Supplementary Material for Faraday Discussions

Electronic Supplementary Information for

Valence Bond Modeling and Density Functional Theory Calculations of Reactivity and Mechanism of Cytochrome P450 Enzymes: Thioether Sulfoxidation

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Reference 47 in Full.

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Table S1. The Mulliken charges and spin densities of the key reaction intermediates in Sulfoxidation of *p-(MeO, Me, H, NO_2)*-TAn by Cpd I.

	Spin Density						Charge					
	Fe	O	SH	Por	Sub [a]	sulfur	Fe	O	SH	Por	Sub	sulfur
1. p-MeO-TAn												
^{4}RC	1.12	0.90	0.50	0.46	0.02	0.01	0.49	-0.42	-0.05	-0.01	-0.01	0.07
^{2}RC	1.24	0.85	-0.54	-0.54	-0.01	-0.01	0.50	-0.42	-0.05	-0.02	-0.01	0.07
$^4TS_{SO}$	1.79	0.50	0.38	-0.02	0.36	0.34	0.49	-0.58	-0.07	-0.36	0.51	0.46
$^2TS_{SO}$	1.33	0.47	-0.25	-0.34	-0.20	-0.19	0.44	-0.48	-0.08	-0.21	0.33	0.31
2. p-Me-TAn												
^{4}RC	1.12	0.90	0.50	0.46	0.02	0.01	0.49	-0.42	-0.05	-0.01	-0.01	0.08
^{2}RC	1.24	0.85	-0.55	-0.54	-0.01	-0.01	0.50	-0.42	-0.05	-0.02	-0.01	0.08
$^4TS_{SO}$	1.78	0.50	0.38	-0.02	0.37	0.34	0.49	-0.58	-0.06	-0.36	0.51	0.46
$^2TS_{SO}$	1.17	0.55	-0.29	-0.36	-0.07	-0.07	0.42	-0.47	-0.07	-0.21	0.32	0.31
3. TAn												
^{4}RC	1.12	0.90	0.50	0.47	0.01	0.01	0.49	-0.42	-0.05	-0.10	0.00	0.08
^{2}RC	1.24	0.85	-0.55	-0.54	0.00	-0.01	0.50	-0.42	-0.05	-0.02	-0.01	0.08
$^4TS_{SO}$	1.79	0.44	0.38	-0.02	0.36	0.33	0.49	-0.58	-0.06	-0.35	0.50	0.47
$^2TS_{SO}$	1.18	0.55	-0.29	-0.37	-0.07	-0.07	0.42	-0.47	-0.07	-0.21	0.33	0.32
^{4}PC	2.54	0.02	0.45	-0.01	0.00	0.00	0.44	-0.61	-0.16	-0.42	0.74	0.84
^{2}PC	1.06	0.00	0.02	-0.08	0.00	0.00	0.21	-0.61	0.03	-0.45	0.83	0.87
4. p-NO_2-TAn												
^{4}RC	1.13	0.89	0.53	0.45	0.00	0.00	0.48	-0.43	-0.03	-0.01	-0.02	0.14
^{2}RC	1.25	0.85	-0.58	-0.52	0.00	0.00	0.49	-0.43	-0.03	-0.01	-0.02	0.14
$^4TS_{SO}$	1.73	0.49	0.37	0.00	0.41	0.26	0.46	-0.58	-0.02	-0.30	0.42	0.52
$^2TS_{SO}$	1.13	0.53	-0.28	-0.38	0.00	-0.02	0.40	-0.49	-0.05	-0.17	0.31	0.40

a. The term "Sub" stands for the substrate *p-X*-Ph-S-Me and "sulfur" stands for the sulfur atom in the substrate.

Table S2. Relative Energies at Various Levels for Sulfoxidation of Pristine TAn by Cpd I of Cytochrome P450

	UB3LYP/B1		UB3LYP/B1 (Gibbs free energy)		UB3LYP/B2//B1		UB3LYP/B2//B1 +ZPE		UB3LYP/B2//B1 +Bulk Polarity		UB3LYP/B2//B1 +Bulk Polarity +ZPE	
	E	E_{rel}	*G*	G_{rel}	*E*	E_{rel}	*E*	E_{rel}	*E*	E_{rel}	*E*	E_{rel}
^{4}RC	-2255.572633	**0.0**	-2255.223591	**0.0**	-2255.988552	**0.0**	-2255.57141	**0.0**	-2256.01161	**0.0**	-2255.59447	**0.0**
^{2}RC	-2255.57272	**-0.1**	-2255.219264	**0.0**	-2255.98875	**-0.1**	-2255.57166	**-0.2**	-2256.01154	**0.0**	-2255.59445	**0.0**
$^4TS_{SO}$	-2255.544536	**17.6**	-2255.192667	**19.4**	-2255.967778	**13.0**	-2255.55135	**12.6**	-2255.98994	**13.6**	-2255.57351	**13.2**
$^2TS_{SO}$	-2255.553871	**11.8**	-2255.20197	**10.8**	-2255.975867	**8.0**	-2255.55966	**7.4**	-2255.99839	**8.3**	-2255.58218	**7.7**
^{4}PC	-2255.610064	**-23.5**	-2255.259405	**-41.9**	-2256.031864	**-27.2**	-2255.6146	**-27.1**	-2256.05733	**-28.7**	-2255.64006	**-28.6**
^{2}PC	-2255.619306	**-29.3**	-2255.263287	**-38.5**	-2256.038623	**-31.4**	-2255.6197	**-30.3**	-2256.06085	**-30.9**	-2255.64192	**-29.8**

* Absolute energies are in a.u. and the relative ones are in kcal/mol.

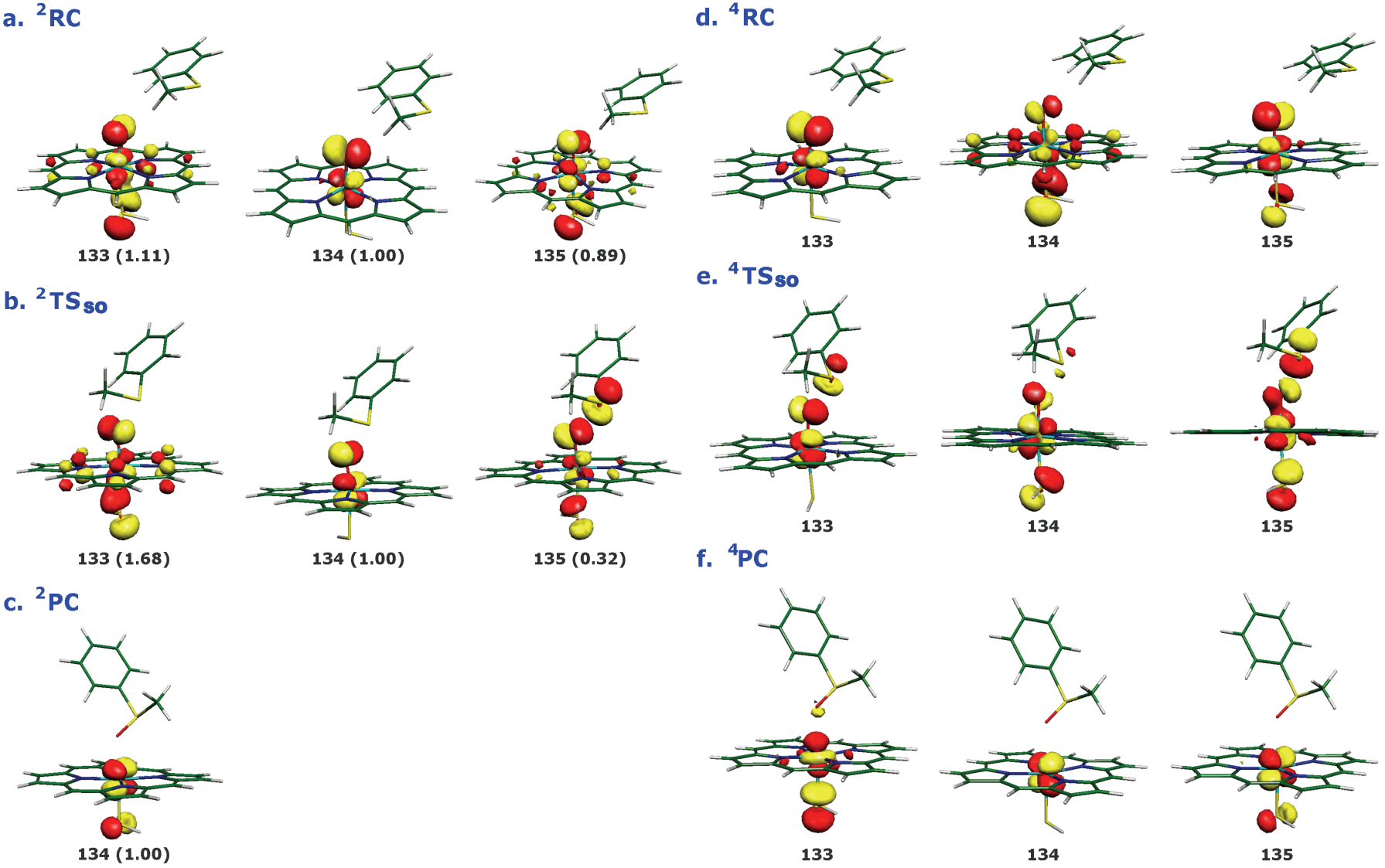

Figure S1. Natural Kohn-Sham orbitals and occupations of the key reaction intermediates during sulfoxidation of the pristine TAn S-oxidation by Cpd I.

Table S3. Relative Energies at Various Levels for Sulfoxidation of *p-(MeO, Me, H, NO_2)*-TAns by Cpd I of Cytochrome P450

	UB3LYP/B1		UB3LYP/B1 (Gibbs free energy)		UB3LYP/B2//B1		UB3LYP/B2//B1 +ZPE		UB3LYP/B2//B1 +Bulk Polarity		UB3LYP/B2//B1 +Bulk Polarity +ZPE	
	E (a.u.)	E_{rel}	G(a.u.)	G_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}
a) p-MeO-TAn												
^{4}RC	-2370.095361	**0.0.**	-2369.71623	**0.0**	-2370.544165	**0.0**	-2370.09436	**0.0**	-2370.56758	**0.0**	-2370.117779	**0.0**
^{2}RC	-2370.095491	**-0.1**	-2369.715439	**0.0**	-2370.544411	**-0.2**	-2370.09457	**-0.1**	-2370.56836	**-0.5**	-2370.11852	**-0.5**
$^4TS_{SO}$	-2370.069163	**16.4**	-2369.687383	**18.1**	-2370.525215	**11.9**	-2370.07608	**11.5**	-2370.54808	**12.2**	-2370.098943	**11.8**
$^2TS_{SO}$	-2370.078551	**10.5**	-2369.696451	**11.9**	-2370.533294	**6.8**	-2370.08457	**6.1**	-2370.55624	**7.1**	-2370.10752	**6.4**
b) p-Me-TAn												
^{4}RC	-2294.892226	**0.0**	-2294.51876	**0.0**	-2295.315673	**0.0**	-2294.871171	**0.0**	-2295.33830	**0.0**	-2294.893799	**0.0**
^{2}RC	-2294.892319	**-0.1**	-2294.518248	**0.0**	-2295.315845	**-0.1**	-2294.871389	**-0.1**	-2295.33833	**-0.02**	-2294.893877	**-0.05**
$^4TS_{SO}$	-2294.864959	**17.1**	-2294.487618	**19.5**	-2295.295728	**12.5**	-2294.851892	**12,1**	-2295.31748	**13.1**	-2294.873640	**12.6**
$^2TS_{SO}$	-2294.874329	**11.2**	-2294.498154	**12.6**	-2295.303928	**7.4**	-2294.860149	**6.9**	-2295.32546	**8.1**	-2294.881677	**7.6**

* Absolute energies are in a.u. and the relative ones are in kcal/mol.

Table S3 (Continued)

	UB3LYP/B1		UB3LYP/B1 (Gibbs free energy)		UB3LYP/B2//B1		UB3LYP/B2//B1 +ZPE		UB3LYP/B2//B1 +Bulk Polarity		UB3LYP/B2//B1 +Bulk Polarity +ZPE	
	E (a.u.)	E_{rel}	G(a.u.)	G_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}
c) TAn												
^{4}RC	-2255.572633	**0.0**	-2255.223591	**0.0**	-2255.988552	**0.0**	-2255.57141	**0.0**	-2256.01161	**0.0**	-2255.59447	**0.0**
^{2}RC	-2255.57272	**-0.1**	-2255.219264	**0.0**	-2255.98875	**-0.1**	-2255.57166	**-0.2**	-2256.01154	**0.0**	-2255.59445	**0.0**
$^4TS_{SO}$	-2255.544536	**17.6**	-2255.192667	**19.4**	-2255.967778	**13.0**	-2255.55135	**12.6**	-2255.98994	**13.6**	-2255.57351	**13.2**
$^2TS_{SO}$	-2255.553871	**11.8**	-2255.20197	**10.8**	-2255.975867	**8.0**	-2255.55966	**7.4**	-2255.99839	**8.3**	-2255.58218	**7.7**
d) p-NO_2-TAn												
^{4}RC	-2460.075318	**0.0**	-2459.723156	**0.0**	-2460.558349	**0.0**	-2460.13834	**0.0**	-2460.58246	**0.0**	-2460.16245	**0.0**
^{2}RC	-2460.075459	**-0.1**	-2459.725542	**0.0**	-2460.558508	**-0.1**	-2460.1385	**-0.1**	-2460.58253	**-0.05**	-2460.162519	**-0.04**
$^4TS_{SO}$	-2460.040521	**21.8**	-2459.689123	**21.4**	-2460.531545	**16.8**	-2460.11235	**16.3**	-2460.55825	**15.2**	-2460.139049	**14.7**
$^2TS_{SO}$	-2460.051276	**15.1**	-2459.698293	**17.1**	-2460.539571	**11.8**	-2460.12005	**11.5**	-2460.56668	**9.9**	-2460.147154	**9.6**

* Absolute energies are in a.u. and the relative ones are in kcal/mol.

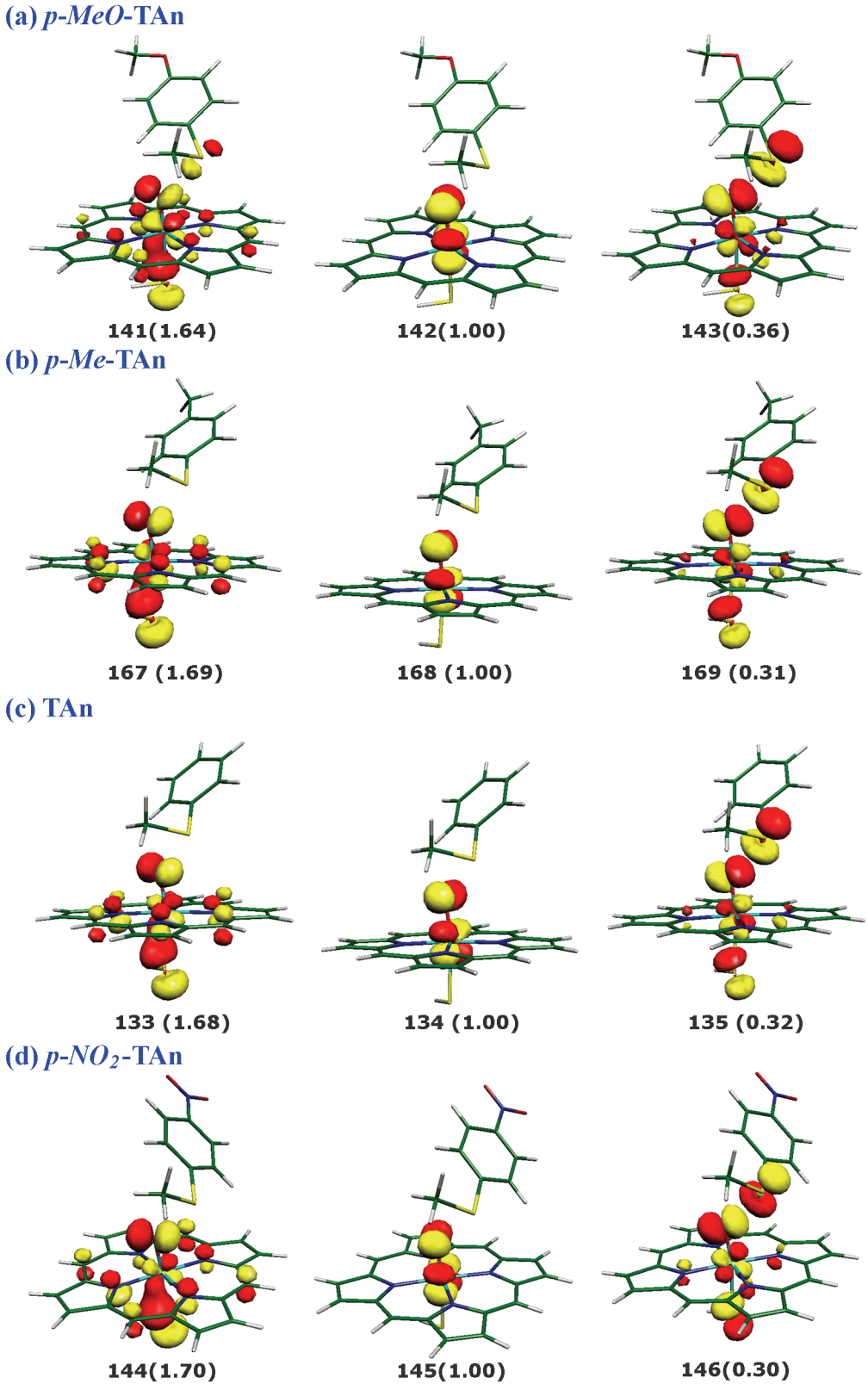

Figure S2. Natural Kohn-Sham orbitals and occupation for the **doublet** transition states $^{2}TS_{S\text{-}O}$ dor sulfoxidation of *p-(MeO, H, Cl, NO_2)*-TAns by Cpd I.

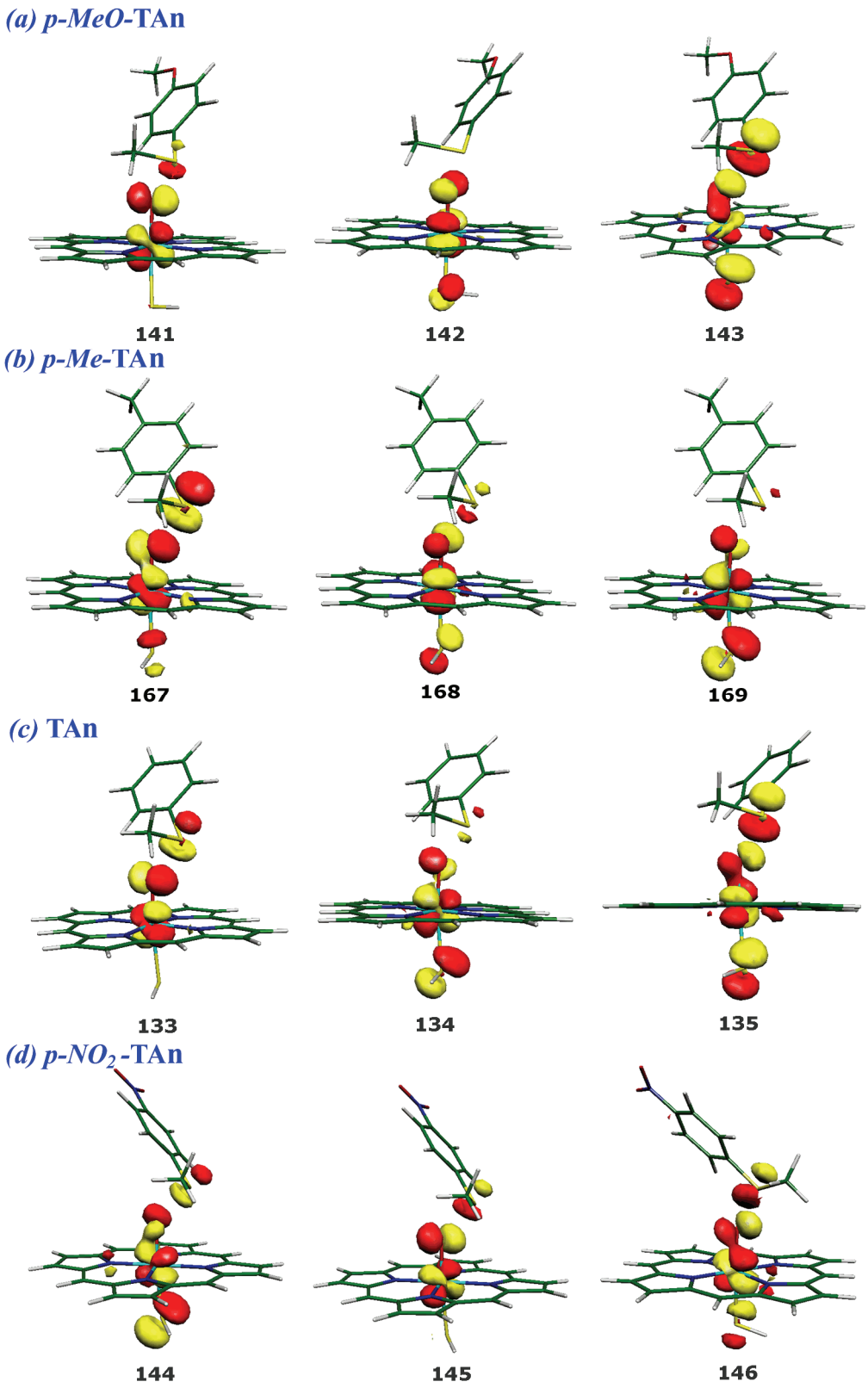

Figure S3. Singly occupied Natural Kohn-Sham orbitals in the **quartet** transition states $^{4}TS_{S\text{-}O}$ for sulfoxidation of *p-(MeO, Me, H, NO_2)*-TAns by Cpd I.

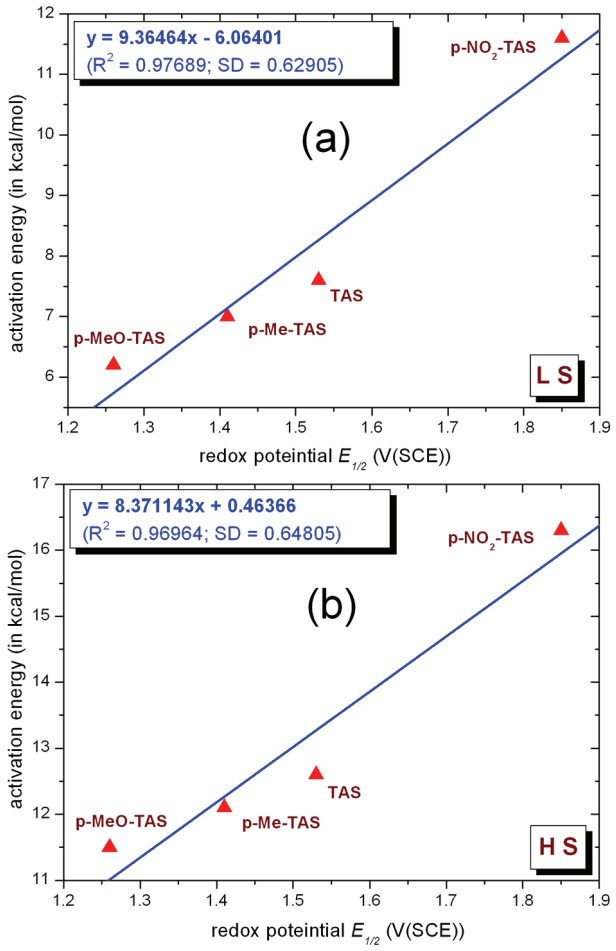

Figure S4. Plots of calculated activation energies for sulfoxidation *vs.* redox potentials ($E_{1/2}$) of *p-X(MeO,Me,H,NO$_2$)*-TAns.

Table S4. Calculated vertical ionization potentials (*IP*s) of the substrates *p-(MeO, Me, H, NO_2)*-TAns and the electron affinity (*EA*) and excitation energies from π_{xz}* orbital to $\sigma^*_{z^2}$ orbital of Cpd I of Cytochrome P450 at the UB3LYP/B2//B1 level.

a) Calculated ionization potentials (Vertical) of the substrate			
	Neutral	Cation radical	***IP (vertical)***
p-MeO-TAn	-784.274861	-784.014126	**163.6**
p-Me-TAn	-709.082125	-708.809473	**171.1**
TAn	-669.753141	-669.47209	**176.4**
p-NO_2-TAn	-874.250872	-873.945194	**191.8**
b) Calculated electron affinity of Cpd I			
	Cpd I	Cpd II	***EA***
HS: ^{4}CpdI → ^{3}CpdII	-1586.13387	-1586.242217	**68.0**
HS: ^{4}CpdI → ^{1}CpdII	-1586.13387	-1586.19463	**38.1**
LS: ^{2}CpdI → ^{3}CpdII	-1586.133974	-1586.241608	**67.5**
LS: ^{2}CpdI → ^{1}CpdII	-1586.133974	-1586.194256	**37.8**
c) excitation energy of Cpd I from π_{xz}* orbital to $\sigma^*_{z^2}$ orbital			
	π* orbital	$\sigma^*_{z^2}$ orbital	***ΔE(π*-$\sigma^*_{z^2}$)***
^{4}CpdI	-0.068	-0.022	**28.9**
^{2}CpdI	-0.068	-0.023	**28.2**

* Absolute energies are in a.u. and *IPs/EAs/excitation energy* are in kcal/mol.

Cartesian coordinates of various reaction species.

A. p-MeO-TAn + Cpd I.

a1. ^{4}RC

Fe	-0.248547000	0.058996000	-0.104289000
N	-0.295493000	0.051897000	1.913945000
N	1.764166000	0.153393000	-0.042275000
N	-2.228657000	-0.331907000	-0.149036000
N	-0.160111000	-0.213285000	-2.101453000
C	-1.409199000	-0.047475000	2.709505000
C	2.625737000	0.186054000	-1.115974000
C	0.752835000	0.278820000	2.762967000
C	2.548416000	0.355712000	1.072147000
C	-3.079775000	-0.383548000	0.921431000
C	0.951795000	-0.127924000	-2.898185000
C	-3.009464000	-0.505142000	-1.257521000
C	-1.218990000	-0.410089000	-2.954742000
C	-1.049342000	0.110399000	4.097519000
C	3.980727000	0.385209000	-0.663287000
C	0.295743000	0.318296000	4.130660000
C	3.932689000	0.492028000	0.690882000
C	-4.436544000	-0.594182000	0.477094000
C	0.589023000	-0.279607000	-4.286510000
C	-4.392998000	-0.668214000	-0.881059000
C	-0.759047000	-0.457259000	-4.321410000
H	-1.746306000	0.065928000	4.923844000
H	4.843430000	0.440426000	-1.313622000
H	0.934000000	0.481387000	4.988660000
H	4.746469000	0.655814000	1.384352000
H	-5.294583000	-0.674480000	1.131110000
H	1.288787000	-0.257178000	-5.111306000
H	-5.207455000	-0.822811000	-1.576165000
H	-1.398160000	-0.609736000	-5.180917000
C	-2.702827000	-0.259364000	2.253421000
C	2.250170000	0.069266000	-2.443920000
C	-2.543595000	-0.543576000	-2.567897000
C	2.081084000	0.430971000	2.373402000
H	-3.488509000	-0.322815000	2.999712000
H	3.036395000	0.122590000	-3.190143000
H	-3.278132000	-0.694597000	-3.352616000
H	2.809853000	0.618425000	3.154478000
O	-0.459363000	1.673574000	-0.195710000
S	0.318536000	-2.430418000	-0.073539000
H	0.926742000	-2.458661000	1.130441000
S	1.616576000	4.285177000	2.684943000
C	-0.171132000	3.983166000	2.431061000
H	-0.546324000	3.596054000	3.381537000
H	-0.685533000	4.916381000	2.191306000
H	-0.347906000	3.239307000	1.651428000
C	2.122998000	4.965688000	1.107784000
C	3.020635000	6.045999000	1.107558000
C	1.706770000	4.434168000	-0.117708000
C	3.495506000	6.575551000	-0.085841000
H	3.341270000	6.476841000	2.051465000
C	2.161027000	4.979751000	-1.321912000
H	1.025561000	3.589184000	-0.153940000
C	3.062809000	6.050091000	-1.311393000
H	4.188371000	7.410882000	-0.093449000
H	1.809442000	4.552163000	-2.253736000
O	3.572809000	6.650746000	-2.429465000
C	3.155785000	6.168583000	-3.694857000
H	3.664087000	6.786686000	-4.437035000
H	3.441164000	5.118805000	-3.844843000
H	2.070271000	6.263750000	-3.829195000

a2. ^{2}RC

Fe	-0.261758000	0.057123000	-0.104201000
N	-0.297339000	0.055544000	1.911711000
N	1.758276000	0.151073000	-0.052244000
N	-2.235705000	-0.336275000	-0.140183000
N	-0.177178000	-0.226947000	-2.102798000
C	-1.407130000	-0.038441000	2.713197000
C	2.612389000	0.195141000	-1.130676000
C	0.756610000	0.280244000	2.755361000
C	2.546013000	0.361459000	1.057428000
C	-3.083827000	-0.383329000	0.933578000
C	0.931051000	-0.133174000	-2.903934000
C	-3.019653000	-0.522808000	-1.245159000
C	-1.237927000	-0.429163000	-2.951287000
C	-1.039963000	0.120217000	4.098976000
C	3.968266000	0.407238000	-0.685694000
C	0.306202000	0.322458000	4.125070000
C	3.927149000	0.511250000	0.668966000
C	-4.440540000	-0.604104000	0.495114000
C	0.563132000	-0.287714000	-4.290801000
C	-4.400667000	-0.690108000	-0.862478000
C	-0.783755000	-0.474477000	-4.320044000
H	-1.732979000	0.079601000	4.928823000
H	4.826640000	0.472056000	-1.340853000
H	0.949311000	0.484483000	4.979652000
H	4.743265000	0.682130000	1.357989000
H	-5.296113000	-0.683592000	1.152455000
H	1.259189000	-0.260660000	-5.118587000
H	-5.216425000	-0.855350000	-1.553587000
H	-1.425557000	-0.631015000	-5.176791000
C	-2.703214000	-0.249111000	2.263337000
C	2.230050000	0.073990000	-2.456561000
C	-2.560076000	-0.566994000	-2.557359000
C	2.083289000	0.432841000	2.360802000
H	-3.486305000	-0.307945000	3.012704000
H	3.011503000	0.133901000	-3.207265000
H	-3.298056000	-0.724700000	-3.337480000
H	2.814219000	0.622164000	3.139455000
O	-0.437743000	1.672778000	-0.219181000
S	0.329814000	-2.438531000	-0.082693000
H	0.952858000	-2.462089000	1.113969000
S	1.590171000	4.296727000	2.687436000
C	-0.187144000	3.964082000	2.401320000
H	-0.579082000	3.598404000	3.353528000
H	-0.707096000	4.883858000	2.124623000
H	-0.336485000	3.197284000	1.638224000
C	2.116071000	4.974351000	1.115632000
C	3.008635000	6.059004000	1.126009000
C	1.719197000	4.438826000	-0.114450000
C	3.497138000	6.588964000	-0.061540000
H	3.314095000	6.493001000	2.073523000
C	2.187180000	4.985161000	-1.313200000
H	1.043673000	3.589651000	-0.159015000
C	3.083452000	6.059702000	-1.292118000
H	4.186056000	7.427606000	-0.061238000
H	1.850294000	4.554424000	-2.248973000
O	3.605823000	6.661439000	-2.404063000
C	3.207786000	6.175851000	-3.674198000
H	3.723538000	6.794897000	-4.410448000
H	3.499280000	5.126999000	-3.818902000
H	2.123789000	6.266496000	-3.823177000

a3. ^{4}TS$_{SO}$

Fe	0.124342000	-0.022430000	-0.139244000
N	-0.514498000	0.198571000	1.752826000
N	1.966839000	0.500970000	0.399547000
N	-1.774694000	-0.606148000	-0.694250000
N	0.775578000	-0.429029000	-2.014965000
C	-1.804275000	0.062426000	2.209493000
C	3.077559000	0.559134000	-0.408242000
C	0.234722000	0.600646000	2.825862000
C	2.386672000	0.857154000	1.657574000
C	-2.886056000	-0.626690000	0.098029000
C	2.042015000	-0.243397000	-2.495840000
C	-2.174026000	-1.015626000	-1.936006000
C	0.017318000	-0.870303000	-3.072180000
C	-1.859848000	0.370453000	3.618596000
C	4.223211000	0.987374000	0.359581000
C	-0.595950000	0.701123000	4.001514000
C	3.796530000	1.168967000	1.638278000
C	-4.035219000	-1.059296000	-0.667859000
C	2.096649000	-0.588288000	-3.895958000
C	-3.592373000	-1.302411000	-1.930940000
C	0.840896000	-0.977829000	-4.253242000
H	-2.758924000	0.334805000	4.219892000
H	5.219865000	1.112704000	-0.043091000
H	-0.242802000	0.993513000	4.981753000
H	4.369650000	1.475864000	2.503436000
H	-5.036887000	-1.164574000	-0.271927000

H	2.986493000	-0.536119000	-4.509650000
H	-4.155016000	-1.648248000	-2.788248000
H	0.488542000	-1.310963000	-5.220790000
C	-2.906605000	-0.311634000	1.452390000
C	3.121792000	0.222596000	-1.752234000
C	-1.345607000	-1.142148000	-3.044702000
C	1.591122000	0.901784000	2.792131000
H	-3.860901000	-0.375207000	1.965661000
H	4.076589000	0.314807000	-2.259836000
H	-1.800313000	-1.483290000	-3.969476000
H	2.061580000	1.201441000	3.722983000
O	-0.299045000	1.638819000	-0.565091000
S	0.491556000	-2.400183000	0.235758000
H	-0.313041000	-2.528067000	1.310846000
S	-1.630631000	2.763086000	-1.624923000
C	-0.376015000	3.060208000	-2.909845000
H	-0.275653000	2.125097000	-3.463140000
H	-0.703536000	3.864435000	-3.572585000
H	0.572839000	3.301883000	-2.431075000
C	-1.577067000	4.269689000	-0.673258000
C	-2.681554000	5.135622000	-0.701812000
C	-0.476654000	4.570295000	0.134705000
C	-2.670372000	6.300579000	0.052549000
H	-3.544535000	4.897557000	-1.316194000
C	-0.459030000	5.743053000	0.888586000
H	0.344619000	3.863780000	0.190287000
C	-1.556846000	6.615276000	0.848380000
H	-3.511480000	6.985623000	0.043126000
H	0.401722000	5.956994000	1.510755000
O	-1.643230000	7.779909000	1.545101000
C	-0.557388000	8.150313000	2.383670000
H	-0.839519000	9.101895000	2.836028000
H	-0.388261000	7.409631000	3.175058000
H	0.368472000	8.283167000	1.810127000

a4. $^{2}TS_{SO}$

Fe	-0.067239000	-0.172013000	-0.257859000
N	0.125010000	0.408382000	1.648696000
N	1.943536000	-0.129128000	-0.501796000
N	-2.045367000	-0.400444000	0.032660000
N	-0.244439000	-0.880027000	-2.156443000
C	-0.864217000	0.536128000	2.591528000
C	2.652381000	-0.411806000	-1.640372000
C	1.298003000	0.720922000	2.289948000
C	2.860759000	0.278526000	0.427319000
C	-2.756750000	-0.162114000	1.180183000
C	0.754072000	-1.054472000	-3.079752000
C	-2.961094000	-0.803620000	-0.906508000
C	-1.414413000	-1.191544000	-2.795362000
C	-0.304706000	0.963722000	3.851919000
C	4.061729000	-0.188290000	-1.418015000
C	1.036918000	1.080857000	3.664161000
C	4.191327000	0.241226000	-0.132718000
C	-4.159381000	-0.423308000	0.962614000
C	0.197492000	-1.497746000	-4.338209000
C	-4.286542000	-0.817409000	-0.333540000
C	-1.148231000	-1.580814000	-4.162357000
H	-0.878691000	1.137459000	4.752576000
H	4.835096000	-0.346828000	-2.158268000
H	1.796030000	1.370741000	4.378684000
H	5.093117000	0.508617000	0.402373000
H	-4.930067000	-0.315298000	1.714406000
H	0.776960000	-1.713970000	-5.226180000
H	-5.184072000	-1.101755000	-0.866999000
H	-1.904721000	-1.880756000	-4.875604000
C	-2.210755000	0.273920000	2.380090000
C	2.105571000	-0.846115000	-2.842780000
C	-2.677433000	-1.154733000	-2.219759000
C	2.565189000	0.675246000	1.726461000
H	-2.886949000	0.415972000	3.216991000
H	2.791302000	-1.032559000	-3.663440000
H	-3.516149000	-1.442789000	-2.845903000
H	3.399127000	0.960604000	2.360020000
O	-0.203737000	1.354963000	-0.946548000
S	0.090137000	-2.517892000	0.369404000
H	1.113008000	-2.861563000	-0.439342000
S	-1.005778000	3.306339000	0.066555000
C	-1.674920000	3.699938000	-1.583078000
H	-2.610457000	3.145152000	-1.675989000
H	-1.863637000	4.772055000	-1.669906000
H	-0.979434000	3.355855000	-2.348905000
C	0.515799000	4.237855000	0.090942000
C	0.665956000	5.282966000	1.016851000
C	1.578046000	3.913497000	-0.759487000
C	1.851083000	6.003971000	1.072339000
H	-0.150235000	5.532651000	1.687702000
C	2.767083000	4.641634000	-0.715322000
H	1.476932000	3.070758000	-1.434832000
C	2.907293000	5.693065000	0.201419000
H	1.982538000	6.817989000	1.777492000
H	3.576120000	4.370123000	-1.382900000
O	4.022238000	6.464136000	0.329031000
C	5.126088000	6.202841000	-0.525474000
H	5.891487000	6.933000000	-0.258859000
H	5.523874000	5.191327000	-0.374884000
H	4.858153000	6.329647000	-1.581975000

B. p-Me-TAn + Cpd I.

b1. ^{4}RC

Fe	-0.274935000	0.129948000	-0.098333000
N	-0.320616000	0.079747000	1.919730000
N	1.729282000	0.334062000	-0.032368000
N	-2.230632000	-0.368862000	-0.152079000
N	-0.171861000	-0.095831000	-2.100246000
C	-1.426170000	-0.101207000	2.712366000
C	2.586787000	0.439449000	-1.104376000
C	0.714204000	0.345315000	2.774517000
C	2.501937000	0.556648000	1.086649000
C	-3.076402000	-0.493439000	0.916673000
C	0.932895000	0.069141000	-2.894323000
C	-3.001193000	-0.560758000	-1.264522000
C	-1.219206000	-0.330658000	-2.958228000
C	-1.074645000	0.045282000	4.103624000
C	3.928778000	0.704596000	-0.647014000
C	0.256501000	0.328032000	4.142285000
C	3.876223000	0.778315000	0.708986000
C	-4.419445000	-0.770249000	0.467021000
C	0.577830000	-0.070863000	-4.285936000
C	-4.373032000	-0.810286000	-0.892492000
C	-0.758332000	-0.321619000	-4.325449000
H	-1.767366000	-0.057006000	4.928383000
H	4.785942000	0.824207000	-1.295906000
H	0.885001000	0.507555000	5.004199000
H	4.679988000	0.973353000	1.405998000
H	-5.270973000	-0.914027000	1.118672000
H	1.274417000	0.009829000	-5.109739000
H	-5.178122000	-0.994732000	-1.591236000
H	-1.388863000	-0.488820000	-5.188550000
C	-2.705851000	-0.377519000	2.251108000
C	2.217995000	0.330036000	-2.434968000
C	-2.534238000	-0.544585000	-2.575203000
C	2.032009000	0.578060000	2.389016000
H	-3.485701000	-0.503282000	2.995634000
H	2.999442000	0.444967000	-3.179210000
H	-3.259780000	-0.718127000	-3.363633000
H	2.749594000	0.789306000	3.174395000
O	-0.575801000	1.731363000	-0.163519000
S	0.419249000	-2.326822000	-0.127326000
H	1.047309000	-2.350357000	1.066675000
S	1.475727000	4.442360000	2.767977000
C	-0.269783000	4.070758000	2.372839000
H	-0.748073000	3.855317000	3.331222000
H	-0.750410000	4.939441000	1.917408000
H	-0.368764000	3.200907000	1.720700000
C	2.159219000	4.910093000	1.183657000
C	3.247427000	5.795308000	1.185245000
C	1.695202000	4.407061000	-0.039361000
C	3.858961000	6.164082000	-0.010716000
H	3.610104000	6.200629000	2.125860000
C	2.308248000	4.801741000	-1.229583000
H	0.872136000	3.700818000	-0.078251000
C	3.396161000	5.683032000	-1.243060000
H	4.702204000	6.850824000	0.014491000
H	1.930495000	4.403272000	-2.168692000
C	4.029731000	6.125854000	-2.541061000
H	3.581680000	7.058406000	-2.907898000
H	5.102631000	6.308948000	-2.423014000
H	3.899634000	5.374726000	-3.326387000

b2. ^{2}RC

Fe	-0.286685000	0.119374000	-0.106529000
N	-0.319559000	0.088806000	1.909886000
N	1.725795000	0.313751000	-0.054058000
N	-2.238249000	-0.374016000	-0.145734000
N	-0.190551000	-0.131889000	-2.108365000
C	-1.421801000	-0.074095000	2.710859000
C	2.574485000	0.420219000	-1.132498000
C	0.723236000	0.353012000	2.756184000
C	2.503956000	0.547746000	1.058200000
C	-3.080984000	-0.480900000	0.927992000
C	0.909688000	0.031944000	-2.909087000
C	-3.013113000	-0.585246000	-1.252626000
C	-1.241140000	-0.375367000	-2.958817000
C	-1.060845000	0.082195000	4.098444000
C	3.918328000	0.695088000	-0.685617000
C	0.273297000	0.351930000	4.126598000
C	3.874854000	0.774256000	0.670471000
C	-4.424971000	-0.765619000	0.487521000
C	0.547653000	-0.119652000	-4.297877000
C	-4.382946000	-0.829526000	-0.871268000
C	-0.787710000	-0.375724000	-4.328605000
H	-1.749585000	-0.005814000	4.928171000
H	4.770405000	0.816562000	-1.340862000
H	0.908568000	0.533804000	4.983036000
H	4.682306000	0.977052000	1.360998000
H	-5.274192000	-0.899035000	1.144360000
H	1.239614000	-0.042371000	-5.125907000
H	-5.190192000	-1.026833000	-1.563960000
H	-1.422210000	-0.551272000	-5.187110000
C	-2.705778000	-0.345817000	2.259144000
C	2.196755000	0.300399000	-2.459821000
C	-2.553671000	-0.586867000	-2.565776000
C	2.040318000	0.576430000	2.362817000
H	-3.483398000	-0.456605000	3.008316000
H	2.972451000	0.414077000	-3.210257000
H	-3.283758000	-0.770894000	-3.347556000
H	2.761756000	0.791504000	3.143648000
O	-0.544240000	1.725147000	-0.200754000
S	0.432132000	-2.343723000	-0.120781000
H	1.060433000	-2.352242000	1.073364000
S	1.442468000	4.435080000	2.764541000
C	-0.293695000	4.057176000	2.335285000
H	-0.787652000	3.831493000	3.283319000
H	-0.770851000	4.926967000	1.878297000
H	-0.376049000	3.191911000	1.674615000
C	2.151459000	4.919569000	1.196496000
C	3.230249000	5.815908000	1.224528000
C	1.716622000	4.419035000	-0.038172000
C	3.861262000	6.198047000	0.043049000
H	3.570039000	6.219374000	2.174443000
C	2.348571000	4.827523000	-1.213870000
H	0.902046000	3.704281000	-0.097032000
C	3.427431000	5.719818000	-1.200920000
H	4.696791000	6.893146000	0.088739000
H	1.993482000	4.431156000	-2.162642000
C	4.082399000	6.176831000	-2.483225000
H	3.649421000	7.120298000	-2.840310000
H	5.155679000	6.346372000	-2.348334000
H	3.954627000	5.439965000	-3.282299000

b3. $^4TS_{SO}$

Fe	1.137491000	0.286979000	0.254839000
N	1.777412000	-1.670617000	0.379835000
N	0.475584000	0.174743000	2.163348000
N	1.976669000	0.421251000	-1.569685000
N	0.557386000	2.188062000	0.150462000
C	2.419390000	-2.387781000	-0.589832000
C	-0.169318000	1.157158000	2.860221000
C	1.629831000	-2.509115000	1.450304000
C	0.512114000	-0.925221000	2.983252000
C	2.594187000	-0.586350000	-2.273990000
C	-0.099388000	2.902856000	1.122688000
C	1.974586000	1.519768000	-2.389129000
C	0.747443000	3.050631000	-0.900530000
C	2.678187000	-3.733064000	-0.124303000
C	-0.540431000	0.675249000	4.169848000
C	2.188721000	-3.807307000	1.143257000
C	-0.117146000	-0.616186000	4.245926000
C	3.006510000	-0.097985000	-3.567702000
C	-0.350228000	4.247740000	0.660241000
C	2.624998000	1.207628000	-3.638209000
C	0.175166000	4.339951000	-0.591043000
H	3.178786000	-4.500482000	-0.700327000
H	-1.057472000	1.261288000	4.918313000
H	2.202342000	-4.649240000	1.823014000
H	-0.215079000	-1.310480000	5.070177000
H	3.521171000	-0.690613000	-4.312884000
H	-0.853415000	5.011576000	1.238562000
H	2.760593000	1.906437000	-4.453290000
H	0.192774000	5.194951000	-1.254202000
C	2.796967000	-1.888931000	-1.832908000
C	-0.444000000	2.433397000	2.380544000
C	1.407332000	2.750960000	-2.082769000
C	1.041848000	-2.168491000	2.662117000
H	3.309864000	-2.566351000	-2.508595000
H	-0.958655000	3.118554000	3.046334000
H	1.484628000	3.537247000	-2.826644000
H	0.994289000	-2.938302000	3.425802000
O	-0.407205000	-0.279211000	-0.384789000
S	3.269354000	0.812616000	1.305658000
H	4.054972000	0.554039000	0.239746000
S	-1.553448000	-1.929913000	-0.725681000
C	-1.092466000	-1.907086000	-2.485123000
H	-0.044052000	-2.206697000	-2.526795000
H	-1.716771000	-2.606762000	-3.045391000
H	-1.192591000	-0.891841000	-2.868380000
C	-3.162832000	-1.159435000	-0.735188000
C	-4.272353000	-1.910510000	-0.333876000
C	-3.316218000	0.186383000	-1.094260000
C	-5.535705000	-1.318371000	-0.314609000
H	-4.151946000	-2.950756000	-0.046775000
C	-4.584734000	0.757173000	-1.077219000
H	-2.438888000	0.771136000	-1.348390000
C	-5.714584000	0.018980000	-0.688484000
H	-6.395152000	-1.908638000	-0.007644000
H	-4.700046000	1.801063000	-1.358709000
C	-7.078605000	0.664958000	-0.648752000
H	-7.874155000	-0.081306000	-0.573115000
H	-7.171483000	1.335713000	0.214157000
H	-7.261601000	1.267044000	-1.544785000

b4. $^2TS_{SO}$

Fe	1.122937000	0.158920000	0.296449000
N	0.344917000	-0.948215000	1.771367000
N	0.278798000	1.831306000	1.065739000
N	2.109828000	-1.463260000	-0.369207000
N	2.013152000	1.310629000	-1.125052000
C	0.545866000	-2.283272000	2.017669000
C	0.350665000	3.107430000	0.571470000
C	-0.486088000	-0.502771000	2.768915000
C	-0.556879000	1.888170000	2.146771000
C	2.082630000	-2.733344000	0.148130000
C	1.849291000	2.655259000	-1.335324000
C	2.936769000	-1.515599000	-1.463606000
C	2.832066000	0.864191000	-2.127028000
C	-0.193104000	-2.695246000	3.187491000
C	-0.453745000	3.999262000	1.374281000
C	-0.835948000	-1.590831000	3.652229000
C	-1.018667000	3.241366000	2.353010000
C	2.912537000	-3.612158000	-0.639699000
C	2.595928000	3.072425000	-2.500863000
C	3.439112000	-2.857363000	-1.642511000
C	3.203760000	1.960455000	-2.993807000
H	-0.200143000	-3.700146000	3.588655000
H	-0.559728000	5.061479000	1.196723000
H	-1.480969000	-1.498440000	4.516103000
H	-1.685377000	3.550974000	3.147089000
H	3.062878000	-4.664210000	-0.436150000
H	2.638123000	4.086927000	-2.875010000
H	4.113212000	-3.161487000	-2.432534000
H	3.850819000	1.871469000	-3.856583000
C	1.355389000	-3.122821000	1.265270000
C	1.083312000	3.499223000	-0.543004000
C	3.259970000	-0.446586000	-2.289632000
C	-0.916315000	0.805471000	2.940568000
H	1.427249000	-4.160638000	1.574417000
H	1.047666000	4.548371000	-0.819436000
H	3.921493000	-0.651488000	-3.125707000

H	-1.580166000	1.002103000	3.776652000
O	-0.150500000	0.011897000	-0.791926000
S	3.118530000	0.610862000	1.610102000
H	3.075899000	1.957915000	1.567497000
S	-1.549009000	-1.833042000	-1.070854000
C	-1.118660000	-1.709965000	-2.837743000
H	-0.141493000	-2.183727000	-2.946953000
H	-1.860878000	-2.230939000	-3.446274000
H	-1.038222000	-0.660527000	-3.121267000
C	-3.115691000	-0.976730000	-1.003358000
C	-4.256931000	-1.681450000	-0.604462000
C	-3.208276000	0.392532000	-1.290323000
C	-5.484239000	-1.023572000	-0.514869000
H	-4.185905000	-2.739029000	-0.369189000
C	-4.442150000	1.031109000	-1.205984000
H	-2.309950000	0.945400000	-1.542139000
C	-5.600655000	0.337437000	-0.821962000
H	-6.364983000	-1.580347000	-0.204947000
H	-4.505220000	2.093853000	-1.427516000
C	-6.934887000	1.041375000	-0.756420000
H	-7.656156000	0.479327000	-0.156604000
H	-6.838169000	2.041661000	-0.322198000
H	-7.365654000	1.165335000	-1.757876000

C. TAn +Cpd I.

c1. ^{4}RC

Fe	-0.284893000	0.147002000	-0.093431000
N	-0.319560000	0.081630000	1.924720000
N	1.715401000	0.388521000	-0.035676000
N	-2.229589000	-0.392885000	-0.140737000
N	-0.186930000	-0.062301000	-2.097340000
C	-1.417740000	-0.124562000	2.721430000
C	2.565252000	0.520192000	-1.111162000
C	0.714566000	0.360079000	2.776444000
C	2.489996000	0.614846000	1.081557000
C	-3.067813000	-0.540570000	0.931169000
C	0.909622000	0.133302000	-2.895713000
C	-3.001142000	-0.594852000	-1.250775000
C	-1.233498000	-0.313511000	-2.951717000
C	-1.062288000	0.019784000	4.111901000
C	3.904552000	0.805209000	-0.658080000
C	0.263747000	0.326087000	4.146171000
C	3.858042000	0.864472000	0.698781000
C	-4.406666000	-0.843307000	0.485993000
C	0.550154000	-0.002927000	-4.286578000
C	-4.365582000	-0.875387000	-0.873924000
C	-0.780291000	-0.283134000	-4.321176000
H	-1.749070000	-0.100232000	4.939242000
H	4.755728000	0.947451000	-1.310213000
H	0.893081000	0.511178000	5.006312000
H	4.661926000	1.067474000	1.393354000
H	-5.252000000	-1.008372000	1.140664000
H	1.240316000	0.099965000	-5.113307000
H	-5.169783000	-1.073155000	-1.570028000
H	-1.411585000	-0.457332000	-5.182327000
C	-2.693872000	-0.423660000	2.264529000
C	2.191616000	0.416615000	-2.440774000
C	-2.541235000	-0.559840000	-2.563638000
C	2.026368000	0.617653000	2.386289000
H	-3.467631000	-0.568986000	3.011848000
H	2.966540000	0.554509000	-3.187907000
H	-3.266809000	-0.743952000	-3.349618000
H	2.744387000	0.834816000	3.169723000
O	-0.619098000	1.742202000	-0.144966000
S	0.464093000	-2.294202000	-0.144326000
H	1.094944000	-2.314230000	1.048265000
S	1.423552000	4.518584000	2.743978000
C	-0.311122000	4.111488000	2.339906000
H	-0.801761000	3.939082000	3.300685000
H	-0.792684000	4.952429000	1.835890000
H	-0.393316000	3.210685000	1.728722000
C	2.133508000	4.917469000	1.153287000
C	3.263173000	5.751326000	1.150012000
C	1.644196000	4.415246000	-0.061117000
C	3.897314000	6.072410000	-0.048727000
H	3.635244000	6.155390000	2.087485000
C	2.278964000	4.757722000	-1.257425000
H	0.787587000	3.749948000	-0.087086000
C	3.405099000	5.581723000	-1.260594000
H	4.769200000	6.720976000	-0.035446000
H	1.885963000	4.366749000	-2.192163000
H	3.892195000	5.842797000	-2.195721000

c2. ^{2}RC

Fe	-0.289501000	0.136655000	-0.111285000
N	-0.309809000	0.100486000	1.905457000
N	1.720344000	0.358412000	-0.070310000
N	-2.233318000	-0.386790000	-0.139586000
N	-0.201590000	-0.108117000	-2.114155000
C	-1.404622000	-0.080446000	2.712745000
C	2.561112000	0.479894000	-1.153515000
C	0.734263000	0.377657000	2.746135000
C	2.502198000	0.599279000	1.038130000
C	-3.067729000	-0.509893000	0.939016000
C	0.891017000	0.074718000	-2.921157000
C	-3.011675000	-0.606863000	-1.242370000
C	-1.253940000	-0.363889000	-2.958898000
C	-1.037581000	0.078341000	4.098438000
C	3.903890000	0.770744000	-0.713721000
C	0.292632000	0.367343000	4.119175000
C	3.867643000	0.844639000	0.642831000
C	-4.409661000	-0.814743000	0.505911000
C	0.522390000	-0.076921000	-4.308206000
C	-4.375039000	-0.874009000	-0.853319000
C	-0.809245000	-0.352477000	-4.331501000
H	-1.719902000	-0.021462000	4.932124000
H	4.750221000	0.906018000	-1.373658000
H	0.930349000	0.556693000	4.972157000
H	4.676623000	1.055763000	1.329045000
H	-5.252560000	-0.963593000	1.167565000
H	1.207858000	0.013637000	-5.140275000
H	-5.183318000	-1.082175000	-1.541616000
H	-1.446543000	-0.534199000	-5.186647000
C	-2.686840000	-0.371567000	2.268217000
C	2.176964000	0.359856000	-2.478935000
C	-2.560516000	-0.596904000	-2.558401000
C	2.045972000	0.618786000	2.345447000
H	-3.458070000	-0.496358000	3.021784000
H	2.946286000	0.487266000	-3.233702000
H	-3.292639000	-0.789407000	-3.336234000
H	2.769360000	0.840990000	3.122521000
O	-0.571508000	1.738525000	-0.200100000
S	0.468429000	-2.315513000	-0.136746000
H	1.100783000	-2.319172000	1.055287000
S	1.370118000	4.498625000	2.765998000
C	-0.349585000	4.083597000	2.308767000
H	-0.863757000	3.889950000	3.253053000
H	-0.825134000	4.929125000	1.806738000
H	-0.407005000	3.192837000	1.680206000
C	2.118219000	4.931699000	1.201752000
C	3.230231000	5.787894000	1.241786000
C	1.675075000	4.434718000	-0.032428000
C	3.892605000	6.136692000	0.066178000
H	3.566138000	6.187712000	2.194598000
C	2.337069000	4.805450000	-1.205302000
H	0.833428000	3.752549000	-0.091269000
C	3.445744000	5.651958000	-1.165394000
H	4.750444000	6.802213000	0.112938000
H	1.979626000	4.418862000	-2.155999000
H	3.954426000	5.934530000	-2.082607000

c3. ^{4}TS$_{SO}$

Fe	0.050135000	-0.016520000	0.005189000
N	0.022805000	-0.016853000	2.068988000
N	2.065354000	-0.115491000	0.045078000
N	-1.964713000	-0.101356000	0.003405000
N	0.072715000	-0.050523000	-1.983294000
C	-1.079659000	0.016541000	2.875416000
C	2.903945000	-0.114493000	-1.034390000
C	1.110137000	-0.030134000	2.896978000
C	2.866519000	-0.116241000	1.160651000
C	-2.796628000	-0.055713000	1.097824000
C	1.181871000	-0.061226000	-2.794500000
C	-2.777713000	-0.126660000	-1.098513000
C	-1.016412000	-0.088297000	-2.819759000
C	-0.678265000	0.033737000	4.265464000

C	4.278968000	-0.132696000	-0.595073000
C	0.681966000	0.003023000	4.278321000
C	4.255186000	-0.134482000	0.765878000
C	-4.174047000	-0.072147000	0.667104000
C	0.778537000	-0.082129000	-4.180813000
C	-4.162291000	-0.119291000	-0.694143000
C	-0.581421000	-0.100851000	-4.196609000
H	-1.360785000	0.055808000	5.105096000
H	5.136468000	-0.140934000	-1.255049000
H	1.348339000	-0.003455000	5.130942000
H	5.089541000	-0.143873000	1.454913000
H	-5.026844000	-0.051369000	1.333209000
H	1.463126000	-0.094208000	-5.018859000
H	-5.002878000	-0.142985000	-1.375282000
H	-1.245941000	-0.130366000	-5.050183000
C	-2.396847000	0.005649000	2.428068000
C	2.499381000	-0.086850000	-2.364569000
C	-2.342867000	-0.127630000	-2.419076000
C	2.435013000	-0.076102000	2.479980000
H	-3.179869000	0.029192000	3.179621000
H	3.274093000	-0.096858000	-3.124360000
H	-3.100127000	-0.156549000	-3.195838000
H	3.199521000	-0.083228000	3.250419000
O	0.057102000	1.751404000	0.035642000
S	0.176680000	-2.434214000	0.240139000
H	-1.084553000	-2.637369000	0.673454000
S	0.112553000	3.362335000	1.274727000
C	-1.617189000	3.748090000	0.862594000
H	-2.221239000	2.975375000	1.340874000
H	-1.883087000	4.736118000	1.245080000
H	-1.749154000	3.692282000	-0.217765000
C	1.019106000	4.501043000	0.237814000
C	1.788412000	5.497523000	0.850852000
C	1.000139000	4.367842000	-1.156494000
C	2.525251000	6.380276000	0.059604000
H	1.805803000	5.582661000	1.933120000
C	1.733047000	5.261746000	-1.935368000
H	0.444646000	3.549808000	-1.602214000
C	2.492995000	6.267834000	-1.331445000
H	3.120864000	7.155925000	0.531826000
H	1.722113000	5.163255000	-3.016947000
H	3.066288000	6.957088000	-1.944493000

c4. $^{2}TS_{SO}$

Fe	0.034010000	-0.253940000	-0.130425000
N	0.110713000	0.039340000	1.849839000
N	2.043857000	-0.490101000	-0.205377000
N	-1.974510000	-0.197979000	-0.035200000
N	-0.049587000	-0.683935000	-2.116735000
C	-0.938600000	0.195818000	2.719737000
C	2.817100000	-0.736681000	-1.309445000
C	1.246887000	0.094750000	2.616733000
C	2.911283000	-0.337852000	0.840796000
C	-2.758775000	-0.006175000	1.074832000
C	1.000471000	-0.902110000	-2.970074000
C	-2.839531000	-0.330694000	-1.093529000
C	-1.181278000	-0.724314000	-2.885678000
C	-0.451917000	0.373507000	4.067404000
C	4.215327000	-0.754523000	-0.945455000
C	0.904997000	0.314232000	4.003148000
C	4.274132000	-0.505044000	0.390527000
C	-4.153848000	-0.012077000	0.708387000
C	0.515904000	-1.095639000	-4.318326000
C	-4.203939000	-0.208839000	-0.637958000
C	-0.838163000	-0.982504000	-4.266620000
H	-1.081753000	0.516564000	4.935517000
H	5.029333000	-0.934750000	-1.635300000
H	1.623434000	0.397315000	4.808007000
H	5.146400000	-0.437913000	1.027297000
H	-4.973867000	0.115071000	1.402816000
H	1.144646000	-1.292670000	-5.176712000
H	-5.074575000	-0.279034000	-1.276814000
H	-1.553965000	-1.069216000	-5.073532000
C	-2.280520000	0.175432000	2.366091000
C	2.337687000	-0.936441000	-2.598526000
C	-2.476904000	-0.555347000	-2.415671000
C	2.545656000	-0.064615000	2.153149000
H	-3.010667000	0.309636000	3.157713000
H	3.068370000	-1.125725000	-3.378673000
H	-3.280641000	-0.627276000	-3.141943000
H	3.344698000	0.015731000	2.883531000
O	0.226849000	1.353792000	-0.587751000
S	-0.186620000	-2.654972000	0.190670000
H	0.890780000	-3.046990000	-0.519077000
S	-0.767506000	3.199788000	0.424422000
C	-1.659224000	3.435662000	-1.147211000
H	-2.515383000	2.759727000	-1.112821000
H	-1.997153000	4.469850000	-1.240476000
H	-1.015927000	3.150466000	-1.979630000
C	0.614192000	4.319916000	0.254060000
C	0.777871000	5.328445000	1.212652000
C	1.548465000	4.170012000	-0.780260000
C	1.866338000	6.197739000	1.124751000
H	0.053789000	5.433637000	2.014724000
C	2.625310000	5.051328000	-0.864897000
H	1.440266000	3.350422000	-1.481754000
C	2.786446000	6.065359000	0.083571000
H	1.989644000	6.981045000	1.866996000
H	3.349382000	4.936371000	-1.666425000
H	3.630653000	6.745225000	0.014483000

c5. ^{4}PC

Fe	0.044485000	-0.379990000	-0.048530000
N	0.021581000	0.013558000	1.944104000
N	2.053815000	-0.346734000	-0.019314000
N	-1.957719000	-0.159746000	-0.094411000
N	0.081217000	-0.413926000	-2.062918000
C	-1.085777000	0.154016000	2.745961000
C	2.897036000	-0.480909000	-1.095453000
C	1.104274000	0.009275000	2.790886000
C	2.861453000	-0.291142000	1.092166000
C	-2.798453000	0.020299000	0.978460000
C	1.188080000	-0.533737000	-2.864880000
C	-2.767017000	-0.238365000	-1.202435000
C	-1.002827000	-0.459443000	-2.903640000
C	-0.688979000	0.266081000	4.127957000
C	4.267155000	-0.514144000	-0.651836000
C	0.669476000	0.171507000	4.155773000
C	4.245045000	-0.397461000	0.705364000
C	-4.169294000	0.046719000	0.535458000
C	0.792411000	-0.645248000	-4.248163000
C	-4.149773000	-0.118334000	-0.817068000
C	-0.567316000	-0.600209000	-4.272159000
H	-1.373283000	0.387590000	4.957571000
H	5.123489000	-0.612909000	-1.305911000
H	1.329539000	0.202094000	5.012732000
H	5.079490000	-0.380360000	1.394043000
H	-5.024441000	0.174968000	1.186213000
H	1.479027000	-0.748777000	-5.078092000
H	-4.985256000	-0.150880000	-1.503995000
H	-1.229647000	-0.657985000	-5.125909000
C	-2.402031000	0.166788000	2.302530000
C	2.502673000	-0.566170000	-2.423967000
C	-2.331198000	-0.385183000	-2.512128000
C	2.428244000	-0.131898000	2.401678000
H	-3.181837000	0.285578000	3.048038000
H	3.281379000	-0.672271000	-3.172073000
H	-3.087185000	-0.436972000	-3.288758000
H	3.184261000	-0.114995000	3.179823000
O	0.111799000	2.136024000	-0.367138000
S	-0.020746000	-2.818530000	0.260264000
H	-1.334235000	-2.871159000	0.563996000
S	0.417133000	3.132117000	0.744773000
C	-1.199465000	3.840000000	1.243027000
H	-1.754411000	3.037320000	1.732896000
H	-1.033123000	4.669406000	1.934789000
H	-1.725740000	4.176472000	0.347058000
C	1.070176000	4.618720000	-0.081177000
C	1.582474000	5.672371000	0.679124000
C	1.098459000	4.645295000	-1.473827000
C	2.104895000	6.788844000	0.025037000
H	1.581009000	5.624945000	1.765492000
C	1.628673000	5.765275000	-2.118103000
H	0.714805000	3.790939000	-2.023102000
C	2.126758000	6.835449000	-1.371791000
H	2.502416000	7.616834000	0.604673000
H	1.655353000	5.800008000	-3.203450000
H	2.540920000	7.703142000	-1.876954000

c6. ^{2}PC

Fe	-0.030301000	-0.256496000	-0.031911000
N	-0.126019000	-0.060403000	1.977492000

N	1.983331000	-0.142321000	0.040769000
N	-2.039226000	-0.215734000	-0.101951000
N	0.070796000	-0.302166000	-2.039918000
C	-1.254350000	0.008956000	2.761513000
C	2.859686000	-0.147458000	-1.015436000
C	0.939130000	-0.090281000	2.847147000
C	2.756203000	-0.152689000	1.175674000
C	-2.917423000	-0.107472000	0.946434000
C	1.194406000	-0.276889000	-2.824364000
C	-2.807694000	-0.350081000	-1.229564000
C	-0.989936000	-0.428259000	-2.897948000
C	-0.890218000	0.043707000	4.156821000
C	4.221225000	-0.141903000	-0.535308000
C	0.469626000	-0.025541000	4.209705000
C	4.157117000	-0.151822000	0.824080000
C	-4.278543000	-0.167704000	0.467124000
C	0.833335000	-0.383375000	-4.219625000
C	-4.210049000	-0.324797000	-0.882809000
C	-0.522431000	-0.483333000	-4.265001000
H	-1.594549000	0.100015000	4.976759000
H	5.098229000	-0.140811000	-1.169362000
H	1.109578000	-0.032726000	5.082548000
H	4.970965000	-0.157571000	1.537509000
H	-5.157395000	-0.104284000	1.095541000
H	1.538830000	-0.386226000	-5.040301000
H	-5.021490000	-0.412723000	-1.593534000
H	-1.163237000	-0.581337000	-5.131619000
C	-2.560231000	0.011597000	2.284355000
C	2.498924000	-0.191146000	-2.355777000
C	-2.328137000	-0.461955000	-2.528236000
C	2.278534000	-0.139855000	2.480141000
H	-3.361526000	0.071577000	3.014270000
H	3.297759000	-0.192001000	-3.090564000
H	-3.061566000	-0.562904000	-3.322047000
H	3.012943000	-0.154432000	3.279339000
O	-0.105357000	1.893179000	-0.269600000
S	0.023477000	-2.501812000	0.058696000
H	-0.895917000	-2.675270000	1.031995000
S	0.523721000	2.826046000	0.779836000
C	-0.898597000	3.681784000	1.549044000
H	-1.436711000	2.926283000	2.124709000
H	-0.530454000	4.474432000	2.204827000
H	-1.533006000	4.087230000	0.758592000
C	1.178052000	4.219628000	-0.180347000
C	1.969778000	5.178067000	0.456832000
C	0.918423000	4.278473000	-1.548459000
C	2.486111000	6.235626000	-0.292492000
H	2.188688000	5.100942000	1.518889000
C	1.446719000	5.338379000	-2.288330000
H	0.324888000	3.495015000	-2.008597000
C	2.223808000	6.315771000	-1.662843000
H	3.100408000	6.989341000	0.190986000
H	1.253399000	5.397254000	-3.355365000
H	2.634365000	7.136120000	-2.244082000

D. p-NO_2-TAn + Cpd I.

d1. ^{4}RC

Fe	-0.164711000	0.163781000	-0.013764000
N	-0.061117000	-0.202564000	1.967240000
N	1.839952000	0.385220000	-0.063782000
N	-2.110019000	-0.369453000	-0.006626000
N	-0.201773000	0.247236000	-2.030034000
C	-1.107953000	-0.502581000	2.802104000
C	2.611335000	0.700058000	-1.161130000
C	1.036843000	-0.074809000	2.773838000
C	2.695815000	0.429387000	1.017300000
C	-2.880263000	-0.651106000	1.089728000
C	0.835282000	0.578986000	-2.863186000
C	-2.952136000	-0.426791000	-1.081757000
C	-1.303011000	0.105091000	-2.840515000
C	-0.654632000	-0.572173000	4.169548000
C	3.979288000	0.928464000	-0.764834000
C	0.679904000	-0.304441000	4.152406000
C	4.032506000	0.753457000	0.582332000
C	-4.247302000	-0.891918000	0.696138000
C	0.380652000	0.645775000	-4.231200000
C	-4.291976000	-0.753236000	-0.657115000
C	-0.945403000	0.344605000	-4.217756000
H	-1.286829000	-0.799193000	5.017610000
H	4.772105000	1.208068000	-1.445004000
H	1.371867000	-0.265447000	4.983117000
H	4.886520000	0.844535000	1.240241000
H	-5.050990000	-1.138532000	1.377089000
H	1.011461000	0.884979000	-5.076773000
H	-5.140019000	-0.861535000	-1.320044000
H	-1.632874000	0.286020000	-5.051049000
C	-2.418878000	-0.715704000	2.398781000
C	2.145533000	0.809037000	-2.461195000
C	-2.579896000	-0.212337000	-2.405571000
C	2.325163000	0.220268000	2.334447000
H	-3.144069000	-0.953334000	3.170661000
H	2.863682000	1.091047000	-3.223817000
H	-3.356104000	-0.295194000	-3.159668000
H	3.102923000	0.293427000	3.087900000
O	-0.491962000	1.747645000	0.194810000
S	0.579395000	-2.237912000	-0.483722000
H	1.286397000	-2.433655000	0.648904000
S	0.243434000	5.949423000	2.097435000
C	-1.132725000	4.801537000	1.754054000
H	-1.860827000	4.982947000	2.547453000
H	-1.593549000	5.020020000	0.788439000
H	-0.813675000	3.758227000	1.784230000
C	1.426002000	5.580817000	0.833024000
C	2.582189000	6.388065000	0.791099000
C	1.277185000	4.540049000	-0.098680000
C	3.575347000	6.153293000	-0.147219000
H	2.699076000	7.199222000	1.503644000
C	2.269805000	4.306713000	-1.043443000
H	0.416754000	3.881592000	-0.083832000
C	3.411915000	5.104363000	-1.057045000
H	4.472226000	6.758987000	-0.186227000
H	2.168965000	3.502150000	-1.758818000
N	4.467118000	4.823100000	-2.023931000
O	5.445874000	5.572199000	-2.047022000
O	4.329706000	3.842510000	-2.765125000

d2. ^{2}RC

Fe	-0.161814000	0.139681000	0.008831000
N	-0.073024000	-0.263670000	1.981750000
N	1.854114000	0.319177000	-0.029224000
N	-2.112210000	-0.352220000	-0.002975000
N	-0.183087000	0.254740000	-2.008042000
C	-1.128862000	-0.556464000	2.807556000
C	2.634594000	0.646299000	-1.115960000
C	1.024710000	-0.172568000	2.794517000
C	2.702866000	0.336576000	1.057136000
C	-2.894309000	-0.638586000	1.084316000
C	0.864889000	0.583234000	-2.828850000
C	-2.949312000	-0.378246000	-1.084197000
C	-1.282047000	0.151363000	-2.826264000
C	-0.682472000	-0.660700000	4.174964000
C	4.002843000	0.853350000	-0.707884000
C	0.657491000	-0.420818000	4.167146000
C	4.045865000	0.654389000	0.636308000
C	-4.262461000	-0.849945000	0.678836000
C	0.419134000	0.684713000	-4.197826000
C	-4.296548000	-0.689134000	-0.672316000
C	-2.412805000	-0.410447000	-4.196968000
H	-1.322495000	-0.890117000	5.016520000
H	4.802275000	1.137945000	-1.378137000
H	1.346933000	-0.411872000	5.000809000
H	4.896653000	0.725557000	1.300776000
H	-5.074170000	-1.094487000	1.350979000
H	1.059135000	0.928091000	-5.035246000
H	-5.142222000	-0.773141000	-1.341793000
H	-1.596969000	0.382427000	-5.034555000
C	-2.442291000	-0.733770000	2.394698000
C	2.177070000	0.782860000	-2.416651000
C	-2.567187000	-0.148140000	-2.402341000
C	2.320254000	0.108372000	2.367857000
H	-3.176590000	-0.969463000	3.158552000
H	2.903086000	1.067942000	-3.170657000
H	-3.341596000	-0.202679000	-3.160860000
H	3.093948000	0.155551000	3.127499000
O	-0.421158000	1.733072000	0.227249000
S	0.557546000	-2.272380000	-0.506209000
H	1.237021000	-2.506144000	0.636165000

S	0.191760000	6.120773000	1.971996000
C	-1.091082000	4.835926000	1.793977000
H	-1.826794000	5.055527000	2.570508000
H	-1.573660000	4.892797000	0.816296000
H	-0.688280000	3.833407000	1.947552000
C	1.389646000	5.691726000	0.741207000
C	2.494206000	6.558351000	0.601418000
C	1.300149000	4.550736000	-0.073391000
C	3.494464000	6.286691000	-0.319260000
H	2.565695000	7.445249000	1.224027000
C	2.300599000	4.279482000	-0.999743000
H	0.478981000	3.848775000	0.013245000
C	3.390515000	5.139705000	-1.112045000
H	4.351644000	6.938517000	-0.433299000
H	2.243261000	3.400014000	-1.625986000
N	4.451895000	4.825792000	-2.062279000
O	5.385327000	5.623507000	-2.171861000
O	4.364406000	3.772165000	-2.704181000

d3. $^{4}TS_{SO}$

Fe	-0.057988000	-0.117288000	-0.005662000
N	-0.073982000	0.029942000	2.051434000
N	1.969890000	-0.019231000	0.030163000
N	-2.045421000	-0.370926000	0.012048000
N	-0.030539000	-0.292615000	-1.983232000
C	-1.174557000	0.028248000	2.862768000
C	2.799447000	0.001469000	-1.055016000
C	1.014778000	0.149925000	2.874009000
C	2.771410000	0.117151000	1.136455000
C	-2.879202000	-0.311749000	1.106235000
C	1.074486000	-0.235301000	-2.799099000
C	-2.853869000	-0.568895000	-1.077911000
C	-1.106685000	-0.503125000	-2.808349000
C	-0.773136000	0.163430000	4.245018000
C	4.171603000	0.141619000	-0.629013000
C	0.586197000	0.235557000	4.251359000
C	4.154120000	0.211353000	0.730799000
C	-4.248310000	-0.491116000	0.688347000
C	0.676880000	-0.393698000	-4.178384000
C	-4.232177000	-0.655233000	-0.663410000
C	-0.672017000	-0.564056000	-4.183981000
H	-1.453509000	0.185599000	5.086312000
H	5.023203000	0.178643000	-1.295528000
H	1.251822000	0.332542000	5.098968000
H	4.988971000	0.316468000	1.411265000
H	-5.099424000	-0.492358000	1.356802000
H	1.359171000	-0.383979000	-5.018130000
H	-5.066764000	-0.815692000	-1.333148000
H	-1.328975000	-0.721563000	-5.029134000
C	-2.487699000	-0.117002000	2.424838000
C	2.387461000	-0.092826000	-2.380492000
C	-2.422824000	-0.642794000	-2.396138000
C	2.338570000	0.191467000	2.454619000
H	-3.269891000	-0.105489000	3.177353000
H	3.155802000	-0.068408000	-3.146248000
H	-3.174091000	-0.807645000	-3.161412000
H	3.100286000	0.293249000	3.221098000
O	-0.185711000	1.646074000	-0.125088000
S	0.312222000	-2.464081000	0.384781000
H	-0.890144000	-2.733149000	0.934639000
S	0.061648000	3.215999000	1.054349000
C	-1.706224000	3.601213000	0.959394000
H	-1.903862000	4.603740000	1.344567000
H	-2.192274000	2.850206000	1.583486000
H	-2.051296000	3.480385000	-0.067815000
C	0.829461000	4.436436000	0.056091000
C	2.235306000	4.519023000	0.164095000
C	0.150302000	5.266214000	-0.857588000
C	2.944619000	5.423579000	-0.608844000
H	2.761840000	3.868309000	0.855477000
C	0.860201000	6.177179000	-1.628009000
H	-0.925273000	5.206566000	-0.968672000
C	2.247929000	6.248916000	-1.496517000
H	4.021666000	5.507805000	-0.538595000
H	0.361154000	6.831443000	-2.331901000
N	2.991217000	7.210492000	-2.308932000
O	4.216259000	7.247706000	-2.173877000
O	2.348845000	7.927273000	-3.079847000

d4. $^{2}TS_{SO}$

Fe	-0.011147000	-0.192623000	-0.227797000
N	0.142089000	0.463624000	1.660994000
N	2.003818000	-0.268351000	-0.399376000
N	-2.009740000	-0.280933000	-0.006491000
N	-0.159923000	-0.957071000	-2.105196000
C	-0.872311000	0.689412000	2.560243000
C	2.736803000	-0.630260000	-1.498054000
C	1.308122000	0.724296000	2.335731000
C	2.908911000	0.127003000	0.547592000
C	-2.749345000	0.044172000	1.102493000
C	0.858730000	-1.225776000	-2.982860000
C	-2.912755000	-0.673933000	-0.963450000
C	-1.322390000	-1.227390000	-2.775587000
C	-0.333166000	1.132110000	3.823426000
C	4.148132000	-0.471458000	-1.232472000
C	1.021334000	1.154046000	3.684198000
C	4.255426000	-0.000099000	0.038960000
C	-4.155130000	-0.148078000	0.840594000
C	0.322378000	-1.687870000	-4.243552000
C	-4.256631000	-0.590234000	-0.442501000
C	-1.031054000	-1.686911000	-4.115761000
H	-0.925973000	1.373312000	4.695948000
H	4.937180000	-0.694375000	-1.938481000
H	1.770691000	1.415981000	4.419700000
H	5.150547000	0.244893000	0.595238000
H	-4.945884000	0.033103000	1.556572000
H	0.919481000	-1.972311000	-5.099933000
H	-5.148732000	-0.848651000	-0.997759000
H	-1.777751000	-1.972560000	-4.844955000
C	-2.223716000	0.499161000	2.304934000
C	2.210258000	-1.082388000	-2.703057000
C	-2.600965000	-1.095339000	-2.249854000
C	2.590680000	0.586984000	1.819198000
H	-2.921311000	0.714325000	3.108014000
H	2.913466000	-1.337159000	-3.489697000
H	-3.431675000	-1.362474000	-2.895700000
H	3.417375000	0.846819000	2.472984000
O	-0.015896000	1.324901000	-0.994321000
S	-0.008374000	-2.496571000	0.497047000
H	1.010231000	-2.939626000	-0.267192000
S	-0.875516000	3.188641000	-0.142951000
C	-1.459289000	3.554095000	-1.820522000
H	-2.363534000	2.956824000	-1.944323000
H	-1.695176000	4.614594000	-1.930297000
H	-0.717388000	3.220303000	-2.546705000
C	0.541783000	4.215096000	0.056929000
C	1.088957000	4.266248000	1.355323000
C	1.151090000	4.936117000	-0.985207000
C	2.216012000	5.033522000	1.609225000
H	0.628761000	3.701904000	2.160288000
C	2.278471000	5.708379000	-0.731367000
H	0.755502000	4.897708000	-1.992510000
C	2.798044000	5.749812000	0.561592000
H	2.650480000	5.090912000	2.599243000
H	2.763491000	6.274411000	-1.516806000
N	3.987228000	6.563210000	0.826715000
O	4.429824000	6.570675000	1.976576000
O	4.473650000	7.190729000	-0.115406000

E. *IP*- and *EA*- related geometries

e1. ^{4}Cpd I

Fe	-0.003000000	-0.001570000	0.020490000
N	2.013010000	-0.003458000	0.003166000
N	0.004354000	2.016731000	0.017351000
N	-0.003209000	-2.000787000	-0.258132000
N	-2.000772000	0.024325000	-0.270674000
C	2.833010000	-1.099360000	-0.013381000
C	-1.085954000	2.846418000	0.035793000
C	2.838249000	1.080835000	0.112778000
C	1.101589000	2.836337000	0.121849000
C	1.087622000	-2.831835000	-0.234869000
C	-2.829259000	1.123138000	-0.221389000
C	-1.094349000	-2.818383000	-0.374658000
C	-2.832911000	-1.066306000	-0.403118000
C	4.215297000	-0.696197000	0.087512000
C	-0.668844000	4.223476000	0.150064000
C	4.218717000	0.662205000	0.164842000

C	0.690216000	4.217545000	0.198120000
C	0.672505000	-4.209142000	-0.347523000
C	-4.206717000	0.715890000	-0.351650000
C	-0.685533000	-4.201129000	-0.433711000
C	-4.209004000	-0.638971000	-0.467568000
H	5.057201000	-1.375610000	0.092906000
H	-1.341941000	5.069879000	0.180377000
H	5.063911000	1.332441000	0.247607000
H	1.366809000	5.057920000	0.278338000
H	1.344902000	-5.056626000	-0.359093000
H	-5.049829000	1.393815000	-0.351851000
H	-1.361321000	-5.040408000	-0.530769000

e2. ^{2}Cpd I

Fe	0.002778000	-0.003266000	0.019947000
N	2.013497000	-0.004821000	0.007219000
N	0.007700000	2.016935000	0.012245000
N	0.000497000	-2.000628000	-0.259269000
N	-2.000267000	0.024387000	-0.279575000
C	2.834285000	-1.100746000	-0.006935000
C	-1.083735000	2.845246000	0.034063000
C	2.839161000	1.080488000	0.111500000
C	1.103756000	2.836897000	0.119105000
C	1.089858000	-2.833047000	-0.230413000
C	-2.828510000	1.122457000	-0.221155000
C	-1.091589000	-2.816860000	-0.380867000
C	-2.832303000	-1.066205000	-0.407231000
C	4.216239000	-0.696715000	0.090083000
C	-0.667474000	4.222516000	0.151082000
C	4.219435000	0.662066000	0.162081000
C	0.691607000	4.217763000	0.198344000
C	0.673858000	-4.209718000	-0.345573000
C	-4.206826000	0.714963000	-0.344074000
C	-0.683732000	-4.199898000	-0.438999000
H	-5.054377000	-1.304586000	-0.580812000
C	2.407921000	-2.417515000	-0.125132000
C	-2.409067000	2.433016000	-0.059021000
C	-2.415817000	-2.386370000	-0.444256000
C	2.419173000	2.406659000	0.161292000
H	3.172431000	-3.188061000	-0.125558000
H	-3.174761000	3.201358000	-0.025278000
H	-3.183386000	-3.147894000	-0.539351000
H	3.188249000	3.167977000	0.245273000
O	-0.090426000	-0.125249000	1.639293000
S	-0.132098000	0.344246000	-2.525313000
H	-0.719799000	-0.830269000	-2.834893000

e3. p-MeO-TAn

S	-0.4353985001	0.6275041545	-0.9078358965
C	-1.1771380094	1.1784646746	0.6600889543
H	-2.2520709061	1.2018998377	0.4789427767
H	-0.9714349064	0.4764893602	1.4694434837
H	-0.8444776840	2.1812537401	0.9317923691
C	1.3152174647	0.5911045698	-0.5480706903
C	1.8849035971	0.9588172826	0.6771654383
C	2.1631373347	0.1645302917	-1.5730965754
C	3.2605216230	0.8997367452	0.8646012244
H	1.2663205538	1.2952077307	1.4986252425
C	3.5433205465	0.1040543264	-1.3916764616
H	1.7464506915	-0.1268616525	-2.5311640771
C	4.1020188266	0.4733218415	-0.1650887456
H	3.7012177640	1.1840717742	1.8127243582
H	4.1643207995	-0.2313491926	-2.2114333442
O	5.4389942794	0.4518048400	0.1202520099
C	6.3400278682	0.0279883555	-0.8919765578
H	7.3338630526	0.0907264081	-0.4515597979
H	6.1440855655	-1.0063634950	-1.1961014534
H	6.2921745951	0.6809940880	-1.7706584034

e4. p-Me-TAn

S	1.230237000	4.876698000	2.768741000
C	-0.198987000	3.833266000	2.336944000
H	-0.703027000	3.618795000	3.281393000
H	-0.894077000	4.356717000	1.676356000
H	0.115880000	2.891286000	1.881965000
C	2.019284000	5.172346000	1.194469000
C	3.192291000	5.945757000	1.212626000
C	1.551487000	4.692686000	-0.032362000
C	3.870587000	6.225523000	0.032893000
H	3.572067000	6.327444000	2.156442000
C	2.245794000	4.982708000	-1.210411000
H	0.650263000	4.092995000	-0.089060000
C	3.412729000	5.749600000	-1.205881000
H	4.776073000	6.826425000	0.074359000
H	1.862674000	4.598768000	-2.152833000
C	4.161907000	6.058313000	-2.480205000
H	4.255323000	7.138832000	-2.639348000
H	5.178827000	5.649152000	-2.457078000
H	3.654968000	5.636638000	-3.352501000

e5. TAn

S	-0.3215526797	0.7338151604	-0.9727003022
C	-1.0998348191	1.4219241422	0.5215895289
H	-2.1455816446	1.5788753073	0.2562649389
H	-1.0494811167	0.7233723039	1.3578376424
H	-0.6588597655	2.3804295242	0.7983935033
C	1.3792392872	0.4982944269	-0.4899924214
C	1.8941301670	0.8074494534	0.7728296702
C	2.2361525287	-0.0351061691	-1.4642821645
C	3.2434570264	0.5850369663	1.0512496965
H	1.2590462925	1.2199677801	1.5454053082
C	3.5779531761	-0.2525987116	-1.1768274779
H	1.8474032173	-0.2785842111	-2.4470776714
C	4.0917111322	0.0560346881	0.0838051638
H	3.6272330866	0.8300665079	2.0355391152
H	4.2255906752	-0.6655415632	-1.9421835295
H	5.1384671815	-0.1144039091	0.3058458181

e6. p-NO_2-TAn

S	-0.3536358671	0.6587350959	-0.9311230082
C	-1.1135100152	1.3305227914	0.5809908529
H	-2.1758028798	1.4164978135	0.3521857663
H	-0.9880815168	0.6524141817	1.4255253846
H	-0.7228035494	2.3202796343	0.8187654770
C	1.3633997423	0.5245547033	-0.5203920643
C	1.9166373971	0.8999513508	0.7120179167
C	2.2053815466	0.0029534663	-1.5194838407
C	3.2795591418	0.7586497090	0.9419121701
H	1.2960415668	1.3037462124	1.4996679109
C	3.5631849099	-0.1397419726	-1.2947441911
H	1.7880914389	-0.2909551046	-2.4755884370
C	4.0902846604	0.2409880768	-0.0611110285
H	3.7184997080	1.0449220583	1.8878066237
H	4.2189104322	-0.5395923629	-2.0557657554
N	5.5317469510	0.0920136755	0.1838114502
O	5.9652637919	0.4395690174	1.2776174738
O	6.2192995161	-0.3716639897	-0.7201328692