Mechanistic aspects of reactive metabolites formation in clomethiazole catalyzed biotransformation by cytochrome P450 enzymes.

Emadeldin M. Kamel[a*], Ahmed M. Tawfeek[b], Ashraf A. El-Bassuony[a], Al Mokhtar Lamsabhi[c,d]
[a]Chemistry Department, Faculty of Science, Beni-Suef University, Beni-Suef 62514, Egypt.
[b]Chemistry Department, College of Science, King Saud University, Riyadh 11451, Saudi Arabia
[c]Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, Campus de Excelencia UAM-CSIC Cantoblanco, Madrid 28049, Spain.
[d]Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, Madrid 28049, Spain.
Email: emad.abdelhameed@science.bsu.edu.eg

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Table S1. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the MBI of P450 by CLM through 4-Me C-H hydroxylation (Path A).

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1 +Bulk Polarity		UB3LYP/BS2//BS1+ZPE +Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
^2RC_A	-2732.37785410	0.00	-2731.95853010	0.00	-2732.83787460	0.00	-2732.41855060	0.00	-2732.85450920	0.00	-2732.43518520	0.00
^4RC_A	-2732.37764523	0.13	-2731.95829223	0.15	-2732.83773160	0.09	-2732.41837860	0.11	-2732.85442790	0.05	-2732.43507490	0.07
$^2TS\text{-}H_A$	-2732.35525142	14.18	-2731.94212942	10.29	-2732.80753550	19.04	-2732.39441350	15.15	-2732.82516130	18.42	-2732.41203930	14.52
$^4TS\text{-}H_A$	-2732.34692967	19.41	-2731.93308067	15.97	-2732.81332610	15.40	-2732.39947710	11.97	-2732.82899190	16.01	-2732.41514290	12.58
$^2INT_A$	-2732.37377151	2.56	-2731.95617351	1.48	-2732.84353800	-3.55	-2732.42594000	-4.64	-2732.860671	-3.87	-2732.44307330	-4.95
$^4INT_A$	-2732.37196076	3.70	-2731.95551276	1.89	-2732.83867140	-0.50	-2732.42222340	-2.30	-2732.853792	0.45	-2732.43734420	-1.35
$^2TS\text{-}reb_A$	-2732.36941590	5.16	-2731.95255490	3.60	-2732.83952350	-1.03	-2732.42266250	-2.69	-2732.8555970	-0.73	-2732.43873600	-2.30
$^2P\text{-}OH_A$	-2732.45693334	-49.62	-2732.03298934	-46.72	-2732.91274100	-46.98	-2732.48879700	-44.08	-2732.942409	-55.16	-2732.51846500	-52.26
$^4P\text{-}OH_A$	-2732.43634133	-36.70	-2732.01542033	-35.70	-2732.89541000	-36.10	-2732.47448900	-35.10	-2732.922596	-42.73	-2732.50167500	-41.72

Table S2. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP-D3BJ level of theory for the MBI of P450 by CLM through 4-Me C-H hydroxylation (Path A).

	UB3LYP-D3BJ/BS1		UB3LYP- D3BJ /BS1+ZPE		UB3LYP- D3BJ /BS2//BS1		UB3LYP D3BJ /BS2//BS1+ZPE		UB3LYP- D3BJ /BS2//BS1 +Bulk Polarity		UB3LYP- D3BJ /BS2//BS1+ZPE+Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
^2RC_A	-2732.55339500	0.00	-2732.13189300	0.00	-2733.01315100	0.00	-2732.59164900	0.00	-2733.02860900	0.00	-2732.60710700	0.00
^4RC_A	-2732.55327000	0.08	-2732.13174200	0.09	-2733.01295200	0.12	-2732.59142400	0.14	-2733.02849600	0.07	-2732.60696800	0.09
$^2TS\text{-}H_A$	-2732.52864140	15.53	-2732.11332040	11.65	-2732.98701235	16.40	-2732.57169135	12.52	-2733.00196130	16.72	-2732.58664030	12.84
$^4TS\text{-}H_A$	-2732.52542310	17.55	-2732.11090010	13.17	-2732.99032610	14.32	-2732.57580310	9.94	-2733.00705410	13.53	-2732.59253110	9.15
$^2INT_A$	-2732.52522300	17.68	-2732.10507900	16.83	-2733.00822700	3.09	-2732.58808300	2.24	-2733.022684	3.72	-2732.60254000	2.87
$^4INT_A$	-2732.54205700	7.11	-2732.12304200	5.55	-2733.01342100	-0.17	-2732.59440600	-1.73	-2733.027502	0.69	-2732.60848700	-0.87
$^2TS\text{-}reb_A$	-2732.54174700	7.23	-2732.12289700	5.55	-2733.01072400	1.52	-2732.59187400	-0.28	-2733.03176800	-2.05	-2732.61291800	-3.73
$^2P\text{-}OH_A$	-2732.62414000	-44.39	-2732.19881800	-42.00	-2733.09375000	-50.58	-2732.66842800	-48.18	-2733.108741	-50.28	-2732.68341900	-47.89
$^4P\text{-}OH_A$	-2732.61285700	-37.31	-2732.18979400	-36.33	-2733.08394400	-44.42	-2732.66088100	-43.44	-2733.097571	-43.27	-2732.67450800	-42.29

Table S3. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the MBI of P450 by CLM through α -methylene C-H hydroxylation (Path B).

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1 +Bulk Polarity		UB3LYP/BS2//BS1+ZPE +Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
^2RC_B	-2732.37975765	0.00	-2731.96030265	0.00	-2732.84004990	0.00	-2732.42059490	0.00	-2732.85639960	0.00	-2732.43694460	0.00
^4RC_B	-2732.37968993	0.04	-2731.96016593	0.09	-2732.83993470	0.07	-2732.42041070	0.12	-2732.85633300	0.04	-2732.43680900	0.09
$^2TS\text{-}H_B$	-2732.34121966	24.18	-2731.92923866	19.49	-2732.807114	20.67	-2732.39513320	15.98	-2732.8232613	20.79	-2732.41128030	16.10
$^4TS\text{-}H_B$	-2732.34026993	24.78	-2731.92795993	20.30	-2732.806961	20.76	-2732.39465050	16.28	-2732.8218826	21.66	-2732.40957260	17.18
$^2INT_B$	-2732.35641677	14.65	-2731.94129077	11.93	-2732.827497	7.88	-2732.41237070	5.16	-2732.843476	8.11	-2732.42834980	5.39
$^4INT_B$	-2732.35631794	14.71	-2731.94026894	12.57	-2732.829715	6.49	-2732.41366570	4.35	-2732.843755	7.93	-2732.42770570	5.80
$^2TS\text{-}reb_B$	-2732.35541748	15.27	-2731.94040648	12.49	-2732.827715	7.74	-2732.41270370	4.95	-2732.841755	9.19	-2732.42674370	6.40
$^4TS\text{-}reb_B$	-2732.35064600	18.27	-2731.93478700	16.01	-2732.827898	7.63	-2732.41203940	5.37	-2732.839357	10.69	-2732.42349800	8.44
$^2P\text{-}OH_B$	-2732.46044136	-50.63	-2732.03837236	-48.99	-2732.931457	-57.36	-2732.50938800	-55.72	-2732.948287	-57.66	-2732.52621800	-56.02
$^4P\text{-}OH_B$	-2732.44416634	-40.42	-2732.03184634	-44.89	-2732.911382	-44.83	-2732.49906200	-49.24	-2732.924823	-42.94	-2732.51250300	-47.41

Table S4. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the MBI of P450 by CLM through β-methylene C-H hydroxylation (Path C).

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1 +Bulk Polarity		UB3LYP/BS2//BS1+ZPE+ Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
^2RC_C	-2732.37970048	0.00	-2731.96038248	0.00	-2732.84131670	0.00	-2732.42199870	0.00	-2732.85715820	0.00	-2732.43784020	0.00
^4RC_C	-2732.37962429	0.05	-2731.96023729	0.09	-2732.84116300	0.10	-2732.42177600	0.14	-2732.85707400	0.05	-2732.43768700	0.10
$^2TS\text{-}H_C$	-2732.34471916	21.95	-2731.93221716	17.67	-2732.80909330	20.22	-2732.39659130	15.94	-2732.82542790	19.91	-2732.41292590	15.63
$^4TS\text{-}H_C$	-2732.34566449	21.36	-2731.93253949	17.47	-2732.81113580	18.94	-2732.39801080	15.05	-2732.82599200	19.56	-2732.41286700	15.67
$^2INT_C$	-2732.38468956	-3.13	-2731.96861556	-5.17	-2732.85526100	-8.75	-2732.43918700	-10.79	-2732.87155130	-9.03	-2732.45547730	-11.07
$^4INT_C$	-2732.38470504	-3.14	-2731.96788804	-4.71	-2732.85695980	-9.82	-2732.44014280	-11.39	-2732.87134810	-8.90	-2732.45453110	-10.47
$^2TS\text{-}reb_C$	-2732.37710556	1.63	-2731.95728556	1.94	-2732.85324500	-7.49	-2732.43342500	-7.17	-2732.86924150	-7.58	-2732.44942150	-7.27
$^4TS\text{-}reb_C$	-2732.37796607	1.09	-2731.95805607	1.46	-2732.85213500	-6.79	-2732.43222500	-6.42	-2732.86733830	-6.39	-2732.44742830	-6.02
$^2P\text{-}OH_C$	-2732.45660800	-48.26	-2732.03414500	-46.29	-2732.92688800	-53.70	-2732.50442500	-51.72	-2732.94069700	-52.42	-2732.51823400	-50.45
$^4P\text{-}OH_C$	-2732.43729300	-36.14	-2732.01785500	-36.06	-2732.90836300	-42.07	-2732.48892500	-42.00	-2732.92232900	-40.90	-2732.50289100	-40.82

Table S5. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the MBI of P450 by CLM through S-oxidation (Path D).

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1+Bulk Polarity		UB3LYP/BS2//BS1+ZPE+Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
$^{2}RC_{D}$	-2732.37995001	0.00	-2731.96048801	0.00	-2732.84044630	0.00	-2732.42098430	0.00	-2732.85694910	0.00	-2732.43748710	0.00
$^{4}RC_{D}$	-2732.37981931	0.08	-2731.96033831	0.09	-2732.84028350	0.10	-2732.42080250	0.11	-2732.85682770	0.08	-2732.43734670	0.09
$^{2}TS\text{-}S_{D}$	-2732.34898659	19.43	-2731.93073859	18.67	-2732.81184680	17.95	-2732.39359880	17.18	-2732.82866760	17.75	-2732.41041960	16.99
$^{4}TS\text{-}S_{D}$	-2732.33887880	25.77	-2731.92094980	24.81	-2732.80410650	22.80	-2732.38617750	21.84	-2732.81914560	23.72	-2732.40121660	22.76
$^{2}P\text{-}S_{D}$	-2732.38780061	-4.93	-2731.96683461	-3.98	-2732.85156400	-6.98	-2732.43059800	-6.03	-2732.86691240	-6.25	-2732.44594640	-5.31
$^{4}P\text{-}S_{D}$	-2732.38550124	-3.48	-2731.96590324	-3.40	-2732.84896210	-5.34	-2732.42936410	-5.26	-2732.86392450	-4.38	-2732.44432650	-4.29

Table S6. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the MBI of P450 by CLM through N-oxidation (Path E).

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1+Bulk Polarity		UB3LYP/BS2//BS1+ZPE+Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
$^{2}RC_{E}$	-2732.37872345	0.00	-2731.95937845	0.00	-2732.84126250	0.00	-2732.42191750	0.00	-2732.85765420	0.00	-2732.43830920	0.00
$^{4}RC_{E}$	-2732.37829146	0.27	-2731.95870946	0.42	-2732.84077250	0.31	-2732.42119050	0.46	-2732.85753440	0.08	-2732.43795240	0.22
$^{2}TS\text{-}N_{E}$	-2732.34677600	20.05	-2731.92704100	20.29	-2732.80933500	20.03	-2732.38960000	20.28	-2732.82913300	17.90	-2732.40939800	18.14
$^{4}TS\text{-}N_{E}$	-2732.33023300	30.43	-2731.91189100	29.80	-2732.80175700	24.79	-2732.38341500	24.16	-2732.81967900	23.83	-2732.40133700	23.20
$^{2}P\text{-}N_{E}$	-2732.40929400	-19.18	-2731.98690400	-17.27	-2732.87407300	-20.59	-2732.45168300	-18.68	-2732.89125400	-21.08	-2732.46886400	-19.17
$^{4}P\text{-}N_{E}$	-2732.38774300	-5.66	-2731.96821400	-5.54	-2732.85386800	-7.91	-2732.43433900	-7.79	-2732.87043600	-8.02	-2732.45090700	-7.91

Table S7. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the MBI of P450 by CLM through C=N epoxidation pathway (oxaziridine Formation) (Path F).

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1+Bulk Polarity		UB3LYP/BS2//BS1+ZPE+ Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
$^{2}RC_F$	-2732.36813820	0.00	-2731.94988820	0.00	-2732.83147450	0.00	-2732.41322450	0.00	-2732.84785610	0.00	-2732.42960610	0.00
$^{4}RC_F$	-2732.36803277	0.07	-2731.94959177	0.19	-2732.83056321	0.57	-2732.41212221	0.69	-2732.84771421	0.09	-2732.42927321	0.21
$^{2}TS\text{-}O_F$	-2732.35138000	10.52	-2731.93329000	10.42	-2732.81855000	8.11	-2732.40046000	8.01	-2732.83377000	8.84	-2732.41568000	8.74
$^{4}TS\text{-}O_F$	-2732.35226700	9.96	-2731.93351300	10.28	-2732.81394600	11.00	-2732.39519200	11.32	-2732.83231200	9.75	-2732.41355800	10.07
$^{2}INT\text{-}O_F$	-2732.38455420	-10.30	-2731.96714220	-10.83	-2732.83914780	-4.82	-2732.42173580	-5.34	-2732.85621	-5.24	-2732.43879800	-5.77
$^{4}INT\text{-}O_F$	-2732.39225700	-15.13	-2731.97328000	-14.68	-2732.83679620	-3.34	-2732.41781920	-2.88	-2732.852521	-2.93	-2732.43354440	-2.47
$^{2}TS\text{-}epo_F$	-2732.38194278	-8.73	-2731.96372866	-8.87	-2732.83598720	-2.83	-2732.41777308	-3.55	-2732.85321500	-3.45	-2732.43500088	-3.59
$^{4}TS\text{-}epo_F$	-2732.38044278	-7.72	-2731.96292878	-8.18	-2732.83423540	-1.73	-2732.41672140	-2.19	-2732.850125	-1.42	-2732.43261050	-1.89
$^{2}P\text{-}epo_F$	-2732.40574133	-23.60	-2731.98741733	-23.55	-2732.85814780	-16.74	-2732.43982380	-16.69	-2732.875725	-17.49	-2732.45740140	-17.44
$^{4}P\text{-}epo_F$	-2732.39745893	-18.40	-2731.98153793	-19.86	-2732.85014560	-11.72	-2732.43422460	-13.18	-2732.868871	-13.19	-2732.45295000	-14.65

Table S8. The electronic energy in Hartree of various species studied in reactive metabolites formation mechanisms.

Structure	EE+ZPE (Hartree)	RE (kcal/mol)
P-epo + -OMe	-1336.809357	0.00
TS-OMe1	-1336.78574	14.82
TS-OMe2	-1336.795599	8.63
P-OMe1	-1336.849909	-25.45
P-OMe2	-1336.866537	-35.88
P-epo + -SMe	-1659.855258	0.00
TS-SMe1	-1659.827451	17.45
TS-SMe2	-1659.834251	13.18
P-SMe1	-1659.890606	-22.18
P-SMe2	-1659.90013	-28.16
P-epo + HOH	-1298.134499	0.00
TS-diol	-1298.095815	24.27
P-diol	-1298.173563	-24.51
TS-R1	-1298.103312	19.57
TS-R2	-1298.099678	21.85
P-R1	-1298.15631	-13.69
P-R2	-1298.15711	-14.19

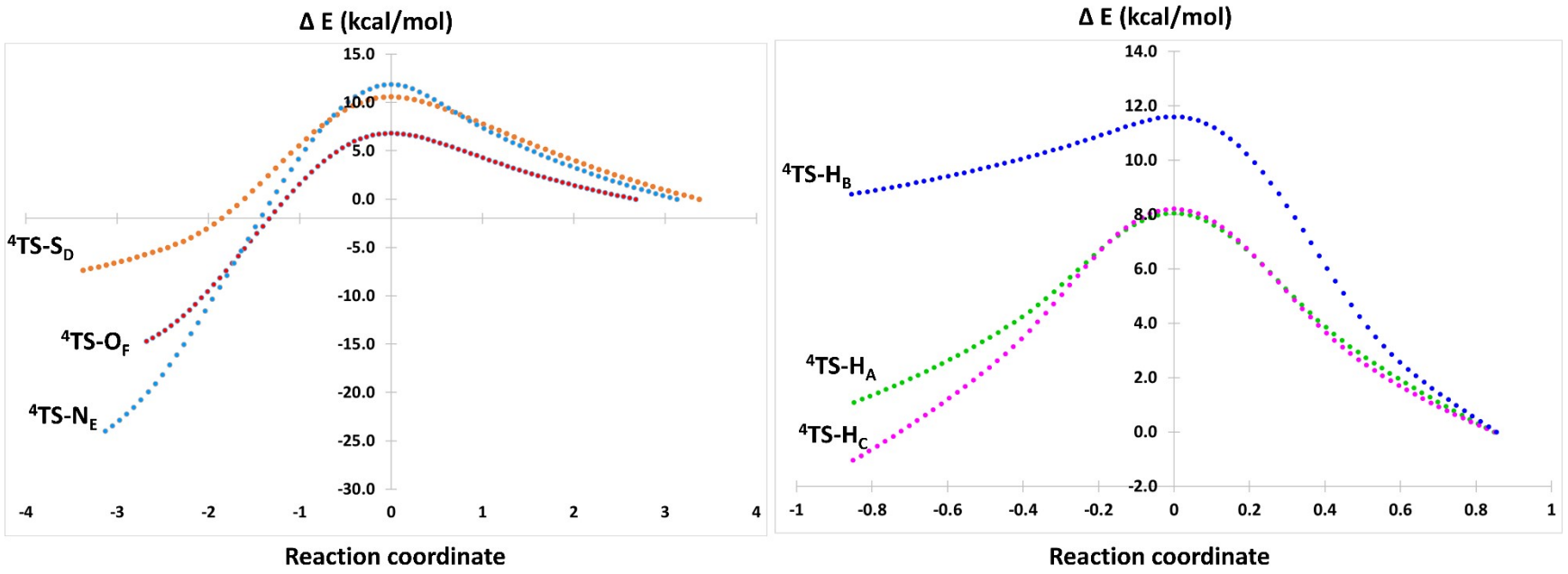

Figure S1. Computed intrinsic reaction coordinate (IRC) of the rate-determining step transition states in paths A, B, and C (right) and D, E, and F (left).

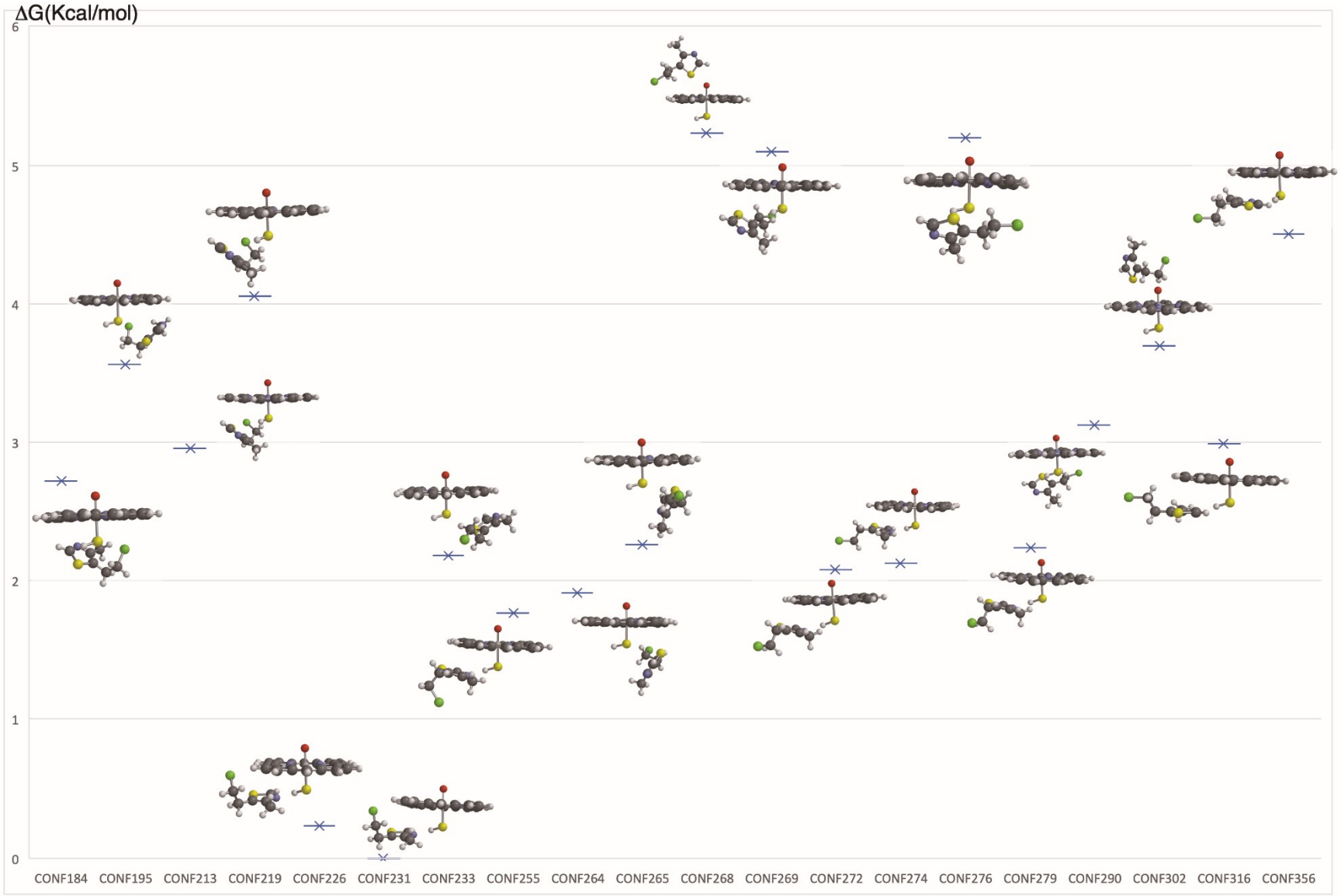

Figure S2. The results of metadynamic simulations to investigate the possible interactions between clomethiazole and P450' active site.

Cartesian coordinates of all structures represented in this study

$^{2}RC_{A}$

Fe	-1.84948	0.00954	-0.05458
O	-0.63845	-0.52971	0.88782
S	-3.80125	1.14848	-1.28977
H	-4.81047	0.44633	-0.72633
N	-2.80715	0.94873	1.46297
C	-4.06285	1.34199	3.36644
C	-3.35211	2.47377	3.11468
H	-4.76228	1.14917	4.16983
H	-3.34739	3.40424	3.66778
N	-0.91444	1.74187	-0.50607
C	-0.92043	2.90026	0.22634
C	-0.0212	3.86744	-0.35584
C	0.53493	3.27691	-1.44763
H	0.14728	4.86334	0.03338
H	1.25858	3.68345	-2.14192
N	-1.12793	-0.8169	-1.74012
C	-0.21353	-0.26858	-2.59714
C	-1.35943	-2.08603	-2.1998
C	0.14334	-1.21358	-3.6272
C	-0.57267	-2.34497	-3.38129
H	0.84913	-1.01771	-4.42381
H	-0.58088	-3.27426	-3.93638
N	-3.00666	-1.61619	0.24407
C	-3.87263	-3.75488	0.11239
H	-4.03957	-4.75214	-0.27408
C	-2.98807	-2.78131	-0.47957
C	-3.70999	0.39044	2.34125
C	-2.564	2.2198	1.93358
C	-0.02415	1.94959	-1.53083
C	-2.22799	-3.00265	-1.61989
H	-2.31422	-3.97551	-2.09449
C	-4.20035	-0.90264	2.26352
H	-4.90385	-1.21511	3.02933
C	-1.67969	3.1238	1.36869
H	-1.57904	4.0908	1.85196
C	0.30589	1.01872	-2.50402
H	1.05033	1.30711	-3.23754
C	-4.42142	-3.16633	1.21016
H	-5.13364	-3.57879	1.9133
C	-3.87249	-1.83393	1.28215
C	4.80214	0.20235	0.24316
C	3.74692	-0.13489	-0.57244
C	4.62937	1.44738	-1.85259

S	5.73867	1.47513	-0.50997
H	4.76476	2.11465	-2.69655
N	3.66345	0.58471	-1.75407
C	5.20642	-0.38657	1.56793
C	6.2684	-1.47759	1.39176
H	4.32808	-0.8134	2.06163
H	5.5962	0.38827	2.23702
H	5.89191	-2.30646	0.78985
H	7.17567	-1.08495	0.92881
Cl	6.7656	-2.17873	2.99415
C	2.70282	-1.17838	-0.28961
H	2.51828	-1.77508	-1.18894
H	3.00991	-1.85421	0.51335
H	1.74719	-0.72605	0.00293

$^{4}RC_{A}$

Fe	-1.8434	0.01256	-0.05169
O	-0.6432	-0.33049	0.99423
S	-3.72963	0.82392	-1.583
H	-4.77094	0.36737	-0.85099
N	-2.72937	1.392	1.12769
C	-3.95486	2.38521	2.82097
C	-3.19123	3.35822	2.2558
H	-4.65859	2.46971	3.63915
H	-3.138	4.4084	2.51267
N	-0.82179	1.48585	-0.9767
C	-0.76108	2.80541	-0.61172
C	0.17817	3.51546	-1.44606
C	0.68975	2.60681	-2.31944
H	0.40112	4.57127	-1.36092
H	1.4238	2.75759	-3.10007
N	-1.18262	-1.30451	-1.42809
C	-0.24955	-1.07584	-2.40082
C	-1.48604	-2.63731	-1.504
C	0.04791	-2.29539	-3.1126
C	-0.72507	-3.26775	-2.55599
H	0.75622	-2.37538	-3.92687
H	-0.78738	-4.31587	-2.81934
N	-3.07734	-1.39852	0.69944
C	-4.0533	-3.4369	1.18318
H	-4.27615	-4.49273	1.09754
C	-3.12867	-2.72095	0.33838
C	-3.65507	1.15965	2.12193
C	-2.42299	2.73241	1.2078
C	0.06393	1.34269	-2.01707
C	-2.39683	-3.2996	-0.68963
H	-2.54091	-4.36137	-0.86583

C	-4.20897	-0.07377	2.42255
H	-4.91931	-0.11379	3.24281
C	-1.49761	3.38813	0.41273
H	-1.34533	4.44747	0.5954
C	0.33479	0.15563	-2.68041
H	1.08436	0.18234	-3.46325
C	-4.55564	-2.53145	2.06659
H	-5.27798	-2.68781	2.85751
C	-3.9392	-1.26483	1.75437
C	4.77483	0.18274	0.14383
C	3.74186	-0.42455	-0.53188
C	4.65484	0.63303	-2.25516
S	5.72854	1.13032	-0.97699
H	4.81137	0.97187	-3.27325
N	3.68769	-0.15345	-1.89
C	5.14384	0.08693	1.5998
C	6.21635	-0.9826	1.83413
H	4.25373	-0.15952	2.18656
H	5.50925	1.0494	1.9742
H	5.86334	-1.97211	1.53853
H	7.13601	-0.75627	1.29135
Cl	6.66555	-1.09159	3.59268
C	2.69245	-1.31892	0.06703
H	2.50373	-2.16776	-0.59798
H	2.99754	-1.70821	1.04236
H	1.73951	-0.79251	0.20244

^{2}TS-H_A

Fe	1.36797	0.26609	-0.16788
O	0.05268	-0.51669	0.64955
S	3.10018	1.74513	-1.08179
H	3.88211	1.83688	0.01744
N	1.14072	1.8207	1.12531
C	0.32306	3.72875	2.14297
C	1.21074	3.16608	3.00567
H	-0.25773	4.63376	2.26748
H	1.50844	3.51097	3.98769
N	2.68323	-0.56542	1.11955
C	3.04108	-0.11308	2.36008
C	3.93246	-1.05191	3.00061
C	4.09691	-2.08671	2.13202
H	4.36069	-0.92299	3.98645
H	4.68991	-2.98395	2.25508
N	1.70396	-1.18886	-1.50377
C	2.48115	-2.30147	-1.31083
C	1.2327	-1.28009	-2.78773
C	2.47965	-3.12818	-2.49452

C	1.70855	-2.48893	-3.41618
H	3.01459	-4.06398	-2.5943
H	1.47596	-2.7916	-4.42915
N	0.19424	1.19959	-1.51455
C	-1.00811	1.7308	-3.41703
H	-1.38461	1.64537	-4.4284
C	-0.08957	0.8052	-2.79958
C	0.28342	2.88074	0.97282
C	1.70602	1.96715	2.36856
C	3.30925	-1.77273	0.96288
C	0.40667	-0.34381	-3.40202
H	0.10928	-0.53801	-4.42825
C	-0.50522	3.11639	-0.14535
H	-1.14272	3.9951	-0.12543
C	2.59917	1.07353	2.94107
H	2.96722	1.30542	3.93614
C	3.21381	-2.58272	-0.16269
H	3.77821	-3.5106	-0.15329
C	-1.28715	2.68391	-2.48596
H	-1.94161	3.54125	-2.57363
C	-0.52379	2.35146	-1.30658
C	-3.53867	-1.38799	0.9575
C	-2.65541	-2.22509	0.29052
C	-3.64031	-3.75813	1.55121
S	-4.51024	-2.32489	2.05815
H	-3.8785	-4.72621	1.97757
N	-2.72374	-3.56268	0.65823
C	-3.67918	0.1022	0.81737
C	-4.71288	0.46779	-0.2538
H	-2.70441	0.52583	0.55433
H	-3.97503	0.55475	1.76972
H	-4.41593	0.10525	-1.23926
H	-5.70211	0.07516	-0.01143
Cl	-4.90083	2.27301	-0.40212
C	-1.66285	-1.79777	-0.68802
H	-1.16785	-2.62078	-1.20116
H	-1.95891	-0.98993	-1.35702
H	-0.68846	-1.1869	-0.0193

^{4}TS-H_A

Fe	-1.46633	0.06958	0.07144
O	0.19084	-0.38446	0.12868
S	-3.74791	0.73697	-0.28555
H	-3.61287	2.05135	0.00085
N	-1.83763	-0.94639	1.74551
C	-2.3492	-2.63703	3.2367
C	-2.06936	-1.52823	3.9709

H	-2.63314	-3.62288	3.58219
H	-2.07418	-1.41107	5.04707
N	-1.13932	1.74644	1.14041
C	-1.15148	1.85676	2.50493
C	-0.78114	3.19297	2.90222
C	-0.52608	3.88487	1.75767
H	-0.72136	3.53663	3.92703
H	-0.21345	4.91536	1.64689
N	-1.16324	1.13715	-1.65181
C	-0.7757	2.44906	-1.75155
C	-1.27065	0.67174	-2.93727
C	-0.62403	2.81957	-3.13867
C	-0.93179	1.71635	-3.87473
H	-0.32294	3.79988	-3.48502
H	-0.93904	1.60441	-4.95148
N	-2.00549	-1.52598	-1.03303
C	-2.3815	-2.9589	-2.80375
H	-2.45708	-3.2953	-3.82991
C	-1.99781	-1.62707	-2.40451
C	-2.21103	-2.26209	1.84788
C	-1.75768	-0.47505	3.03174
C	-0.74492	2.97247	0.66208
C	-1.6516	-0.61651	-3.29067
H	-1.68944	-0.85163	-4.35
C	-2.4611	-3.11048	0.77972
H	-2.75735	-4.12939	1.00926
C	-1.44707	0.82699	3.39151
H	-1.42208	1.05979	4.45168
C	-0.57102	3.30331	-0.67607
H	-0.25114	4.31631	-0.89921
C	-2.61117	-3.66206	-1.66112
H	-2.91376	-4.69585	-1.55385
C	-2.36573	-2.76063	-0.56216
C	3.88808	0.17097	0.17997
C	3.06613	0.80722	-0.74261
C	4.18365	2.58828	-0.03943
S	4.94223	1.33914	0.92634
H	4.50297	3.62081	0.04858
N	3.24627	2.18283	-0.83449
C	3.92633	-1.29091	0.52668
C	4.93511	-2.04291	-0.35008
H	2.9267	-1.71617	0.39093
H	4.18938	-1.43468	1.57996
H	4.67533	-1.97384	-1.40785
H	5.94983	-1.66619	-0.20804
Cl	4.97704	-3.81301	0.06167

C	2.0297	0.16487	-1.53636
H	1.65392	0.77648	-2.35418
H	2.21119	-0.87275	-1.81936
H	0.97964	-0.02081	-0.7177

$^{2}INT_{A}$

Fe	-1.46196	0.09002	-0.25416
O	-0.0658	0.07565	0.93767
S	-3.39028	-0.06542	-1.67079
H	-2.98526	-1.09425	-2.44963
N	-1.8481	-1.85171	0.15634
C	-1.80225	-4.16406	0.18266
C	-2.63781	-3.76911	1.1797
H	-1.52718	-5.16925	-0.10977
H	-3.19585	-4.38304	1.87507
N	-2.76937	0.67603	1.18133
C	-3.45474	-0.14644	2.03693
C	-4.29081	0.63183	2.92097
C	-4.11354	1.93746	2.57949
H	-4.93113	0.21692	3.68891
H	-4.57569	2.8165	3.01025
N	-1.1741	2.02846	-0.73025
C	-1.7675	3.13182	-0.17593
C	-0.3252	2.50116	-1.69232
C	-1.27967	4.33535	-0.80423
C	-0.37789	3.94283	-1.74699
H	-1.59393	5.33884	-0.54723
H	0.19971	4.55789	-2.42522
N	-0.20433	-0.499	-1.71527
C	1.373	-0.45724	-3.40408
H	2.04949	-0.04305	-4.14086
C	0.53444	0.32234	-2.5218
C	-1.30465	-2.95968	-0.44148
C	-2.65617	-2.3237	1.16014
C	-3.16223	1.95398	1.49398
C	0.48528	1.71371	-2.50913
H	1.12075	2.23504	-3.21902
C	-0.37949	-2.92845	-1.47636
H	-0.0143	-3.88126	-1.84651
C	-3.38629	-1.5367	2.04084
H	-3.98111	-2.05579	2.78679
C	-2.70165	3.10052	0.85638
H	-3.09518	4.05292	1.19931
C	1.12515	-1.76584	-3.11882
H	1.55619	-2.65004	-3.57063
C	0.14011	-1.77605	-2.06138
C	4.10589	0.33407	1.19314

C	3.72657	1.61211	0.71842
C	5.87204	2.04092	1.12144
S	5.79779	0.34815	1.61333
H	6.80783	2.58532	1.19417
N	4.77201	2.55081	0.69471
C	3.28035	-0.91405	1.31248
C	3.55924	-1.86491	0.13706
H	2.21241	-0.665	1.32941
H	3.51543	-1.43416	2.24865
H	3.14535	-1.4775	-0.79527
H	4.62783	-2.04982	0.01177
Cl	2.79976	-3.49601	0.40756
C	2.44766	1.99363	0.31251
H	2.28874	3.01967	0.00183
H	1.60028	1.31551	0.35845
H	-0.29496	0.72221	1.62749

$^4INT_A$

Fe	-1.51374	0.02164	-0.15021
O	0.17728	0.29349	0.46157
S	-3.77143	-0.47762	-0.8627
H	-3.4914	-1.44799	-1.76183
N	-1.43162	-1.94509	0.26166
C	-1.02998	-4.2224	0.14602
C	-1.51578	-3.96407	1.38884
H	-0.72434	-5.17128	-0.27534
H	-1.69696	-4.65809	2.19951
N	-2.35318	0.38976	1.65007
C	-2.5525	-0.52234	2.65259
C	-3.16267	0.11143	3.79789
C	-3.34516	1.41968	3.47102
H	-3.42171	-0.39579	4.71842
H	-3.78095	2.21009	4.06856
N	-1.72851	1.98149	-0.60725
C	-2.27567	2.97215	0.15891
C	-1.32728	2.58299	-1.76851
C	-2.21668	4.23782	-0.53033
C	-1.62066	3.99553	-1.73155
H	-2.5832	5.17662	-0.13539
H	-1.39933	4.6947	-2.52774
N	-0.75867	-0.36026	-1.98656
C	0.12409	-0.06429	-4.10255
H	0.43849	0.45259	-5.00025
C	-0.47617	0.57025	-2.95108
C	-0.96584	-2.95692	-0.54657
C	-1.75888	-2.54128	1.45534
C	-2.83359	1.58614	2.13198

C	-0.74089	1.93159	-2.85249
H	-0.47337	2.54707	-3.70669
C	-0.46241	-2.78066	-1.82581
H	-0.10105	-3.66395	-2.34322
C	-2.25247	-1.87945	2.57111
H	-2.45908	-2.48284	3.45021
C	-2.80596	2.78692	1.43632
H	-3.21583	3.66033	1.93497
C	0.19879	-1.39333	-3.81789
H	0.58812	-2.19538	-4.43167
C	-0.3548	-1.55974	-2.49362
C	4.27445	0.54438	0.90545
C	3.9805	1.7831	0.29187
C	6.02516	2.26104	1.03266
S	5.87536	0.60222	1.60581
H	6.93074	2.82429	1.23333
N	5.01311	2.73105	0.39218
C	3.45377	-0.71341	0.91936
C	3.85475	-1.62258	-0.25105
H	2.38671	-0.47215	0.84211
H	3.59972	-1.2587	1.85899
H	3.58469	-1.1755	-1.20899
H	4.92357	-1.8442	-0.24378
Cl	3.00774	-3.23495	-0.17231
C	2.79585	2.12507	-0.3673
H	2.70906	3.11693	-0.79557
H	1.95095	1.44652	-0.42186
H	0.13161	1.0224	1.10432

^{2}TS-reb$_{A}$

Fe	1.41431	0.21435	0.34656
S	2.89215	0.94054	2.04272
H	4.006	1.05131	1.28492
N	-0.00215	0.30014	1.77999
C	-1.72158	1.02776	3.13007
C	-1.46457	-0.26712	3.46698
H	-2.46237	1.69933	3.54478
H	-1.94842	-0.87727	4.21912
N	1.75358	-1.73006	0.8004
C	1.13303	-2.4632	1.78394
C	1.71123	-3.78218	1.85041
C	2.70285	-3.82818	0.91819
H	1.39582	-4.55652	2.53809
H	3.36911	-4.64805	0.68183
N	2.92605	0.1655	-0.9829
C	3.72627	-0.90948	-1.28258
C	3.29543	1.17512	-1.83758

C	4.64978	-0.55624	-2.33147
C	4.38252	0.7344	-2.67535
H	5.3921	-1.22554	-2.7474
H	4.86051	1.34375	-3.43183
N	0.99936	2.11842	-0.18588
C	1.05462	4.17832	-1.21807
H	1.3764	4.95595	-1.89911
C	1.63662	2.85866	-1.14597
C	-0.80898	1.37256	2.06805
C	-0.39454	-0.71767	2.61195
C	2.73551	-2.53725	0.27713
C	2.70573	2.42909	-1.91913
H	3.11348	3.12672	-2.64377
C	-0.79409	2.59991	1.4183
H	-1.49902	3.35255	1.75604
C	0.12843	-2.00429	2.62285
H	-0.27408	-2.70177	3.35047
C	3.65066	-2.16655	-0.69732
H	4.36363	-2.91571	-1.02633
C	0.07113	4.22621	-0.27866
H	-0.58395	5.05059	-0.02728
C	0.05045	2.93602	0.36972
C	-1.61202	-0.27213	-2.49189
H	-0.9414	-0.47713	-3.31546
H	-1.68073	0.74324	-2.13164
O	0.18281	-0.32002	-0.93996
H	0.21499	-1.29406	-0.95094
C	-3.34021	-3.32696	-2.16227
C	-2.50442	-1.27071	-2.06785
C	-3.46426	-1.14711	-1.04618
S	-4.33338	-2.64717	-0.87609
H	-3.4886	-4.35399	-2.47829
N	-2.45993	-2.53501	-2.66902
C	-3.75757	0.05618	-0.19995
H	-2.84959	0.66063	-0.10916
H	-4.0373	-0.24046	0.81669
C	-4.88274	0.90489	-0.80575
H	-4.61468	1.27531	-1.79665
H	-5.81796	0.34615	-0.87432
Cl	-5.23074	2.36736	0.21999
^{2}P-OH$_{A}$			
Fe	1.60186	0.3812	-0.15899
O	-0.24572	-0.63641	0.50609
S	3.56368	1.27353	-0.74848
H	3.33222	2.53694	-0.32427
N	1.65657	1.21949	1.66487

C	1.45053	2.68651	3.43932
C	2.16751	1.61829	3.88226
H	1.1531	3.57359	3.98425
H	2.57937	1.44417	4.86836
N	2.49579	-1.28809	0.54405
C	3.02724	-1.44337	1.80138
C	3.68768	-2.72242	1.90797
C	3.55584	-3.33682	0.70035
H	4.18252	-3.08725	2.79925
H	3.92142	-4.30876	0.39401
N	1.38529	-0.54084	-1.94386
C	1.85005	-1.78023	-2.3152
C	0.85088	0.01715	-3.08086
C	1.58351	-2.0166	-3.71325
C	0.96743	-0.90021	-4.18928
H	1.84726	-2.92141	-4.24618
H	0.61879	-0.69891	-5.19444
N	0.53464	1.95511	-0.81896
C	-0.53365	3.45062	-2.22042
H	-0.95394	3.85237	-3.13391
C	0.11727	2.16719	-2.11128
C	1.14023	2.43064	2.05265
C	2.28892	0.70594	2.76867
C	2.82055	-2.43101	-0.14821
C	0.26439	1.27349	-3.16491
H	-0.11678	1.58066	-4.1342
C	0.43782	3.30165	1.22993
H	0.09301	4.23552	1.66342
C	2.93482	-0.52198	2.83564
H	3.39685	-0.78878	3.78135
C	2.50745	-2.67377	-1.47944
H	2.82379	-3.62073	-1.90574
C	-0.50409	4.01472	-0.98128
H	-0.89312	4.97534	-0.66791
C	0.17216	3.0801	-0.11532
C	-3.77985	-1.33183	0.78935
C	-2.49107	-1.48034	0.34138
C	-2.92772	-3.62672	0.64995
S	-4.44488	-2.91586	1.12563
H	-2.78004	-4.70005	0.68202
N	-2.02148	-2.77726	0.27054
C	-4.5922	-0.0783	0.96633
C	-5.47272	0.20458	-0.25704
H	-3.91917	0.77047	1.12724
H	-5.22639	-0.15028	1.85641
H	-4.87126	0.35195	-1.15589

H	-6.18552	-0.60298	-0.43474
Cl	-6.4463	1.71761	-0.02201
C	-1.52984	-0.404	-0.08631
H	-1.43451	-0.38992	-1.17961
H	-1.84772	0.58648	0.24102
H	-0.03087	-1.57921	0.37366
^{4}P-OH$_A$			
Fe	1.64647	0.35371	-0.18659
O	-0.30505	-0.59601	0.57648
S	3.71206	1.14519	-0.87968
H	3.35476	2.43226	-1.09201
N	1.95672	0.80535	1.84256
C	2.14624	1.9558	3.82292
C	2.73329	0.73791	4.004
H	2.0495	2.76305	4.53837
H	3.21007	0.3532	4.89702
N	2.41039	-1.51026	0.11482
C	3.03743	-1.94587	1.25902
C	3.58545	-3.26375	1.02468
C	3.28675	-3.60225	-0.2619
H	4.12504	-3.84674	1.76056
H	3.5331	-4.51702	-0.78629
N	1.01373	-0.24065	-2.11636
C	1.34273	-1.41034	-2.74109
C	0.41603	0.56526	-3.04518
C	0.89798	-1.36334	-4.11897
C	0.32367	-0.13941	-4.30763
H	1.02559	-2.15859	-4.84297
H	-0.10901	0.2614	-5.21599
N	0.70406	2.13211	-0.44083
C	-0.32021	3.95304	-1.39994
H	-0.80923	4.55987	-2.15179
C	0.14358	2.5989	-1.6074
C	1.66916	1.99021	2.45357
C	2.61466	0.02485	2.74641
C	2.55145	-2.49635	-0.83456
C	0.00487	1.87942	-2.79936
H	-0.46055	2.40849	-3.62655
C	1.04374	3.06961	1.8227
H	0.88267	3.96063	2.42334
C	3.11694	-1.25043	2.4698
H	3.637	-1.75635	3.27857
C	2.04786	-2.4574	-2.13842
H	2.24643	-3.32983	-2.75469
C	-0.03252	4.28369	-0.10846
H	-0.23931	5.21486	0.40415

C	0.61297	3.13756	0.49328
C	-3.86348	-1.243	0.86625
C	-2.57009	-1.39891	0.43454
C	-3.0281	-3.54365	0.72631
S	-4.54535	-2.82338	1.18647
H	-2.88895	-4.61821	0.75483
N	-2.11051	-2.69924	0.36291
C	-4.66838	0.01626	1.03546
C	-5.52379	0.31194	-0.20253
H	-3.99096	0.85848	1.2122
H	-5.31934	-0.05409	1.91349
H	-4.90477	0.45524	-1.09003
H	-6.24168	-0.48758	-0.39533
Cl	-6.48589	1.83472	0.01876
C	-1.59461	-0.32788	0.02148
H	-1.52308	-0.28102	-1.07323
H	-1.89211	0.65746	0.38456
H	-0.12257	-1.54548	0.44213

$^{2}RC_{B}$

Fe	1.22808	0.1238	-0.27476
O	0.31429	-0.11118	1.05095
S	2.98379	0.46726	-2.12208
H	3.00002	1.81959	-2.11096
N	2.75168	0.96918	0.75604
C	4.03119	2.48264	1.95075
C	4.57431	1.2523	2.15184
H	4.35711	3.4367	2.34485
H	5.44068	0.98609	2.74362
N	2.15278	-1.66556	-0.12896
C	3.24282	-1.97046	0.64322
C	3.52884	-3.38377	0.57415
C	2.59887	-3.93127	-0.25305
H	4.34305	-3.87304	1.093
H	2.48587	-4.96491	-0.55337
N	-0.10646	-0.67339	-1.55241
C	-0.2143	-1.98761	-1.91762
C	-1.15121	-0.02703	-2.15829
C	-1.35509	-2.17943	-2.77947
C	-1.94013	-0.95797	-2.92774
H	-1.65085	-3.12779	-3.20935
H	-2.81308	-0.69229	-3.51012
N	0.48109	1.9607	-0.64529
C	-0.93261	3.66816	-1.29961
H	-1.76557	4.15187	-1.79325
C	-0.64916	2.25515	-1.36496
C	2.88619	2.2987	1.09272

C	3.7682	0.31207	1.41208
C	1.73959	-2.8536	-0.68084
C	-1.41402	1.33489	-2.06818
H	-2.29231	1.70897	-2.58441
C	2.03266	3.3117	0.68914
H	2.25361	4.31665	1.03596
C	3.98806	-1.0551	1.37646
H	4.82509	-1.44052	1.95042
C	0.64634	-3.00651	-1.51885
H	0.43461	-4.00683	-1.88365
C	0.03865	4.2249	-0.52496
H	0.16999	5.26288	-0.24701
C	0.91031	3.14909	-0.11884
C	-3.8701	0.09246	1.3282
C	-4.60673	0.44293	0.21988
C	-3.86806	2.46217	0.73945
S	-3.12243	1.52136	1.99645
H	-3.71693	3.5343	0.68562
N	-4.59547	1.78796	-0.1027
C	-3.6346	-1.27308	1.91692
C	-2.4745	-1.98841	1.21616
H	-4.54395	-1.87697	1.81908
H	-3.41887	-1.20212	2.98799
H	-2.67798	-2.13112	0.15369
H	-1.53002	-1.45343	1.33104
Cl	-2.23224	-3.6559	1.91638
C	-5.39941	-0.4914	-0.65084
H	-4.88462	-0.67451	-1.6027
H	-5.56196	-1.46019	-0.1696
H	-6.37409	-0.05162	-0.88618

^4RC_B

Fe	1.24492	-0.12159	0.26612
O	0.29899	0.11713	-1.0384
S	2.9719	-0.4604	2.12575
H	2.98297	-1.8128	2.12398
N	2.76184	-0.97035	-0.75959
C	4.0516	-2.49172	-1.93347
C	4.59962	-1.26349	-2.13373
H	4.37961	-3.44814	-2.32003
H	5.47279	-1.00151	-2.71732
N	2.16859	1.66576	0.11715
C	3.26376	1.96745	-0.64867
C	3.55315	3.37991	-0.57958
C	2.62036	3.93041	0.24245
H	4.37145	3.86655	-1.09442
H	2.50881	4.96454	0.5417

N	-0.09436	0.68223	1.54296
C	-0.20394	1.99762	1.90042
C	-1.14085	0.03859	2.14756
C	-1.34859	2.19418	2.75658
C	-1.93349	0.97327	2.90926
H	-1.64662	3.14486	3.17971
H	-2.80883	0.7103	3.48928
N	0.49045	-1.95702	0.63929
C	-0.92892	-3.65903	1.29588
H	-1.76341	-4.13937	1.79024
C	-0.64069	-2.24676	1.35993
C	2.89839	-2.30235	-1.08805
C	3.7881	-0.31849	-1.40653
C	1.75609	2.85559	0.66716
C	-1.40337	-1.32382	2.06196
H	-2.28229	-1.6959	2.57866
C	2.04036	-3.31314	-0.68908
H	2.26188	-4.31894	-1.033
C	4.01093	1.04815	-1.3751
H	4.85342	1.42918	-1.94396
C	0.6603	3.01336	1.50076
H	0.44981	4.0154	1.86159
C	0.03995	-4.21985	0.52124
H	0.16767	-5.25851	0.24417
C	0.91539	-3.14726	0.11466
C	-3.89661	-0.10071	-1.31446
C	-4.62606	-0.45167	-0.20158
C	-3.88565	-2.46981	-0.72309
S	-3.14957	-1.52865	-1.98553
H	-3.73178	-3.54155	-0.66902
N	-4.60979	-1.79634	0.12241
C	-3.66753	1.26463	-1.9062
C	-2.50506	1.98361	-1.21309
H	-4.57766	1.86661	-1.80398
H	-3.45784	1.19273	-2.9784
H	-2.70304	2.12815	-0.14983
H	-1.56016	1.45031	-1.33154
Cl	-2.26977	3.64999	-1.91827
C	-5.41638	0.48159	0.67241
H	-4.89881	0.66397	1.62289
H	-5.58077	1.45074	0.19255
H	-6.39018	0.04128	0.91045

^{2}TS-H_B

Fe	0.99991	-0.25821	0.42754
O	0.10988	-0.02834	-1.06682
S	2.60635	-0.66761	2.23012

H	2.73976	-2.00381	2.0721
N	2.50145	-1.04072	-0.69691
C	3.79906	-2.46436	-1.97794
C	4.32366	-1.21688	-2.10874
H	4.13713	-3.38919	-2.42773
H	5.18439	-0.90439	-2.68612
N	1.88466	1.54931	0.3794
C	2.98519	1.89424	-0.36307
C	3.30687	3.28766	-0.16324
C	2.39603	3.77949	0.71912
H	4.13131	3.80339	-0.63863
H	2.31301	4.78352	1.11478
N	-0.40016	0.48733	1.65814
C	-0.49152	1.7596	2.15783
C	-1.46245	-0.19959	2.18706
C	-1.65178	1.88808	3.00637
C	-2.26055	0.66928	3.01876
H	-1.94317	2.79396	3.52254
H	-3.15478	0.36592	3.5479
N	0.22712	-2.11618	0.62346
C	-1.21026	-3.85168	1.13304
H	-2.06114	-4.36072	1.56763
C	-0.92556	-2.44408	1.28498
C	2.65316	-2.34329	-1.10564
C	3.50529	-0.33404	-1.30802
C	1.5072	2.69094	1.04491
C	-1.71583	-1.55511	2.00553
H	-2.60488	-1.95701	2.48187
C	1.80845	-3.38554	-0.75366
H	2.03999	-4.3698	-1.15008
C	3.7184	1.03073	-1.16953
H	4.55722	1.45734	-1.71154
C	0.40693	2.78887	1.88474
H	0.21974	3.75104	2.35212
C	-0.21418	-4.36831	0.36198
H	-0.0783	-5.38929	0.02862
C	0.67144	-3.27274	0.0445
C	-3.28533	0.3374	-1.62428
C	-4.28882	0.46754	-0.69132
C	-4.30144	-1.73733	-0.84743
S	-3.0331	-1.3518	-1.96975
H	-4.59115	-2.7669	-0.66836
N	-4.85403	-0.71668	-0.25765
C	-2.47294	1.41624	-2.28913
C	-1.38375	1.97846	-1.39313
H	-3.14239	2.23852	-2.58574

H	-2.01723	1.04787	-3.21439
H	-1.68997	2.26741	-0.38841
H	-0.48191	0.93372	-1.15594
Cl	-0.46972	3.30008	-2.1476
C	-4.80267	1.75766	-0.11557
H	-5.8944	1.72744	-0.04073
H	-4.40805	1.91995	0.8956
H	-4.51959	2.61965	-0.72758

^{4}TS-H_B

Fe	1.05487	-0.29701	0.38144
O	0.10737	-0.00508	-1.05133
S	2.31193	-0.49457	2.44924
H	3.52815	-0.17877	1.94951
N	2.62649	-0.84782	-0.7174
C	4.11239	-2.08129	-1.98622
C	4.50874	-0.7818	-2.05613
H	4.55993	-2.94979	-2.45232
H	5.35207	-0.36094	-2.58868
N	1.75977	1.60921	0.46739
C	2.84167	2.10025	-0.21541
C	3.01399	3.50642	0.0637
C	2.02156	3.86062	0.92394
H	3.79782	4.12554	-0.35363
H	1.81902	4.83176	1.35688
N	-0.4502	0.25966	1.63843
C	-0.6874	1.5008	2.17197
C	-1.46585	-0.54492	2.08362
C	-1.88781	1.4793	2.97283
C	-2.37486	0.20817	2.91376
H	-2.28834	2.33131	3.50736
H	-3.25989	-0.19892	3.38533
N	0.43264	-2.20062	0.45407
C	-0.8297	-4.09154	0.85937
H	-1.63822	-4.69942	1.24524
C	-0.70001	-2.66759	1.0672
C	2.9324	-2.11115	-1.15523
C	3.57851	-0.01914	-1.25686
C	1.23582	2.67495	1.16557
C	-1.59007	-1.90306	1.81171
H	-2.44832	-2.41451	2.23634
C	2.19947	-3.25492	-0.86946
H	2.55851	-4.19379	-1.28002
C	3.67411	1.34951	-1.03788
H	4.49002	1.87306	-1.52707
C	0.09798	2.62945	1.9565
H	-0.2087	3.55078	2.44232

C	0.24465	-4.47821	0.1198
H	0.50133	-5.46884	-0.23315
C	1.02376	-3.28797	-0.12906
C	-3.3227	0.31389	-1.60243
C	-4.33217	0.4231	-0.67323
C	-4.31796	-1.78031	-0.84964
S	-3.04935	-1.36915	-1.96326
H	-4.59716	-2.81476	-0.68213
N	-4.88536	-0.77187	-0.25358
C	-2.5232	1.40816	-2.25787
C	-1.44204	1.9812	-1.35862
H	-3.20414	2.22249	-2.55059
H	-2.06248	1.05194	-3.18554
H	-1.75	2.26042	-0.3514
H	-0.51302	0.94171	-1.12067
Cl	-0.54976	3.31995	-2.109
C	-4.86647	1.7009	-0.08916
H	-5.9596	1.66443	-0.0405
H	-4.4968	1.84648	0.9337
H	-4.57336	2.57434	-0.67966

$^{2}INT_{B}$

Fe	1.42235	-0.37944	-0.13454
O	-0.07392	0.55811	0.26364
S	3.40379	-1.49452	-0.97785
H	2.80233	-2.56237	-1.54946
N	0.8888	-0.43363	-2.08926
C	-0.10241	-1.00066	-4.10175
C	0.55046	0.17669	-4.29416
H	-0.6804	-1.57565	-4.81385
H	0.622	0.76755	-5.19838
N	2.49048	1.31314	-0.45697
C	2.54576	2.027	-1.62587
C	3.3887	3.18879	-1.46553
C	3.85432	3.16278	-0.18704
H	3.59417	3.91366	-2.24278
H	4.51784	3.86296	0.30406
N	2.07523	-0.388	1.76698
C	2.9144	0.50507	2.37718
C	1.73811	-1.30287	2.72758
C	3.11194	0.14886	3.7611
C	2.376	-0.97595	3.9804
H	3.73232	0.69679	4.45865
H	2.26875	-1.54426	4.89545
N	0.43668	-2.11332	0.14931
C	-0.51492	-3.95631	1.1702
H	-0.76158	-4.65624	1.95831

C	0.31589	-2.78551	1.33579
C	0.10167	-1.36711	-2.71965
C	1.1616	0.52724	-3.03249
C	3.28503	1.99174	0.43519
C	0.91775	-2.41114	2.53181
H	0.74027	-3.0483	3.39338
C	-0.44749	-2.48257	-2.10337
H	-1.0606	-3.13769	-2.71522
C	1.91056	1.6754	-2.81343
H	2.03763	2.3482	-3.65647
C	3.49117	1.61076	1.75505
H	4.14274	2.23613	2.35816
C	-0.89478	-3.98073	-0.13652
H	-1.51883	-4.704	-0.64566
C	-0.29561	-2.82314	-0.76008
C	-4.08852	0.66126	0.14315
C	-5.44915	0.75125	-0.03059
C	-5.35353	-1.40284	0.45977
S	-3.66666	-0.98275	0.56302
H	-5.68637	-2.41834	0.64532
N	-6.15285	-0.427	0.14602
C	-3.04014	1.73819	0.04733
C	-2.95935	2.53858	1.31073
H	-3.26829	2.4061	-0.79599
H	-2.05484	1.29171	-0.17004
H	-3.20805	2.1244	2.28111
H	0.20722	1.36164	0.73526
Cl	-1.84114	3.87347	1.37484
C	-6.21672	1.99172	-0.3906
H	-6.95373	2.22592	0.38656
H	-5.55954	2.85723	-0.50645
H	-6.77055	1.84502	-1.3255

$^4INT_B$

Fe	-1.48278	-0.27241	0.31886
O	-0.05299	0.28191	-0.61693
S	-3.37224	-1.00093	1.42656
H	-3.07525	-0.51458	2.65205
N	-0.77059	0.51887	2.0287
C	0.42747	0.83017	3.97249
C	-0.22054	1.99854	3.70828
H	1.08661	0.59551	4.79852
H	-0.20398	2.92231	4.27241
N	-2.40517	1.48942	-0.10314
C	-2.38495	2.63149	0.66005
C	-3.21293	3.64281	0.05216
C	-3.75339	3.09039	-1.06897

H	-3.3587	4.63831	0.45158
H	-4.4348	3.53839	-1.78082
N	-2.34684	-1.1042	-1.29551
C	-3.19306	-0.49139	-2.18748
C	-2.13804	-2.37527	-1.76823
C	-3.54857	-1.41338	-3.23663
C	-2.89499	-2.57935	-2.97736
H	-4.20648	-1.17731	-4.06318
H	-2.90487	-3.49997	-3.54663
N	-0.50314	-1.98269	0.69314
C	0.30209	-4.1369	0.53906
H	0.44804	-5.13141	0.13729
C	-0.54279	-3.13027	-0.05679
C	0.09066	-0.08491	2.91152
C	-0.95565	1.80262	2.48432
C	-3.25781	1.7394	-1.15117
C	-1.30102	-3.3247	-1.2003
H	-1.23551	-4.29152	-1.68863
C	0.6002	-1.37053	2.79738
H	1.27278	-1.71461	3.5763
C	-1.70686	2.78806	1.85993
H	-1.77089	3.75423	2.34994
C	-3.62381	0.82604	-2.12856
H	-4.30171	1.16617	-2.90462
C	0.8368	-3.58803	1.66322
H	1.51441	-4.03663	2.37826
C	0.31994	-2.24403	1.75835
C	4.23063	0.33479	-0.54539
C	5.56928	0.6084	-0.39466
C	5.73504	-1.58925	-0.58556
S	4.0107	-1.389	-0.73359
H	6.18635	-2.57426	-0.63228
N	6.40855	-0.49133	-0.41438
C	3.06351	1.28587	-0.58827
C	2.92964	1.93788	-1.92995
H	3.18567	2.05972	0.18371
H	2.12563	0.76277	-0.33889
H	3.25378	1.46104	-2.84777
H	-0.26096	1.14835	-1.01404
Cl	1.67	3.12092	-2.14947
C	6.18128	1.96823	-0.21196
H	6.87826	2.1886	-1.02911
H	5.42395	2.75592	-0.19113
H	6.75573	2.00926	0.72091

^{2}TS-reb$_{B}$

Fe	1.27042981	0.26638484	0.38982073

O	-0.14928419	-0.33989416	-0.64947627
S	3.19638957	0.99678845	1.67888579
H	2.60186057	1.97045145	2.40403679
N	0.59562200	-0.93994100	1.80845200
C	-0.45559900	-1.80466400	3.66844800
C	0.34376400	-2.78500800	3.16577800
H	-1.10026900	-1.83789200	4.53754700
H	0.49088200	-3.79194700	3.53502000
N	2.44146100	-1.12553400	-0.36610600
C	2.59296700	-2.39361500	0.13387100
C	3.51824300	-3.13639500	-0.68529000
C	3.90698700	-2.30768800	-1.69319300
H	3.81221000	-4.16224000	-0.50359400
H	4.58685500	-2.51140500	-2.51058300
N	1.77023100	1.53452400	-1.16497700
C	2.66228800	1.24497100	-2.17072100
C	1.42073400	2.85411500	-1.32572900
C	2.84249400	2.40064200	-3.01299500
C	2.07575200	3.39700600	-2.48922200
H	3.48843200	2.43229100	-3.88115700
H	1.96133700	4.41499300	-2.83931700
N	0.13307400	1.79847000	1.15650100
C	-0.91718000	3.82114500	1.49922400
H	-1.19488200	4.85413000	1.33220400
C	-0.01148400	3.07340900	0.66427700
C	-0.28115200	-0.64899400	2.82095200
C	1.00545100	-2.23268500	2.00807000
C	3.22211000	-1.05472900	-1.49147100
C	0.58855500	3.57556100	-0.48275700
H	0.39060500	4.61140000	-0.73908200
C	-0.88498600	0.58152700	3.03633900
H	-1.56060100	0.66903900	3.88110100
C	1.93498100	-2.91577100	1.23836700
H	2.16096900	-3.93993200	1.51712300
C	3.33119900	0.04140700	-2.33679200
H	4.00127700	-0.04629000	-3.18591000
C	-1.33483300	2.97821000	2.48471400
H	-2.02751700	3.17587600	3.29276100
C	-0.68431700	1.71295600	2.25799900
C	-3.75742136	-0.61176000	-0.72006187
C	-5.11172236	-0.61588400	-0.96113287
C	-4.82098536	1.57536200	-0.91442487
S	-3.18986336	1.04170400	-0.62501487
H	-5.05864936	2.63280800	-0.96119887
N	-5.70172136	0.63241400	-1.06580887
C	-2.81865936	-1.77507300	-0.55389187

C	-1.82174536	-1.87659200	-1.66595387
H	-3.41159536	-2.70030700	-0.50546487
H	-2.27629136	-1.71263800	0.39940013
H	-1.94409536	-1.34381700	-2.60129387
H	-0.09370919	0.18218184	-1.47046527
Cl	-0.85719236	-3.30416500	-1.78190487
C	-6.00469036	-1.81528200	-1.11679187
H	-6.49426436	-1.80039000	-2.09750887
H	-5.46026836	-2.75807900	-1.02196087
H	-6.79897036	-1.80002800	-0.36138287

^{4}TS-reb$_B$

Fe	1.22545	0.31151	0.35737
O	-0.19426	-0.29477	-0.68193
S	3.10032	0.95628	1.62966
H	2.50579	1.92994	2.35481
N	0.59562	-0.93994	1.80845
C	-0.4556	-1.80466	3.66845
C	0.34376	-2.78501	3.16578
H	-1.10027	-1.83789	4.53755
H	0.49088	-3.79195	3.53502
N	2.44146	-1.12553	-0.36611
C	2.59297	-2.39362	0.13387
C	3.51824	-3.1364	-0.68529
C	3.90699	-2.30769	-1.69319
H	3.81221	-4.16224	-0.50359
H	4.58685	-2.51141	-2.51058
N	1.77023	1.53452	-1.16498
C	2.66229	1.24497	-2.17072
C	1.42073	2.85412	-1.32573
C	2.84249	2.40064	-3.013
C	2.07575	3.39701	-2.48922
H	3.48843	2.43229	-3.88116
H	1.96134	4.41499	-2.83932
N	0.13307	1.79847	1.1565
C	-0.91718	3.82115	1.49922
H	-1.19488	4.85413	1.3322
C	-0.01148	3.07341	0.66428
C	-0.28115	-0.64899	2.82095
C	1.00545	-2.23269	2.00807
C	3.22211	-1.05473	-1.49147
C	0.58856	3.57556	-0.48276
H	0.39061	4.6114	-0.73908
C	-0.88499	0.58153	3.03634
H	-1.5606	0.66904	3.8811
C	1.93498	-2.91577	1.23837
H	2.16097	-3.93993	1.51712

C	3.3312	0.04141	-2.33679
H	4.00128	-0.04629	-3.18591
C	-1.33483	2.97821	2.48471
H	-2.02752	3.17588	3.29276
C	-0.68432	1.71296	2.258
C	-3.73513	-0.6006	-0.70173
C	-5.08943	-0.60472	-0.9428
C	-4.7987	1.58653	-0.8961
S	-3.16758	1.05287	-0.60669
H	-5.03636	2.64397	-0.94287
N	-5.67943	0.64358	-1.04748
C	-2.79637	-1.76391	-0.53556
C	-1.79946	-1.86543	-1.64763
H	-3.38931	-2.68914	-0.48714
H	-2.254	-1.70147	0.41773
H	-1.92181	-1.33265	-2.58297
H	-0.13869	0.22731	-1.50292
Cl	-0.83491	-3.293	-1.76358
C	-5.9824	-1.80412	-1.09846
H	-6.47198	-1.78923	-2.07918
H	-5.43798	-2.74692	-1.00363
H	-6.77668	-1.78886	-0.34305

^{2}P-OH$_{B}$

Fe	1.68514	0.20238	-0.41049
O	-1.44318	-0.90051	1.00319
S	3.13765	0.45497	-2.07444
H	3.24883	1.80235	-2.01689
N	2.63077	1.36677	0.90738
C	3.45424	3.21051	2.04508
C	4.22028	2.14408	2.40241
H	3.53092	4.23854	2.37537
H	5.05549	2.11349	3.09042
N	2.58232	-1.41522	0.36208
C	3.6515	-1.41261	1.22922
C	4.11967	-2.75656	1.46174
C	3.32528	-3.58126	0.72856
H	4.94397	-3.01623	2.11361
H	3.36039	-4.66014	0.64935
N	0.44129	-1.03272	-1.41537
C	0.54145	-2.40741	-1.55228
C	-0.51101	-0.64341	-2.34267
C	-0.38326	-2.88283	-2.54328
C	-1.03017	-1.78919	-3.03873
H	-0.50976	-3.92215	-2.81735
H	-1.79359	-1.74916	-3.8053
N	0.51605	1.75537	-0.89358

C	-1.00336	3.09767	-2.01618
H	-1.79424	3.36335	-2.70598
C	-0.4735	1.76734	-1.853
C	2.47474	2.72213	1.1089
C	3.70139	1.00156	1.69374
C	2.37948	-2.74022	0.03904
C	-0.93566	0.65967	-2.54692
H	-1.71156	0.82236	-3.28848
C	1.52596	3.51511	0.48394
H	1.50697	4.57138	0.73369
C	4.18931	-0.28798	1.83434
H	5.03626	-0.43297	2.49775
C	1.42631	-3.20975	-0.84993
H	1.38534	-4.27944	-1.02762
C	-0.33195	3.89818	-1.14422
H	-0.45247	4.96002	-0.97128
C	0.61681	3.05918	-0.45782
C	-4.28797	0.06205	1.14414
C	-5.55193	0.29531	0.6506
C	-4.78146	2.36164	0.49054
S	-3.38191	1.55977	1.14039
H	-4.75908	3.42282	0.26672
N	-5.8159	1.60304	0.28209
C	-3.69685	-1.22376	1.65505
C	-2.52448	-1.71742	0.80842
H	-4.46973	-1.99482	1.66643
H	-3.33186	-1.11495	2.68343
H	-2.79113	-1.83484	-0.24507
H	-0.80244	-1.00788	0.27247
Cl	-2.13739	-3.48623	1.33367
C	-6.66073	-0.7057	0.47995
H	-6.97038	-0.75563	-0.57055
H	-6.37197	-1.71047	0.7978
H	-7.54051	-0.40219	1.05914
^{4}P-OH$_B$			
Fe	1.42235	-0.37944	-0.13454
O	-1.07802	1.22013	0.64299
S	3.40379	-1.49452	-0.97785
H	2.80233	-2.56237	-1.54946
N	0.8888	-0.43363	-2.08926
C	-0.10241	-1.00066	-4.10175
C	0.55046	0.17669	-4.29416
H	-0.6804	-1.57565	-4.81385
H	0.622	0.76755	-5.19838
N	2.49048	1.31314	-0.45697
C	2.54576	2.027	-1.62587

C	3.3887	3.18879	-1.46553
C	3.85432	3.16278	-0.18704
H	3.59417	3.91366	-2.24278
H	4.51784	3.86296	0.30406
N	2.07523	-0.388	1.76698
C	2.9144	0.50507	2.37718
C	1.73811	-1.30287	2.72758
C	3.11194	0.14886	3.7611
C	2.376	-0.97595	3.9804
H	3.73232	0.69679	4.45865
H	2.26875	-1.54426	4.89545
N	0.43668	-2.11332	0.14931
C	-0.51492	-3.95631	1.1702
H	-0.76158	-4.65624	1.95831
C	0.31589	-2.78551	1.33579
C	0.10167	-1.36711	-2.71965
C	1.1616	0.52724	-3.03249
C	3.28503	1.99174	0.43519
C	0.91775	-2.41114	2.53181
H	0.74027	-3.0483	3.39338
C	-0.44749	-2.48257	-2.10337
H	-1.0606	-3.13769	-2.71522
C	1.91056	1.6754	-2.81343
H	2.03763	2.3482	-3.65647
C	3.49117	1.61076	1.75505
H	4.14274	2.23613	2.35816
C	-0.89478	-3.98073	-0.13652
H	-1.51883	-4.704	-0.64566
C	-0.29561	-2.82314	-0.76008
C	-3.73351	0.64905	-0.42772
C	-5.05509	0.89528	-0.14068
C	-5.07138	-1.28479	0.22905
S	-3.40389	-1.05511	-0.21747
H	-5.44836	-2.26913	0.48485
N	-5.80286	-0.2103	0.22426
C	-2.6487	1.61189	-0.83292
C	-2.06531	2.31222	0.35558
H	-3.05375	2.35556	-1.53449
H	-1.84971	1.07841	-1.37553
H	-2.57284	2.40445	1.30895
H	-0.64294	0.76736	1.38651
Cl	-0.83147	3.51273	0.08566
C	-5.73924	2.23201	-0.19203
H	-6.15009	2.49072	0.79096
H	-5.05388	3.02823	-0.49324
H	-6.57961	2.20853	-0.89595

$^{2}RC_{C}$

Fe	-1.27847	-0.17264	0.19813
O	0.24403	-0.00496	-0.35415
S	-3.78562	-0.2848	0.73761
H	-3.89729	0.92014	1.3414
N	-2.00515	1.32431	-0.95474
C	-2.48249	3.43044	-1.7857
C	-2.73673	2.54023	-2.78164
H	-2.5871	4.50762	-1.80023
H	-3.09742	2.73404	-3.78361
N	-1.81122	-1.50002	-1.22892
C	-2.25466	-1.21791	-2.49465
C	-2.41291	-2.43451	-3.25466
C	-2.06056	-3.45872	-2.43176
H	-2.75654	-2.47922	-4.2801
H	-2.05262	-4.52088	-2.64015
N	-0.85181	-1.69298	1.44552
C	-0.85445	-3.02843	1.1489
C	-0.41138	-1.597	2.73856
C	-0.40608	-3.79864	2.28353
C	-0.12937	-2.90677	3.27364
H	-0.3233	-4.87773	2.30289
H	0.22858	-3.09959	4.27678
N	-1.01831	1.13774	1.70791
C	-0.37962	2.07504	3.72164
H	-0.02348	2.12266	4.7427
C	-0.54431	0.85798	2.96477
C	-2.01409	2.66877	-0.65399
C	-2.42799	1.23047	-2.26205
C	-1.6805	-2.86597	-1.17241
C	-0.26537	-0.41222	3.45012
H	0.09779	-0.4862	4.47072
C	-1.61187	3.21705	0.55236
H	-1.65689	4.29737	0.64784
C	-2.53086	0.05304	-2.98422
H	-2.87102	0.12711	-4.01255
C	-1.24176	-3.58038	-0.06804
H	-1.19268	-4.66105	-0.16153
C	-0.75384	3.0964	2.90376
H	-0.76738	4.15856	3.11121
C	-1.14832	2.49941	1.65116
C	4.01015	-0.08039	-0.34084
C	5.35224	-0.31655	-0.53598
C	4.6219	-2.34746	-1.01012
S	3.11537	-1.55268	-0.65593
H	4.64413	-3.39458	-1.29279

N	5.68499	-1.60596	-0.91119
C	3.32334	1.20109	0.04959
C	2.76526	1.93751	-1.17231
H	4.04148	1.84877	0.56273
H	2.50017	1.00705	0.74366
H	3.52961	2.09236	-1.93572
H	1.91031	1.40697	-1.59127
Cl	2.16393	3.59908	-0.71432
C	6.47187	0.67495	-0.38177
H	6.96953	0.84751	-1.34382
H	6.12299	1.63935	-0.00361
H	7.23126	0.28696	0.30664
^4RC_C			
Fe	-1.28579	-0.16721	0.19167
O	0.25272	-0.02499	-0.32758
S	-3.77798	-0.29881	0.74143
H	-3.90889	0.92838	1.29442
N	-2.01194	1.28944	-1.00052
C	-2.51694	3.36774	-1.88397
C	-2.7638	2.44922	-2.85573
H	-2.63428	4.44289	-1.92593
H	-3.12962	2.61278	-3.86122
N	-1.79887	-1.53731	-1.19942
C	-2.24457	-1.29449	-2.47228
C	-2.39359	-2.53272	-3.19818
C	-2.0341	-3.53085	-2.34681
H	-2.73673	-2.60864	-4.22192
H	-2.01874	-4.59836	-2.52534
N	-0.85238	-1.6544	1.48551
C	-0.83884	-2.99618	1.22332
C	-0.4188	-1.51977	2.77678
C	-0.38608	-3.73231	2.37904
C	-0.12401	-2.81217	3.34696
H	-0.29052	-4.80948	2.42625
H	0.23236	-2.97489	4.35597
N	-1.03808	1.18454	1.66886
C	-0.41625	2.17788	3.66102
H	-0.06635	2.25429	4.68248
C	-0.57088	0.94012	2.93587
C	-2.03734	2.64149	-0.73407
C	-2.43915	1.15706	-2.30356
C	-1.65914	-2.90079	-1.10418
C	-0.28822	-0.31481	3.4572
H	0.06868	-0.35847	4.48178
C	-1.64013	3.22668	0.45637
H	-1.69503	4.30877	0.52173

C	-2.53068	-0.0392	-2.99545
H	-2.87245	0.00527	-4.02494
C	-1.21761	-3.58236	0.01953
H	-1.15967	-4.66466	-0.04593
C	-0.78972	3.17542	2.81406
H	-0.80909	4.24265	2.99298
C	-1.1745	2.54302	1.57583
C	4.02785	-0.08121	-0.33615
C	5.36992	-0.30878	-0.5413
C	4.64975	-2.34608	-1.00351
S	3.14065	-1.56044	-0.63975
H	4.67687	-3.39389	-1.28317
N	5.70845	-1.59704	-0.91526
C	3.33543	1.19678	0.05583
C	2.7642	1.92629	-1.16417
H	4.05281	1.85051	0.56228
H	2.5185	0.99916	0.75623
H	3.52211	2.08313	-1.93356
H	1.90952	1.38937	-1.57557
Cl	2.15654	3.5857	-0.70715
C	6.48384	0.69084	-0.39879
H	6.97633	0.85947	-1.36416
H	6.13031	1.65569	-0.02618
H	7.24862	0.31282	0.28925

^{2}TS-H_C

Fe	-1.02676	0.22244	0.39185
O	-0.21669	0.01811	-1.12082
S	-2.32189	0.96152	2.36163
H	-1.34912	0.81353	3.29019
N	0.17399	1.7357	0.98433
C	1.936	2.94032	1.87663
C	1.17719	3.81137	1.15859
H	2.84251	3.13684	2.43437
H	1.33058	4.87222	1.00772
N	-2.22233	1.55902	-0.57063
C	-1.98047	2.89292	-0.75257
C	-3.01744	3.48668	-1.56772
C	-3.89132	2.49092	-1.87208
H	-3.05705	4.53049	-1.8519
H	-4.79826	2.54447	-2.46062
N	-2.35995	-1.23464	0.00049
C	-3.50199	-1.12965	-0.74375
C	-2.26937	-2.54954	0.36687
C	-4.15479	-2.41318	-0.84903
C	-3.38689	-3.29791	-0.15645
H	-5.07697	-2.59439	-1.38615

H	-3.54468	-4.35827	-0.00719
N	0.07809	-1.05936	1.47173
C	0.86276	-2.98802	2.47936
H	0.89905	-4.03043	2.76927
C	-0.16282	-2.39958	1.65281
C	1.3112	1.64584	1.75297
C	0.08357	3.05358	0.59939
C	-3.38229	1.28991	-1.24783
C	-1.2495	-3.09545	1.1368
H	-1.30712	-4.15733	1.35576
C	1.79857	0.47347	2.31139
H	2.7083	0.54337	2.89972
C	-0.90252	3.58861	-0.21775
H	-0.83441	4.6486	-0.44383
C	-3.98347	0.04163	-1.32381
H	-4.90736	-0.03159	-1.88994
C	1.72218	-1.98369	2.81033
H	2.61072	-2.03152	3.4267
C	1.21773	-0.78599	2.18466
C	3.08794	-0.26288	-1.33561
C	3.36307	1.02862	-1.77399
C	5.09506	0.80182	-0.41711
S	4.3258	-0.7467	-0.18941
H	6.0097	1.0479	0.11007
N	4.49347	1.60423	-1.2481
C	1.96234	-1.09804	-1.73614
C	2.04555	-2.56903	-1.38641
H	1.68759	-0.9372	-2.78266
H	0.84095	-0.57716	-1.22114
H	2.96199	-3.01946	-1.78252
H	2.00981	-2.74073	-0.30838
Cl	0.68026	-3.52003	-2.10832
C	2.51085	1.79473	-2.74452
H	2.60982	1.3999	-3.76517
H	1.45276	1.73505	-2.46859
H	2.82378	2.84143	-2.75639

^{4}TS-H_C

Fe	-1.08298	0.26746	0.37421
O	-0.20116	-0.01424	-1.06862
S	-2.21831	0.48548	2.47697
H	-1.39823	1.39608	3.0476
N	-0.10426	1.99432	0.73947
C	1.50638	3.52937	1.35619
C	0.54781	4.20683	0.66621
H	2.41681	3.9116	1.79956
H	0.50668	5.26187	0.42731

N	-2.48181	1.25754	-0.64658
C	-2.50769	2.60203	-0.91914
C	-3.66903	2.92821	-1.71437
C	-4.3475	1.76713	-1.91136
H	-3.91658	3.92322	-2.06158
H	-5.27057	1.60711	-2.45373
N	-2.15272	-1.42697	0.22069
C	-3.31921	-1.59693	-0.47621
C	-1.81751	-2.66691	0.71163
C	-3.74302	-2.97434	-0.41286
C	-2.81133	-3.63748	0.32414
H	-4.63675	-3.36516	-0.88214
H	-2.77881	-4.68744	0.58501
N	0.30811	-0.72869	1.5023
C	1.45103	-2.38337	2.63533
H	1.67184	-3.36776	3.02811
C	0.29656	-2.05925	1.83034
C	1.09318	2.14773	1.3943
C	-0.44665	3.2374	0.27632
C	-3.60394	0.73057	-1.23324
C	-0.68544	-2.96731	1.45437
H	-0.56039	-3.99763	1.77247
C	1.8114	1.13426	2.01785
H	2.74017	1.41319	2.50558
C	-1.5713	3.52857	-0.48706
H	-1.72087	4.56339	-0.77944
C	-3.99906	-0.59616	-1.15981
H	-4.91575	-0.87475	-1.6702
C	2.15544	-1.2287	2.79291
H	3.07699	-1.06926	3.33765
C	1.43129	-0.2002	2.0844
C	3.12996	-0.23874	-1.30422
C	3.35962	1.10372	-1.60426
C	5.14722	0.77107	-0.3449
S	4.42236	-0.81341	-0.26462
H	6.07575	0.9813	0.17368
N	4.49654	1.64582	-1.05765
C	2.01357	-1.05803	-1.75227
C	2.1062	-2.54542	-1.48754
H	1.7261	-0.83563	-2.78442
H	0.88138	-0.57827	-1.20229
H	3.01625	-2.97491	-1.92046
H	2.08591	-2.7722	-0.41893
Cl	0.72856	-3.45603	-2.23637
C	2.46252	1.95124	-2.45829
H	2.64795	3.00699	-2.2456

H	2.6562	1.78505	-3.52738
H	1.40839	1.72662	-2.26899
$^2INT_C$			
Fe	-1.48413	0.11667	-0.21415
O	0.18968	-0.03651	0.49126
S	-3.7456	0.55219	-0.92693
H	-4.32258	-0.57968	-0.46297
N	-1.40837	2.11891	0.0628
C	-1.51094	4.20828	1.04626
C	-1.02708	4.38336	-0.21247
H	-1.70061	4.95575	1.80596
H	-0.7346	5.30367	-0.70159
N	-0.73978	0.37359	-2.06662
C	-0.37624	1.54389	-2.67038
C	0.13976	1.29157	-3.99613
C	0.08165	-0.05496	-4.18398
H	0.49225	2.05437	-4.67856
H	0.37569	-0.62862	-5.05372
N	-1.65695	-1.87019	-0.51247
C	-1.26197	-2.55139	-1.63416
C	-2.1519	-2.81754	0.34578
C	-1.51218	-3.96445	-1.47915
C	-2.06715	-4.13005	-0.2467
H	-1.28867	-4.71723	-2.22428
H	-2.39082	-5.04609	0.23051
N	-2.32471	-0.12965	1.61456
C	-3.24832	-1.03835	3.53217
H	-3.64162	-1.79181	4.20254
C	-2.74335	-1.29945	2.20566
C	-1.7469	2.79086	1.20785
C	-0.9596	3.07119	-0.81448
C	-0.47206	-0.61623	-2.97271
C	-2.66516	-2.55328	1.61442
H	-3.02353	-3.40032	2.1918
C	-2.25486	2.20702	2.36242
H	-2.47282	2.87048	3.19422
C	-0.48441	2.80763	-2.09306
H	-0.16124	3.65588	-2.68934
C	-0.71031	-1.97237	-2.77368
H	-0.4523	-2.64248	-3.58882
C	-3.11742	0.29954	3.74305
H	-3.38415	0.87182	4.62237
C	-2.53968	0.85832	2.54303
C	4.18113	0.08376	0.35042
C	4.0271	1.48135	0.59174
C	6.18555	1.32721	1.04917

S	5.87499	-0.34703	0.65503
H	7.17871	1.64784	1.34187
N	5.15712	2.13362	0.97556
C	3.19761	-0.8029	-0.05842
C	3.40361	-2.2463	-0.27587
H	2.17701	-0.42978	-0.14352
H	0.17984	-0.78763	1.1099
H	2.75249	-2.64321	-1.05451
H	4.43972	-2.52389	-0.47477
Cl	2.93402	-3.24167	1.24298
C	2.74376	2.23238	0.42228
H	2.56472	2.46856	-0.63698
H	1.87867	1.65219	0.76177
H	2.79997	3.17635	0.9705

$^4INT_C$

Fe	-1.53419	-0.04419	0.25963
O	-0.02473	-0.14833	-0.71978
S	-3.51716	0.06824	1.42919
H	-3.13242	0.95973	2.36894
N	-2.54126	-1.2817	-0.96088
C	-3.794	-2.11728	-2.70483
C	-3.36073	-3.18114	-1.97411
H	-4.40412	-2.11589	-3.59894
H	-3.54144	-4.23493	-2.1431
N	-0.88456	-1.60873	1.332
C	-1.13269	-2.9343	1.08157
C	-0.48769	-3.75296	2.07937
C	0.13357	-2.90533	2.94372
H	-0.52589	-4.83447	2.10378
H	0.7133	-3.14522	3.82585
N	-0.67874	1.2234	1.57361
C	0.05333	0.87776	2.68269
C	-0.60864	2.59302	1.4728
C	0.56781	2.06331	3.32001
C	0.15952	3.12553	2.56935
H	1.1702	2.06455	4.21952
H	0.35915	4.17817	2.72362
N	-2.11216	1.54031	-0.8766
C	-2.49618	3.68426	-1.63223
H	-2.44439	4.76485	-1.66708
C	-1.86875	2.86867	-0.62274
C	-3.26886	-0.93298	-2.07334
C	-2.57052	-2.65192	-0.8914
C	-0.1278	-1.56558	2.47587
C	-1.16144	3.36583	0.46129
H	-1.02967	4.44092	0.52429

C	-3.45055	0.35376	-2.55795
H	-4.06019	0.47193	-3.44781
C	-1.91654	-3.43055	0.05194
H	-2.02979	-4.50728	-0.02033
C	0.30833	-0.41626	3.11539
H	0.90243	-0.53625	4.01553
C	-3.14376	2.83717	-2.47891
H	-3.73475	3.07817	-3.35319
C	-2.9128	1.50022	-1.99207
C	4.15869	-0.42723	-0.62183
C	3.96269	-1.76743	-1.06082
C	6.14616	-1.65626	-1.39954
S	5.88051	-0.03762	-0.79033
H	7.13884	-1.97738	-1.69311
N	5.08429	-2.41473	-1.48188
C	3.19795	0.44664	-0.12834
C	3.4625	1.82217	0.32382
H	2.16096	0.11884	-0.1369
H	-0.05028	0.56067	-1.38858
H	2.78613	2.13568	1.11892
H	4.49802	2.00091	0.6166
Cl	3.14717	3.08298	-1.03834
C	2.64837	-2.48868	-1.04543
H	2.45676	-2.93631	-0.05967
H	1.80631	-1.82436	-1.26151
H	2.67137	-3.29967	-1.77846
^{2}TS-reb$_C$			
Fe	-1.21777	0.08762	0.29338
O	0.68203	0.32013	-0.66385
S	-3.38906	-0.31552	1.35005
H	-4.14937	-0.26378	0.23277
N	-0.45144	-1.11514	1.71962
C	0.31316	-2.98755	2.83983
C	0.56906	-1.91131	3.63449
H	0.51927	-4.03305	3.03147
H	1.03025	-1.88859	4.61398
N	-0.85204	1.67633	1.47146
C	-0.25056	1.68909	2.6999
C	-0.14032	3.04315	3.19448
C	-0.68624	3.84772	2.24297
H	0.29592	3.3213	4.14539
H	-0.79138	4.92525	2.24916
N	-2.11368	1.26603	-1.09076
C	-2.21494	2.63267	-1.03098
C	-2.70004	0.89732	-2.27075
C	-2.88313	3.13844	-2.20774

C	-3.18564	2.05816	-2.97949
H	-3.08835	4.18366	-2.40083
H	-3.68878	2.03275	-3.93792
N	-1.71421	-1.52378	-0.83882
C	-2.46472	-2.89559	-2.54665
H	-2.93538	-3.18001	-3.47935
C	-2.35665	-1.54101	-2.05768
C	-0.32478	-2.47959	1.64561
C	0.09271	-0.7492	2.91932
C	-1.12805	2.98039	1.17313
C	-2.8163	-0.41629	-2.72658
H	-3.30466	-0.56958	-3.68472
C	-0.75476	-3.27196	0.59031
H	-0.57402	-4.33968	0.67065
C	0.186	0.56016	3.38345
H	0.64057	0.71275	4.35802
C	-1.75799	3.42648	0.01388
H	-1.91266	4.49768	-0.07978
C	-1.87511	-3.69427	-1.61529
H	-1.76126	-4.77097	-1.62608
C	-1.41034	-2.82779	-0.55531
C	3.50706	0.48562	0.6962
C	3.87137	-0.89583	0.54428
C	3.64954	-0.86481	2.73556
S	3.27571	0.79749	2.42154
H	3.66074	-1.24586	3.74982
N	3.93759	-1.60715	1.68761
C	2.64552	1.1834	-0.13132
C	3.03048	2.70332	0.17892
H	3.31755	1.21933	-1.00143
H	0.55846	0.26581	-1.62572
H	2.62375	3.34472	-0.60198
H	2.43326	2.83799	1.08334
Cl	4.45677	3.63315	0.62447
C	4.12509	-1.56998	-0.7638
H	3.21106	-2.06527	-1.1223
H	4.45089	-0.86629	-1.53515
H	4.88805	-2.34331	-0.63867

^{4}TS-reb$_C$

Fe	1.36493	-0.10348	0.00083
O	-0.51187	0.05554	-0.04989
S	3.73613	-0.18683	0.02209
H	3.88445	-1.07307	1.03202
N	1.59158	1.29657	-1.42958
C	1.77281	2.3513	-3.4696
C	1.79576	3.31976	-2.51211

H	1.83445	2.46381	-4.54452
H	1.87973	4.39158	-2.63876
N	1.35054	1.33748	1.41997
C	1.46506	2.68796	1.21571
C	1.43928	3.38205	2.48174
C	1.32635	2.43151	3.44895
H	1.5084	4.45633	2.59562
H	1.2838	2.56299	4.52268
N	1.26708	-1.51848	1.4336
C	1.19856	-1.30747	2.78943
C	1.16943	-2.87569	1.24633
C	1.08437	-2.56948	3.4764
C	1.06683	-3.54086	2.52084
H	1.01874	-2.68003	4.55137
H	0.98317	-4.61247	2.64983
N	1.25652	-1.5394	-1.42132
C	1.21625	-3.58652	-2.48228
H	1.16914	-4.66195	-2.59689
C	1.19117	-2.89736	-1.21629
C	1.63563	1.08976	-2.78529
C	1.67364	2.65349	-1.23943
C	1.28137	1.15454	2.77604
C	1.14132	-3.52598	0.01931
H	1.07832	-4.60939	0.02835
C	1.53237	-0.14005	-3.42216
H	1.5959	-0.14954	-4.5055
C	1.61376	3.30913	-0.0167
H	1.69428	4.39139	-0.02594
C	1.20866	-0.07142	3.42233
H	1.15799	-0.06484	4.50652
C	1.32353	-2.63411	-3.44969
H	1.38362	-2.76657	-4.52241
C	1.36561	-1.35819	-2.77998
C	-3.55934	-0.18045	0.04445
C	-3.87941	-1.40042	0.68661
C	-5.12172	-1.66913	-1.11979
S	-4.4394	-0.10629	-1.4864
H	-5.81785	-2.14003	-1.8041
N	-4.74886	-2.20407	0.01564
C	-2.67117	0.79566	0.50166
C	-2.41947	2.09062	-0.17058
H	-2.2963	0.68893	1.51174
H	-0.80635	-0.59478	-0.71302
H	-1.45541	2.50666	0.10804
H	-2.50066	2.03472	-1.25643
Cl	-3.67981	3.35535	0.3511

C	-3.30471	-1.84027	1.99967
H	-3.67078	-2.8411	2.2382
H	-2.20849	-1.85986	1.96565
H	-3.59385	-1.16252	2.81347
^{2}P-OH$_C$			
Fe	-1.30838	-0.13943	-0.41405
O	0.61375	-0.1616	0.8952
S	-3.19453	-0.30444	-1.59122
H	-2.7364	-1.11796	-2.57038
N	-2.28312	-0.41668	1.32166
C	-3.37432	-1.42557	3.09299
C	-3.52852	-0.08268	3.24197
H	-3.74203	-2.22196	3.72759
H	-4.05145	0.45526	4.02247
N	-1.51781	1.84404	-0.18504
C	-2.19658	2.50859	0.80938
C	-2.20751	3.9271	0.54635
C	-1.54474	4.11345	-0.62784
H	-2.6712	4.66862	1.18441
H	-1.34795	5.04027	-1.15152
N	-0.15389	0.14544	-2.03903
C	0.05911	1.34591	-2.67771
C	0.47416	-0.80702	-2.80998
C	0.85053	1.14504	-3.8668
C	1.11144	-0.18963	-3.94675
H	1.15854	1.9335	-4.54178
H	1.67476	-0.72279	-4.70214
N	-0.89256	-2.11634	-0.51802
C	-0.24165	-4.20421	-1.27314
H	0.24239	-4.94603	-1.89564
C	-0.18143	-2.78233	-1.4948
C	-2.59544	-1.62512	1.89238
C	-2.85056	0.53795	2.12835
C	-1.12148	2.80978	-1.07978
C	0.4757	-2.17267	-2.55511
H	1.00572	-2.81333	-3.25311
C	-2.20646	-2.87061	1.41753
H	-2.53824	-3.74136	1.97476
C	-2.80588	1.90643	1.90168
H	-3.30757	2.55163	2.61627
C	-0.39277	2.58381	-2.2396
H	-0.145	3.44801	-2.84817
C	-1.01124	-4.39824	-0.16552
H	-1.28605	-5.33251	0.30756
C	-1.41758	-3.09556	0.29741
C	3.04287	-0.18	0.93417

C	4.11855	-0.42624	0.11187
C	4.81862	-1.55423	1.88362
S	3.29253	-0.96629	2.4818
H	5.4502	-2.17837	2.50615
N	5.1155	-1.20772	0.66828
C	1.80745	0.62363	0.6628
C	1.63022	1.85075	1.56502
H	1.82324	0.95423	-0.38009
H	0.7892	-1.08431	0.63458
H	0.6688	2.32091	1.36157
H	1.69195	1.5772	2.61954
Cl	2.9144	3.08308	1.24696
C	4.32779	0.0772	-1.28828
H	4.74429	-0.72366	-1.90721
H	3.40436	0.43235	-1.75169
H	5.04906	0.90348	-1.29315

^{4}P-OH$_{C}$

Fe	-1.39783	-0.09447	-0.43798
O	0.72877	-0.29323	0.89074
S	-3.35692	-0.12137	-1.67928
H	-3.22104	-1.36291	-2.19942
N	-2.19653	-0.99077	1.27889
C	-3.05986	-2.54319	2.74034
C	-3.41466	-1.31035	3.20323
H	-3.29111	-3.50975	3.17026
H	-3.99438	-1.07031	4.08576
N	-1.81401	1.74414	0.32053
C	-2.58076	2.00091	1.43048
C	-2.78814	3.42897	1.54545
C	-2.14307	4.01409	0.49695
H	-3.35002	3.91	2.33613
H	-2.07122	5.06818	0.26054
N	-0.18692	0.79799	-1.90993
C	-0.1199	2.13926	-2.17571
C	0.47269	0.15032	-2.91899
C	0.65111	2.35474	-3.38146
C	1.0186	1.12296	-3.84237
H	0.86663	3.32165	-3.81856
H	1.59058	0.88695	-4.73106
N	-0.72296	-1.93548	-1.04932
C	0.07545	-3.62984	-2.38731
H	0.58596	-4.11581	-3.20927
C	-0.01682	-2.20003	-2.20486
C	-2.30278	-2.33065	1.52298
C	-2.87643	-0.34107	2.26971
C	-1.53247	2.95128	-0.27297

C	0.55103	-1.2406	-3.04795
H	1.09536	-1.61993	-3.90831
C	-1.78999	-3.32894	0.68892
H	-1.96692	-4.35704	0.99238
C	-3.05438	1.04408	2.33331
H	-3.63378	1.42157	3.17133
C	-0.7427	3.1321	-1.41214
H	-0.60715	4.15732	-1.74485
C	-0.58054	-4.2138	-1.34271
H	-0.71051	-5.27027	-1.14416
C	-1.08349	-3.15045	-0.50448
C	3.15796	-0.28806	0.89131
C	4.25595	-0.39541	0.06949
C	4.95133	-1.73203	1.69098
S	3.39601	-1.26958	2.32348
H	5.58723	-2.41843	2.2392
N	5.26357	-1.21926	0.53959
C	1.90483	0.51525	0.70442
C	1.72373	1.66142	1.70776
H	1.90487	0.93924	-0.3055
H	0.8418	-1.12722	0.39887
H	0.75282	2.13136	1.55168
H	1.79935	1.30244	2.73538
Cl	2.98567	2.93667	1.48405
C	4.47497	0.29689	-1.24657
H	4.97048	-0.38747	-1.94209
H	3.54169	0.64268	-1.69846
H	5.12906	1.16806	-1.11939
^2RC_D			
Fe	1.62983	0.08139	0.21584
O	0.66639	-0.35827	-1.01941
S	3.31904	1.02252	1.90904
H	2.54016	1.99793	2.42952
N	0.11336	0.78444	1.34679
C	-1.58448	2.11408	2.17611
C	-1.72018	0.8863	2.74987
H	-2.18837	2.99997	2.32562
H	-2.45713	0.55566	3.47063
N	1.51718	-1.68669	1.16809
C	0.56282	-2.07567	2.07032
C	0.76857	-3.44935	2.46081
C	1.86467	-3.88598	1.78278
H	0.14916	-3.99002	3.16477
H	2.3343	-4.86074	1.81241
N	3.32287	-0.52506	-0.70208
C	3.88693	-1.77602	-0.64549

C	4.06626	0.18038	-1.61233
C	5.02159	-1.85528	-1.53345
C	5.12942	-0.64189	-2.13831
H	5.64091	-2.73325	-1.66476
H	5.85754	-0.31355	-2.8688
N	1.93244	1.94769	-0.50849
C	2.67319	3.70925	-1.81179
H	3.28547	4.24744	-2.52389
C	2.86666	2.3275	-1.44583
C	-0.43963	2.03634	1.3014
C	-0.65926	0.06397	2.22149
C	2.32089	-2.77735	0.97964
C	3.84822	1.50434	-1.97304
H	4.51403	1.93469	-2.71469
C	0.03588	3.09767	0.53606
H	-0.50515	4.03693	0.59917
C	-0.45288	-1.26587	2.56284
H	-1.14132	-1.70959	3.2756
C	3.42935	-2.8229	0.13998
H	3.9761	-3.75957	0.08914
C	1.6058	4.16082	-1.10039
H	1.15783	5.1462	-1.1082
C	1.1386	3.05482	-0.30091
C	-4.20164	-0.55581	-1.5112
C	-4.27171	-1.81619	-2.05781
C	-2.06401	-1.63864	-1.99098
S	-2.524	-0.09913	-1.31635
H	-1.01369	-1.88214	-2.09544
N	-3.05173	-2.41266	-2.32724
C	-5.30926	0.35757	-1.06105
C	-5.46647	0.32493	0.4627
H	-6.25311	0.05501	-1.52524
H	-5.11929	1.3895	-1.37816
H	-5.73431	-0.67309	0.81395
H	-4.55446	0.64877	0.96768
Cl	-6.79119	1.44491	1.01964
C	-5.5163	-2.5921	-2.38657
H	-5.56429	-3.51405	-1.7945
H	-6.42694	-2.01782	-2.19562
H	-5.51165	-2.8894	-3.4415

^4RC_D

Fe	1.6498	0.11553	0.18686
O	0.69249	-0.34026	-1.04962
S	2.93432	0.76374	2.30367
H	2.67779	2.09145	2.2815
N	0.14002	0.73483	1.37752

C	-1.5782	1.99133	2.28636
C	-1.67305	0.74075	2.8145
H	-2.20248	2.85427	2.48001
H	-2.38909	0.36587	3.53461
N	1.60481	-1.68377	1.10031
C	0.66426	-2.13712	1.98836
C	0.9175	-3.51625	2.32941
C	2.02709	-3.89258	1.6388
H	0.31783	-4.10087	3.01506
H	2.52859	-4.85178	1.63677
N	3.34212	-0.41752	-0.76951
C	3.94432	-1.64472	-0.75534
C	4.06368	0.34518	-1.64781
C	5.07881	-1.66107	-1.64738
C	5.15223	-0.42172	-2.20458
H	5.72274	-2.51554	-1.81118
H	5.86945	-0.04428	-2.92203
N	1.85442	1.99972	-0.50712
C	2.52225	3.81788	-1.76803
H	3.11122	4.39673	-2.46779
C	2.77307	2.4388	-1.4265
C	-0.45499	1.97852	1.38163
C	-0.60605	-0.03984	2.23809
C	2.44548	-2.74574	0.86947
C	3.80407	1.67499	-1.95625
H	4.46186	2.15671	-2.67334
C	-0.05038	3.05812	0.61404
H	-0.62093	3.97712	0.7079
C	-0.37734	-1.37896	2.50872
H	-1.05377	-1.87043	3.2011
C	3.53553	-2.73049	0.0128
H	4.1142	-3.64527	-0.07236
C	1.43484	4.20647	-1.04781
H	0.94382	5.17098	-1.03223
C	1.02663	3.06327	-0.26782
C	-4.16823	-0.56291	-1.53186
C	-4.234	-1.81604	-2.09536
C	-2.02704	-1.62613	-2.03909
S	-2.4922	-0.09865	-1.34078
H	-0.97599	-1.86189	-2.15345
N	-3.01208	-2.40133	-2.38018
C	-5.27838	0.33713	-1.0617
C	-5.42939	0.27704	0.46189
H	-6.22264	0.03824	-1.52743
H	-5.09451	1.37529	-1.36154
H	-5.69314	-0.7278	0.79641

H	-4.51629	0.59415	0.96923
Cl	-6.75496	1.38329	1.04351
C	-5.47585	-2.59488	-2.42753
H	-5.51476	-3.52516	-1.84797
H	-6.38878	-2.02884	-2.22339
H	-5.47559	-2.87761	-3.48647

^{2}TS-S_D

Fe	1.12209	-0.28145	-0.41318
O	0.23722	0.23028	0.98912
S	2.6469	-1.159	-2.04353
H	2.30855	-0.32972	-3.05729
N	0.37958	-2.15051	-0.17615
C	0.00586	-4.30885	0.55596
C	-0.96272	-4.02227	-0.35478
H	0.15976	-5.22406	1.11328
H	-1.77119	-4.65196	-0.70367
N	-0.25788	0.12451	-1.8039
C	-1.26662	-0.71578	-2.21899
C	-2.06575	-0.07431	-3.23474
C	-1.52104	1.15651	-3.44531
H	-2.92255	-0.52545	-3.71847
H	-1.83791	1.92419	-4.13982
N	1.94322	1.52876	-0.74126
C	1.53143	2.49631	-1.62448
C	3.04314	2.04384	-0.1009
C	2.39333	3.65011	-1.54136
C	3.32954	3.37019	-0.59362
H	2.28321	4.54677	-2.13791
H	4.14859	3.98998	-0.25139
N	2.5776	-0.72936	0.92999
C	4.38222	-0.53821	2.35879
H	5.23328	-0.08548	2.85136
C	3.57036	0.11185	1.35332
C	0.83655	-3.13093	0.66218
C	-0.71711	-2.67103	-0.806
C	-0.39276	1.27068	-2.55549
C	3.78793	1.3984	0.87854
H	4.62695	1.94517	1.29859
C	1.93734	-3.01974	1.50334
H	2.18556	-3.88153	2.11552
C	-1.48967	-2.00479	-1.75043
H	-2.33556	-2.5414	-2.1691
C	0.43865	2.38019	-2.47405
H	0.21988	3.2189	-3.12807
C	3.867	-1.78421	2.5304
H	4.20459	-2.56976	3.19432

C	2.73784	-1.89284	1.63347
C	-2.68248	0.90138	1.71595
C	-2.7558	1.39524	2.99502
C	-0.95196	2.52162	2.36225
S	-1.31112	1.61852	0.89597
H	-0.09588	3.18543	2.39449
N	-1.76615	2.31532	3.34288
C	-3.54802	-0.10963	1.01676
C	-4.39867	0.52466	-0.08852
H	-4.20798	-0.58593	1.74791
H	-2.92871	-0.90305	0.58256
H	-5.06026	1.29783	0.30612
H	-3.78149	0.94622	-0.88401
Cl	-5.46679	-0.71726	-0.88188
C	-3.77248	1.05388	4.04309
H	-4.3238	1.95161	4.34732
H	-4.49244	0.30802	3.69838
H	-3.27305	0.66627	4.93881

^{4}TS- S_D

Fe	-1.11191	0.49525	-0.26153
O	0.09879	-0.47246	0.6559
S	-2.7548	1.60972	-1.59205
H	-1.95362	2.02672	-2.59713
N	-0.63501	2.10394	0.79787
C	-0.60591	3.75936	2.40559
C	0.41296	4.02131	1.54391
H	-0.90597	4.31409	3.28543
H	1.12327	4.83797	1.56617
N	0.29344	0.96878	-1.65759
C	1.19138	1.99907	-1.57642
C	2.08794	1.96718	-2.70517
C	1.71922	0.89923	-3.46893
H	2.89123	2.67242	-2.87458
H	2.1575	0.55098	-4.39564
N	-1.58435	-1.17545	-1.37985
C	-1.03609	-1.55893	-2.57679
C	-2.54998	-2.09638	-1.08492
C	-1.66659	-2.77238	-3.04319
C	-2.60284	-3.10951	-2.11427
H	-1.4154	-3.28256	-3.96446
H	-3.28346	-3.95149	-2.11661
N	-2.5893	0.07339	0.99901
C	-4.32536	-0.99134	2.08246
H	-5.07655	-1.74348	2.28729
C	-3.41184	-1.03217	0.96828
C	-1.2566	2.56083	1.93224

C	0.38384	2.99053	0.53309
C	0.60502	0.27228	-2.80178
C	-3.39224	-2.04372	0.02042
H	-4.11592	-2.84467	0.1359
C	-2.35028	1.9659	2.54185
H	-2.74606	2.43537	3.4367
C	1.24062	2.94336	-0.55451
H	2.00431	3.71154	-0.62236
C	-0.01934	-0.88871	-3.2439
H	0.33007	-1.31502	-4.17928
C	-4.04936	0.14314	2.78271
H	-4.52449	0.51285	3.68233
C	-2.95839	0.79709	2.10576
C	2.59126	-1.58547	1.25728
C	2.65907	-2.59005	2.19111
C	0.89476	-3.35806	1.08175
S	1.24023	-1.88243	0.17735
H	0.06425	-3.99024	0.79025
N	1.69061	-3.58544	2.07874
C	3.41294	-0.33698	1.10653
C	4.30272	-0.37116	-0.14003
H	4.04305	-0.21226	1.99222
H	2.75303	0.53687	1.05607
H	4.98462	-1.22323	-0.1253
H	3.71419	-0.39295	-1.05919
Cl	5.3414	1.12073	-0.24124
C	3.65119	-2.72072	3.30838
H	4.23229	-3.64416	3.19813
H	4.34697	-1.87929	3.34665
H	3.12884	-2.78413	4.27018

$^2P\text{-}S_D$

Fe	1.0944	0.24355	0.49705
O	-0.13992	0.08235	-1.36616
S	2.42472	0.54834	2.27855
H	3.19422	1.53531	1.7657
N	0.9598	2.21135	0.12066
C	1.35412	4.35388	-0.65568
C	0.31849	4.43027	0.22291
H	1.81948	5.15051	-1.22222
H	-0.24708	5.30219	0.52627
N	-0.56156	0.31859	1.64443
C	-1.22078	1.46104	2.0283
C	-2.29288	1.13742	2.94007
C	-2.26737	-0.21322	3.11273
H	-2.96348	1.86232	3.38414
H	-2.90903	-0.8267	3.73275

N	1.13423	-1.75728	0.76105
C	0.32037	-2.51992	1.56855
C	2.11419	-2.60914	0.30249
C	0.77794	-3.88608	1.59184
C	1.89228	-3.94153	0.80953
H	0.3027	-4.686	2.1452
H	2.52032	-4.79646	0.5922
N	2.64956	0.13513	-0.7726
C	4.45529	-0.66301	-1.97455
H	5.17917	-1.3741	-2.35238
C	3.39056	-0.98497	-1.05267
C	1.75154	2.96659	-0.70866
C	0.07788	3.08785	0.70068
C	-1.17409	-0.71309	2.31366
C	3.15441	-2.25767	-0.54808
H	3.84211	-3.0446	-0.84345
C	2.80309	2.47912	-1.47229
H	3.35099	3.18839	-2.0851
C	-0.92808	2.74783	1.59615
H	-1.54779	3.55362	1.9775
C	-0.77609	-2.04309	2.27404
H	-1.33837	-2.75499	2.8705
C	4.34752	0.66521	-2.24944
H	4.96489	1.27298	-2.89883
C	3.2218	1.15568	-1.49024
C	-2.68522	-1.11307	-1.60259
C	-2.971	-2.38773	-1.24435
C	-0.76086	-2.71956	-1.44657
S	-0.95308	-1.01788	-2.06523
H	0.20477	-3.21146	-1.48788
N	-1.8697	-3.29086	-1.18256
C	-3.59049	0.06752	-1.81309
C	-3.39722	1.13706	-0.73255
H	-4.63287	-0.26647	-1.81198
H	-3.40724	0.51709	-2.79661
H	-3.61498	0.74736	0.26247
H	-2.38728	1.54513	-0.74014
Cl	-4.53502	2.52646	-1.0131
C	-4.30907	-2.97497	-0.92081
H	-4.26189	-3.47281	0.05479
H	-5.09897	-2.2215	-0.89311
H	-4.5798	-3.74095	-1.65747
^4P-S_D			
Fe	1.544	0.13507	-0.10615
O	-1.06927	0.03346	0.37755
S	3.96367	0.29394	-0.39161

H	3.92733	0.55897	-1.7176
N	1.08739	-0.04154	-2.06003
C	0.82216	-0.89515	-4.19055
C	0.68331	0.45815	-4.27845
H	0.75952	-1.63183	-4.98145
H	0.4854	1.05937	-5.15682
N	1.19827	2.11906	-0.21828
C	0.93284	2.85086	-1.34908
C	0.86941	4.25739	-1.03133
C	1.11007	4.36893	0.30287
H	0.66864	5.04241	-1.74925
H	1.1471	5.26449	0.90987
N	1.69695	0.28269	1.89067
C	1.75932	1.44222	2.62593
C	1.8732	-0.74406	2.7877
C	1.99116	1.139	4.01498
C	2.05917	-0.21759	4.11586
H	2.08085	1.87921	4.7998
H	2.21785	-0.82103	5.00058
N	1.4791	-1.88607	0.06358
C	1.70189	-4.02882	0.89841
H	1.84387	-4.81817	1.6258
C	1.68083	-2.62151	1.2083
C	1.06737	-1.20039	-2.80562
C	0.84887	0.98271	-2.94837
C	1.31595	3.03062	0.8018
C	1.86297	-2.09699	2.48017
H	2.01723	-2.79753	3.29482
C	1.22092	-2.48554	-2.30409
H	1.18249	-3.308	-3.01145
C	0.77101	2.33083	-2.62423
H	0.57425	3.02956	-3.43123
C	1.59024	2.72579	2.12594
H	1.66276	3.55084	2.82738
C	1.5331	-4.13846	-0.4507
H	1.50607	-5.03595	-1.05576
C	1.40405	-2.79811	-0.96407
C	-3.67781	-0.83871	-0.03559
C	-4.17649	-2.02527	0.3827
C	-2.02376	-2.66143	0.4315
S	-1.91683	-1.01255	-0.33967
H	-1.13846	-3.28552	0.51719
N	-3.22145	-3.06113	0.61781
C	-4.35829	0.46702	-0.32998
C	-4.07199	1.49409	0.77467
H	-5.43879	0.31568	-0.41861

H	-4.01577	0.87256	-1.28926
H	-4.4561	1.15589	1.73864
H	-3.00442	1.69735	0.86292
Cl	-4.89525	3.07023	0.40724
C	-5.60671	-2.39207	0.62833
H	-5.71611	-2.79336	1.64289
H	-6.27971	-1.53955	0.5121
H	-5.92235	-3.18305	-0.06261

^4RC_E

Fe	1.6498	0.11553	0.18686
O	0.69249	-0.34026	-1.04962
S	2.93432	0.76374	2.30367
H	2.67779	2.09145	2.2815
N	0.14002	0.73483	1.37752
C	-1.5782	1.99133	2.28636
C	-1.67305	0.74075	2.8145
H	-2.20248	2.85427	2.48001
H	-2.38909	0.36587	3.53461
N	1.60481	-1.68377	1.10031
C	0.66426	-2.13712	1.98836
C	0.9175	-3.51625	2.32941
C	2.02709	-3.89258	1.6388
H	0.31783	-4.10087	3.01506
H	2.52859	-4.85178	1.63677
N	3.34212	-0.41752	-0.76951
C	3.94432	-1.64472	-0.75534
C	4.06368	0.34518	-1.64781
C	5.07881	-1.66107	-1.64738
C	5.15223	-0.42172	-2.20458
H	5.72274	-2.51554	-1.81118
H	5.86945	-0.04428	-2.92203
N	1.85442	1.99972	-0.50712
C	2.52225	3.81788	-1.76803
H	3.11122	4.39673	-2.46779
C	2.77307	2.4388	-1.4265
C	-0.45499	1.97852	1.38163
C	-0.60605	-0.03984	2.23809
C	2.44548	-2.74574	0.86947
C	3.80407	1.67499	-1.95625
H	4.46186	2.15671	-2.67334
C	-0.05038	3.05812	0.61404
H	-0.62093	3.97712	0.7079
C	-0.37734	-1.37896	2.50872
H	-1.05377	-1.87043	3.2011
C	3.53553	-2.73049	0.0128
H	4.1142	-3.64527	-0.07236

C	1.43484	4.20647	-1.04781
H	0.94382	5.17098	-1.03223
C	1.02663	3.06327	-0.26782
C	-3.76395	-1.07701	-1.52553
C	-2.57816	-0.40932	-1.7262
C	-1.72648	-2.33985	-1.04976
S	-3.42936	-2.70163	-0.96893
H	-1.00618	-3.1024	-0.77949
N	-1.43451	-1.13814	-1.4475
C	-5.17646	-0.61629	-1.7624
C	-5.72988	-1.18549	-3.07293
H	-5.20953	0.47689	-1.8043
H	-5.83094	-0.91938	-0.937
H	-5.15175	-0.84087	-3.93211
H	-5.74064	-2.27705	-3.06436
Cl	-7.44922	-0.65361	-3.35609
C	-2.40571	1.00467	-2.20579
H	-1.86932	1.0253	-3.16219
H	-3.36189	1.51739	-2.34127
H	-1.80572	1.57847	-1.49021

$^{2}RC_{E}$

Fe	1.62983	0.08139	0.21584
O	0.66639	-0.35827	-1.01941
S	3.31904	1.02252	1.90904
H	2.54016	1.99793	2.42952
N	0.11336	0.78444	1.34679
C	-1.58448	2.11408	2.17611
C	-1.72018	0.8863	2.74987
H	-2.18837	2.99997	2.32562
H	-2.45713	0.55566	3.47063
N	1.51718	-1.68669	1.16809
C	0.56282	-2.07567	2.07032
C	0.76857	-3.44935	2.46081
C	1.86467	-3.88598	1.78278
H	0.14916	-3.99002	3.16477
H	2.3343	-4.86074	1.81241
N	3.32287	-0.52506	-0.70208
C	3.88693	-1.77602	-0.64549
C	4.06626	0.18038	-1.61233
C	5.02159	-1.85528	-1.53345
C	5.12942	-0.64189	-2.13831
H	5.64091	-2.73325	-1.66476
H	5.85754	-0.31355	-2.8688
N	1.93244	1.94769	-0.50849
C	2.67319	3.70925	-1.81179
H	3.28547	4.24744	-2.52389

C	2.86666	2.3275	-1.44583
C	-0.43963	2.03634	1.3014
C	-0.65926	0.06397	2.22149
C	2.32089	-2.77735	0.97964
C	3.84822	1.50434	-1.97304
H	4.51403	1.93469	-2.71469
C	0.03588	3.09767	0.53606
H	-0.50515	4.03693	0.59917
C	-0.45288	-1.26587	2.56284
H	-1.14132	-1.70959	3.2756
C	3.42935	-2.8229	0.13998
H	3.9761	-3.75957	0.08914
C	1.6058	4.16082	-1.10039
H	1.15783	5.1462	-1.1082
C	1.1386	3.05482	-0.30091
C	-3.53605	-0.126	-2.66071
C	-2.17176	-0.00403	-2.78758
C	-2.19143	-1.68513	-1.34418
S	-3.9025	-1.42381	-1.54607
H	-1.84682	-2.47072	-0.68276
N	-1.42573	-0.89199	-2.03149
C	-4.63554	0.63269	-3.35296
C	-5.24033	-0.19108	-4.49455
H	-4.24305	1.57105	-3.75707
H	-5.43004	0.90192	-2.6474
H	-4.49659	-0.41492	-5.2613
H	-5.67129	-1.12579	-4.13092
Cl	-6.58799	0.71076	-5.32516
C	-1.42709	0.97931	-3.64644
H	-0.83408	0.45654	-4.40662
H	-2.09719	1.67571	-4.15783
H	-0.72541	1.561	-3.0377
^{2}TS-N_E			
Fe	1.50807	0.09169	0.27794
O	0.33278	0.08459	-0.94806
S	3.47255	0.3243	1.5552
H	2.93214	0.00222	2.75263
N	2.68216	0.81845	-1.22102
C	4.056	0.96422	-3.06412
C	3.71207	2.23427	-2.71795
H	4.69165	0.63404	-3.8759
H	4.00577	3.16503	-3.18639
N	1.00876	1.98914	0.79433
C	1.41709	3.14043	0.1737
C	0.83043	4.28815	0.82771
C	0.06777	3.81223	1.84888

H	0.99807	5.31621	0.53234
H	-0.52032	4.36687	2.56922
N	0.47172	-0.60708	1.81457
C	-0.27857	0.12624	2.70966
C	0.33954	-1.9247	2.19631
C	-0.89722	-0.75194	3.66921
C	-0.51382	-2.01986	3.35303
H	-1.53484	-0.42279	4.48003
H	-0.77301	-2.94651	3.84952
N	2.08232	-1.79541	-0.20073
C	2.34147	-4.08806	-0.20741
H	2.22504	-5.11617	0.11166
C	1.73453	-2.94923	0.44414
C	3.40489	0.08394	-2.12158
C	2.84793	2.13309	-1.56473
C	0.19023	2.37226	1.81932
C	0.91735	-3.01851	1.56596
H	0.724	-3.99917	1.98998
C	3.51179	-1.30067	-2.13531
H	4.13398	-1.74407	-2.90655
C	2.26908	3.21728	-0.91867
H	2.50106	4.20646	-1.30117
C	-0.42272	1.50582	2.71517
H	-1.04511	1.9399	3.49161
C	3.0637	-3.59882	-1.25114
H	3.66432	-4.14174	-1.96995
C	2.90043	-2.16262	-1.2365
C	-2.56078	0.1887	-1.01205
C	-3.71395	-0.52175	-1.24315
C	-1.74169	-1.88709	-0.70172
H	-1.00344	-2.65127	-0.49353
C	-2.36339	1.67331	-1.06139
H	-2.16285	2.06855	-0.05934
H	-3.24136	2.18216	-1.46765
C	-5.09396	-0.01145	-1.55695
H	-5.01733	0.94307	-2.08756
H	-5.61971	-0.70118	-2.22592
N	-1.48387	-0.61608	-0.70216
S	-3.39796	-2.23808	-1.06814
C	-5.92337	0.18645	-0.28251
H	-6.05812	-0.75181	0.25909
H	-5.46154	0.91783	0.38299
Cl	-7.58295	0.80655	-0.67563
H	-1.49033	1.90775	-1.67663

^{4}TS- N_E

Fe	1.4667	0.14627	0.28221

O	0.35343	-0.00116	-1.1158
S	2.78625	0.23874	2.39408
H	3.49415	-0.89684	2.19864
N	2.31205	1.74831	-0.52461
C	3.70625	3.13322	-1.73791
C	2.79375	3.92797	-1.11768
H	4.52109	3.42215	-2.38957
H	2.70421	5.00643	-1.15242
N	0.16912	1.32632	1.30695
C	0.07621	2.68835	1.23102
C	-1.00726	3.16016	2.06055
C	-1.56977	2.05898	2.63309
H	-1.28516	4.19965	2.1817
H	-2.40323	2.01006	3.32273
N	0.61522	-1.51394	1.1728
C	-0.44305	-1.5255	2.04087
C	0.98774	-2.81677	0.9986
C	-0.75594	-2.88446	2.42297
C	0.13248	-3.68799	1.77471
H	-1.54651	-3.16753	3.10662
H	0.22287	-4.76632	1.81785
N	2.84185	-1.04067	-0.57135
C	3.99954	-2.89146	-1.32216
H	4.26665	-3.93384	-1.44277
C	2.90194	-2.41447	-0.51496
C	3.40367	1.77321	-1.35783
C	1.92996	3.05855	-0.35323
C	-0.83098	0.91475	2.15367
C	2.04777	-3.24263	0.20175
H	2.23688	-4.31093	0.15145
C	4.12997	0.66633	-1.76843
H	4.97235	0.83678	-2.43156
C	0.89519	3.50356	0.45413
H	0.71622	4.57378	0.49154
C	-1.12191	-0.40066	2.49502
H	-1.94492	-0.56191	3.18507
C	4.59279	-1.79558	-1.87019
H	5.44612	-1.75182	-2.53505
C	3.85666	-0.64608	-1.40219
C	-2.32842	0.0892	-1.64713
C	-3.50934	-0.60396	-1.55518
C	-1.48515	-1.98623	-1.33845
H	-0.72686	-2.74506	-1.2012
C	-2.12577	1.5579	-1.85418
H	-1.67979	2.00908	-0.96264
H	-3.07031	2.06226	-2.07376

C	-4.91777	-0.07592	-1.5925
H	-4.95389	0.82349	-2.21552
H	-5.59494	-0.80368	-2.05214
N	-1.2207	-0.7282	-1.53268
S	-3.18486	-2.30825	-1.29433
C	-5.42184	0.26633	-0.1849
H	-5.44812	-0.61583	0.45769
H	-4.80048	1.03033	0.28556
Cl	-7.11322	0.92157	-0.24252
H	-1.42891	1.72771	-2.68058

^{2}P-N_E

Fe	1.39975	0.1112	0.4092
O	0.24996	0.00454	-1.38721
S	2.78368	0.30547	2.18102
H	1.9827	-0.25349	3.11698
N	1.86006	1.98057	-0.18291
C	2.89618	3.81216	-1.13922
C	1.89323	4.285	-0.35225
H	3.60039	4.36918	-1.74429
H	1.59967	5.31245	-0.17686
N	-0.18384	0.79662	1.46138
C	-0.49972	2.11777	1.66282
C	-1.64429	2.22853	2.5368
C	-2.00884	0.95917	2.8717
H	-2.0916	3.16327	2.85139
H	-2.81314	0.63797	3.522
N	0.87206	-1.76709	0.9286
C	-0.15712	-2.16324	1.75069
C	1.55002	-2.91311	0.58792
C	-0.13824	-3.59543	1.91754
C	0.92096	-4.06109	1.19655
H	-0.84325	-4.15658	2.51816
H	1.26211	-5.08277	1.08437
N	2.90956	-0.5842	-0.72812
C	4.43633	-2.00603	-1.72128
H	4.92834	-2.93591	-1.97763
C	3.28931	-1.89496	-0.84673
C	2.87218	2.3716	-1.02004
C	1.25192	3.13237	0.24198
C	-1.08348	0.07281	2.2069
C	2.66538	-2.97783	-0.24067
H	3.08776	-3.9611	-0.42587
C	3.76798	1.51674	-1.64779
H	4.52514	1.96181	-2.28607
C	0.16214	3.20432	1.1008
H	-0.20673	4.19415	1.35324

C	-1.08353	-1.31051	2.33994
H	-1.8459	-1.75565	2.97232
C	4.74131	-0.74483	-2.12754
H	5.53676	-0.42074	-2.78671
C	3.78283	0.13589	-1.49834
C	-2.09798	0.23457	-1.58533
C	-3.22676	-0.52882	-1.61591
C	-1.16156	-1.85477	-1.36865
H	-0.36077	-2.56885	-1.26063
C	-1.93409	1.70909	-1.73209
H	-2.87923	2.17552	-2.02063
H	-1.17716	1.92372	-2.49295
C	-4.65786	-0.07322	-1.68336
H	-4.72049	0.85449	-2.26111
H	-5.27563	-0.81208	-2.20499
N	-0.93514	-0.5476	-1.42944
S	-2.82952	-2.22908	-1.46154
C	-5.22776	0.16626	-0.2787
H	-5.23897	-0.75283	0.31027
H	-4.65635	0.92405	0.26037
Cl	-6.94111	0.75243	-0.36983
H	-1.58453	2.15962	-0.79855
$^4P\text{-}N_E$			
Fe	1.43676	0.13381	0.39721
O	0.14062	0.08102	-1.37064
S	2.95951	0.40787	2.13944
H	2.42437	-0.49774	2.98961
N	0.08192	1.53881	1.21555
C	-0.86506	3.52874	1.86105
C	-1.53008	2.53127	2.51597
H	-1.035	4.59654	1.92617
H	-2.34685	2.62696	3.22107
N	0.43562	-1.3615	1.35952
C	-0.60254	-1.2014	2.25046
C	-0.9559	-2.49224	2.79921
C	-0.11814	-3.41256	2.24019
H	-1.74331	-2.66032	3.52359
H	-0.08681	-4.48075	2.41648
N	2.62883	-1.31659	-0.56905
C	2.62021	-2.65955	-0.34344
C	3.64625	-1.04809	-1.43593
C	3.66668	-3.2886	-1.12905
C	4.302	-2.28929	-1.80615
H	3.88611	-4.34914	-1.14433
H	5.14233	-2.37322	-2.48424
N	2.38007	1.6097	-0.61134

C	3.86226	2.75441	-1.93848
H	4.67622	2.92488	-2.632
C	3.43573	1.45105	-1.46913
C	0.15768	2.89161	1.05316
C	-0.91313	1.2826	2.11113
C	0.76005	-2.6997	1.33854
C	4.01136	0.23456	-1.8555
H	4.84642	0.30081	-2.54758
C	1.09916	3.54011	0.24567
H	1.04279	4.62473	0.20812
C	-1.2344	0.00295	2.57999
H	-2.04186	-0.06437	3.30433
C	1.74585	-3.29951	0.54393
H	1.85348	-4.37605	0.64704
C	3.05183	3.67738	-1.34909
H	3.07032	4.75402	-1.4639
C	2.11717	2.95125	-0.51252
C	-2.20959	0.20969	-1.56991
C	-3.30949	-0.59489	-1.56497
C	-1.1974	-1.82931	-1.24624
H	-0.37184	-2.50759	-1.09661
C	-2.09749	1.68378	-1.76476
H	-3.07042	2.11668	-2.00966
H	-1.39125	1.90185	-2.5723
C	-4.75648	-0.19967	-1.67397
H	-4.84999	0.67701	-2.32304
H	-5.33947	-1.00054	-2.14116
N	-1.01729	-0.52058	-1.38177
S	-2.85158	-2.26904	-1.31846
C	-5.35197	0.12398	-0.29768
H	-5.31909	-0.74134	0.36699
H	-4.82924	0.95619	0.17697
Cl	-7.09342	0.60699	-0.44626
H	-1.70773	2.16414	-0.86238
^2RC_F			
Fe	-1.84948	0.00954	-0.05458
O	-0.63845	-0.52971	0.88782
S	-3.80125	1.14848	-1.28977
H	-4.81047	0.44633	-0.72633
N	-2.80715	0.94873	1.46297
C	-4.06285	1.34199	3.36644
C	-3.35211	2.47377	3.11468
H	-4.76228	1.14917	4.16983
H	-3.34739	3.40424	3.66778
N	-0.91444	1.74187	-0.50607
C	-0.92043	2.90026	0.22634

C	-0.0212	3.86744	-0.35584
C	0.53493	3.27691	-1.44763
H	0.14728	4.86334	0.03338
H	1.25858	3.68345	-2.14192
N	-1.12793	-0.8169	-1.74012
C	-0.21353	-0.26858	-2.59714
C	-1.35943	-2.08603	-2.1998
C	0.14334	-1.21358	-3.6272
C	-0.57267	-2.34497	-3.38129
H	0.84913	-1.01771	-4.42381
H	-0.58088	-3.27426	-3.93638
N	-3.00666	-1.61619	0.24407
C	-3.87263	-3.75488	0.11239
H	-4.03957	-4.75214	-0.27408
C	-2.98807	-2.78131	-0.47957
C	-3.70999	0.39044	2.34125
C	-2.564	2.2198	1.93358
C	-0.02415	1.94959	-1.53083
C	-2.22799	-3.00265	-1.61989
H	-2.31422	-3.97551	-2.09449
C	-4.20035	-0.90264	2.26352
H	-4.90385	-1.21511	3.02933
C	-1.67969	3.1238	1.36869
H	-1.57904	4.0908	1.85196
C	0.30589	1.01872	-2.50402
H	1.05033	1.30711	-3.23754
C	-4.42142	-3.16633	1.21016
H	-5.13364	-3.57879	1.9133
C	-3.87249	-1.83393	1.28215
C	4.17636	0.00756	1.39398
C	3.85593	-1.09933	0.6426
C	1.92923	-0.89483	1.72292
S	2.81053	0.44826	2.39624
H	0.91088	-1.10043	2.03361
N	2.57914	-1.59878	0.846
C	5.44699	0.81419	1.40527
C	5.3455	2.02657	0.47307
H	6.28326	0.18357	1.08843
H	5.68127	1.15951	2.41812
H	5.18571	1.72069	-0.56228
H	4.53993	2.69905	0.77384
Cl	6.87636	3.00755	0.49804
C	4.75373	-1.79674	-0.34054
H	4.19481	-2.03742	-1.25081
H	5.61153	-1.178	-0.6183
H	5.14058	-2.74051	0.06327

$4RC_F$

Fe	-1.8434	0.01256	-0.05169
O	-0.6432	-0.33049	0.99423
S	-3.72963	0.82392	-1.583
H	-4.77094	0.36737	-0.85099
N	-2.72937	1.392	1.12769
C	-3.95486	2.38521	2.82097
C	-3.19123	3.35822	2.2558
H	-4.65859	2.46971	3.63915
H	-3.138	4.4084	2.51267
N	-0.82179	1.48585	-0.9767
C	-0.76108	2.80541	-0.61172
C	0.17817	3.51546	-1.44606
C	0.68975	2.60681	-2.31944
H	0.40112	4.57127	-1.36092
H	1.4238	2.75759	-3.10007
N	-1.18262	-1.30451	-1.42809
C	-0.24955	-1.07584	-2.40082
C	-1.48604	-2.63731	-1.504
C	0.04791	-2.29539	-3.1126
C	-0.72507	-3.26775	-2.55599
H	0.75622	-2.37538	-3.92687
H	-0.78738	-4.31587	-2.81934
N	-3.07734	-1.39852	0.69944
C	-4.0533	-3.4369	1.18318
H	-4.27615	-4.49273	1.09754
C	-3.12867	-2.72095	0.33838
C	-3.65507	1.15965	2.12193
C	-2.42299	2.73241	1.2078
C	0.06393	1.34269	-2.01707
C	-2.39683	-3.2996	-0.68963
H	-2.54091	-4.36137	-0.86583
C	-4.20897	-0.07377	2.42255
H	-4.91931	-0.11379	3.24281
C	-1.49761	3.38813	0.41273
H	-1.34533	4.44747	0.5954
C	0.33479	0.15563	-2.68041
H	1.08436	0.18234	-3.46325
C	-4.55564	-2.53145	2.06659
H	-5.27798	-2.68781	2.85751
C	-3.9392	-1.26483	1.75437
C	4.27204	-0.64429	1.30368
C	3.73976	0.55001	1.73111
C	2.06944	-0.77009	2.35486
S	3.15636	-1.94357	1.66537
H	1.1188	-1.07655	2.777

N	2.48847	0.45892	2.32011
C	5.60337	-0.91302	0.65516
C	6.65348	-1.33174	1.69007
H	5.94578	-0.0119	0.13742
H	5.51632	-1.69706	-0.10494
H	6.82163	-0.54503	2.4276
H	6.36548	-2.24873	2.20756
Cl	8.25903	-1.66265	0.90338
C	4.3791	1.90449	1.60274
H	4.22435	2.47738	2.52265
H	5.45495	1.83136	1.42082

^{2}TS-O_F

Fe	1.46525	-0.05287	-0.14186
O	-0.10446	0.50052	0.21084
S	3.85897	-0.33228	-0.77831
H	4.34053	-0.62287	0.45176
N	1.45005	1.1859	-1.75156
C	1.04512	2.0417	-3.85979
C	1.52327	3.06182	-3.09816
H	0.74858	2.05729	-4.90083
H	1.70168	4.09098	-3.38244
N	2.27108	1.45251	0.9638
C	2.48398	2.75169	0.56844
C	2.96852	3.53772	1.67848
C	3.03264	2.70559	2.75239
H	3.21984	4.58927	1.6243
H	3.34735	2.93127	3.76337
N	1.67782	-1.30556	1.41259
C	2.09382	-0.98479	2.68263
C	1.43996	-2.65955	1.42764
C	2.097	-2.15886	3.5206
C	1.69682	-3.20003	2.73888
H	2.38337	-2.17032	4.56459
H	1.58365	-4.24206	3.00938
N	0.89305	-1.58549	-1.29449
C	0.25757	-3.67925	-2.03542
H	0.05896	-4.74272	-1.99967
C	0.74072	-2.8948	-0.92537
C	0.9992	0.87582	-3.00689
C	1.76855	2.5171	-1.7821
C	2.58786	1.40836	2.29985
C	1.00842	-3.40449	0.33801
H	0.85411	-4.46825	0.49089
C	0.56363	-0.38006	-3.40759
H	0.23821	-0.48646	-4.43828
C	2.24939	3.25053	-0.70419

H	2.45679	4.30316	-0.87138
C	2.49716	0.27959	3.10195
H	2.79035	0.38488	4.14236
C	0.11552	-2.82247	-3.08347
H	-0.2165	-3.03664	-4.09148
C	0.52302	-1.51977	-2.61068
C	-3.64869	0.2208	0.3234
C	-4.94234	0.89605	-0.03355
H	-5.25308	0.60018	-1.04072
H	-4.82098	1.98471	-0.04564
C	-1.43048	-0.44216	1.18335
H	-0.72802	-0.71275	1.96081
S	-2.57309	0.88893	1.51502
N	-1.93742	-1.36087	0.35881
C	-3.12212	-0.97326	-0.17026
C	-6.05426	0.52864	0.958
H	-6.24501	-0.5459	0.96465
H	-5.81164	0.85402	1.97116
Cl	-7.62304	1.33404	0.51396
C	-3.76324	-1.85548	-1.20662
H	-3.01523	-2.1615	-1.94462
H	-4.1577	-2.7699	-0.74572
H	-4.5869	-1.35879	-1.72664

^{4}TS- O_F

Fe	1.50299	0.00025	0.15817
O	-0.10894	-0.4547	-0.13224
S	3.7491	0.83814	0.49214
H	4.34025	0.1916	-0.53798
N	0.98394	1.73644	1.05772
C	0.3661	3.92705	1.43878
C	0.24534	3.26406	2.62133
H	0.16718	4.9695	1.22559
H	-0.06624	3.64963	3.58383
N	1.47087	-0.9367	1.92121
C	1.05471	-0.41724	3.12018
C	1.12962	-1.42473	4.15299
C	1.60796	-2.55351	3.56524
H	0.85663	-1.2658	5.18845
H	1.80723	-3.51769	4.01523
N	2.22413	-1.65389	-0.72358
C	2.46932	-2.86144	-0.12325
C	2.48219	-1.83461	-2.06121
C	2.90614	-3.82711	-1.10242
C	2.90805	-3.19176	-2.3058
H	3.16642	-4.85423	-0.88065
H	3.1736	-3.58762	-3.27783

N	1.66926	1.00128	-1.61617
C	1.99448	1.48871	-3.84979
H	2.23431	1.32507	-4.89276
C	2.02159	0.4674	-2.83018
C	0.82015	2.96347	0.46579
C	0.63322	1.896	2.37026
C	1.81726	-2.23892	2.17097
C	2.38008	-0.85863	-3.04401
H	2.62825	-1.14961	-4.06029
C	1.03071	3.24986	-0.87535
H	0.8598	4.27198	-1.19859
C	0.65615	0.89419	3.33411
H	0.35576	1.16535	4.34166
C	2.29584	-3.1363	1.22735
H	2.53217	-4.14012	1.56679
C	1.6303	2.64765	-3.23456
H	1.50609	3.63139	-3.66889
C	1.42782	2.33514	-1.84078
C	-3.65475	-0.22388	-0.2581
C	-4.93987	-0.8408	0.21494
H	-5.24243	-0.39007	1.16557
H	-4.81069	-1.9129	0.39897
C	-1.4509	0.31291	-1.23627
H	-0.75547	0.45834	-2.05205
S	-2.58253	-1.06722	-1.33877
N	-1.959	1.34877	-0.56478
C	-3.13479	1.04081	0.02941
C	-6.06381	-0.64138	-0.81068
H	-6.26372	0.41755	-0.98328
H	-5.82696	-1.11928	-1.76287
Cl	-7.62145	-1.37856	-0.23067
C	-3.77981	2.07298	0.91298
H	-4.17114	2.90378	0.31238
H	-4.60605	1.66298	1.49978
H	-3.03471	2.49109	1.59713
^{2}INT-O_F			
Fe	-1.55143	-0.15797	0.18957
O	0.03284	0.2955	-0.69588
S	-3.59355	-0.84457	1.15294
H	-3.38565	-0.39888	2.4125
N	-1.59948	-1.89915	-0.82593
C	-1.9387	-3.51173	-2.45051
C	-1.26302	-4.10611	-1.43163
H	-2.27409	-3.94674	-3.3831
H	-0.92808	-5.13216	-1.35128
N	-0.62812	-1.06226	1.74531

C	-0.229	-2.37187	1.80201
C	0.39085	-2.65643	3.07422
C	0.35966	-1.50131	3.79294
H	0.79107	-3.61951	3.36332
H	0.72964	-1.31896	4.79361
N	-1.57163	1.56341	1.25005
C	-1.08708	1.78627	2.51038
C	-2.07404	2.76305	0.82601
C	-1.28657	3.16112	2.89549
C	-1.90112	3.77099	1.8432
H	-0.98937	3.58874	3.84433
H	-2.21288	4.8033	1.75037
N	-2.53637	0.72755	-1.33585
C	-3.54274	2.3254	-2.66889
H	-3.91879	3.29469	-2.96978
C	-2.8949	2.04555	-1.40745
C	-2.13632	-2.13335	-2.06535
C	-1.05723	-3.09112	-0.4235
C	-0.27231	-0.51157	2.95563
C	-2.68371	2.98807	-0.40731
H	-3.03119	3.99827	-0.6036
C	-2.76027	-1.1738	-2.85224
H	-3.13278	-1.49257	-3.82131
C	-0.40731	-3.30693	0.78585
H	-0.02282	-4.30637	0.96631
C	-0.48159	0.81534	3.31007
H	-0.14082	1.12578	4.29351
C	-3.57065	1.15239	-3.35753
H	-3.97403	0.95581	-4.34247
C	-2.93699	0.16706	-2.51162
C	3.63815	0.39968	-0.89107
C	5.05887	0.04598	-1.23501
H	5.43515	0.6999	-2.02873
H	5.11895	-0.9831	-1.60842
C	1.13465	0.77973	-0.13381
H	1.05591	1.02737	0.93231
S	2.61409	-0.68737	-0.02971
N	1.75476	1.82987	-0.85591
C	3.00023	1.64539	-1.2045
C	5.97148	0.17716	-0.00936
H	5.99317	1.20082	0.36923
H	5.65825	-0.4945	0.79098
Cl	7.69621	-0.25939	-0.41059
H	3.0493	3.60302	-2.05778
H	4.61922	3.0764	-1.40987
H	4.03579	2.41976	-2.94245

^{2}TS-epo$_{F}$

Fe	-1.55143	-0.15797	0.18957
O	0.03284	0.2955	-0.69588
S	-3.59355	-0.84457	1.15294
H	-3.38565	-0.39888	2.4125
N	-1.59948	-1.89915	-0.82593
C	-1.9387	-3.51173	-2.45051
C	-1.26302	-4.10611	-1.43163
H	-2.27409	-3.94674	-3.3831
H	-0.92808	-5.13216	-1.35128
N	-0.62812	-1.06226	1.74531
C	-0.229	-2.37187	1.80201
C	0.39085	-2.65643	3.07422
C	0.35966	-1.50131	3.79294
H	0.79107	-3.61951	3.36332
H	0.72964	-1.31896	4.79361
C	-1.08708	1.78627	2.51038
C	-2.07404	2.76305	0.82601
C	-1.28657	3.16112	2.89549
C	-1.90112	3.77099	1.8432
H	-0.98937	3.58874	3.84433
H	-2.21288	4.8033	1.75037
N	-2.53637	0.72755	-1.33585
C	-3.54274	2.3254	-2.66889
H	-3.91879	3.29469	-2.96978
C	-2.8949	2.04555	-1.40745
C	-2.13632	-2.13335	-2.06535
C	-1.05723	-3.09112	-0.4235
C	-0.27231	-0.51157	2.95563
C	-2.68371	2.98807	-0.40731
H	-3.03119	3.99827	-0.6036
C	-2.76027	-1.1738	-2.85224
H	-3.13278	-1.49257	-3.82131
C	-0.40731	-3.30693	0.78585
H	-0.02282	-4.30637	0.96631
C	-0.48159	0.81534	3.31007
H	-0.14082	1.12578	4.29351
C	-3.57065	1.15239	-3.35753
H	-3.97403	0.95581	-4.34247
C	-2.93699	0.16706	-2.51162
C	3.63815	0.39968	-0.89107
C	5.05887	0.04598	-1.23501
H	5.43515	0.6999	-2.02873
H	5.11895	-0.9831	-1.60842
C	1.13465	0.77973	-0.13381
H	1.05591	1.02737	0.93231

S	2.61409	-0.68737	-0.02971
N	1.75476	1.82987	-0.85591
C	3.00023	1.64539	-1.2045
C	5.97148	0.17716	-0.00936
H	5.99317	1.20082	0.36923
H	5.65825	-0.4945	0.79098
Cl	7.69621	-0.25939	-0.41059
C	3.71966	2.74886	-1.9451
H	3.0493	3.60302	-2.05778
H	4.61922	3.0764	-1.40987
H	4.03579	2.41976	-2.94245

^{4}TS-epo$_{F}$

S	2.89215	0.94054	2.04272
H	4.006	1.05131	1.28492
N	-0.00215	0.30014	1.77999
C	-1.72158	1.02776	3.13007
C	-1.46457	-0.26712	3.46698
H	-2.46237	1.69933	3.54478
H	-1.94842	-0.87727	4.21912
N	1.75358	-1.73006	0.8004
C	1.13303	-2.4632	1.78394
C	1.71123	-3.78218	1.85041
C	2.70285	-3.82818	0.91819
H	1.39582	-4.55652	2.53809
H	3.36911	-4.64805	0.68183
N	2.92605	0.1655	-0.9829
C	3.72627	-0.90948	-1.28258
C	3.29543	1.17512	-1.83758
C	4.64978	-0.55624	-2.33147
C	4.38252	0.7344	-2.67535
H	5.3921	-1.22554	-2.7474
H	4.86051	1.34375	-3.43183
N	0.99936	2.11842	-0.18588
C	1.05462	4.17832	-1.21807
H	1.3764	4.95595	-1.89911
C	1.63662	2.85866	-1.14597
C	-0.80898	1.37256	2.06805
C	-0.39454	-0.71767	2.61195
C	2.73551	-2.53725	0.27713
C	2.70573	2.42909	-1.91913
H	3.11348	3.12672	-2.64377
C	-0.79409	2.59991	1.4183
H	-1.49902	3.35255	1.75604
C	0.12843	-2.00429	2.62285
H	-0.27408	-2.70177	3.35047
C	3.65066	-2.16655	-0.69732

H	4.36363	-2.91571	-1.02633
C	0.07113	4.22621	-0.27866
H	-0.58395	5.05059	-0.02728
C	0.05045	2.93602	0.36972
C	-2.31616	-3.88172	-0.87721
H	-1.35796	-4.29946	-1.10577
H	-2.67192	-4.28926	0.04596
O	0.20989	-0.51887	-0.96011
C	-1.21416	-0.55073	-1.21988
C	-2.20287	-2.48642	-0.76033
C	-3.06088	-1.64187	-0.03168
S	-2.52464	0.00849	-0.18418
N	-1.17042	-1.82025	-1.43271
C	-4.26169	-2.02875	0.77977
H	-4.69462	-2.94459	0.36526
H	-5.03953	-1.26013	0.7166
C	-3.89287	-2.25387	2.25171
H	-3.16559	-3.05991	2.36269
H	-3.49443	-1.34755	2.71144
Cl	-5.35088	-2.7299	3.23133
H	-3.00491	-4.11924	-1.66087
H	-1.36297	-0.07583	-2.1671

^{2}P-epo$_{F}$

Fe	1.47798	0.01647	-0.41613
O	-0.64005	0.08645	0.41204
S	3.47069	-0.00549	-1.42355
H	4.17735	0.63627	-0.46466
N	0.53933	0.50122	-2.12839
C	-0.48646	0.40243	-4.1991
C	-0.27113	1.71648	-3.92061
H	-0.94423	-0.03608	-5.07684
H	-0.51835	2.58325	-4.52051
N	1.60057	1.96099	0.09482
C	1.28158	3.02852	-0.71207
C	1.60608	4.26852	-0.05058
C	2.13173	3.94403	1.16291
H	1.44523	5.25195	-0.47404
H	2.49428	4.60499	1.9401
N	2.23151	-0.46199	1.38843
C	2.69172	0.38774	2.36837
C	2.50679	-1.73239	1.83498
C	3.25664	-0.36534	3.46103
C	3.1462	-1.68047	3.1273
H	3.68136	0.07116	4.35625
H	3.45963	-2.54828	3.69387
N	1.13651	-1.92323	-0.81702

C	1.19681	-4.2312	-0.70589
H	1.41208	-5.21548	-0.30932
C	1.55157	-2.98994	-0.05934
C	0.02663	-0.34821	-3.07798
C	0.3666	1.76874	-2.62574
C	2.13597	2.50446	1.24147
C	2.19954	-2.9081	1.1652
H	2.47403	-3.84163	1.64705
C	0.01091	-1.73258	-2.98713
H	-0.42528	-2.28665	-3.81272
C	0.71585	2.94487	-1.9769
H	0.51741	3.87791	-2.49555
C	2.63658	1.77512	2.31261
H	3.03729	2.32949	3.15581
C	0.56315	-3.90339	-1.86503
H	0.15352	-4.56173	-2.62079
C	0.53976	-2.46158	-1.93052
C	-3.34327	-0.16099	1.54226
C	-4.83888	-0.17366	1.39156
H	-5.30672	0.42004	2.18547
H	-5.21301	-1.19653	1.49366
C	-0.94379	0.53471	1.70713
H	-0.11506	0.93092	2.28725
S	-2.53181	1.37532	1.94099
N	-1.10342	-0.88285	1.58815
C	-2.47973	-1.19028	1.3762
C	-5.26517	0.38631	0.0277
H	-4.94278	1.4204	-0.10281
H	-4.86807	-0.21586	-0.79099
Cl	-7.0717	0.37399	-0.13541
C	-2.76643	-2.61753	1.02292
H	-2.32439	-2.86363	0.04952
H	-2.31284	-3.28926	1.76082
H	-3.83873	-2.82302	0.97794
^{4}P-epo$_F$			
Fe	1.47798	0.01647	-0.41613
O	-1.98418	-0.14912	1.44915
S	3.47069	-0.00549	-1.42355
H	4.17735	0.63627	-0.46466
N	0.53933	0.50122	-2.12839
C	-0.48646	0.40243	-4.1991
C	-0.27113	1.71648	-3.92061
H	-0.94423	-0.03608	-5.07684
H	-0.51835	2.58325	-4.52051
N	1.60057	1.96099	0.09482
C	1.28158	3.02852	-0.71207

C	1.60608	4.26852	-0.05058
C	2.13173	3.94403	1.16291
H	1.44523	5.25195	-0.47404
H	2.49428	4.60499	1.9401
N	2.23151	-0.46199	1.38843
C	2.69172	0.38774	2.36837
C	2.50679	-1.73239	1.83498
C	3.25664	-0.36534	3.46103
C	3.1462	-1.68047	3.1273
H	3.68136	0.07116	4.35625
H	3.45963	-2.54828	3.69387
N	1.13651	-1.92323	-0.81702
C	1.19681	-4.2312	-0.70589
H	1.41208	-5.21548	-0.30932
C	1.55157	-2.98994	-0.05934
C	0.02663	-0.34821	-3.07798
C	0.3666	1.76874	-2.62574
C	2.13597	2.50446	1.24147
C	2.19954	-2.9081	1.1652
H	2.47403	-3.84163	1.64705
C	0.01091	-1.73258	-2.98713
H	-0.42528	-2.28665	-3.81272
C	0.71585	2.94487	-1.9769
H	0.51741	3.87791	-2.49555
C	2.63658	1.77512	2.31261
H	3.03729	2.32949	3.15581
C	0.56315	-3.90339	-1.86503
H	0.15352	-4.56173	-2.62079
C	0.53976	-2.46158	-1.93052
C	-4.66659	-0.35302	2.52655
C	-6.16221	-0.3657	2.37585
H	-6.63005	0.22801	3.16975
H	-6.53633	-1.38856	2.47795
C	-2.26711	0.34268	2.69142
H	-1.43838	0.73889	3.27153
S	-3.85513	1.18328	2.92528
N	-2.42674	-1.07488	2.57244
C	-3.80305	-1.38231	2.36049
C	-6.58849	0.19428	1.01199
H	-6.2661	1.22837	0.88148
H	-6.1914	-0.40789	0.1933
Cl	-8.39502	0.18196	0.84888
C	-4.08975	-2.80956	2.00721
H	-3.64772	-3.05566	1.03381
H	-3.63616	-3.4813	2.74511
H	-5.16205	-3.01505	1.96222

P-epo

C	-0.23522	-0.00519	-0.43594
C	-1.07476	1.03289	-0.23693
C	-2.66021	-0.78763	-0.00081
S	-1.06226	-1.57441	-0.34585
N	-2.48814	0.69424	-0.02212
C	1.21923	-0.01602	-0.70879
C	2.00978	-0.17076	0.58896
H	1.52234	0.92248	-1.23165
H	1.49168	-0.82755	-1.42345
H	1.78445	0.63478	1.31337
H	1.82333	-1.14479	1.08098
Cl	3.75771	-0.08285	0.1997
C	-0.77943	2.48323	-0.24971
H	-0.94151	2.92608	0.74851
H	0.25409	2.70169	-0.55018
H	-1.45244	3.02192	-0.93959
O	-2.65659	-0.05281	1.23326
H	-3.57354	-1.29185	-0.31123

TS-OMe1

C	0.3432	0.45819	0.62813
C	-0.32828	1.45603	0.01144
C	-2.1919	0.08906	0.46345
O	-2.96558	-1.90987	-0.00822
C	-2.50905	-2.44333	-1.21927
H	-2.5138	-3.56431	-1.24476
H	-3.10011	-2.14159	-2.12082
H	-1.44854	-2.17315	-1.46473
N	-1.74957	1.27011	-0.01876
S	-0.81043	-0.932	1.03852
H	-3.20679	-0.00724	0.78019
O	-2.58146	2.28553	-0.4531
C	1.8246	0.31518	0.79222
H	2.30113	1.29885	0.87191
H	2.07009	-0.26524	1.68844
C	2.35119	-0.41067	-0.44394
H	2.22987	0.16725	-1.35652
H	1.95293	-1.41731	-0.54346
Cl	4.28775	-0.66909	-0.30446
C	0.13867	2.7513	-0.57584
H	0.73751	3.33509	0.13231
H	0.71798	2.60488	-1.49582
H	-0.81256	3.25868	-0.80238

TS-OMe2

C	-0.06724	-1.19233	0.46681
C	-0.80981	-0.15651	1.13024

C	-2.61893	0.11596	-0.51371
O	-0.49262	1.73704	-0.52718
C	-0.73386	3.11495	-0.72681
H	-1.81801	3.36113	-0.70811
H	-0.26357	3.79344	0.02143
H	-0.38093	3.48255	-1.71969
N	-1.8654	0.43409	0.63166
S	-0.75005	-2.30927	-0.65462
C	1.44815	-1.12856	0.58222
H	1.77614	-0.72839	1.5428
H	1.89883	-2.10766	0.41198
C	1.86476	-0.1533	-0.53804
H	1.30196	0.78745	-0.50184
H	1.80129	-0.62776	-1.51463
Cl	3.7582	0.26755	-0.3487
C	-0.19828	0.59255	2.30513
H	0.44664	-0.02087	2.93911
H	0.3591	1.43348	1.87349
H	-1.01419	1.00539	2.90456
H	-2.09478	0.45463	-1.41417
O	-3.77637	-0.3156	-0.48405

P-OMe1

C	0.43729	0.20085	-0.5697
C	-0.39444	1.22587	-0.19219
C	-2.07177	-0.57459	-0.52821
S	-0.43523	-1.2679	-0.98224
N	-1.77756	0.87509	-0.22306
C	1.91191	0.18737	-0.65474
C	2.51854	-0.44218	0.5983
H	2.30249	1.2242	-0.78807
H	2.25705	-0.35839	-1.56391
H	2.21535	0.08843	1.52031
H	2.24871	-1.5104	0.70556
Cl	4.30518	-0.34209	0.47262
C	-0.0098	2.60023	0.19968
H	0.69273	2.59654	1.04656
H	0.46755	3.13832	-0.63368
H	-0.88833	3.19933	0.50711
O	-2.35066	-1.28515	0.65137
H	-2.86136	-0.66799	-1.30175
O	-2.70621	1.65536	0.04838
C	-3.69203	-1.10573	1.17699
H	-3.63864	-1.64554	2.1301
H	-3.89886	-0.04024	1.33864
H	-4.42142	-1.56073	0.50316

P-OMe2

C	-0.23522	-0.00519	-0.43594
C	-1.07476	1.03289	-0.23693
C	-2.66021	-0.78763	-0.00081
S	-1.06226	-1.57441	-0.34585
N	-2.48814	0.69424	-0.02212
C	1.21923	-0.01602	-0.70879
C	2.00978	-0.17076	0.58896
H	1.52234	0.92248	-1.23165
H	1.49168	-0.82755	-1.42345
H	1.78445	0.63478	1.31337
H	1.82333	-1.14479	1.08098
Cl	3.75771	-0.08285	0.1997
C	-0.77943	2.48323	-0.24971
H	-0.94151	2.92608	0.74851
H	0.25409	2.70169	-0.55018
H	-1.45244	3.02192	-0.93959
O	-2.65659	-0.05281	1.23326
H	-3.57354	-1.29185	-0.31123
O	-3.19971	1.67966	-0.66517
C	-4.34994	2.37265	-0.1736
H	-4.26729	2.49403	0.88627
H	-4.41292	3.33414	-0.63887
H	-5.23028	1.80832	-0.4004

TS-SMe2

C	0.42139	-1.18429	0.10069
C	-0.51413	-0.60598	1.03153
C	-2.68428	-1.10822	-0.0547
C	-2.55496	3.38648	-0.64249
H	-3.51912	3.19577	-0.15981
H	-2.12854	4.30522	-0.22722
H	-2.71103	3.50612	-1.71871
N	-1.79739	-0.47855	0.82002
S	-0.02947	-1.99373	-1.35018
C	1.90777	-0.95892	0.34872
H	2.14287	-0.85258	1.40964
H	2.48745	-1.78069	-0.07516
C	2.25717	0.33789	-0.38861
H	1.71245	1.20663	-0.02616
H	2.16071	0.22495	-1.4651
Cl	4.1355	0.75708	-0.10832
C	0.01091	0.0405	2.31195
H	0.55795	-0.68198	2.93104
H	0.6652	0.88956	2.0906
H	-0.85212	0.41176	2.86544
H	-2.98872	-0.44505	-0.87089
O	-3.19327	-2.21418	0.17291

S	-1.39341	1.91676	-0.2922	P-SMe1
C	-0.23522	-0.00519	-0.43594	
C	-1.07476	1.03289	-0.23693	
C	-2.66021	-0.78763	-0.00081	
S	-1.06226	-1.57441	-0.34585	
N	-2.48814	0.69424	-0.02212	
C	1.21923	-0.01602	-0.70879	
C	2.00978	-0.17076	0.58896	
H	1.52234	0.92248	-1.23165	
H	1.49168	-0.82755	-1.42345	
H	1.78445	0.63478	1.31337	
H	1.82333	-1.14479	1.08098	
Cl	3.75771	-0.08285	0.1997	
C	-0.77943	2.48323	-0.24971	
H	-0.94151	2.92608	0.74851	
H	0.25409	2.70169	-0.55018	
H	-1.45244	3.02193	-0.93959	
H	-3.57354	-1.29185	-0.31123	
O	-3.19971	1.67966	-0.66517	
C	-3.97738	-1.68501	2.06896	
H	-3.76259	-1.59458	3.11327	
H	-4.77389	-1.01924	1.80968	
H	-4.26824	-2.69128	1.85048	
S	-2.81124	-1.35083	1.31178	

P-SMe1

6	0	-0.71479	0.34042	0.36652
6	0	-0.71119	1.69268	0.22746
6	0	1.4669	1.21846	-0.28541
16	0	0.87247	-0.36637	0.00828
7	0	0.56308	2.18736	-0.14031
6	0	-1.88251	-0.54122	0.70389
6	0	-2.65362	-0.91797	-0.55919
1	0	-2.55665	-0.03542	1.40096
1	0	-1.53575	-1.45391	1.19711
1	0	-3.04876	-0.04185	-1.06873
1	0	-2.04204	-1.49869	-1.24572
17	0	-4.1116	-1.96657	-0.17491
6	0	-1.78917	2.70506	0.40995
1	0	-2.69463	2.24783	0.81326
1	0	-1.44259	3.49604	1.08012
1	0	-2.0281	3.1952	-0.53904
1	0	2.50582	1.3953	-0.50911
8	0	0.77077	3.45183	-0.28771
6	0	4.0171	-1.96916	1.01771
1	0	4.43224	-2.98051	0.94595
1	0	4.70913	-1.36834	1.61623

1	0	3.07707	-2.03864	1.57919
16	0	3.75362	-1.23245	-0.65194

P-SMe2

C	-0.23522	-0.00519	-0.43594
C	-1.07476	1.03289	-0.23693
C	-2.66021	-0.78763	-0.00081
S	-1.06226	-1.57441	-0.34585
N	-2.48814	0.69424	-0.02212
C	1.21923	-0.01602	-0.70879
C	2.00978	-0.17076	0.58896
H	1.52234	0.92248	-1.23165
H	1.49168	-0.82755	-1.42345
H	1.78445	0.63478	1.31337
H	1.82333	-1.14479	1.08098
Cl	3.75771	-0.08285	0.1997
C	-0.77943	2.48323	-0.24971
H	-0.94151	2.92608	0.74851
H	0.25409	2.70169	-0.55018
H	-1.45244	3.02192	-0.93959
S	-3.37301	1.91966	-0.82178
C	-4.83586	2.30471	0.11641
H	-4.63123	3.1211	0.77711
H	-5.62673	2.57588	-0.55134
H	-5.12898	1.44859	0.68742
O	-2.81124	-1.35083	1.31178
H	-1.94481	-1.51384	1.69168

TS-diol

C	-0.16378	0.06554	-0.62447
C	0.79385	0.98724	-0.40271
C	2.2022	-0.90045	-0.34424
H	1.97019	-0.92473	2.03923
O	2.82778	-1.01416	1.53536
N	2.10258	0.45033	-0.35955
S	0.58974	-1.63324	-0.73035
H	3.10384	-1.41455	-0.62549
O	3.15305	1.11242	0.37346
C	-1.64815	0.22673	-0.72686
H	-1.88269	1.27465	-0.93798
H	-2.05865	-0.37607	-1.54386
C	-2.31351	-0.18721	0.59172
H	-2.03579	0.46143	1.41957
H	-2.14748	-1.23476	0.83472
Cl	-4.20623	-0.00641	0.42258
C	0.68594	2.46689	-0.19842
H	0.75613	2.99755	-1.15525
H	-0.2481	2.74172	0.29565

H	1.54842	2.74843	0.41426
H	3.16015	0.07631	1.23701

P-diol

C	0.13736	-0.00325	-0.5139
C	-0.72392	1.02515	-0.38136
C	-2.35751	-0.81889	-0.30744
S	-0.65973	-1.57562	-0.45588
N	-2.14198	0.67	-0.33423
C	1.60578	0.01457	-0.7081
C	2.32584	-0.23104	0.61585
H	1.92982	0.98705	-1.14724
H	1.91892	-0.7453	-1.46177
H	2.04149	0.50629	1.3894
H	2.13829	-1.24723	1.01287
Cl	4.09197	-0.0745	0.33816
C	-0.41558	2.47537	-0.3376
H	-0.92478	2.96201	0.5123
H	0.6603	2.67235	-0.23656
H	-0.76632	2.98187	-1.25176
H	-3.00645	-1.13382	-1.15842
O	-2.66772	1.19361	0.88337
H	-3.57342	1.55055	0.6037
O	-2.98906	-1.27382	0.8356
H	-2.6094	-0.87722	1.66588

TS-R1

C	0.02455	-0.13038	-0.33516
C	-0.73993	1.02189	-0.25593
C	-2.82548	0.06491	-0.80568
S	-0.53022	-1.74987	0.17391
N	-2.11713	0.81711	0.0406
C	1.49235	-0.0459	-0.72777
C	2.3539	-0.17257	0.5309
H	1.72314	0.88952	-1.24332
H	1.72235	-0.881	-1.39486
H	2.20385	0.64235	1.23591
H	2.23395	-1.14302	1.00421
Cl	4.20089	-0.05975	0.03842
C	-0.26458	2.45388	-0.22156
H	0.82316	2.51702	-0.27365
H	-0.68274	3.04617	-1.04557
H	-0.58469	2.91701	0.72163
H	-2.86718	0.37528	-1.84208
O	-2.47728	0.56985	1.49167
H	-3.17966	1.27399	1.64394
O	-3.39582	-1.06858	-0.47705
H	-2.764	-1.50448	0.24822

TS-R2

C	0.07488	0.08103	-0.4424
C	-0.74772	1.13816	-0.29912
C	-2.38348	-0.68402	-0.58854
S	-0.69075	-1.5931	-0.1533
N	-2.10648	0.70195	0.0396
C	1.55046	0.12091	-0.72421
C	2.32607	-0.23992	0.54921
H	1.84948	1.11872	-1.05682
H	1.80147	-0.59546	-1.51295
H	2.17706	0.48251	1.34824
H	2.12657	-1.25376	0.88911
Cl	4.19303	-0.19415	0.16417
C	-0.465	2.60794	-0.33749
H	-0.67482	3.04127	0.6485
H	0.57833	2.8046	-0.59187
H	-1.10617	3.11037	-1.0711
H	-2.29842	-0.56873	-1.67516
O	-2.08775	0.46626	1.54372
H	-2.86282	-0.20568	1.55562
O	-3.64002	-0.81908	-0.04584
H	-3.38391	0.62053	-0.07661

P-R1

C	-0.09863	0.15868	-0.19736
C	0.89431	-0.62565	0.25551
C	3.32168	-0.26964	-0.31032
S	0.17322	1.86351	-0.55903
N	2.21174	-0.12073	0.61503
C	-1.47061	-0.30947	-0.55125
C	-2.51482	0.28527	0.38824
H	-1.52674	-1.42398	-0.52738
H	-1.70893	-0.03984	-1.60719
H	-2.29069	0.07781	1.45019
H	-2.62655	1.37877	0.25318
Cl	-4.10469	-0.46552	0.01686
C	0.82012	-2.10397	0.44598
H	1.06955	-2.39822	1.47632
H	-0.178	-2.50506	0.21498
H	1.54601	-2.61554	-0.21691
O	2.14416	1.22453	1.06449
H	2.46092	1.16537	2.02931
H	0.56328	2.32547	0.65317
O	3.41046	-1.27072	-0.9796
H	4.06786	0.53604	-0.23701

P-R2

C	0.33073	-0.04601	-0.60421

C	1.27878	-0.88678	-0.12502
C	0.36736	2.58585	0.48736
S	0.77541	1.60515	-0.97174
N	2.55812	-0.36606	0.28049
C	-1.09362	-0.40696	-0.85422
C	-1.89702	-0.32333	0.44143
H	-1.17039	-1.4303	-1.28787
H	-1.54736	0.25443	-1.62711
H	-1.51885	-1.01322	1.21665
H	-1.90205	0.70129	0.86769
Cl	-3.59767	-0.78431	0.08675
C	1.03446	-2.33415	0.14314
H	0.84039	-2.50958	1.21307
H	0.16755	-2.72382	-0.41185
H	1.90586	-2.95185	-0.13528
H	0.71177	3.6204	0.35975
O	3.54216	-1.39109	0.32537
H	3.66056	-1.55956	1.31629
O	-0.21685	2.13706	1.42855
H	2.97295	0.32604	-0.36389