2.12802 H -0.87442 -3.38066 -1.86579 H -1.66852 -1.81300 -1.99506 H -0.46676 -2.30058 -3.18766 C 0.77006 -0.36531 -2.05000 H -0.08934 0.29914 -2.12667 H 1.57501 0.16221 -1.54641 H 1.11510 -0.60696 -3.05659 C 3.68235 1.26378 -0.33697 C 3.20506 0.38009 0.67290 C 1.14665 1.78225 0.89040 C 1.65857 2.65484 -0.12379 C 2.88771 2.36154 -0.71327 H 3.26745 3.03202 -1.47877 H 1.74335 0.22091 2.22490 C 5.28347 -0.84485 0.53462 H 5.91736 -1.65257 0.88142 C 4.03868 -0.66474 1.09786 H 3.69937 -1.32849 1.88403 C 5.74651 0.00903 -0.48650 H 6.72407 -0.15437 -0.92285 C 4.96070 1.04676 -0.91345 H 5.30639 1.71887 -1.69072 C -0.72375 3.27376 1.17829 H -1.66287 3.50274 1.66477 C -0.05011 2.12829 1.53103 H -0.47004 1.46813 2.27734 C -0.23461 4.12830 0.16532 H -0.79886 5.01113 -0.10664 C 0.93088 3.82635 -0.47667 H 1.31776 4.46645 -1.26115		

INT1b′ (singlet) B3LYP+IDSCRF-D3/TZP-DKH(-dfg)	C	1.35516	1.33154	0.00003	**R1b** (singlet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C	1.39930	-1.32432	-0.05341
	C	-0.01310	1.08147	0.00012		C	0.03923	-1.07150	-0.18395
	C	2.26144	0.27568	-0.00007		C	2.29589	-0.27064	0.10256
	H	-0.72419	1.89816	0.00018		H	-0.66144	-1.88979	-0.30043
	H	3.32704	0.47269	-0.00014		H	3.35658	-0.46831	0.20447
	C	-0.48487	-0.22760	0.00008		C	-0.44445	0.23766	-0.15587
	C	1.79360	-1.03497	-0.00011		C	1.82242	1.03609	0.13238
	H	2.49358	-1.86244	-0.00021		H	2.51301	1.86170	0.26057
	C	0.42649	-1.28383	-0.00002		C	0.45914	1.28625	0.00840
	H	0.06511	-2.30780	-0.00006		H	0.09446	2.30776	0.04291
	H	1.71481	2.35408	0.00006		H	1.76209	-2.34565	-0.07521
	C	-1.96729	-0.52714	0.00024		C	-1.92176	0.51054	-0.32213
	H	-2.23070	-1.18181	0.85942		H	-2.19913	0.43343	-1.37706
	H	-2.23071	-1.18292	-0.85808		H	-2.14716	1.53585	-0.00375
	O	-2.83044	0.51489	-0.00035		O	-2.76070	-0.42892	0.34891
						H	-2.53135	-0.42812	1.28927
TS1b (quintet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C	-2.13899	2.95212	0.07006	**TS1b** (septet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C	-2.13690	2.95344	0.06843
	C	-1.53460	2.34598	-1.19190		C	-1.53288	2.34576	-1.19294
	C	-0.10046	1.82180	-1.02519		C	-0.09929	1.82017	-1.02561
	N	-0.08093	0.90185	0.21564		N	-0.08138	0.90075	0.21558
	C	-0.71103	1.41405	1.53257		C	-0.71124	1.41438	1.53207
	C	-2.11615	1.93373	1.20600		C	-2.11565	1.93562	1.20490
	H	-3.16981	3.25227	-0.13120		H	-3.16727	3.25479	-0.13332
	H	-1.60774	3.86308	0.35460		H	-1.60459	3.86388	0.35268
	H	-1.51574	3.07635	-2.00430		H	-1.51321	3.07538	-2.00600
	H	-2.17338	1.52564	-1.52639		H	-2.17242	1.52574	-1.52676
	H	-2.52297	2.36498	2.12373		H	-2.52203	2.36796	2.12231
	H	-2.75909	1.08882	0.94649		H	-2.75964	1.09137	0.94578
	O	1.13867	0.41455	0.48011		O	1.13713	0.41115	0.48109
	Fe	2.61538	-0.60195	-0.02681		Fe	2.61576	-0.60211	-0.02676
	Cl	4.00958	0.67520	-1.18055		Cl	4.00717	0.67392	-1.18507
	Cl	3.46872	-1.34476	1.86740		Cl	3.47368	-1.33845	1.86791
	Cl	1.87345	-2.31201	-1.29498		Cl	1.87374	-2.31582	-1.29019

	C	-4.86897	-1.64255	0.84593	C	-4.87075	-1.64136	0.84628
	C	-3.48942	-1.77780	0.78951	C	-3.49126	-1.77716	0.78983
	C	-5.56734	-1.09362	-0.22659	C	-5.56892	-1.09209	-0.22620
	H	-2.95151	-2.22262	1.61605	H	-2.95351	-2.22226	1.61632
	H	-6.64463	-0.98949	-0.17784	H	-6.64617	-0.98753	-0.17743
	C	-2.78612	-1.36383	-0.34889	C	-2.78781	-1.36344	-0.34857
	C	-4.87791	-0.69366	-1.36894	C	-4.87934	-0.69235	-1.36854
	H	-5.41839	-0.28692	-2.21535	H	-5.41966	-0.28533	-2.21491
	C	-3.49977	-0.82872	-1.43059	C	-3.50125	-0.82794	-1.43022
	H	-2.97093	-0.53709	-2.33101	H	-2.97231	-0.53645	-2.33062
	H	-5.40458	-1.97258	1.72819	H	-5.40648	-1.97122	1.72854
	C	-1.32200	-1.44478	-0.42630	C	-1.32373	-1.44484	-0.42591
	H	-0.91176	-1.53936	-1.43292	H	-0.91337	-1.54002	-1.43244
	H	-0.84686	-0.19793	-0.14045	H	-0.84844	-0.19806	-0.14044
	O	-0.72938	-2.27335	0.48366	O	-0.73129	-2.27291	0.48453
	H	0.17912	-2.46484	0.17512	H	0.17744	-2.46410	0.17638
	C	0.17415	2.49182	2.17340	C	0.17510	2.49139	2.17260
	H	-0.15139	2.61964	3.20662	H	-0.15077	2.62036	3.20556
	H	1.21635	2.17781	2.18285	H	1.21686	2.17594	2.18278
	H	0.10053	3.45947	1.68748	H	0.10307	3.45881	1.68598
	C	-0.78141	0.22886	2.49707	C	-0.78351	0.22976	2.49716
	H	-1.38169	-0.58662	2.10845	H	-1.38399	-0.58550	2.10838
	H	0.21349	-0.15073	2.72330	H	0.21086	-0.15043	2.72467
	H	-1.24160	0.57267	3.42448	H	-1.24443	0.57448	3.42387
	C	0.92653	2.95112	-0.87306	C	0.92884	2.94845	-0.87354
	H	0.61246	3.72640	-0.18174	H	0.61466	3.72497	-0.18368
	H	1.89057	2.55633	-0.55846	H	1.89199	2.55299	-0.55710
	H	1.05964	3.41690	-1.85043	H	1.06397	3.41279	-1.85131
	C	0.28731	0.99298	-2.25175	C	0.28765	0.99046	-2.25185
	H	1.30390	0.61266	-2.18733	H	1.30362	0.60861	-2.18722
	H	-0.39117	0.16182	-2.42607	H	-0.39211	0.16035	-2.42616
	H	0.23695	1.64317	-3.12613	H	0.23852	1.64052	-3.12639

TS1b-O (quintet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 0.85406 3.99697 -0.26801 C 0.75187 3.40991 1.13527 C -0.17300 2.18266 1.21575 N 0.23729 1.25388 0.12210 C 0.51008 1.66727 -1.28611 C 1.38252 2.93415 -1.22467 H 1.52949 4.85610 -0.26078 H -0.11618 4.37335 -0.60199 H 0.38583 4.15219 1.84831 H 1.75255 3.11431 1.46623 H 1.47111 3.32718 -2.24002 H 2.38809 2.64341 -0.90563 O -0.35535 0.02663 0.21662 Fe -2.10207 -0.88331 -0.17989 Cl -3.84965 0.36487 -0.62332 Cl -1.53945 -2.18754 -1.86197 Cl -2.26269 -1.95393 1.78914 C 4.18946 -1.93075 -1.02931 C 2.97384 -2.23545 -0.44269 C 4.96569 -0.87943 -0.54062 H 2.36167 -3.04043 -0.82653 H 5.91453 -0.64356 -1.00744 C 2.51908 -1.49471 0.66195 C 4.52143 -0.13573 0.54996 H 5.12645 0.67554 0.93666 C 3.30902 -0.43813 1.14818 H 2.97343 0.13169 2.00523 H 4.53722 -2.50989 -1.87642 C 1.22063 -1.75206 1.25626 H 1.06881 -1.41323 2.28532 H 0.44461 -0.77258 0.67376 O 0.64247 -2.94495 0.93874 H -0.25430 -2.98080 1.32281	**TS1b-O** (septet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 0.83695 4.04517 -0.26683 C 0.72090 3.46647 1.13895 C -0.18312 2.22260 1.21267 N 0.27461 1.29210 0.14105 C 0.52804 1.70552 -1.26970 C 1.38839 2.98138 -1.20965 H 1.50313 4.91161 -0.25612 H -0.13245 4.40924 -0.61675 H 0.33026 4.20756 1.84033 H 1.72069 3.19037 1.48868 H 1.48477 3.36821 -2.22682 H 2.39283 2.70274 -0.87670 O -0.35818 0.06532 0.22228 Fe -2.05736 -0.87758 -0.18551 Cl -3.81137 0.31648 -0.72198 Cl -1.48460 -2.26204 -1.78770 Cl -2.34158 -1.93890 1.76010 C 4.14707 -1.98601 -1.02581 C 2.93151 -2.27068 -0.42860 C 4.94023 -0.94143 -0.55019 H 2.30764 -3.07205 -0.80088 H 5.88928 -0.72155 -1.02436 C 2.49194 -1.51486 0.67195 C 4.51133 -0.18307 0.53712 H 5.12876 0.62389 0.91323 C 3.29812 -0.46347 1.14326 H 2.97068 0.12190 1.99311 H 4.48194 -2.57628 -1.87050 C 1.19024 -1.74800 1.27371 H 1.05852 -1.40237 2.30499 H 0.43656 -0.78523 0.69399 O 0.61824 -2.96141 0.99176 H -0.27916 -2.98924 1.36937

	C -0.77779 1.91578 -2.08822 H -0.51482 2.14146 -3.12334 H -1.41406 1.03182 -2.10240 H -1.36397 2.74571 -1.70153 C 1.30473 0.54601 -1.96378 H 2.22008 0.33291 -1.41414 H 0.71682 -0.36768 -2.04156 H 1.57376 0.86183 -2.97334 C -1.65055 2.59518 1.13699 H -1.88244 3.16968 0.24375 H -2.30328 1.72529 1.15335 H -1.89567 3.20987 2.00542 C 0.05379 1.46502 2.55148 H -0.60817 0.60584 2.66032 H 1.08740 1.13083 2.64330 H -0.15220 2.15633 3.37004		C -0.75551 1.94090 -2.08196 H -0.48793 2.16658 -3.11601 H -1.38244 1.05038 -2.09984 H -1.35472 2.76529 -1.70383 C 1.33575 0.59073 -1.94367 H 2.24756 0.38172 -1.38643 H 0.75496 -0.32754 -2.02366 H 1.61019 0.90597 -2.95215 C -1.66626 2.60882 1.10912 H -1.89341 3.18633 0.21662 H -2.30294 1.72646 1.10805 H -1.94129 3.21181 1.97686 C 0.03657 1.52135 2.55879 H -0.61529 0.65426 2.66658 H 1.07308 1.19920 2.66285 H -0.18733 2.21531 3.37067
P1b (singlet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C -1.32792 -1.32414 -0.00007 C 0.03919 -1.10204 0.00019 C -2.21050 -0.24328 -0.00021 H 0.74330 -1.92515 0.00031 H -3.27970 -0.42116 -0.00041 C 0.53236 0.20701 0.00032 C -1.72591 1.06070 -0.00010 H -2.41479 1.89688 -0.00021 C -0.35515 1.28521 0.00016 H 0.03269 2.29872 0.00026 H -1.71371 -2.33672 -0.00015 C 1.98516 0.46440 0.00064 H 2.26529 1.53885 -0.00060 O 2.84295 -0.39233 -0.00060	**INT1b** (doublet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C -1.34043 -1.34200 -0.00004 C 0.01699 -1.08030 0.00014 C -2.27228 -0.30131 -0.00020 H 0.73130 -1.89259 0.00035 H -3.33310 -0.51662 -0.00051 C 0.49248 0.25834 0.00018 C -1.82030 1.02275 -0.00009 H -2.53591 1.83642 -0.00008 C -0.46943 1.30434 0.00010 H -0.13011 2.33412 0.00028 H -1.68395 -2.36990 -0.00003 C 1.85987 0.56647 0.00000 H 2.22174 1.58683 0.00005 O 2.78234 -0.43599 -0.00007 H 3.66989 -0.06012 -0.00010

INT1b′ (doublet) B3LYP+IDSCRF-D3a/TZP-DKH(-dfg)	C 1.35516 1.33154 0.00003 C -0.01310 1.08147 0.00012 C 2.26144 0.27568 -0.00007 H -0.72419 1.89816 0.00018 H 3.32704 0.47269 -0.00014 C -0.48487 -0.22760 0.00008 C 1.79360 -1.03497 -0.00011 H 2.49358 -1.86244 -0.00021 C 0.42649 -1.28383 -0.00002 H 0.06511 -2.30780 -0.00006 H 1.71481 2.35408 0.00006 C -1.96729 -0.52714 0.00024 H -2.23070 -1.18181 0.85942 H -2.23071 -1.18292 -0.85808 O -2.83044 0.51489 -0.00035		
R1a (singlet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C 0.00000 1.41019 0.77308 C 1.24206 -0.69876 0.30182 C 1.24209 0.69884 0.30176 C -1.24206 0.69884 0.30167 C -1.24207 -0.69877 0.30185 C 0.00000 -1.41002 0.77334 H -0.00001 -2.44586 0.43755 H 0.00001 -1.43489 1.86894 H 0.00002 2.44596 0.43707 C 3.49635 0.69462 -0.56537 H 4.36590 1.23800 -0.90652 C 2.36982 1.38625 -0.13495 H 2.36376 2.46841 -0.14363 C 3.49628 -0.69473 -0.56541 H 4.36578 -1.23818 -0.90658 C 2.36969 -1.38626 -0.13498 H 2.36357 -2.46842 -0.14356 C -3.49630 0.69459 -0.56549	**R2** (quintet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C 4.02064 0.00013 0.22032 C 3.38052 -1.23528 -0.38866 C 1.87499 -1.33503 -0.13428 N 1.25343 0.00168 -0.38909 C 1.87581 1.33919 -0.13916 C 3.38273 1.23745 -0.38701 H 5.08901 -0.00058 0.01008 H 3.91738 -0.00065 1.30538 H 3.83075 -2.14765 -0.00006 H 3.55248 -1.22698 -1.46664 H 3.83283 2.14855 0.00483 H 3.55860 1.23139 -1.46438 O 0.01222 0.00179 -0.70070 Fe -1.79595 -0.01382 -0.03480 Cl -2.70356 -1.82250 -0.85219 Cl -1.65053 -0.06641 2.14508 Cl -2.67389 1.84328 -0.77371 C 1.56858 1.75867 1.30187

	H -4.36582 1.23794 -0.90679 C -2.36974 1.38624 -0.13518 H -2.36365 2.46839 -0.14395 C -3.49632 -0.69477 -0.56527 H -4.36585 -1.23821 -0.90637 C -2.36976 -1.38630 -0.13476 H -2.36369 -2.46846 -0.14320 H -0.00005 1.43531 1.86867		H 1.92242 2.77875 1.43877 H 0.49940 1.73632 1.49526 H 2.06484 1.12481 2.03089 C 1.25889 2.33864 -1.11144 H 1.35874 1.99300 -2.13829 H 0.20886 2.51710 -0.90205 H 1.79831 3.27824 -1.00982 C 1.57597 -1.74768 1.31039 H 2.07592 -1.10986 2.03351 H 0.50836 -1.72471 1.51030 H 1.93165 -2.76670 1.45012 C 1.25125 -2.33769 -1.09872 H 0.20189 -2.51276 -0.88337 H 1.34603 -1.99669 -2.12761 H 1.78831 -3.27828 -0.99556
TS1a (quintet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C 1.40817 -3.70278 -0.09056 C 1.55280 -2.57102 -1.09824 C 0.30163 -1.70058 -1.23119 N -0.08198 -1.25252 0.18086 C -0.25927 -2.31988 1.26097 C 1.02039 -3.15424 1.27566 H 2.35359 -4.23807 -0.01078 H 0.67268 -4.43077 -0.43114 H 1.77484 -2.96426 -2.09035 H 2.39602 -1.94084 -0.81303 H 0.87254 -3.96269 1.99154 H 1.83571 -2.54002 1.65915 O -1.09667 -0.37567 0.18428 Fe -2.77369 0.37314 -0.05846 Cl -2.53601 1.97482 -1.54970 Cl -4.18760 -1.14789 -0.80991 Cl -3.42291 1.09235 1.93154 C 1.85092 0.44884 1.07487	**TS1a-O** (quintet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C 3.98844 2.43865 0.25134 C 2.88590 2.67805 -0.76521 C 2.06389 1.42190 -1.07197 N 1.62273 0.87612 0.24284 C 2.55782 0.65072 1.37781 C 3.36739 1.94210 1.54520 H 4.53139 3.36553 0.43499 H 4.71742 1.72225 -0.12851 H 3.29034 3.04615 -1.70823 H 2.20936 3.44334 -0.37953 H 4.12740 1.75984 2.30503 H 2.70129 2.71623 1.93187 O 0.71629 -0.16740 0.10198 Fe 0.64789 -2.06810 -0.44847 Cl -0.94136 -1.96289 -1.95433 Cl 2.43240 -3.01890 -1.27650 Cl 0.07534 -3.08117 1.41005 C -1.50678 0.71502 1.11934

H	0.96582	-0.49282	0.56969	H	-0.38812	0.22459	0.52423
C	-1.49910	-3.17635	1.00086	C	3.48429	-0.55737	1.21480
H	-1.73093	-3.70516	1.92318	H	4.05778	-0.68221	2.13242
H	-2.35783	-2.56506	0.73956	H	2.92023	-1.47343	1.06135
H	-1.35180	-3.91815	0.22625	H	4.18592	-0.45011	0.39466
C	-0.45752	-1.61555	2.59932	C	1.72474	0.44069	2.64065
H	0.39248	-1.00102	2.87486	H	1.04675	1.27722	2.79495
H	-1.35293	-1.00005	2.59407	H	1.15278	-0.48302	2.59436
H	-0.56978	-2.38051	3.36477	H	2.39254	0.38145	3.49861
C	-0.83575	-2.43853	-1.93588	C	2.86640	0.44612	-1.93612
H	-0.91479	-3.47871	-1.64320	H	3.80260	0.13861	-1.48322
H	-1.79363	-1.95439	-1.77352	H	2.29192	-0.44677	-2.16309
H	-0.62561	-2.41398	-3.00372	H	3.09698	0.93320	-2.88276
C	0.61863	-0.44090	-2.02397	C	0.82407	1.83622	-1.85753
H	-0.25699	0.19137	-2.14190	H	0.20160	0.97685	-2.09721
H	1.40506	0.13029	-1.54651	H	0.23790	2.55904	-1.29828
H	0.97157	-0.73978	-3.00924	H	1.13987	2.29380	-2.79397
C	3.71129	0.99556	-0.48961	C	-2.39692	2.24549	-0.60142
C	3.20572	0.21472	0.55370	C	-1.61027	2.05170	0.54427
C	1.21941	1.73073	0.76957	C	-2.60566	-0.21276	0.86016
C	1.72225	2.54641	-0.25325	C	-3.41017	-0.02865	-0.27180
C	2.90462	2.11957	-1.07620	C	-3.06827	1.06455	-1.23942
H	3.55791	2.97763	-1.24119	H	-3.95187	1.38025	-1.79226
H	2.55492	1.82907	-2.07240	H	-2.37654	0.64106	-1.97902
H	1.73767	0.14639	2.11136	H	-1.11790	0.68337	2.13421
C	5.28349	-1.02147	0.63572	C	-1.04817	4.39924	0.55986
H	5.89672	-1.78884	1.08525	H	-0.53255	5.23581	1.00828
C	4.01509	-0.77708	1.11799	C	-0.93761	3.13926	1.11165
H	3.63985	-1.35055	1.95457	H	-0.33970	2.98489	1.99828
C	5.77119	-0.26439	-0.42480	C	-1.83342	4.58724	-0.57153
H	6.76400	-0.44646	-0.80998	H	-1.92909	5.57237	-1.00515
C	4.99193	0.73916	-0.96957	C	-2.50372	3.51589	-1.14241
H	5.38482	1.34757	-1.77349	H	-3.11808	3.67097	-2.01908

	C -0.48046 3.37770 1.25432 H -1.34204 3.68930 1.82501 C 0.11400 2.16417 1.51402 H -0.27896 1.53074 2.29626 C 0.02512 4.18511 0.24202 H -0.43646 5.13841 0.02939 C 1.11814 3.77086 -0.49781 H 1.51255 4.40913 -1.27746		C -3.95067 -2.10296 1.51477 H -4.16249 -2.90732 2.20363 C -2.88460 -1.25930 1.74304 H -2.25610 -1.39959 2.61072 C -4.75085 -1.91213 0.39414 H -5.58998 -2.56834 0.21226 C -4.47946 -0.88062 -0.49072 H -5.10685 -0.73655 -1.35998
P2 (sextet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	Fe 1.67885 0.01729 -0.00756 Cl 2.72834 1.73997 -0.88349 Cl 1.49288 0.21940 2.18326 O 0.00681 -0.00699 -0.85712 N -1.36927 0.00037 -0.86109 C -1.93067 -1.33104 -0.29857 C -1.85581 -1.26647 1.22115 H -2.32870 -2.17096 1.60353 H -0.81134 -1.29941 1.52751 C -2.51277 -0.02382 1.81060 H -2.37782 -0.02949 2.89090 H -3.58928 -0.03608 1.63775 C -3.35484 -1.53895 -0.81222 H -4.10075 -0.95616 -0.28957 H -3.60057 -2.58792 -0.66760 H -3.43124 -1.33384 -1.88015 C -1.06549 -2.45312 -0.85700 H -1.07273 -2.45086 -1.94721 H -1.49347 -3.39508 -0.52088 H -0.03856 -2.39890 -0.51948 C -1.93061 1.32566 -0.27974 C -1.88388 1.24246 1.24075 H -2.39132 2.12842 1.62255 H -0.84805 1.30263 1.56709 C -3.34509 1.54902 -0.81359	**P2-O** (sextet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C 4.08481 0.07203 0.40380 C 3.53263 -1.18406 -0.25071 C 2.00514 -1.29977 -0.13430 N 1.49195 -0.02137 -0.68762 C 1.88514 1.28022 -0.10192 C 3.41992 1.29964 -0.19792 H 5.16190 0.12633 0.24609 H 3.93416 0.04090 1.48293 H 3.96545 -2.08121 0.19190 H 3.79634 -1.18177 -1.30972 H 3.76763 2.21152 0.28782 H 3.69065 1.36900 -1.25272 O 0.01722 -0.09927 -0.76420 Fe -1.83844 0.13264 0.07762 Cl -2.83444 -0.45347 -1.77955 Cl -2.11573 -1.26634 1.71174 Cl -2.22672 2.20217 0.59113 H -0.13988 -0.23462 -1.70787 C 1.42216 1.53802 1.33558 H 1.53556 2.59862 1.55433 H 0.37041 1.29845 1.47319 H 1.99761 0.98492 2.06918 C 1.33610 2.37619 -1.01321 H 1.57560 2.15765 -2.05235 H 0.26050 2.48939 -0.90894

	H -4.10074 0.95937 -0.31274 H -3.58931 2.59604 -0.65280 H -3.40613 1.36433 -1.88628 C -1.05013 2.45348 -0.80122 H -1.03820 2.47625 -1.89089 H -1.47667 3.39043 -0.44941 H -0.02919 2.38559 -0.44835 Cl 2.67670 -1.87980 -0.50708 H -1.61987 0.00887 -1.85304		H 1.79687 3.32530 -0.74417 C 1.59109 -1.64685 1.29753 H 2.08561 -1.03455 2.04302 H 0.51709 -1.56429 1.43570 H 1.86637 -2.68291 1.49097 C 1.53173 -2.41492 -1.06530 H 0.47010 -2.61684 -0.94083 H 1.72755 -2.15355 -2.10431 H 2.07228 -3.33045 -0.83300
INT1a (doublet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C 0.00000 1.39302 0.17751 C 1.27166 -0.70120 0.06368 C 1.24506 0.70510 0.09607 C -1.24506 0.70512 0.09604 C -1.27167 -0.70119 0.06371 C 0.00000 -1.48849 0.23465 H -0.00000 -2.34429 -0.44235 H 0.00001 -1.91456 1.24441 H 0.00001 2.47358 0.21732 C 3.65596 0.74316 -0.11714 H 4.57961 1.29982 -0.18546 C 2.45813 1.40885 0.01020 H 2.43603 2.49019 0.03705 C 3.67389 -0.64701 -0.16638 H 4.61001 -1.17524 -0.27483 C 2.48565 -1.35351 -0.07422 H 2.50217 -2.43547 -0.10706 C -3.65595 0.74316 -0.11720 H -4.57960 1.29981 -0.18559 C -2.45813 1.40886 0.01009 H -2.43602 2.49021 0.03685 C -3.67390 -0.64702 -0.16632 H -4.61002 -1.17526 -0.27470 C -2.48565 -1.35351 -0.07410	**TS2** (sextet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C 1.30858 -3.87309 -0.40056 C 1.51376 -2.66519 -1.30106 C 0.30465 -1.72554 -1.34235 N -0.03574 -1.39110 0.07746 C -0.28439 -2.50520 1.04782 C 0.94876 -3.41231 1.00315 H 2.21949 -4.47168 -0.37154 H 0.52910 -4.52108 -0.80077 H 1.73095 -2.97351 -2.32445 H 2.38047 -2.10181 -0.94631 H 0.76242 -4.26311 1.65920 H 1.79689 -2.86554 1.42257 O -1.07185 -0.47918 0.11813 Fe -2.65774 0.35732 -0.03423 Cl -2.39112 2.01788 -1.51655 Cl -4.27123 -1.01846 -0.73232 Cl -3.16100 1.16823 2.00435 C 1.89237 0.65383 1.20881 H 1.22964 -0.16989 0.73947 C -1.56781 -3.29887 0.78111 H -1.80370 -3.88453 1.66870 H -2.40458 -2.63527 0.58181 H -1.47316 -3.98852 -0.05054 C -0.39430 -1.88299 2.43824

	H -2.50218 -2.43548 -0.10686		H 0.49893 -1.31356 2.68386 H -1.25901 -1.22855 2.51262 H -0.49683 -2.67869 3.17456 C -0.85148 -2.34049 -2.13912 H -1.00686 -3.38990 -1.91318 H -1.78123 -1.80948 -1.95517 H -0.62201 -2.26343 -3.20123 C 0.71337 -0.42372 -2.02866 H -0.11545 0.27762 -2.08032 H 1.54108 0.04730 -1.50335 H 1.04611 -0.64767 -3.04140 C 3.79130 1.20278 -0.31946 C 3.25337 0.39647 0.71527 C 1.26871 1.92838 0.82813 C 1.84805 2.71855 -0.20866 C 3.06595 2.32612 -0.75626 H 3.49564 2.93567 -1.54316 H 1.79158 0.45497 2.27518 C 5.25588 -0.94500 0.64618 H 5.83408 -1.77320 1.03025 C 4.01259 -0.67537 1.18641 H 3.62513 -1.29115 1.98577 C 5.78196 -0.15937 -0.39287 H 6.75220 -0.39170 -0.80480 C 5.06000 0.90444 -0.87066 H 5.44726 1.52792 -1.66429 C -0.51406 3.53272 0.98452 H -1.44625 3.83733 1.43677 C 0.08495 2.36529 1.41449 H -0.38857 1.77476 2.18461 C 0.04923 4.31422 -0.04341 H -0.45134 5.21401 -0.36609 C 1.21290 3.91519 -0.63678

			H 1.66371 4.49106 -1.43280
P1a (singlet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C 0.00000 1.39934 0.00007 C -1.21668 -0.71793 0.00008 C -1.21668 0.71793 0.00007 C 1.21668 0.71793 0.00007 C 1.21668 -0.71793 0.00007 C -0.00000 -1.39934 0.00008 H -0.00001 -2.48238 0.00008 H 0.00000 2.48238 0.00007 C -3.64087 0.71022 0.00005 H -4.58206 1.24122 0.00005 C -2.46551 1.40218 0.00006 H -2.46376 2.48410 0.00005 C -3.64087 -0.71022 0.00006 H -4.58206 -1.24122 0.00006 C -2.46550 -1.40218 0.00007 H -2.46376 -2.48409 0.00007 C 3.64087 0.71022 0.00006 H 4.58206 1.24123 0.00007 C 2.46551 1.40218 0.00007 H 2.46376 2.48410 0.00009 C 3.64087 -0.71022 0.00005 H 4.58207 -1.24122 0.00004 C 2.46551 -1.40218 0.00005 H 2.46376 -2.48410 0.00006	**R1b** (singlet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C -1.35755 -1.30482 -0.05190 C -0.00728 -1.02791 0.10330 C -2.27991 -0.26441 -0.12541 H 0.71029 -1.83530 0.15706 H -3.33190 -0.48041 -0.24473 C 0.44091 0.29120 0.18700 C -1.84341 1.05083 -0.04335 H -2.55441 1.86284 -0.10041 C -0.48786 1.32478 0.11007 H -0.14881 2.35035 0.17287 H -1.69411 -2.33009 -0.11238 C 1.90923 0.58249 0.33136 H 2.32134 0.05148 1.18702 H 2.05828 1.65168 0.49628 O 2.67302 0.13312 -0.78775 H 2.27909 0.51192 -1.57975
TS1b (quintet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C -2.11220 2.96088 0.02374 C -1.49896 2.35092 -1.22686 C -0.06959 1.84162 -1.03743 N -0.06960 0.92102 0.18291 C -0.69837 1.42604 1.48523	**TS1b-O** (quintet) B2GP-PLYP+ IDSCRF/TZP-DKH(-dfg)	C -0.73705 4.04513 0.22106 C -0.68383 3.42994 -1.16681 C 0.20166 2.18169 -1.23780 N -0.25017 1.28146 -0.14358 C -0.43404 1.73360 1.26160

	C	-2.09687	1.94668	1.15721		C	-1.27276	3.01525	1.20054
	H	-3.13901	3.25796	-0.18541		H	-1.38670	4.92018	0.21312
	H	-1.58160	3.86835	0.30925		H	0.24964	4.39419	0.52631
	H	-1.47303	3.07408	-2.04210		H	-0.31134	4.14295	-1.90217
	H	-2.12705	1.52419	-1.55952		H	-1.69628	3.15157	-1.46686
	H	-2.49883	2.38036	2.07300		H	-1.32785	3.42158	2.21047
	H	-2.74061	1.10520	0.89727		H	-2.28778	2.74293	0.90462
	O	1.15272	0.42977	0.45625		O	0.36938	0.04058	-0.21652
	Fe	2.62312	-0.60927	0.02576		Fe	2.02632	-0.93087	0.18947
	Cl	4.09871	0.60217	-1.06724		Cl	3.83359	0.21060	0.57898
	Cl	3.37750	-1.33514	1.95083		Cl	1.48966	-2.19344	1.88107
	Cl	1.92361	-2.32908	-1.22727		Cl	2.16360	-2.11307	-1.69100
	C	-4.82738	-1.63535	0.97289		C	-4.22857	-1.79805	1.15422
	C	-3.45453	-1.75902	0.83620		C	-3.03442	-2.11775	0.53909
	C	-5.58226	-1.05230	-0.03541		C	-4.99157	-0.73229	0.69139
	H	-2.87054	-2.22857	1.61312		H	-2.43069	-2.93682	0.89920
	H	-6.65241	-0.95476	0.07609		H	-5.92310	-0.48398	1.17891
	C	-2.82231	-1.29881	-0.31621		C	-2.59501	-1.37686	-0.55932
	C	-4.96057	-0.61072	-1.19524		C	-4.56008	0.00941	-0.39789
	H	-5.54539	-0.17738	-1.99350		H	-5.15574	0.83280	-0.76419
	C	-3.58915	-0.73650	-1.33515		C	-3.36664	-0.30961	-1.02029
	H	-3.11170	-0.41230	-2.24984		H	-3.03491	0.26058	-1.87582
	H	-5.31079	-1.99881	1.86803		H	-4.56821	-2.37650	2.00103
	C	-1.35566	-1.38252	-0.47772		C	-1.31042	-1.66495	-1.19596
	H	-1.01980	-1.45951	-1.51089		H	-1.20073	-1.32862	-2.22925
	H	-0.84062	-0.16870	-0.17435		H	-0.47409	-0.77768	-0.64684
	O	-0.74757	-2.26742	0.36018		O	-0.80966	-2.90670	-0.93480
	H	0.14270	-2.45667	0.00533		H	0.07041	-2.97891	-1.34170
	C	0.17413	2.49744	2.14032		C	0.87342	1.96949	2.02159
	H	-0.15269	2.59393	3.17381		H	0.63743	2.21230	3.05675
	H	1.21747	2.19562	2.14216		H	1.49204	1.07519	2.03595
	H	0.08356	3.47185	1.67655		H	1.46363	2.78296	1.61284
	C	-0.77752	0.24067	2.44022		C	-1.24076	0.66762	1.99860

	H -1.34065 -0.58494 2.02218		H -2.17058 0.46231 1.47440
	H 0.21445 -0.11251 2.70729		H -0.68126 -0.25848 2.10504
	H -1.28422 0.57328 3.34402		H -1.47735 1.03428 2.99650
	C 0.93252 2.98370 -0.86662		C 1.68322 2.56165 -1.18772
	H 0.58765 3.75845 -0.19369		H 1.93770 3.16525 -0.32316
	H 1.89279 2.60926 -0.52442		H 2.31859 1.68084 -1.18424
	H 1.08000 3.43737 -1.84467		H 1.92525 3.13768 -2.07997
	C 0.35201 1.03066 -2.25797		C -0.06407 1.47160 -2.56367
	H 1.38041 0.69037 -2.18525		H 0.56890 0.59516 -2.68313
	H -0.29570 0.17858 -2.43524		H -1.10723 1.17148 -2.63424
	H 0.28273 1.68251 -3.12659		H 0.14977 2.15595 -3.38280