

Mechanistic insights into chloramphenicol-mediated inactivation of cytochrome P450 enzymes and their active site mutants.

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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 secondary amine hydroxylation of chloramphenicol by P450 (Cpd I) by HAT mechanism.

	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 _H	-3417.531146	0.00	-3417.005725	0.00	-3418.754758	0.00	-3418.229337	0.00	-3418.778710	0.00	-3418.253289	0.00
⁴ RC _H	-3417.528216	1.84	-3417.003287	1.53	-3418.752321	1.53	-3418.227392	1.22	-3418.776744	1.23	-3418.251815	0.93
² TS _H	-3417.509421	13.63	-3416.987057	11.71	-3418.718921	22.49	-3418.196557	20.57	-3418.742421	22.77	-3418.220057	20.85
⁴ TS _H	-3417.510479	12.97	-3416.989019	10.48	-3418.717479	23.39	-3418.198019	19.65	-3418.740479	23.99	-3418.221019	20.25
² INT _H	-3417.523530	4.78	-3417.009527	-2.39	-3418.746122	5.42	-3418.222119	4.53	-3418.756194	14.13	-3418.242191	6.96
⁴ INT _H	-3417.532300	-0.72	-3417.011417	-3.57	-3418.744208	6.62	-3418.223325	3.77	-3418.765555	8.26	-3418.244672	5.41
² TS-reb _H	-3417.480388	31.85	-3416.958016	29.94	-3418.708231	29.20	-3418.185859	27.28	-3418.729772	30.71	-3418.207400	28.80
⁴ TS-reb _H	-3417.476469	34.31	-3416.953862	32.54	-3418.708539	29.00	-3418.185932	27.24	-3418.729505	30.88	-3418.206898	29.11
² P-OH	-3417.522315	5.54	-3416.996747	5.63	-3418.764395	-6.05	-3418.238827	-5.95	-3418.787917	-5.78	-3418.262349	-5.68
⁴ P-OH	-3417.524411	4.23	-3416.999297	4.03	-3418.767039	-7.71	-3418.241925	-7.90	-3418.792359	-8.56	-3418.267245	-8.76

Table S2. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for the secondary amine hydroxylation of chloramphenicol by P450 (Cpd I) by OAR mechanism.

	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 TS _O	-3417.531146	0.00	-3417.005725	0.00	-3418.7547579	0.00	-3418.2293369	0.00	-3418.77871030	0.00	-3418.25328930	0.00
⁴ TS _O	-3417.528216	1.84	-3417.003287	1.53	-3418.7523214	1.53	-3418.2273924	1.22	-3418.77674390	1.23	-3418.25181490	0.93
² INT _O	-3417.475698	34.79	-3416.950785	34.48	-3418.697986	35.62	-3418.175622	33.71	-3418.721278	36.04	-3418.198914	34.12
⁴ INT _O	-3417.445694	53.62	-3416.923842	51.38	-3418.675834	49.53	-3418.154374	47.04	-3418.69931	49.82	-3418.17785	47.34
² TS-reb _O	-3417.48701	27.70	-3416.960535	28.36	-3418.72179	20.69	-3418.197787	19.80	-3418.745983	20.54	-3418.23198	13.37
⁴ TS-reb _O	-3417.478229	33.21	-3416.953291	32.90	-3418.695224	37.36	-3418.174341	34.51	-3418.722436	35.31	-3418.201553	32.46

Table S3. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for C-H hydroxylation of chloramphenicol by P450 (Cpd I) through dichloromethane oxidation (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
² RC ₁	-3417.506344	0.00	-3416.982004	0.00	-3418.733393	0.00	-3418.209053	0.00	-3418.760815	0.00	-3418.236475	0.00
⁴ RC ₁	-3417.506306	0.02	-3416.981916	0.06	-3418.733215	0.11	-3418.208825	0.14	-3418.760691	0.08	-3418.236301	0.11
² TS-H ₁	-3417.472789	21.06	-3416.955000	16.95	-3418.705472	17.52	-3418.187683	13.41	-3418.730882	18.78	-3418.213093	14.67
⁴ TS-H ₁	-3417.472181	21.44	-3416.953881	17.65	-3418.705771	17.33	-3418.187471	13.54	-3418.730774	18.85	-3418.212474	15.06
² INT ₁	-3417.513620	-4.57	-3416.990816	-5.53	-3418.751320	-11.25	-3418.228516	-12.21	-3418.773686	-8.08	-3418.250882	-9.04
⁴ INT ₁	-3417.511647	-3.33	-3416.987909	-3.71	-3418.751647	-11.45	-3418.227909	-11.83	-3418.779116	-11.48	-3418.255378	-11.86
² TS-reb ₁	-3417.482987	14.63	-3416.960999	13.13	-3418.719534	8.58	-3418.197546	7.08	-3418.744938	9.89	-3418.222950	8.38
⁴ TS-reb ₁	-3417.480536	16.20	-3416.958324	14.86	-3418.725861	4.73	-3418.203649	3.39	-3418.749993	6.79	-3418.227781	5.46
² P-OH ₁	-3417.567042	-38.09	-3417.041801	-37.52	-3418.816109	-51.91	-3418.290868	-51.34	-3418.844834	-52.72	-3418.319593	-52.16
⁴ P-OH ₁	-3417.553096	-29.34	-3417.029579	-29.85	-3418.803125	-43.76	-3418.279608	-44.27	-3418.832515	-44.99	-3418.308998	-45.51

Table S4. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for C-H hydroxylation of chloramphenicol by P450 (Cpd I) through 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
² RC ₂	-3417.518405	0.00	-3416.994121	0.00	-3418.744103	0.00	-3418.219819	0.00	-3418.766443	0.00	-3418.242159	0.00
⁴ RC ₂	-3417.520272	-1.17	-3416.993467	0.41	-3418.746027	-1.21	-3418.219222	0.37	-3418.768272	-1.15	-3418.241467	0.43
² TS-H ₂	-3417.477291	25.80	-3416.954502	24.86	-3418.701457	26.76	-3418.178668	25.82	-3418.726320	25.18	-3418.203531	24.24
⁴ TS-H ₂	-3417.475889	26.68	-3416.957589	22.92	-3418.701189	26.93	-3418.182889	23.17	-3418.717889	30.47	-3418.199589	26.71
² INT ₂	-3417.516126	1.43	-3416.993322	0.50	-3418.746199	-1.32	-3418.223395	-2.24	-3418.769017	-1.62	-3418.246213	-2.54
⁴ INT ₂	-3417.516120	1.43	-3416.992333	1.12	-3418.746195	-1.31	-3418.222408	-1.62	-3418.769018	-1.62	-3418.245231	-1.93
² TS-reb ₂	-3417.495214	15.72	-3416.968226	15.84	-3418.721717	15.25	-3418.194729	15.37	-3418.740273	17.57	-3418.213285	17.68
⁴ TS-reb ₂	-3417.490681	17.40	-3416.968469	16.10	-3418.713418	19.25	-3418.191206	17.95	-3418.738121	17.77	-3418.215909	16.47
² P-OH ₂	-3417.588235	-43.82	-3417.059416	-40.97	-3418.817932	-46.33	-3418.289113	-43.48	-3418.841224	-46.93	-3418.312405	-44.08
⁴ P-OH ₂	-3417.579096	-38.08	-3417.055579	-38.56	-3418.808010	-40.10	-3418.284493	-40.58	-3418.829096	-39.32	-3418.305579	-39.80

Table S5. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for C-H hydroxylation of chloramphenicol by P450 (Cpd I) through 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 ₃	-3417.510151	0.00	-3416.986161	0.00	-3418.769545	0.00	-3418.245555	0.00	-3418.775611	0.00	-3418.251621	0.00
⁴ RC ₃	-3417.509939	0.13	-3416.985983	0.11	-3418.769423	0.08	-3418.245467	0.06	-3418.775054	0.35	-3418.251098	0.33
² TS-H ₃	-3417.485291	15.60	-3416.961612	15.41	-3418.744625	15.64	-3418.220946	15.44	-3418.754142	13.47	-3418.230463	13.28
⁴ TS- H ₃	-3417.480889	18.36	-3416.958059	17.63	-3418.740889	17.98	-3418.218059	17.25	-3418.751424	15.18	-3418.228594	14.45
² INT ₃	-3417.520481	-6.48	-3416.997544	-7.14	-3418.782556	-8.16	-3418.259619	-8.83	-3418.789462	-8.69	-3418.266525	-9.35
⁴ INT ₃	-3417.520476	-6.48	-3416.997535	-7.14	-3418.781476	-7.49	-3418.258535	-8.14	-3418.788237	-7.92	-3418.265296	-8.58
² TS-reb ₃	-3417.514139	-2.64	-3416.992108	-3.84	-3418.774265	-3.04	-3418.252234	-4.25	-3418.781151	-3.83	-3418.259120	-5.03
⁴ TS-reb ₃	-3417.507851	1.44	-3416.985823	0.21	-3418.770142	-0.37	-3418.248114	-1.61	-3418.775654	-0.03	-3418.253626	-1.26
² P-OH ₃	-3417.580354	-44.05	-3417.054883	-43.12	-3418.845012	-47.36	-3418.319541	-46.43	-3418.852637	-48.33	-3418.327166	-47.40
⁴ P-OH ₃	-3417.565701	-34.86	-3417.041026	-34.43	-3418.840126	-44.29	-3418.315451	-43.86	-3418.847125	-44.88	-3418.322450	-44.45

Table S6. Relative energy (RE) (in kcal/mol) and atomic energy (in a.u.) at the B3LYP level of theory for C-H hydroxylation of chloramphenicol by P450 (Cpd I) through 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 ₄	-3417.511360	0.00	-3416.987420	0.00	-3418.744103	0.00	-3418.220163	0.00	-3418.770141	0.00	-3418.246201	0.00
⁴ RC ₄	-3417.510643	0.45	-3416.986883	0.34	-3418.743468	0.40	-3418.219708	0.29	-3418.769406	0.46	-3418.245646	0.35
² TS-H ₄	-3417.483235	17.65	-3416.945656	26.21	-3418.700199	27.55	-3418.182620	23.56	-3418.725654	27.92	-3418.208075	23.92
⁴ TS- H ₄	-3417.466339	28.25	-3416.948843	24.21	-3418.695587	30.44	-3418.178091	26.40	-3418.723452	29.30	-3418.205956	25.25
² INT ₄	-3417.499623	7.37	-3416.976586	6.80	-3418.735919	5.14	-3418.212882	4.57	-3418.764068	3.81	-3418.240031	3.87
⁴ INT ₄	-3417.497662	8.60	-3416.976675	6.74	-3418.734758	5.86	-3418.213771	4.01	-3418.761435	5.46	-3418.240448	3.61
² TS-reb ₄	-3417.504139	4.08	-3416.977008	6.20	-3418.737259	3.90	-3418.210128	6.01	-3418.762365	4.42	-3418.235234	6.53
⁴ TS-reb ₄	-3417.496108	9.57	-3416.975857	7.26	-3418.734400	6.09	-3418.214149	3.77	-3418.759356	6.77	-3418.239105	4.45
² P-OH ₄	-3417.584322	-45.78	-3417.057161	-43.76	-3418.828705	-53.09	-3418.301544	-51.07	-3418.853076	-52.04	-3418.325915	-50.02
⁴ P-OH ₄	-3417.572130	-38.13	-3417.046476	-37.06	-3418.808541	-40.44	-3418.282887	-39.36	-3418.838246	-42.74	-3418.312592	-41.66

Table S7. UB3LYP/BS1-calculated Mulliken group spin densities and group charges for the species in the N-hydroxylation of CP by the P450 mechanism through the HAT pathway.

	Spin densities					Charge				
	Fe	O	Por	CP	SH	Fe	O	Por	CP	SH
² RC _H	1.40	0.73	-0.62	0.01	-0.51	0.53	-0.5	0.04	-0.06	-0.01
⁴ RC _H	1.23	0.79	0.51	0.01	0.45	0.52	-0.49	0.03	-0.05	-0.02
² TS _H	1.76	0.42	-0.78	-0.28	-0.13	0.48	-0.62	0.22	-0.07	0
⁴ TS _H	1.69	0.44	0.31	0.29	0.28	0.44	-0.61	0.2	0.04	-0.06
² INT _H	1.13	0.01	-0.34	1	-0.8	0.93	-0.75	-0.61	0.42	0.01
⁴ INT _H	2.64	0.18	0.19	-0.84	0.83	0.79	-0.72	-0.26	0.27	-0.08
² TS-reb _H	1.23	0.06	-0.58	0.41	-0.12	0.32	-0.56	-0.06	0.25	0.04
⁴ TS-reb _H	2.15	0.05	0.00	0.51	0.30	0.42	-0.57	-0.2	0.3	0.06
² P-OH	1.29	0.00	-0.15	0.00	-0.14	0.34	-0.45	-0.4	0.48	0.04
⁴ P-OH	2.48	0.00	0.04	0.00	0.48	0.54	-0.46	-0.42	0.48	-0.14

Table S8. UB3LYP/BS1-calculated Mulliken group spin densities and group charges for the species in the N-hydroxylation of CP by the P450 mechanism through the OAR pathway.

	Spin densities					Charge				
	Fe	O	Por	CP	SH	Fe	O	Por	CP	SH
² TS _O	1.14	0.14	-0.22	0.01	-0.06	0.36	-0.41	-0.30	0.33	0.02
⁴ TS _O	2.97	0.31	-0.28	0.09	-0.09	0.50	-0.41	-0.30	0.29	-0.09
² INT _O	1.08	0.00	-0.09	0.01	0.00	0.32	-0.40	-0.50	0.56	0.03
⁴ INT _O	2.56	0.03	-0.02	0.00	0.44	0.53	-0.39	-0.48	0.51	-0.17
² TS-reb _O	1.22	0.00	-0.13	0.00	-0.10	0.29	-0.44	-0.40	0.47	0.07
⁴ TS-reb _O	3.06	0.00	-0.01	0.00	-0.05	0.55	-0.43	-0.54	0.45	-0.03

Table S9. UB3LYP/BS1-calculated Mulliken group spin densities and group charges for the species in dichloromethylene oxidation of CP by the P450(Path B).

	Spin densities					Charge				
	Fe	O	Por	CP	SH	Fe	O	Por	CP	SH
² RC ₁	1.24	0.86	-0.56	0.00	-0.54	0.52	-0.38	-0.07	-0.01	-0.06
⁴ RC ₁	1.11	0.92	0.48	0.00	0.49	0.51	-0.38	-0.06	-0.01	-0.06
² TS-H ₁	1.94	0.23	-0.40	-0.46	-0.32	0.51	-0.61	-0.1	0.17	0.02
⁴ TS-H ₁	1.25	0.55	0.31	0.52	0.37	0.46	-0.58	-0.1	0.17	0.05
² INT ₁	0.82	0.19	0.41	-0.96	0.55	0.54	-0.63	-0.23	0.39	-0.07
⁴ INT ₁	1.84	0.26	-0.13	1.00	0.02	0.48	-0.66	-0.28	0.42	0.05
² TS-reb ₁	0.91	0.14	0.46	-0.80	0.29	0.42	-0.6	-0.16	0.35	-0.01
⁴ TS-reb ₁	2.14	0.03	-0.10	0.76	0.18	0.5	-0.59	-0.29	0.38	0.01
² P-OH ₁	1.30	0.00	-0.15	0.00	-0.14	0.35	-0.51	-0.38	0.51	0.02
⁴ P-OH ₁	2.96	0.00	0.03	0.00	0.01	0.57	-0.51	-0.49	0.49	-0.07

Table S10. UB3LYP/BS1-calculated Mulliken group spin densities and group charges for the species in C-H hydroxylation of CP by the P450 (Path C).

	Spin densities					Charge				
	Fe	O	Por	CP	SH	Fe	O	Por	CP	SH
² RC ₂	1.24	0.86	-0.53	0.00	-0.57	0.50	-0.38	-0.09	0.00	-0.04
⁴ RC ₂	1.10	0.93	0.45	0.00	0.52	0.49	-0.37	-0.63	0.55	-0.04
² TS-H ₂	1.06	0.46	-0.62	0.54	-0.44	0.46	-0.58	-0.12	0.26	-0.02
⁴ TS-H ₂	0.92	0.72	0.35	0.59	0.42	0.42	-0.54	-0.13	0.23	0.03
² INT ₂	0.84	0.19	0.42	-1	0.54	0.49	-0.61	-0.24	0.39	-0.04
⁴ INT ₂	1.79	0.29	-0.12	1.0	0.03	0.44	-0.62	-0.31	0.44	0.05
² TS-reb ₂	0.92	0.16	0.43	-0.77	0.26	0.44	-0.58	-0.17	0.33	-0.01
⁴ TS-reb ₂	2.23	0.04	-0.13	0.73	0.14	0.51	-0.56	-0.31	0.35	0.01
² P-OH ₂	1.25	0	-0.13	0	-0.12	0.37	-0.54	-0.37	0.51	0.03
⁴ P-OH ₂	3.07	0.00	0.01	0.00	-0.09	0.54	-0.60	-0.59	0.67	-0.03

Table S11. UB3LYP/BS1-calculated Mulliken group spin densities and group charges for the species in β -Hydroxymethylene oxidation of CP by the P450 (Path D).

	Spin densities					Charge				
	Fe	O	Por	CP	SH	Fe	O	Por	CP	SH
² RC ₃	1.32	0.79	-0.56	0.00	-0.56	0.51	-0.43	-0.04	-0.03	-0.01
⁴ RC ₃	1.18	0.84	0.47	0.01	0.50	0.50	-0.43	-0.03	-0.03	-0.02
² TS-H ₃	1.91	0.24	-0.48	-0.41	-0.26	0.51	-0.62	-0.1	0.15	0.05
⁴ TS-H ₃	1.23	0.53	0.34	0.51	0.39	0.48	-0.59	-0.1	0.16	0.05
² INT ₃	1.95	0.20	-0.13	-0.99	-0.03	0.49	-0.69	-0.25	0.37	0.08
⁴ INT ₃	1.95	0.20	-0.13	1.00	-0.03	0.49	-0.69	-0.25	0.37	0.08
² TS-reb ₃	1.12	-0.07	-0.55	0.63	-0.13	0.37	-0.70	-0.22	0.58	-0.03
⁴ TS-reb ₃	2.36	0.00	-0.12	0.69	0.07	0.49	-0.68	-0.33	0.53	-0.01
² P-OH ₃	1.30	0.00	-0.15	0.00	-0.14	0.35	-0.63	-0.39	0.65	0.02
⁴ P-OH ₃	3.14	0.00	-0.05	0.00	-0.09	0.57	-0.64	-0.50	0.64	-0.07

Table S12. UB3LYP/BS1-calculated Mulliken group spin densities and group charges for the species in α -Hydroxymethylene oxidation of CP by the P450 (Path E).

	Spin densities					Charge				
	Fe	O	Por	CP	SH	Fe	O	Por	CP	SH
² RC ₄	1.30	0.81	-0.56	0.00	-0.55	0.53	-0.43	-0.03	-0.04	-0.03
⁴ RC ₄	1.17	0.85	0.47	0.01	0.50	0.51	-0.42	-0.03	-0.03	-0.03
² TS-H ₄	1.9	0.26	-0.46	-0.44	-0.26	0.42	-0.45	-0.29	0.26	0.06
⁴ TS-H ₄	1.25	0.66	0.15	0.55	0.39	0.44	-0.51	-0.26	0.29	0.04
² INT ₄	1.88	0.16	-0.15	-0.90	0.02	0.38	-0.58	-0.30	0.41	0.07
⁴ INT ₄	0.92	0.12	0.63	1.00	0.34	0.45	-0.71	-0.03	0.32	-0.02
² TS-reb ₄	0.95	0.12	0.43	-0.75	0.25	0.44	-0.62	-0.18	0.37	-0.01
⁴ TS-reb ₄	2.26	0.04	-0.13	0.80	0.04	0.48	-0.67	-0.30	0.48	0.02
² P-OH ₄	1.10	0.00	-0.09	0.00	-0.01	0.37	-0.62	-0.54	0.75	0.04
⁴ P-OH ₄	3.14	0.00	-0.04	0.00	-0.10	0.56	-0.60	-0.51	0.59	-0.04

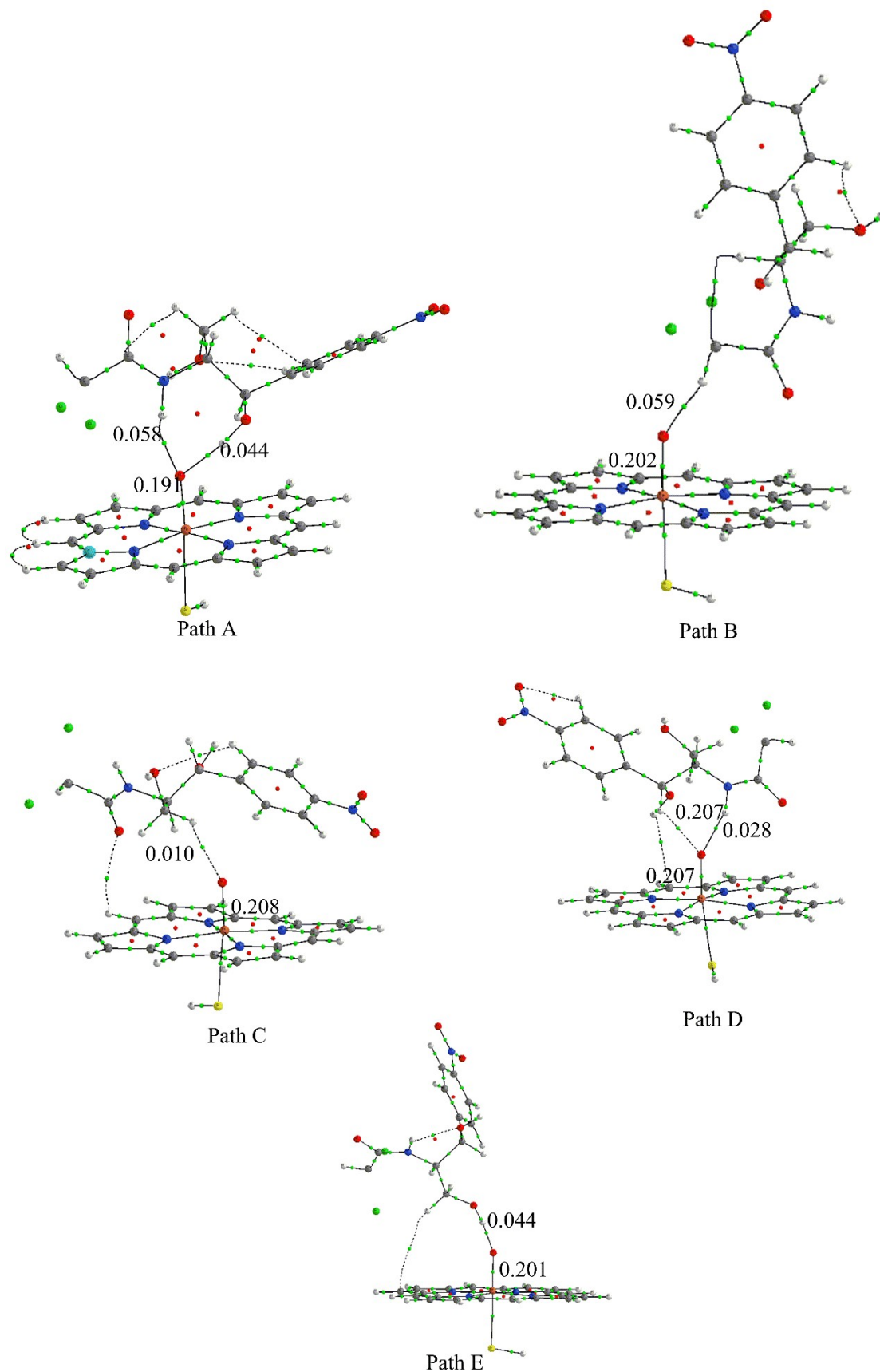


Figure S1. Molecular representation of the electronic density of some BCPs (in a.u.) of the intermediates of Paths A-E. 8

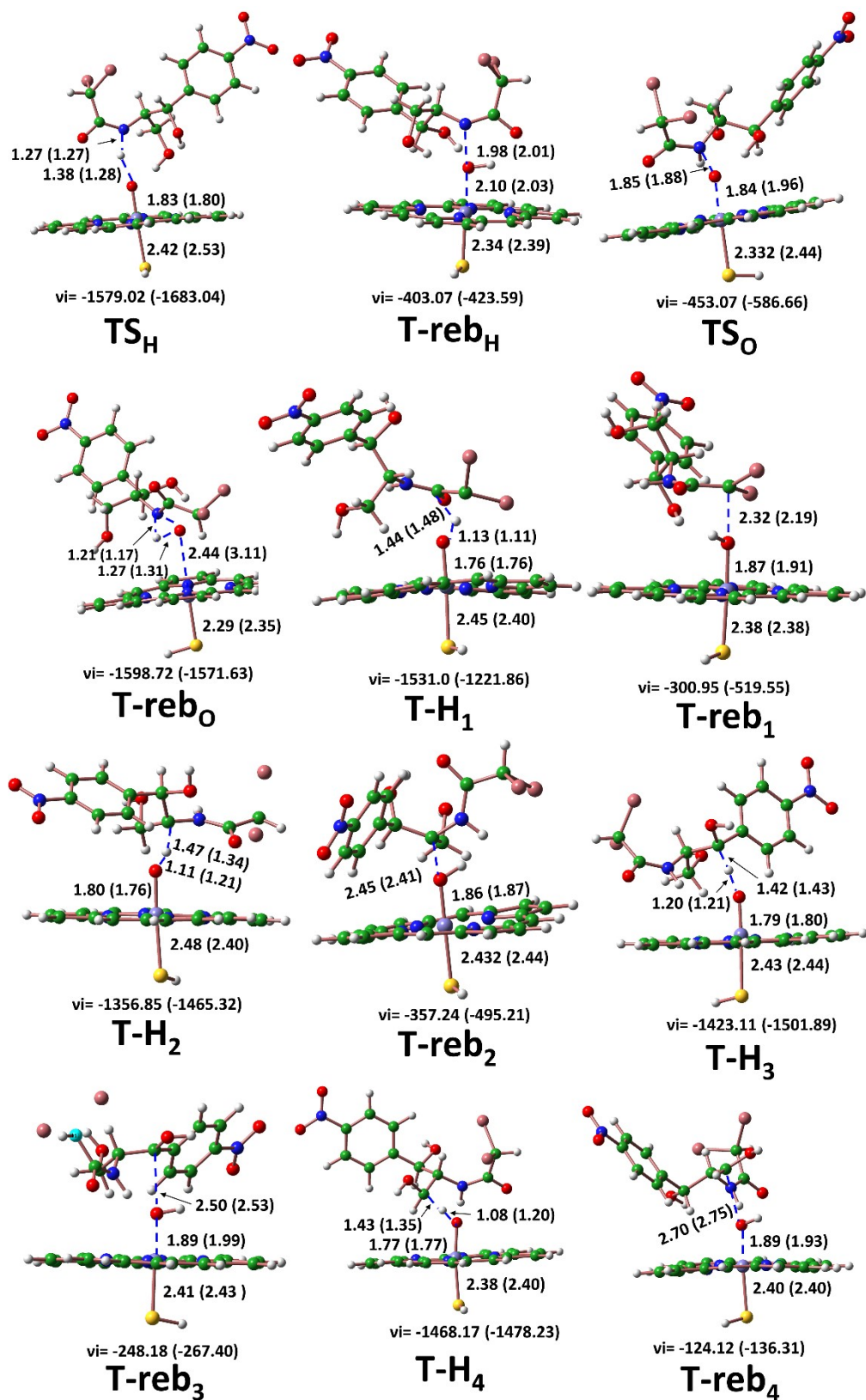


Figure S2. Structures of transition states in all pathways in this study. Cartesian coordinates of all structures discussed in this study.

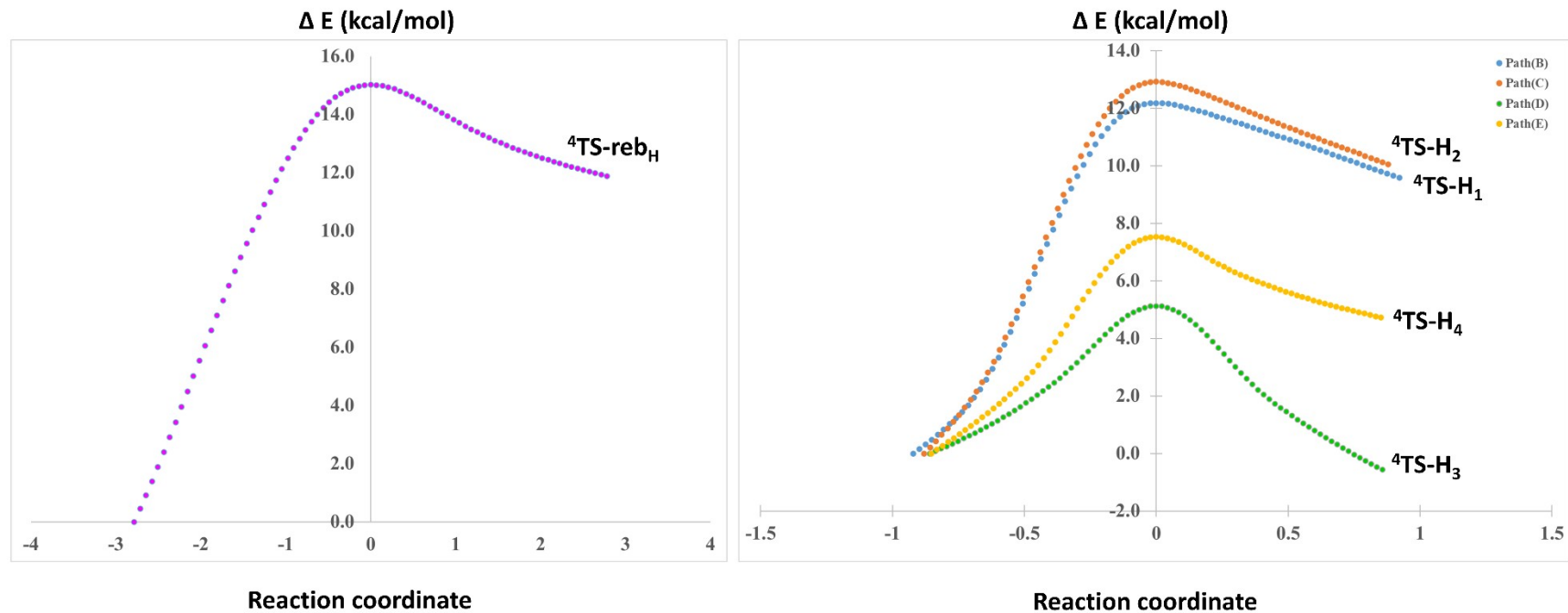


Figure S3. Computed intrinsic reaction coordinate (IRC) of the rate-determining step transition states in paths A (left) and B, C, D, and E (right).

HAT pathway**⁴RC_H**

Fe	1.73681000	-1.22140000	0.21357800
O	0.90661000	0.13520000	-0.28150200
S	2.85596900	-3.27608700	1.15608800
H	2.10463200	-4.23471500	0.50264500
N	1.29337700	-2.24432200	-1.46953000
C	0.15803300	-3.46090400	-3.08562300
C	1.29805900	-2.98451400	-3.66862800
H	-0.61926400	-4.06629100	-3.52765800
H	1.64082000	-3.12378900	-4.68320300
N	3.46869100	-0.61050800	-0.61541500
C	3.88100700	-0.81271500	-1.92036900
C	5.13780500	-0.13530300	-2.15420900
C	5.48324800	0.47615800	-0.98343800
H	5.67052000	-0.13720500	-3.09356400
H	6.35472100	1.07741700	-0.77126500
N	2.30750800	-0.43398700	1.97653200
C	3.44523600	0.32441900	2.22018000
C	1.59643400	-0.44374700	3.16596100
C	3.44484400	0.78790100	3.58961400
C	2.30341800	0.31735500	4.17166200
H	4.22261000	1.39331900	4.03093400
H	1.96004800	0.45872300	5.18571800
N	0.14637600	-2.06779300	1.12245000
C	-1.52371600	-2.55136400	2.66375800
H	-2.05640300	-2.55287800	3.60311900
C	-0.27611400	-1.85946000	2.43258300
C	0.15773300	-2.99681800	-1.71740400
C	2.00144300	-2.22232500	-2.66232700
C	4.43942100	0.17608500	-0.02803900
C	0.38959200	-1.09443400	3.37352100
H	-0.06140900	-1.00846400	4.35604000
C	-0.83370900	-3.28163800	-0.78643800
H	-1.67378800	-3.88029600	-1.12069200
C	3.20393900	-1.56430800	-2.86907500
H	3.64805600	-1.63762600	-3.85604000
C	4.43259300	0.60697200	1.29230200
H	5.26551300	1.21880800	1.62085300
C	-1.86742000	-3.16749800	1.49534700
H	-2.73881500	-3.77037900	1.28716200
C	-0.83588900	-2.86107800	0.53093800
C	1.49043400	4.10176900	-1.01306900
H	1.67567500	5.11636900	-1.34725400
C	-1.91310000	2.42932000	-0.38616700
C	-2.15562000	0.89439100	-0.30207200

H	-2.37754900	2.79890700	-1.30904000
H	-1.69261200	0.53397900	0.62366400
Cl	2.34372600	3.93413600	0.65211700
Cl	2.29094300	2.97164100	-2.26713200
C	-0.01387500	3.88358900	-0.90204800
O	-0.74919200	4.85731100	-1.20523800
N	-0.46218300	2.68585800	-0.48201700
C	-2.52433500	3.20611500	0.78390900
H	-3.61778600	3.18423500	0.71018600
H	-2.19260900	4.24678900	0.72813200
O	-2.09999400	2.57311400	2.03372700
H	-2.00450600	3.23741900	2.74139600
O	-1.55688200	0.24232000	-1.44860400
H	-0.59099800	0.11966300	-1.27424000
C	-3.63233400	0.54508500	-0.28573200
C	-4.36397000	0.58203900	0.91642600
C	-4.27940100	0.16695100	-1.47508200
C	-5.71938000	0.25584000	0.93351200
H	-3.86209100	0.87777500	1.83185500
C	-5.63488200	-0.16097400	-1.47195500
H	-3.69972000	0.11473700	-2.38742600
C	-6.33838600	-0.11231000	-0.26485900
H	-6.29764400	0.27631800	1.84782900
H	-6.15016100	-0.45414300	-2.37715000
N	-7.75728300	-0.46351700	-0.25257300
O	-8.30050200	-0.80291700	-1.34473900
O	-8.37745500	-0.41349800	0.85070000
H	0.18811600	1.92694700	-0.26709900
² RC _H			
Fe	1.67871800	-1.21713800	0.26988500
O	0.91055100	0.12772200	-0.34590600
S	3.05573300	-3.05921700	1.34072900
H	2.35874800	-3.16788700	2.52947000
N	0.07277300	-1.81300700	1.33793300
C	-1.57116400	-1.95567300	2.96915800
C	-1.98486600	-2.71865600	1.91356000
H	-2.07451200	-1.78103500	3.90845900
H	-2.89527000	-3.29101900	1.81621100
N	1.12307700	-2.42835500	-1.23601300
C	-0.04804400	-3.16317400	-1.32525700
C	-0.11642400	-3.83325000	-2.60381300
C	1.01874100	-3.50323500	-3.28800200
H	-0.93146700	-4.46643600	-2.92118300
H	1.32010000	-3.81385000	-4.27733700
N	3.41752300	-0.84446300	-0.67659400
C	3.77486800	-1.25501500	-1.95383200

C	4.44275800	-0.01989900	-0.24301400
C	5.05244500	-0.68244900	-2.31748600
C	5.46243500	0.08153400	-1.26409200
H	5.55339000	-0.85142700	-3.25912400
H	6.36608500	0.66500700	-1.16978300
N	2.37496700	-0.24137300	1.89903800
C	3.62267400	1.15142200	3.27585600
H	4.44115000	1.77874600	3.59629800
C	3.54903500	0.49850000	1.98843000
C	-0.29085600	-1.39181000	2.60700500
C	-0.96173800	-2.62565900	0.89764000
C	1.78793200	-2.62878600	-2.43175500
C	4.50014300	0.61082300	0.99006100
H	5.36273200	1.23653200	1.19038300
C	0.46630900	-0.56174100	3.42539800
H	0.05385400	-0.31080600	4.39665300
C	-1.01533300	-3.25554300	-0.33618700
H	-1.88849900	-3.86279400	-0.54788000
C	3.02139000	-2.08427200	-2.76604700
H	3.42455000	-2.32741300	-3.74314100
C	2.48892600	0.82340900	3.96166100
H	2.19558700	1.12801400	4.95544200
C	1.70388500	-0.03447300	3.10323700
C	1.52168200	4.03853500	-1.23881400
H	1.71294800	5.03432500	-1.62261000
C	-1.88365500	2.39594100	-0.52002100
C	-2.12290200	0.86310200	-0.40977000
H	-2.36259900	2.76027700	-1.43711600
H	-1.64843600	0.51909200	0.51649300
Cl	2.36144300	3.95465800	0.44212200
Cl	2.32387800	2.84054900	-2.42412600
C	0.01665300	3.83080600	-1.11478300
O	-0.71788900	4.79134600	-1.44924400
N	-0.42860400	2.65024900	-0.63356100
C	-2.45224000	3.18283100	0.67188200
H	-3.53750900	3.08871100	0.71016500
H	-2.19915700	4.24210300	0.56028100
O	-1.97407300	2.65812000	1.94867600
H	-1.01241300	2.82493200	2.02582600
O	-1.53787300	0.18559100	-1.54900300
H	-0.57552200	0.04362700	-1.36996800
C	-3.59807700	0.51445700	-0.36110100
C	-4.29720700	0.53701200	0.86056900
C	-4.27629300	0.15325000	-1.53811300
C	-5.65285700	0.21358500	0.90891500
H	-3.77234200	0.81429700	1.76898100

C	-5.63196400	-0.17213900	-1.50360200
H	-3.72125600	0.11030100	-2.46633100
C	-6.30324000	-0.13749400	-0.27775300
H	-6.20685900	0.22418400	1.83826100
H	-6.17143700	-0.45303600	-2.39851500
N	-7.72212900	-0.48801800	-0.23292400
O	-8.29493300	-0.80699600	-1.31591900
O	-8.31113900	-0.45845900	0.88772600
H	0.22079600	1.87466300	-0.46991800
⁴TS_H			
Fe	2.30966456	-0.82693949	0.14062331
O	0.99078156	0.30699251	-0.42108369
S	4.00212100	-2.39198600	0.88456500
H	5.06590500	-1.89638500	0.15642200
N	1.07663100	-2.00807900	1.19623600
C	-0.26288700	-2.80853400	2.90759500
C	-0.46939700	-3.61411700	1.82291300
H	-0.71746200	-2.86944500	3.88512000
H	-1.12627500	-4.46694700	1.73677500
N	2.01071900	-2.04451500	-1.49396100
C	1.15043800	-3.12970900	-1.57124800
C	1.18104700	-3.68198900	-2.90633900
C	2.06810200	-2.93756300	-3.63022800
H	0.59495200	-4.52914000	-3.23032800
H	2.35476000	-3.05476000	-4.66481200
N	3.76087500	0.11789500	-0.90438000
C	4.10234900	-0.05408500	-2.23942400
C	4.49254100	1.20969900	-0.45528700
C	5.09421300	0.92499800	-2.61777000
C	5.33551600	1.70118400	-1.51960400
H	5.52883000	1.00415900	-3.60325100
H	6.00517600	2.54336700	-1.42760300
N	2.66200900	0.29785000	1.71810800
C	3.49148300	1.93521700	3.13053600
H	4.08293200	2.77747300	3.45745200
C	3.55759500	1.35460300	1.81010200
C	0.69798000	-1.80417100	2.51639400
C	0.35888400	-3.11048600	0.75250400
C	2.59409500	-1.92250700	-2.74602600
C	4.40709900	1.78093300	0.80358800
H	5.04295600	2.63379300	1.01108600
C	1.14257100	-0.77959000	3.33704900
H	0.75097200	-0.74177400	4.34713100
C	0.38851000	-3.63216700	-0.53052900
H	-0.23778400	-4.49268000	-0.73625200
C	3.56315400	-0.99825100	-3.09758100

H	3.92804500	-1.01534500	-4.11827900
C	2.56948200	1.21992700	3.84128100
H	2.26044600	1.35667900	4.86712400
C	2.06125500	0.18938600	2.96507700
C	-0.99411556	4.25258449	-1.04748331
H	-0.35189556	5.05179349	-1.39970231
C	-1.97391556	1.70218249	0.39388669
C	-1.98756056	0.16490849	-0.09765831
H	-2.64240756	2.25594049	-0.27256731
Cl	-1.84903600	3.60188100	-2.53806000
Cl	-2.29593700	5.13720200	0.09883300
C	-0.13515256	3.22621549	-0.30304731
O	1.11091644	3.45397449	-0.35773231
N	-0.61516656	2.17794149	0.41098769
C	-2.49353056	1.78550249	1.85720369
H	-3.51915056	1.42099649	1.91158769
H	-2.47055756	2.83363849	2.17576569
O	-1.71838856	0.94979749	2.74961269
H	-0.77265056	1.19857549	2.66730369
C	-3.40273556	-0.36108651	-0.15575731
C	-3.98618556	-0.96458151	0.97451769
C	-4.14063156	-0.26832951	-1.34925031
C	-5.28891256	-1.46024451	0.92125169
H	-3.41064756	-1.04769251	1.89084169
C	-5.44391556	-0.75803851	-1.41505331
H	-3.66895056	0.16602949	-2.22140131
C	-6.00161756	-1.34656351	-0.27537631
H	-5.75406656	-1.93113151	1.77705369
H	-6.02781256	-0.69858551	-2.32400831
N	-7.36709356	-1.86855751	-0.33919831
O	-7.99800856	-1.76116251	-1.43088431
O	-7.85209956	-2.40295251	0.70108869
H	0.33762994	1.39229113	0.12656569
H	-1.54433421	0.07363244	-1.06725569
O	-1.23497237	-0.54484858	0.88963897
H	-1.50363301	-0.23847887	1.75886797
²TS_H			
Fe	2.30966456	-0.82693949	0.14062331
O	0.99078156	0.30699251	-0.42108369
S	4.00212100	-2.39198600	0.88456500
H	5.06590500	-1.89638500	0.15642200
N	1.07663100	-2.00807900	1.19623600
C	-0.26288700	-2.80853400	2.90759500
C	-0.46939700	-3.61411700	1.82291300
H	-0.71746200	-2.86944500	3.88512000
H	-1.12627500	-4.46694700	1.73677500

N	2.01071900	-2.04451500	-1.49396100
C	1.15043800	-3.12970900	-1.57124800
C	1.18104700	-3.68198900	-2.90633900
C	2.06810200	-2.93756300	-3.63022800
H	0.59495200	-4.52914000	-3.23032800
H	2.35476000	-3.05476000	-4.66481200
N	3.76087500	0.11789500	-0.90438000
C	4.10234900	-0.05408500	-2.23942400
C	4.49254100	1.20969900	-0.45528700
C	5.09421300	0.92499800	-2.61777000
C	5.33551600	1.70118400	-1.51960400
H	5.52883000	1.00415900	-3.60325100
H	6.00517600	2.54336700	-1.42760300
N	2.66200900	0.29785000	1.71810800
C	3.49148300	1.93521700	3.13053600
H	4.08293200	2.77747300	3.45745200
C	3.55759500	1.35460300	1.81010200
C	0.69798000	-1.80417100	2.51639400
C	0.35888400	-3.11048600	0.75250400
C	2.59409500	-1.92250700	-2.74602600
C	4.40709900	1.78093300	0.80358800
H	5.04295600	2.63379300	1.01108600
C	1.14257100	-0.77959000	3.33704900
H	0.75097200	-0.74177400	4.34713100
C	0.38851000	-3.63216700	-0.53052900
H	-0.23778400	-4.49268000	-0.73625200
C	3.56315400	-0.99825100	-3.09758100
H	3.92804500	-1.01534500	-4.11827900
C	2.56948200	1.21992700	3.84128100
H	2.26044600	1.35667900	4.86712400
C	2.06125500	0.18938600	2.96507700
C	-0.99411556	4.25258449	-1.04748331
H	-0.35189556	5.05179349	-1.39970231
C	-1.97391556	1.70218249	0.39388669
C	-1.98756056	0.16490849	-0.09765831
H	-2.64240756	2.25594049	-0.27256731
Cl	-1.84903600	3.60188100	-2.53806000
Cl	-2.29593700	5.13720200	0.09883300
C	-0.13515256	3.22621549	-0.30304731
O	1.11091644	3.45397449	-0.35773231
N	-0.61516656	2.17794149	0.41098769
C	-2.49353056	1.78550249	1.85720369
H	-3.51915056	1.42099649	1.91158769
H	-2.47055756	2.83363849	2.17576569
O	-1.71838856	0.94979749	2.74961269
H	-0.77265056	1.19857549	2.66730369

C	-3.40273556	-0.36108651	-0.15575731
C	-3.98618556	-0.96458151	0.97451769
C	-4.14063156	-0.26832951	-1.34925031
C	-5.28891256	-1.46024451	0.92125169
H	-3.41064756	-1.04769251	1.89084169
C	-5.44391556	-0.75803851	-1.41505331
H	-3.66895056	0.16602949	-2.22140131
C	-6.00161756	-1.34656351	-0.27537631
H	-5.75406656	-1.93113151	1.77705369
H	-6.02781256	-0.69858551	-2.32400831
N	-7.36709356	-1.86855751	-0.33919831
O	-7.99800856	-1.76116251	-1.43088431
O	-7.85209956	-2.40295251	0.70108869
H	0.33762994	1.39229113	0.12656569
H	-1.54433421	0.07363244	-1.06725569
O	-1.23497237	-0.54484858	0.88963897
H	-1.50363301	-0.23847887	1.75886797
²INT_H			
Fe	2.13033900	-0.96599700	0.18218200
O	1.69796900	0.23091300	-1.11079700
S	3.04101000	-2.62478500	2.39634500
H	1.76978300	-3.00858200	2.78817300
N	0.40096900	-1.98569400	0.23346300
C	-1.78278500	-2.62508100	0.70643900
C	-1.36886100	-3.36455300	-0.36681200
H	-2.73568400	-2.65684900	1.21422900
H	-1.91714200	-4.12035500	-0.91015900
N	2.82629400	-2.23206900	-1.24788400
C	2.08134300	-3.16929500	-1.94384500
C	2.88187100	-3.76529100	-2.99474600
C	4.11113900	-3.17725800	-2.93754400
H	2.53413900	-4.53116400	-3.67263300
H	4.97506900	-3.36350600	-3.55859500
N	4.01431100	-0.23656100	0.37106500
C	5.10210700	-0.48282400	-0.45071800
C	4.42364300	0.75154500	1.25188500
C	6.21528400	0.36324300	-0.07223100
C	5.79653000	1.12570000	0.97811500
H	7.18211500	0.35550200	-0.55386800
H	6.35167500	1.86868700	1.53195900
N	1.59748400	-0.01610400	1.87045900
C	1.57864900	1.45334200	3.67018200
H	1.94514000	2.17746900	4.38304400
C	2.35189300	0.92347600	2.57209600
C	-0.68208300	-1.76673900	1.07786500
C	-0.01202700	-2.96419500	-0.66223600

C	4.06866000	-2.21797100	-1.85244700
C	3.65360700	1.28815300	2.27286000
H	4.11693100	2.03944800	2.90362800
C	-0.69835700	-0.87558000	2.14274600
H	-1.60913900	-0.81453400	2.72915100
C	0.76432500	-3.50670200	-1.67589300
H	0.30664900	-4.26667800	-2.30038100
C	5.13002300	-1.40381800	-1.48404700
H	6.05102100	-1.49459900	-2.04968700
C	0.35320500	0.84560200	3.63659900
H	-0.47848300	0.98006100	4.31316000
C	0.35989900	-0.06585100	2.51710000
C	0.29534500	4.16148000	-0.74971700
C	-1.92190000	1.13852700	-0.89802400
C	-3.33536700	1.76460500	-1.07980400
H	-3.45964000	1.92599700	-2.15388800
Cl	1.75831800	4.68973400	0.11646300
Cl	0.02426900	4.84538500	-2.36610400
C	-0.45720400	2.99022800	-0.33082700
O	-0.71913700	2.86247600	1.02613100
N	-0.89599100	2.15850200	-1.19767400
C	-1.68081200	-0.01206200	-1.87716000
H	-2.36777500	-0.83572300	-1.68395900
H	-0.65623300	-0.37712100	-1.75097100
O	-1.89824500	0.39637000	-3.25132100
H	-1.24380300	1.09705700	-3.46015600
O	-3.35843600	3.03075000	-0.36990600
H	-4.15943000	3.52812200	-0.62880600
C	-4.42171400	0.82740100	-0.57747500
C	-5.04780900	-0.07483000	-1.45710900
C	-4.80636000	0.85410400	0.77528500
C	-6.03767200	-0.94392700	-0.99693600
H	-4.75525900	-0.09253500	-2.50234500
C	-5.79186600	-0.00977200	1.24893300
H	-4.33704300	1.57142700	1.43811000
C	-6.39396600	-0.89913300	0.35333500
H	-6.53625200	-1.64020900	-1.65829300
H	-6.10167700	-0.00652200	2.28553900
N	-7.43544700	-1.80352600	0.84343400
O	-7.70324600	-1.79093900	2.08050500
O	-8.02416300	-2.54557300	0.00454900
H	0.90901400	0.81719000	-1.13722100
H	-0.17824000	3.47170700	1.56492800
H	-1.83841100	0.75224300	0.11615200
⁴ INT _H			
Fe	2.50540100	-0.90253000	0.33304700

O	1.55719500	-0.25412700	-1.05096800
S	3.84566100	-1.63922300	2.16540500
H	2.79977900	-2.20101200	2.93986800
N	0.98904500	-2.08259900	0.97268600
C	-0.92661300	-2.86728100	2.00808100
C	-0.48452200	-3.85630500	1.17283900
H	-1.78834200	-2.87808300	2.66005600
H	-0.91387400	-4.83389700	1.00785000
N	3.18476500	-2.38407000	-0.84126800
C	2.59627500	-3.62359700	-1.02678900
C	3.36071600	-4.38428300	-1.99292900
C	4.40526900	-3.60049300	-2.38762600
H	3.11326300	-5.38491600	-2.31655800
H	5.18550600	-3.82955300	-3.09790500
N	4.11746400	0.20212000	-0.14236000
C	5.09709900	-0.10959700	-1.07127700
C	4.41533200	1.47222900	0.32568100
C	6.03754200	0.98399200	-1.17535800
C	5.61813800	1.95841200	-0.31632800
H	6.90163500	0.98522700	-1.82271200
H	6.06872200	2.91948100	-0.11828200
N	1.87272700	0.55434300	1.61451100
C	1.80033700	2.47242000	2.88587800
H	2.09958200	3.43492500	3.27449200
C	2.52323000	1.74587900	1.85979600
C	-0.00956300	-1.75842700	1.88040900
C	0.70863600	-3.36634600	0.52479100
C	4.29509700	-2.34750000	-1.66651800
C	3.68329700	2.18841900	1.25570200
H	4.05536200	3.16831200	1.53714800
C	-0.10242500	-0.56992600	2.58470300
H	-0.92416400	-0.45922300	3.28170600
C	1.45339400	-4.08522700	-0.39968200
H	1.11035200	-5.08305600	-0.64941800
C	5.18630400	-1.29498000	-1.78278500
H	6.01411800	-1.40893100	-2.47371200
C	0.73742200	1.69528200	3.26293300
H	-0.00980200	1.89786900	4.01589900
C	0.79023500	0.48951700	2.47034200
C	0.21222900	3.54266300	-0.90097200
C	-2.40157500	0.90219800	-0.54923200
C	-3.72578500	1.47530200	-1.13822600
H	-3.62148400	1.46908000	-2.22542500
Cl	0.86067900	4.94130700	0.01467600
Cl	0.80135900	3.36138900	-2.56171300
C	-0.77464300	2.68529500	-0.33475700

O	-1.16780100	2.89107800	0.97790500
N	-1.30550400	1.74258000	-1.06000500
C	-2.14240400	-0.52706900	-1.04698400
H	-2.91196500	-1.21277200	-0.68582900
H	-1.17163200	-0.87264000	-0.68515900
O	-2.21282600	-0.58779200	-2.50077300
H	-1.50238300	-0.01599900	-2.86176600
O	-3.81824400	2.83868500	-0.63187800
H	-4.50621100	3.33077100	-1.12051600
C	-4.95289200	0.66315900	-0.75333100
C	-5.37438600	-0.40730900	-1.56660700
C	-5.67354800	0.97200000	0.41172300
C	-6.49771100	-1.15852800	-1.22067200
H	-4.80425200	-0.65881000	-2.45475600
C	-6.79984500	0.22983300	0.76786400
H	-5.35153400	1.80855000	1.02069800
C	-7.19618600	-0.82666600	-0.05575300
H	-6.83930700	-1.98453700	-1.83027900
H	-7.36993400	0.45435800	1.65942900
N	-8.37883400	-1.60843000	0.31166500
O	-8.99857800	-1.29075500	1.36860000
O	-8.71849600	-2.56742500	-0.44017100
H	0.75441100	0.30580800	-1.05350200
H	-0.47407700	3.30942800	1.53336900
H	-2.47782100	0.92381100	0.54140900
²TS-reb_H			
Fe	2.18521000	-0.98130300	0.14937000
O	0.52138500	0.13572400	-0.46874800
S	4.06397500	-2.29380900	0.61206400
H	4.31056900	-1.82263100	1.88755400
N	1.25254100	-2.61203400	-0.57895300
C	0.12476700	-4.63770500	-0.69148200
C	0.50407000	-4.32109400	-1.96451300
H	-0.42868700	-5.50097800	-0.35312600
H	0.33194300	-4.87919900	-2.87289500
N	2.91268400	-0.62251400	-1.69830800
C	2.66068100	-1.32357200	-2.87118000
C	3.44084800	-0.77159200	-3.95549100
C	4.19361800	0.24143900	-3.43118800
H	3.41986000	-1.13216700	-4.97326500
H	4.90447500	0.87728600	-3.93791500
N	3.12381500	0.63463300	0.86888400
C	4.06713000	1.40140600	0.19378000
C	3.01446300	1.18981000	2.13413700
C	4.56325700	2.44480600	1.06348300
C	3.90169200	2.32400300	2.25631500

H	5.30844600	3.17514000	0.78429100
H	4.00312900	2.93319700	3.14219100
N	1.41130600	-1.31049000	1.95922700
C	0.78537600	-1.10230800	4.18725500
H	0.68739700	-0.66268600	5.16870800
C	1.48392800	-0.49066400	3.07866900
C	0.58807200	-3.57062800	0.16820900
C	1.22116700	-3.06700100	-1.89291900
C	3.86702400	0.33117200	-2.02561100
C	2.19875300	0.69631700	3.14710800
H	2.17089300	1.24614500	4.08099000
C	0.34218600	-3.48969800	1.53250700
H	-0.21663800	-4.30241500	1.98336200
C	1.85000000	-2.44863200	-2.96303100
H	1.74744300	-2.91166600	-3.93869500
C	4.41552300	1.25029100	-1.14152700
H	5.15756800	1.93489200	-1.53863500
C	0.31534800	-2.30720700	3.74684000
H	-0.25027600	-3.04561700	4.29557400
C	0.69727000	-2.43150400	2.35707700
C	1.04759800	3.31807200	0.02229700
H	2.01496000	3.20195500	0.49760200
C	-2.03523500	1.06773800	0.21731000
C	-2.88478100	0.83900300	-1.07061300
H	-2.51700600	1.85831100	0.81320800
H	-2.42819900	0.00802200	-1.62280500
Cl	1.32369200	3.11064900	-1.80813800
Cl	0.55253700	5.10029300	0.35695800
C	-0.01217200	2.40052300	0.63390200
O	-0.17985700	2.46080400	1.87295800
N	-0.75659500	1.63658600	-0.24690600
C	-1.93182500	-0.17700400	1.11926700
H	-2.89829200	-0.36496600	1.58897600
H	-1.18803100	0.00706100	1.90026700
O	-1.61790300	-1.36362200	0.35239500
H	-0.75579600	-1.18988400	-0.09783600
O	-2.85102100	2.04524300	-1.87327700
H	-1.91722000	2.34946200	-1.89914300
C	-4.33280600	0.50587400	-0.77985800
C	-4.70395500	-0.81044000	-0.44360200
C	-5.31723100	1.50673100	-0.84562800
C	-6.03342200	-1.12085400	-0.16250100
H	-3.94171400	-1.58158500	-0.39850700
C	-6.65111200	1.20755500	-0.56839900
H	-5.02404900	2.50624000	-1.13847600
C	-6.99120600	-0.10416400	-0.22670600

H	-6.33907700	-2.12568000	0.09722400
H	-7.42373700	1.96349500	-0.61674800
N	-8.38773000	-0.42514200	0.06471400
O	-9.24345600	0.50515100	-0.00386200
O	-8.67574500	-1.61901600	0.37409000
H	0.68355500	0.36151300	-1.41098100
⁴TS-reb_H			
Fe	2.26228800	-0.92292400	-0.14327500
O	0.94833500	0.61371800	0.05552500
S	3.83483700	-2.69386500	-0.43166500
H	4.24975200	-2.78960200	0.88194400
N	0.85929800	-2.23051800	0.47569500
C	-0.43491200	-3.63158700	1.79296300
C	-0.80001900	-3.84905400	0.49389300
H	-0.82144100	-4.09966400	2.68608700
H	-1.54493800	-4.53100600	0.11138800
N	1.71176900	-1.21725900	-2.03670100
C	0.75038800	-2.11580400	-2.49853200
C	0.67153100	-2.04584800	-3.93572500
C	1.57374200	-1.10508000	-4.34804600
H	-0.00163000	-2.63684200	-4.53867700
H	1.78634600	-0.77744400	-5.35485400
N	3.56455900	0.48626100	-0.73865200
C	3.82601400	0.88523100	-2.04586000
C	4.47285200	1.17815100	0.06166000
C	4.88675400	1.86368100	-2.05478200
C	5.28513500	2.04218100	-0.76093700
H	5.26992900	2.33915800	-2.94542100
H	6.05859300	2.69368500	-0.38207700
N	2.85273400	-0.66223300	1.76354900
C	3.94688400	0.10388000	3.65644700
H	4.64361100	0.66947700	4.25736700
C	3.84278000	0.19838400	2.22085200
C	0.60930400	-2.63424100	1.78123600
C	0.01375000	-2.98367100	-0.32767200
C	2.22211300	-0.58723800	-3.16916500
C	4.60265400	1.04880200	1.43144300
H	5.34836000	1.66074200	1.92597500
C	1.27862200	-2.18678900	2.90737400
H	0.96205700	-2.57593300	3.86777900
C	-0.03808300	-2.93383700	-1.71024500
H	-0.75284300	-3.57633200	-2.21112200
C	3.19832100	0.39475000	-3.17641700
H	3.49944100	0.79839500	-4.13615300
C	3.00824300	-0.80016500	4.07225700
H	2.78526800	-1.11909200	5.07969900

C	2.32054100	-1.27388900	2.89589900
C	-0.83369300	4.33461200	-0.11403900
H	-0.20172800	5.14958000	-0.44912200
C	-1.72942400	1.44763900	0.87885100
C	-1.93228400	0.13699100	0.02424700
H	-2.47352400	2.17979500	0.53648800
H	-1.36091000	-0.64396700	0.53274700
Cl	-2.15528500	4.13220300	-1.42154400
Cl	-1.59373700	4.88460700	1.50379800
C	0.03477000	3.08052300	0.00868900
O	1.19978600	3.18884700	-0.48155600
N	-0.39895300	1.98600000	0.64462900
C	-1.89906100	1.18881100	2.38316600
H	-2.90414500	0.82337300	2.60004400
H	-1.74172900	2.12583600	2.92991800
O	-0.99050000	0.15541400	2.84837300
H	-0.08154100	0.37035100	2.54744500
O	-1.43616700	0.33394000	-1.31334900
H	-0.45342300	0.39371600	-1.23589200
C	-3.38837600	-0.25763700	-0.04899200
C	-3.94528400	-1.09799400	0.93228900
C	-4.20016300	0.21513300	-1.09531900
C	-5.29415300	-1.44999900	0.88530800
H	-3.31333700	-1.48412900	1.72569700
C	-5.54934700	-0.13030700	-1.15560400
H	-3.75469500	0.83418000	-1.86368700
C	-6.07962100	-0.95666200	-0.15974900
H	-5.74059000	-2.09607800	1.62950400
H	-6.19070600	0.22230000	-1.95251100
N	-7.49442800	-1.32444500	-0.21771800
O	-8.19188000	-0.87020500	-1.17097500
O	-7.95356600	-2.07962700	0.68892700
H	1.49753900	1.40645100	-0.21317800
²P-OH			
Fe	-1.66855500	-1.54280800	0.36036900
S	-2.80402000	-3.37470600	1.13545800
H	-1.99717700	-3.65634400	2.22294300
N	0.16104700	-2.32896900	0.62763500
C	2.03039600	-3.68862500	0.36357000
C	2.13183400	-3.10538100	1.59557800
H	2.71329400	-4.38144300	-0.10624500
H	2.91227600	-3.22829200	2.33231100
N	-1.49453600	-0.64026500	2.14655900
C	-0.48076000	-0.79542200	3.09484900
C	-0.82726500	-0.10209100	4.31274200
C	-2.05846300	0.45789400	4.11936000

H	-0.20525800	-0.06321300	5.19508800
H	-2.63983300	1.04986300	4.81090000
N	-3.32248900	-0.48032500	-0.01943000
C	-4.04904700	0.26936800	0.89849600
C	-4.06262800	-0.44179200	-1.19630600
C	-5.25424200	0.78146900	0.28349100
C	-5.25907400	0.34874200	-1.00994100
H	-5.98199200	1.40078400	0.78665200
H	-5.99394600	0.53795400	-1.77843700
N	-1.64820600	-2.13291300	-1.55275600
C	-2.29185300	-2.62872000	-3.73432900
H	-2.87651300	-2.60060500	-4.64199000
C	-2.60777000	-1.89070700	-2.53309300
C	0.80973400	-3.20600700	-0.23962100
C	0.96666600	-2.26976600	1.76566300
C	-2.47568700	0.12359600	2.77825700
C	-3.72527100	-1.08970200	-2.37165800
H	-4.39581200	-0.98314900	-3.21727100
C	0.37732800	-3.54020700	-1.51208800
H	0.98565800	-4.23500200	-2.08103200
C	0.67646800	-1.53811400	2.90909900
H	1.37839200	-1.59347000	3.73483800
C	-3.66561500	0.53415500	2.20151800
H	-4.33381700	1.13579700	2.80768800
C	-1.15293500	-3.33680900	-3.48115700
H	-0.61645400	-4.00142300	-4.14221100
C	-0.75255500	-3.03042700	-2.12668100
C	-1.36497500	4.45504000	-0.46788900
H	-1.31889800	5.53319200	-0.57341500
C	1.50838000	1.95235800	-1.17713000
C	1.89043500	0.85145200	-0.14943700
H	2.23374300	2.77085900	-1.15234800
H	1.39566800	-0.07600700	-0.45064000
Cl	-2.76784700	3.89409200	-1.56065300
Cl	-1.73793100	4.14243700	1.33926800
C	-0.02028600	3.89621600	-0.90159700
O	0.83109200	4.70078000	-1.34837800
N	0.22621900	2.56474200	-0.80789200
C	1.44583800	1.37648300	-2.60525300
H	2.44369200	1.07977100	-2.93551800
H	1.07445200	2.15506900	-3.28253300
O	0.64152000	0.17095200	-2.68536300
H	-0.26750800	0.33730200	-2.35740800
O	1.35725300	1.28084300	1.14802700
H	1.43202200	0.54928300	1.79774700
C	3.38913300	0.62970900	-0.09800600

C	3.97420800	-0.39366400	-0.86405900
C	4.20516500	1.45225200	0.69926200
C	5.35512700	-0.59260100	-0.84504100
H	3.34354600	-1.03718200	-1.46874300
C	5.58560900	1.26052600	0.73239700
H	3.74707600	2.23044600	1.29883100
C	6.14087900	0.23895100	-0.04391900
H	5.82591500	-1.37417100	-1.42641000
H	6.23192200	1.88061300	1.33939000
N	7.59067800	0.02885800	-0.01083900
O	8.28538000	0.78595400	0.72631900
O	8.07400300	-0.90015000	-0.72037900
O	-0.80669100	1.67152300	-0.38208300
H	-0.52758000	1.43050000	0.54386600
⁴P-OH			
Fe	-1.08824800	-1.97713900	0.11327200
S	-1.83452800	-4.29516000	0.22034000
H	-2.84797800	-4.12078300	1.14388200
N	0.39306100	-2.05640300	1.51158200
C	2.32169800	-2.75357900	2.61018700
C	1.44252400	-2.33155900	3.56940500
H	3.32038300	-3.14251300	2.74421900
H	1.58262400	-2.30867800	4.64011700
N	-2.31053400	-1.20349800	1.50658500
C	-2.09260600	-1.15207100	2.88347100
C	-3.27942500	-0.68019200	3.55259400
C	-4.21791000	-0.43464700	2.58870400
H	-3.36750100	-0.54858200	4.62095200
H	-5.22283800	-0.05939700	2.71305700
N	-2.34312900	-1.30299600	-1.31335300
C	-3.63805700	-0.82532100	-1.13156000
C	-2.17776100	-1.41908400	-2.69123000
C	-4.27517900	-0.62050200	-2.41093000
C	-3.37495700	-0.98364700	-3.37166100
H	-5.27917300	-0.24447300	-2.54042800
H	-3.49613100	-0.96734300	-4.44464200
N	0.29396800	-2.33537500	-1.30010500
C	1.26836900	-2.84236800	-3.34634000
H	1.36761500	-2.94303300	-4.41702700
C	0.09444600	-2.33821200	-2.67990900
C	1.66994100	-2.60187900	1.33446400
C	0.23778600	-1.91940600	2.89527300
C	-3.61639600	-0.75037600	1.31742800
C	-1.04963400	-1.90429800	-3.32750500
H	-1.05963000	-1.94277600	-4.41049700
C	2.22077400	-2.96194300	0.11785900

H	3.22482100	-3.37092300	0.12048100
C	-0.91343300	-1.48649000	3.52926300
H	-0.89501600	-1.41201900	4.61073300
C	-4.23765200	-0.58132500	0.09181200
H	-5.25543800	-0.20864500	0.08996100
C	2.18367300	-3.15066500	-2.37681500
H	3.17727200	-3.55635300	-2.49919000
C	1.58276000	-2.83130600	-1.10585200
C	-2.08024700	4.40047700	0.70978400
H	-2.02051600	5.35008100	1.22962400
C	0.80245300	2.57100000	-1.12777500
C	1.23970500	1.16370500	-0.59951900
H	1.49979400	3.34184600	-0.78881200
H	0.98431600	0.42559800	-1.36547700
Cl	-3.38509000	4.61994900	-0.60556100
Cl	-2.61496000	3.15425000	1.99833500
C	-0.70402700	4.10963000	0.13313000
O	0.19421400	4.96592000	0.30616200
N	-0.49100300	2.96363300	-0.56409500
C	0.73846300	2.57844600	-2.66679700
H	1.72952600	2.37916700	-3.08323100
H	0.41378700	3.57133700	-3.00288500
O	-0.12474500	1.53551600	-3.18730700
H	-1.00071300	1.59249900	-2.74557200
O	0.44242700	0.89187500	0.60213700
H	0.60201400	-0.02141700	0.93892600
C	2.72539500	1.10916400	-0.30900500
C	3.59993500	0.48698000	-1.21604300
C	3.24358200	1.69350400	0.86184800
C	4.97348400	0.45259500	-0.96993400
H	3.20330000	0.01686700	-2.11017400
C	4.61184000	1.66170600	1.12345500
H	2.56588300	2.16216700	1.56631000
C	5.45860700	1.04090600	0.19951400
H	5.66359300	-0.02179100	-1.65496800
H	5.03034500	2.10453700	2.01749700
N	6.89797800	0.99816100	0.47037900
O	7.31955600	1.53366600	1.53545300
O	7.64601200	0.42544400	-0.37403200
O	-1.55211100	2.01560900	-0.72674200
H	-1.30673000	1.30705500	-0.06676300

OAR pathway

²TS₀

Fe	2.02907	-1.01456	0.09997
O	0.74175	0.42431	-0.52723

S	3.59486	-2.64259	0.51012
H	3.01394	-3.2031	1.63262
N	0.51827	-2.3394	0.27253
C	-1.12044	-3.7571	1.11015
C	-0.9841	-4.03808	-0.22009
H	-1.7847	-4.21765	1.82716
H	-1.5191	-4.76976	-0.80782
N	2.13874	-1.34293	-1.87748
C	1.42622	-2.29658	-2.58916
C	1.825	-2.26885	-3.98246
C	2.77829	-1.30021	-4.10777
H	1.41784	-2.91203	-4.74896
H	3.31038	-0.99445	-4.99688
N	3.47902	0.37747	-0.06972
C	4.14541	0.76277	-1.22273
C	4.0631	1.08282	0.96917
C	5.16023	1.7446	-0.89872
C	5.11363	1.93758	0.45294
H	5.82227	2.20364	-1.61877
H	5.72544	2.59074	1.05832
N	1.80729	-0.57461	2.06772
C	2.30421	0.16149	4.21309
H	2.80548	0.7041	5.00162
C	2.65676	0.23939	2.81502
C	-0.17769	-2.70348	1.42039
C	0.0399	-3.15809	-0.74099
C	2.9792	-0.72842	-2.79156
C	3.68757	1.01535	2.30378
H	4.24711	1.62142	3.00819
C	0.02113	-2.16432	2.68383
H	-0.58042	-2.55614	3.49708
C	0.46078	-3.14061	-2.06296
H	-0.01573	-3.83733	-2.74415
C	3.90463	0.26059	-2.49254
H	4.5047	0.64897	-3.3086
C	1.26053	-0.71713	4.32206
H	0.74775	-1.03825	5.21754
C	0.96443	-1.19462	2.99218
C	0.46825	3.7999	-1.33594
H	1.44002	4.28187	-1.29309
C	-1.9797	1.89672	-0.4467
C	-2.44307	0.43734	-0.74728
H	-1.97024	2.43461	-1.39652
H	-2.18128	-0.19175	0.11061
Cl	0.39055	2.84639	-2.89996
Cl	-0.47244	4.90314	-0.25736

C	0.22991	3.1098	-0.00521
O	0.66652	3.61527	1.02385
N	-0.53719	1.84952	0.08365
C	-2.77857	2.66965	0.60022
H	-3.83391	2.68974	0.31331
H	-2.41923	3.70353	0.67595
O	-2.57636	1.94967	1.85243
H	-2.86317	2.4672	2.62838
O	-2.13617	-0.05486	-2.06734
H	-2.77912	-0.78639	-2.2518
C	-3.93703	0.34917	-0.99352
C	-4.82874	0.20401	0.08547
C	-4.4378	0.39131	-2.30518
C	-6.20253	0.11741	-0.13621
H	-4.43928	0.15826	1.09707
C	-5.81046	0.30545	-2.54066
H	-3.73803	0.46151	-3.12761
C	-6.67435	0.17387	-1.45066
H	-6.9051	0.00011	0.67816
H	-6.21683	0.33292	-3.54309
N	-8.11668	0.0855	-1.69011
O	-8.52756	0.13819	-2.88494
O	-8.88063	-0.03569	-0.68845
H	-0.57422	1.58353	1.08897
⁴ TS ₀			
Fe	-2.06555600	-1.00711200	-0.00635600
O	-0.86136700	0.44290500	0.52162400
S	-3.75150300	-2.75434400	-0.21823900
H	-2.89738400	-3.84073500	-0.24190600
N	-0.48786700	-2.39804800	-0.34948600
C	1.13397700	-3.70038700	-1.35904200
C	1.21907300	-3.91703500	-0.00784100
H	1.73523700	-4.14256500	-2.14054700
H	1.90321900	-4.56750000	0.51772700
N	-1.89541100	-1.32435300	1.96160700
C	-1.04129500	-2.22188700	2.59968700
C	-1.31032800	-2.19171000	4.02225600
C	-2.32506900	-1.29918800	4.23013500
H	-0.78434100	-2.78365400	4.75696300
H	-2.79081000	-1.02970800	5.16686700
N	-3.66692200	0.30267700	0.30339700
C	-4.16452600	0.68924800	1.52645800
C	-4.29481300	1.05714400	-0.65936600
C	-5.18050700	1.71169000	1.32601100
C	-5.26129200	1.93793500	-0.02191100
H	-5.74685200	2.18709400	2.11395300

H	-5.90247500	2.63574400	-0.54084800
N	-2.08495000	-0.61602000	-1.99082200
C	-2.88354000	0.03192800	-4.06085700
H	-3.49096200	0.54173600	-4.79450200
C	-3.03491000	0.17512700	-2.62955800
C	0.06464000	-2.74105900	-1.56880800
C	0.20012500	-3.09563500	0.61976200
C	-2.70312000	-0.75595800	2.94106800
C	-4.00835100	0.97191300	-2.02041200
H	-4.60879300	1.58262700	-2.68711800
C	-0.37237100	-2.23206700	-2.79105500
H	0.10615500	-2.61951200	-3.68531500
C	-0.07576900	-3.01504200	1.98735800
H	0.52637400	-3.63311400	2.64567400
C	-3.72695300	0.17064000	2.74402900
H	-4.22835200	0.52625400	3.63889100
C	-1.87095100	-0.86324300	-4.28077700
H	-1.49526100	-1.22239300	-5.22809900
C	-1.38183400	-1.28897800	-2.98815600
C	-0.43892100	3.74433000	0.50772300
H	-1.33540900	4.34660400	0.60533900
C	1.57959300	1.52837300	-0.46213100
C	2.02270800	0.14864700	0.13122200
H	1.83924600	2.29172400	0.27207400
H	1.58959300	-0.63877400	-0.49647500
Cl	0.01597900	3.15764400	2.19515200
Cl	0.87318300	4.95298700	-0.14063800
C	-0.70469100	2.69301700	-0.55562700
O	-1.65147300	2.89372000	-1.33292800
N	0.09456300	1.54180100	-0.67302300
C	2.21174200	1.87761200	-1.81341800
H	3.30254000	1.86721900	-1.72546900
H	1.89220500	2.87711600	-2.13189400
O	1.74521400	0.85618300	-2.74757400
H	1.95235700	1.09356300	-3.67136200
O	1.54078600	0.05650800	1.48185400
C	3.53103900	-0.00641800	0.15941000
C	4.21744800	-0.53060500	-0.95154000
C	4.25342100	0.35891200	1.30799400
C	5.60410300	-0.67430700	-0.92766300
H	3.65700900	-0.82424500	-1.83278900
C	5.64111500	0.22105000	1.34549800
H	3.70891600	0.72128700	2.17029300
C	6.29827900	-0.29090400	0.22337300
H	6.15010100	-1.07922400	-1.76942500
H	6.21536500	0.49519100	2.22064100

N	7.75433600	-0.43757600	0.25456700
O	8.36753500	-0.09078400	1.30526200
O	8.32966600	-0.90172300	-0.77318700
H	-0.17667800	0.98381800	-1.49015200
H	0.54447600	0.11243800	1.43080600
²INT_o			
Fe	2.02907300	-1.01455900	0.09997000
O	0.69818000	0.47301100	-0.54845900
S	3.59485600	-2.64258800	0.51011700
H	3.01393700	-3.20310100	1.63261600
N	0.51827300	-2.33940300	0.27252600
C	-1.12044100	-3.75709800	1.11015100
C	-0.98409600	-4.03808400	-0.22008700
H	-1.78469800	-4.21764900	1.82715500
H	-1.51909600	-4.76975800	-0.80781600
N	2.13874200	-1.34292800	-1.87748300
C	1.42621600	-2.29657500	-2.58916000
C	1.82500400	-2.26885300	-3.98245700
C	2.77828900	-1.30021200	-4.10777300
H	1.41783700	-2.91203300	-4.74895900
H	3.31038400	-0.99445200	-4.99688000
N	3.47902100	0.37747000	-0.06971600
C	4.14541100	0.76277000	-1.22273100
C	4.06310100	1.08282100	0.96917000
C	5.16023400	1.74460100	-0.89871900
C	5.11363200	1.93757500	0.45294400
H	5.82226500	2.20363500	-1.61877300
H	5.72543800	2.59073800	1.05831500
N	1.80728700	-0.57461000	2.06772000
C	2.30421000	0.16149300	4.21309100
H	2.80548300	0.70410400	5.00161700
C	2.65676200	0.23938800	2.81501600
C	-0.17769200	-2.70348000	1.42038500
C	0.03990100	-3.15809200	-0.74099200
C	2.97920000	-0.72841800	-2.79156200
C	3.68757200	1.01535300	2.30378400
H	4.24710900	1.62142400	3.00818700
C	0.02113000	-2.16431500	2.68382900
H	-0.58042100	-2.55613700	3.49708400
C	0.46077900	-3.14061200	-2.06295900
H	-0.01572700	-3.83732600	-2.74414500
C	3.90462700	0.26059100	-2.49253900
H	4.50470200	0.64897300	-3.30859600
C	1.26052800	-0.71713200	4.32206000
H	0.74774800	-1.03825300	5.21753700
C	0.96442800	-1.19462000	2.99217800

C	0.73657400	3.49822900	-0.69879700
H	1.70850300	3.98030600	-0.73664300
C	-1.54238300	1.40636500	0.21539400
C	-2.07945600	0.02993400	-0.28646100
H	-1.69658200	2.12640700	-0.59042000
H	-1.67705500	-0.75535900	0.36288400
Cl	0.35731000	2.88169400	-2.38326300
Cl	-0.47243800	4.90314200	-0.25736100
C	0.73250700	2.54718100	0.48416000
O	1.35876900	2.84105500	1.49733700
N	-0.02841800	1.28044200	0.45285000
C	-2.12249600	1.93424100	1.52553500
H	-3.21192400	1.99165000	1.44611400
H	-1.73650900	2.93788900	1.74341800
O	-1.70836200	0.97854500	2.54653100
H	-1.83922400	1.32158600	3.45063400
O	-1.63921100	-0.15020900	-1.64760800
H	-0.64882400	-0.11294600	-1.63065900
C	-3.59462600	-0.03547400	-0.26882100
C	-4.27695100	-0.41463800	0.90212500
C	-4.32550500	0.26295700	-1.43060100
C	-5.66947200	-0.48117100	0.92179200
H	-3.71030900	-0.65771400	1.79485000
C	-5.71943000	0.19997900	-1.42426700
H	-3.78642000	0.51276200	-2.33502400
C	-6.37214800	-0.16758900	-0.24503700
H	-6.21365000	-0.77550100	1.80937900
H	-6.30134900	0.42295900	-2.30880100
N	-7.83531900	-0.23357100	-0.23033000
O	-8.45632100	0.05317000	-1.29397300
O	-8.40572500	-0.57102900	0.84781200
H	0.11377800	0.81471600	1.37246400
⁴INT₀			
Fe	2.17612100	-1.05258500	0.12028400
O	0.62761200	0.70873200	-0.63758800
S	3.89002400	-2.77394000	0.63605800
H	3.14157600	-3.89180700	0.31673800
N	0.65473900	-2.36312400	-0.00639100
C	-1.03153900	-3.85558300	0.55071200
C	-0.80723700	-3.98216600	-0.79268900
H	-1.74452600	-4.38918000	1.16233500
H	-1.30339400	-4.63647700	-1.49442400
N	2.41537900	-1.14841200	-1.88207900
C	1.74605300	-1.98325600	-2.76497600
C	2.27984200	-1.81472800	-4.09999600
C	3.27952200	-0.88797000	-4.01847200

H	1.92946700	-2.34780700	-4.97176800
H	3.91110100	-0.51261600	-4.81042100
N	3.58207200	0.37906800	0.22576600
C	4.39351000	0.81883000	-0.81133700
C	4.00940200	1.04943200	1.36285100
C	5.35382200	1.77429600	-0.30755800
C	5.11798300	1.91517000	1.03201000
H	6.10497100	2.26412300	-0.91001600
H	5.63594800	2.54510700	1.74039200
N	1.66782800	-0.67795500	2.05688700
C	1.84892300	-0.05147100	4.28502900
H	2.21821700	0.46212500	5.16098900
C	2.37160100	0.12810100	2.95135800
C	-0.12655900	-2.84216200	1.04162900
C	0.24011800	-3.05204300	-1.14137500
C	3.36856000	-0.47746900	-2.63314900
C	3.44988600	0.93511700	2.62784700
H	3.89751100	1.51641500	3.42629300
C	-0.07774700	-2.39914400	2.35602200
H	-0.73849100	-2.87905100	3.06984300
C	0.73970000	-2.87275400	-2.42296800
H	0.30911700	-3.47373000	-3.21613000
C	4.29242900	0.42893700	-2.13854000
H	4.99365600	0.86429500	-2.84223200
C	0.85932000	-0.99369800	4.21021100
H	0.26343400	-1.40282200	5.01349100
C	0.76156400	-1.40240900	2.82909400
C	0.41775700	3.70249800	-0.76858800
H	1.34086400	4.26609100	-0.85793400
C	-1.66436400	1.46467500	0.21209000
C	-2.11579900	0.05875500	-0.29133900
H	-1.90047500	2.18452400	-0.57314400
H	-1.65431000	-0.70034600	0.35093900
Cl	-0.03291500	3.10958800	-2.44502000
Cl	-0.86201600	4.98219200	-0.18267100
C	0.58796800	2.71499900	0.37305500
O	1.34242400	2.99250000	1.30001200
N	-0.14169500	1.43633500	0.39284300
C	-2.23378500	1.92347600	1.55233500
H	-3.32683300	1.90980600	1.51129200
H	-1.90643800	2.94500300	1.78266000
O	-1.72185700	0.97381700	2.53506100
H	-1.85222200	1.27947600	3.45244700
O	-1.67976000	-0.08613800	-1.65790600
H	-0.69443500	0.04777500	-1.65006200
C	-3.62275500	-0.10682400	-0.25415700

C	-4.26582400	-0.52807100	0.92465700
C	-4.38501500	0.14511500	-1.40672100
C	-5.65120800	-0.68098200	0.96137800
H	-3.67409600	-0.73501100	1.81041300
C	-5.77206100	-0.00472800	-1.38359000
H	-3.87253100	0.42889500	-2.31660800
C	-6.38627000	-0.41193900	-0.19664300
H	-6.16539500	-1.00775100	1.85549400
H	-6.37761200	0.18183000	-2.26067200
N	-7.84217500	-0.56816500	-0.16395000
O	-8.49251400	-0.32336100	-1.22054300
O	-8.37762300	-0.93727800	0.92176800
H	0.05314000	0.96866700	1.29947600
²TS-rebo			
Fe	2.37182800	-1.21141000	0.07965700
O	-0.03333100	0.62074300	-0.65858200
S	4.05347700	-2.82042600	0.43509000
H	3.55613600	-3.38467600	1.59505000
N	1.06519700	-2.33960500	-1.08901500
C	-0.50252300	-3.91139100	-1.74196000
C	0.15993300	-3.50736400	-2.86855700
H	-1.29956800	-4.63643300	-1.66304900
H	0.00666000	-3.83853300	-3.88532300
N	3.24731200	-0.52039300	-1.59531600
C	3.06756100	-1.01569200	-2.88175700
C	4.01315500	-0.37452400	-3.77424100
C	4.74606200	0.50555700	-3.03058100
H	4.08332800	-0.57189500	-4.83387500
H	5.53130000	1.16811600	-3.36381700
N	3.21516600	0.38645900	1.14738900
C	4.22929600	1.21357700	0.68851000
C	3.11270000	0.60488600	2.51381900
C	4.73913300	2.00812600	1.78741300
C	4.05076700	1.63516700	2.91018400
H	5.52585400	2.74340800	1.70344600
H	4.17206200	2.00602900	3.91757800
N	1.27599800	-1.67268300	1.71240400
C	0.58377300	-1.89399600	3.90960100
H	0.53741900	-1.72501600	4.97624100
C	1.45396700	-1.17578900	3.00245200
C	0.07534300	-3.18775700	-0.62487300
C	1.15242100	-2.53360600	-2.45433300
C	4.26463400	0.42536100	-1.66572500
C	2.29015800	-0.12294900	3.36772300
H	2.31115900	0.14178300	4.42002200
C	-0.25680200	-3.35162500	0.71530500

H	-1.03215600	-4.07378900	0.94909400
C	2.09644700	-1.92852700	-3.27913900
H	2.07407300	-2.18993500	-4.33190500
C	4.71122900	1.22449300	-0.61804700
H	5.51123500	1.92189600	-0.84283200
C	-0.11773000	-2.80873900	3.16676600
H	-0.85691900	-3.51854300	3.50953000
C	0.30070800	-2.66339000	1.78995300
C	1.08972800	3.10038400	-0.30397700
H	1.71108800	2.21341500	-0.33935700
C	-2.24085400	1.43083100	0.55576900
C	-2.77532700	0.44412300	-0.52384500
H	-2.69109400	2.41231900	0.38340900
H	-2.28815500	-0.52274300	-0.36976000
Cl	0.63505300	3.48613600	-2.08320400
Cl	2.07199200	4.47884900	0.42230800
C	-0.20996300	2.90597500	0.45068900
O	-0.79936000	3.78434200	1.08299300
N	-0.75547100	1.59521900	0.38189200
C	-2.47000000	0.98927400	1.99949100
H	-3.54350400	0.92985400	2.20794800
H	-2.01661600	1.71572600	2.68325600
O	-1.84251500	-0.31899000	2.10490500
H	-1.56561100	-0.55317500	3.01178600
O	-2.45019400	0.97842300	-1.82544700
H	-1.47867700	0.86227500	-1.94485900
C	-4.27793300	0.27481500	-0.43302200
C	-4.83190600	-0.65907400	0.46214800
C	-5.12704700	1.03970800	-1.24997200
C	-6.21376400	-0.81975300	0.55504900
H	-4.17294100	-1.26086400	1.08006500
C	-6.51140200	0.88741300	-1.16805400
H	-4.68696900	1.72769800	-1.96012400
C	-7.03545400	-0.03864000	-0.26218900
H	-6.66060000	-1.53442400	1.23334700
H	-7.18341300	1.46395300	-1.78992100
N	-8.48751000	-0.20337000	-0.17016800
O	-9.21797700	0.50715200	-0.91926700
O	-8.94060400	-1.04778900	0.65679800
H	-0.13788700	0.63059500	0.64766200
⁴TS-rebo			
Fe	2.37182800	-1.21141000	0.07965700
O	-0.03333100	0.62074300	-0.65858200
S	4.05347700	-2.82042600	0.43509000
H	3.55613600	-3.38467600	1.59505000
N	1.06519700	-2.33960500	-1.08901500

C	-0.50252300	-3.91139100	-1.74196000
C	0.15993300	-3.50736400	-2.86855700
H	-1.29956800	-4.63643300	-1.66304900
H	0.00666000	-3.83853300	-3.88532300
N	3.24731200	-0.52039300	-1.59531600
C	3.06756100	-1.01569200	-2.88175700
C	4.01315500	-0.37452400	-3.77424100
C	4.74606200	0.50555700	-3.03058100
H	4.08332800	-0.57189500	-4.83387500
H	5.53130000	1.16811600	-3.36381700
N	3.21516600	0.38645900	1.14738900
C	4.22929600	1.21357700	0.68851000
C	3.11270000	0.60488600	2.51381900
C	4.73913300	2.00812600	1.78741300
C	4.05076700	1.63516700	2.91018400
H	5.52585400	2.74340800	1.70344600
H	4.17206200	2.00602900	3.91757800
N	1.27599800	-1.67268300	1.71240400
C	0.58377300	-1.89399600	3.90960100
H	0.53741900	-1.72501600	4.97624100
C	1.45396700	-1.17578900	3.00245200
C	0.07534300	-3.18775700	-0.62487300
C	1.15242100	-2.53360600	-2.45433300
C	4.26463400	0.42536100	-1.66572500
C	2.29015800	-0.12294900	3.36772300
H	2.31115900	0.14178300	4.42002200
C	-0.25680200	-3.35162500	0.71530500
H	-1.03215600	-4.07378900	0.94909400
C	2.09644700	-1.92852700	-3.27913900
H	2.07407300	-2.18993500	-4.33190500
C	4.71122900	1.22449300	-0.61804700
H	5.51123500	1.92189600	-0.84283200
C	-0.11773000	-2.80873900	3.16676600
H	-0.85691900	-3.51854300	3.50953000
C	0.30070800	-2.66339000	1.78995300
C	1.08972800	3.10038400	-0.30397700
H	1.71108800	2.21341500	-0.33935700
C	-2.24085400	1.43083100	0.55576900
C	-2.77532700	0.44412300	-0.52384500
H	-2.69109400	2.41231900	0.38340900
H	-2.28815500	-0.52274300	-0.36976000
Cl	0.63505300	3.48613600	-2.08320400
Cl	2.07199200	4.47884900	0.42230800
C	-0.20996300	2.90597500	0.45068900
O	-0.79936000	3.78434200	1.08299300
N	-0.75547100	1.59521900	0.38189200

C	-2.47000000	0.98927400	1.99949100
H	-3.54350400	0.92985400	2.20794800
H	-2.01661600	1.71572600	2.68325600
O	-1.84251500	-0.31899000	2.10490500
H	-1.56561100	-0.55317500	3.01178600
O	-2.45019400	0.97842300	-1.82544700
H	-1.47867700	0.86227500	-1.94485900
C	-4.27793300	0.27481500	-0.43302200
C	-4.83190600	-0.65907400	0.46214800
C	-5.12704700	1.03970800	-1.24997200
C	-6.21376400	-0.81975300	0.55504900
H	-4.17294100	-1.26086400	1.08006500
C	-6.51140200	0.88741300	-1.16805400
H	-4.68696900	1.72769800	-1.96012400
C	-7.03545400	-0.03864000	-0.26218900
H	-6.66060000	-1.53442400	1.23334700
H	-7.18341300	1.46395300	-1.78992100
N	-8.48751000	-0.20337000	-0.17016800
O	-9.21797700	0.50715200	-0.91926700
O	-8.94060400	-1.04778900	0.65679800
H	-0.13788700	0.63059500	0.64766200

C-H hydroxylation through Path B

²RC₁

Fe	-3.56839400	-0.18751500	-0.03475100
O	-2.01840700	-0.40902600	0.49509200
S	-5.98708300	0.45067000	-0.64407400
H	-5.71009800	1.29107600	-1.70633700
N	-3.00464100	0.15600400	-1.93954200
C	-2.13029900	1.15903000	-3.83904800
C	-2.27455800	-0.16948400	-4.11869700
H	-1.74589600	1.94213300	-4.47524700
H	-2.03753200	-0.69288900	-5.03328300
N	-3.88247800	-2.12449500	-0.47637500
C	-3.58562200	-2.76331400	-1.66693500
C	-3.87467300	-4.17646300	-1.55786800
C	-4.34871000	-4.38909100	-0.29477800
H	-3.73075300	-4.89546200	-2.35092500
H	-4.67101000	-5.31706600	0.15419600
N	-4.39444000	-0.47302200	1.78478000
C	-4.79485500	-1.68219000	2.33548800
C	-4.56198700	0.47263000	2.78267200
C	-5.22888900	-1.48379500	3.70121000
C	-5.08194400	-0.15540500	3.97817000
H	-5.59406100	-2.26782200	4.34818900
H	-5.30391600	0.36686900	4.89715100

N	-3.53574600	1.80561100	0.31413400
C	-3.54493600	3.86149000	1.39506900
H	-3.69367900	4.58216100	2.18575400
C	-3.82243700	2.44723400	1.51469700
C	-2.58488900	1.35709100	-2.48108000
C	-2.81343800	-0.79487400	-2.93094900
C	-4.35175600	-3.10702800	0.37533300
C	-4.28605000	1.82651800	2.66094100
H	-4.45826500	2.45048600	3.53139800
C	-2.60607900	2.58352900	-1.82982600
H	-2.22702600	3.44093500	-2.37388600
C	-3.08992600	-2.14673100	-2.80702800
H	-2.89761000	-2.77589900	-3.66970000
C	-4.77690100	-2.90229700	1.68150700
H	-5.12112400	-3.76985600	2.23452500
C	-3.07365000	4.07528100	0.13217900
H	-2.75678700	5.00504200	-0.31686200
C	-3.05470200	2.79505900	-0.53936700
C	0.95567500	0.24237600	0.31222900
H	-0.13131500	0.15391800	0.27737200
C	3.93346900	1.14373800	-0.06605900
C	4.93944900	0.69808400	-1.16560100
H	3.65028700	0.26297600	0.51129200
H	5.19571000	1.58360200	-1.76083100
Cl	1.61466800	-1.45961600	-0.08483000
Cl	1.35816900	0.69184000	2.10509800
C	1.43408100	1.32878700	-0.64291800
O	0.55865400	1.89729300	-1.33596500
N	2.73932700	1.70953800	-0.69638800
H	2.90864700	2.50178200	-1.30596100
C	4.54984100	2.18056000	0.87499300
H	5.39563800	1.75136100	1.42389400
H	3.78680600	2.50943900	1.58732400
O	4.99595700	3.28850100	0.02711400
H	5.17475200	4.08640600	0.56005300
O	4.21645800	-0.26711200	-1.97637100
H	4.72902100	-0.48690900	-2.78017300
C	6.21402300	0.09710300	-0.59630400
C	7.35124500	0.89897100	-0.38803300
C	6.26502200	-1.27103200	-0.27492800
C	8.52148400	0.34979200	0.13493500
H	7.30704500	1.95666400	-0.62639200
C	7.42865900	-1.83334100	0.24960200
H	5.39028400	-1.88569800	-0.45233400
C	8.54261800	-1.01258500	0.44621000
H	9.40793700	0.94795100	0.29948200

H	7.48769200	-2.88330200	0.50434900
N	9.77007900	-1.59642200	0.99146300
O	9.77447500	-2.83237500	1.25995300
O	10.76515100	-0.83470600	1.16764500
⁴RC₁			
Fe	-3.57262900	-0.17881300	-0.03526200
O	-2.02264700	-0.42287700	0.49178600
S	-5.98168200	0.40077800	-0.66954800
H	-5.71303100	1.27259900	-1.70823700
N	-2.99077700	0.17568300	-1.93291500
C	-2.10921600	1.19382600	-3.82114700
C	-2.24186200	-0.13419200	-4.10814700
H	-1.72543600	1.98268100	-4.45055700
H	-1.99373400	-0.65156700	-5.02322000
N	-3.85843000	-2.12358800	-0.48749600
C	-3.54564800	-2.75278400	-1.67829600
C	-3.81223300	-4.17118200	-1.57567100
C	-4.28817700	-4.39593600	-0.31544500
H	-3.65234700	-4.88502200	-2.37032600
H	-4.59675600	-5.33067000	0.12912900
N	-4.40649500	-0.48519100	1.77671700
C	-4.79541400	-1.70240100	2.31892100
C	-4.60139100	0.45437400	2.77498500
C	-5.24830900	-1.51462900	3.68001500
C	-5.12566100	-0.18488700	3.96246200
H	-5.60906100	-2.30612200	4.32036200
H	-5.36692200	0.33116800	4.88008800
N	-3.56145100	1.80597000	0.32183700
C	-3.62494800	3.86090100	1.40341500
H	-3.79832900	4.57807300	2.19225000
C	-3.87813500	2.44195500	1.51849400
C	-2.57689000	1.38205700	-2.46614000
C	-2.78562100	-0.76948800	-2.92760900
C	-4.31573400	-3.11585900	0.35856100
C	-4.34516000	1.81270200	2.65854100
H	-4.53831000	2.43297600	3.52724500
C	-2.62001900	2.60530000	-1.81019400
H	-2.24736700	3.47027800	-2.34668600
C	-3.05161100	-2.12407600	-2.81280500
H	-2.84796600	-2.74653400	-3.67777300
C	-4.75349200	-2.92042000	1.66209700
H	-5.08954500	-3.79419100	2.21038000
C	-3.13991000	4.08432400	0.14745000
H	-2.83448400	5.02024700	-0.29670600
C	-3.08834000	2.80557800	-0.52488800
C	0.95752900	0.22313600	0.31015700

H	-0.12905200	0.13255400	0.27332900
C	3.93201500	1.14344900	-0.05065000
C	4.94133000	0.71392600	-1.15357000
H	3.65183400	0.25527600	0.51678000
H	5.19366100	1.60663900	-1.73963100
Cl	1.62118900	-1.47118800	-0.11088500
Cl	1.35756900	0.64808100	2.10933400
C	1.43278600	1.32392200	-0.63003900
O	0.55589600	1.89701200	-1.31737800
N	2.73634700	1.71120300	-0.67632400
H	2.90305600	2.51207800	-1.27528000
C	4.54273800	2.17286300	0.90211200
H	5.39000700	1.74173200	1.44718400
H	3.77762900	2.49079600	1.61717100
O	4.98453700	3.29178300	0.06643700
H	5.15875700	4.08494500	0.60790000
O	4.22392000	-0.24666700	-1.97466000
H	4.73828600	-0.45585100	-2.78013500
C	6.21834100	0.11373700	-0.58889800
C	7.35147300	0.91914400	-0.37209300
C	6.27573200	-1.25705500	-0.28017700
C	8.52387800	0.37085200	0.14694300
H	7.30234200	1.97880100	-0.60053000
C	7.44156000	-1.81850200	0.24042300
H	5.40426000	-1.87441300	-0.46420900
C	8.55130800	-0.99419400	0.44574800
H	9.40725700	0.97176700	0.31786200
H	7.50542500	-2.87044800	0.48563000
N	9.78100100	-1.57704800	0.98706100
O	9.79090100	-2.81526000	1.24474000
O	10.77230800	-0.81225700	1.17087800
²TS-H₁			
Fe	-2.18263000	-0.92094300	0.19822400
O	-0.88274000	0.05644300	-0.46957400
S	-3.89758000	-2.40152200	1.12327900
H	-3.96692000	-3.27863800	0.05842400
N	-3.33042900	0.62092200	0.75719700
C	-4.21018500	2.41857700	1.92670600
C	-4.94944900	2.27838600	0.78866000
H	-4.31701400	3.15310800	2.71053300
H	-5.78227300	2.87773600	0.45239900
N	-3.16407500	-1.02900900	-1.55002400
C	-4.22819500	-0.24097000	-1.95585000
C	-4.59918300	-0.58260000	-3.31143000
C	-3.74569000	-1.56437400	-3.72727900
H	-5.40119600	-0.11419700	-3.86241500

H	-3.71431000	-2.06408600	-4.68424200
N	-1.16845600	-2.59402600	-0.28172100
C	-1.12005200	-3.20154900	-1.52679800
C	-0.30351600	-3.30896300	0.53449800
C	-0.20147200	-4.31783000	-1.48957100
C	0.29086100	-4.39213700	-0.21749200
H	0.01890600	-4.95760700	-2.33137800
H	0.99865300	-5.10114200	0.18618100
N	-1.35201400	-0.94866100	2.04035600
C	-0.05828300	-1.51905200	3.87371200
H	0.60190300	-2.10228300	4.49961400
C	-0.47867400	-1.90123400	2.54350700
C	-3.21083600	1.37390200	1.91684300
C	-4.39266200	1.16542400	0.05259700
C	-2.85478900	-1.85073400	-2.62411800
C	-0.00617700	-3.00810400	1.85369600
H	0.68326000	-3.66475900	2.37308500
C	-2.32278600	1.12577500	2.94939900
H	-2.32570800	1.81155700	3.78873800
C	-4.82007700	0.76011400	-1.20141300
H	-5.65352800	1.29459500	-1.64303000
C	-1.88508900	-2.84072800	-2.62595100
H	-1.74818900	-3.40747100	-3.54022400
C	-0.66757400	-0.32479600	4.16149100
H	-0.60643300	0.25682500	5.06997900
C	-1.48376200	0.02152500	3.01964900
C	-0.52759300	2.48973200	-1.14683200
H	-0.82422700	1.11561200	-0.85047200
C	2.08522100	1.59153500	0.33415400
C	3.49247800	2.24395100	0.39771100
H	1.89728100	1.28587000	-0.69378200
H	3.62892100	2.63766800	1.41381600
Cl	-2.10080700	3.21781400	-1.72274100
Cl	0.68634600	2.48871400	-2.53943500
C	-0.07423700	3.03270200	0.19395400
O	-0.83014600	3.80370200	0.83233300
N	1.08600000	2.58170600	0.75164100
H	1.21292200	2.91651400	1.70084700
C	1.96351400	0.36193700	1.23368600
H	2.67511000	-0.41388900	0.93037000
H	0.94836600	-0.02530700	1.13395600
O	2.24749800	0.79419700	2.60484700
H	1.70236300	0.28333400	3.23600800
O	3.45572900	3.33146800	-0.56806900
H	4.22635600	3.92123400	-0.44421800
C	4.62283400	1.27445900	0.09245200

C	5.23606600	0.54789100	1.13018300
C	5.06405900	1.09565900	-1.23021000
C	6.26984000	-0.34608800	0.85563700
H	4.88076800	0.67355600	2.14785200
C	6.09667200	0.20369000	-1.51941500
H	4.59680700	1.67052500	-2.02090500
C	6.68632900	-0.50564300	-0.46949100
H	6.75552200	-0.91279900	1.63897500
H	6.44907600	0.05057800	-2.53093300
N	7.77063300	-1.44328500	-0.76438700
O	8.13894100	-1.57152200	-1.96811700
O	8.28595700	-2.08239800	0.19907400
⁴TS- H₁			
Fe	2.16229000	0.97399800	0.18623900
O	0.88547600	-0.00870300	-0.51572100
S	3.94226100	2.18121800	1.26105100
H	4.88805800	2.08944900	0.25844100
N	3.28016500	-0.66217200	0.67484300
C	4.12865300	-2.50516000	1.80051300
C	4.83718700	-2.38235500	0.64257800
H	4.22837700	-3.25245200	2.57296900
H	5.63511200	-3.01018300	0.27500300
N	3.15164600	1.08572700	-1.56301600
C	4.15437600	0.24479500	-2.02495800
C	4.51785300	0.61301600	-3.37470800
C	3.71816100	1.66106200	-3.73465600
H	5.27565400	0.11580900	-3.96199100
H	3.69568400	2.19515600	-4.67311000
N	1.15293400	2.63729400	-0.25346400
C	1.14647200	3.30192500	-1.46936500
C	0.31344300	3.35681900	0.58172000
C	0.26034000	4.44595800	-1.40058100
C	-0.24366400	4.48674000	-0.13356400
H	0.07382600	5.12614800	-2.21855000
H	-0.92947700	5.20413200	0.29263800
N	1.36195400	0.96610900	2.02621800
C	0.10566200	1.51082200	3.89422400
H	-0.53663800	2.08753500	4.54437400
C	0.50571400	1.91486100	2.56578000
C	3.16712300	-1.42243000	1.82717900
C	4.29930600	-1.23926100	-0.06583800
C	2.86738400	1.95446400	-2.60324500
C	0.03362100	3.03928600	1.90083400
H	-0.63436300	3.69858300	2.44460900
C	2.30790300	-1.15350000	2.87960200
H	2.30537300	-1.84984500	3.71052200

C	4.70728800	-0.81646600	-1.32051900
H	5.49788400	-1.37848300	-1.80531100
C	1.92522100	2.97347400	-2.56668700
H	1.81535000	3.58217500	-3.45768300
C	0.70754800	0.30401900	4.14651600
H	0.65289600	-0.29624100	5.04318700
C	1.49859000	-0.02990800	2.98505200
C	0.56443400	-2.49324300	-1.10893600
H	0.89618500	-1.07689800	-0.81970400
C	-2.06324000	-1.53793100	0.36082300
C	-3.45862300	-2.21721900	0.41950000
H	-1.87229900	-1.23658300	-0.66722600
H	-3.59541500	-2.60382700	1.43824900
Cl	2.07622600	-3.32402100	-1.70345400
Cl	-0.65315800	-2.40052300	-2.49527000
C	0.09712300	-2.99176400	0.24102200
O	0.84090500	-3.76027700	0.89830800
N	-1.04935000	-2.50364900	0.79797100
H	-1.16893500	-2.81070300	1.75763600
C	-1.97237500	-0.29908700	1.25057400
H	-2.70231800	0.45693700	0.94152500
H	-0.96700100	0.11210800	1.14900500
O	-2.24709100	-0.72654900	2.62517000
H	-1.69927700	-0.21311800	3.25183100
O	-3.39088700	-3.31291900	-0.53527500
H	-4.14828500	-3.91935100	-0.41066000
C	-4.60527600	-1.27395000	0.09497400
C	-5.24520600	-0.55347200	1.12078300
C	-5.03486000	-1.11259400	-1.23380300
C	-6.29351500	0.31773400	0.82860000
H	-4.90057400	-0.66612400	2.14367600
C	-6.08185400	-0.24362500	-1.54064100
H	-4.54708700	-1.68307600	-2.01523400
C	-6.69773300	0.46041400	-0.50221900
H	-6.79964600	0.87935700	1.60259500
H	-6.42561300	-0.10419900	-2.55709800
N	-7.79757200	1.37361100	-0.81560200
O	-8.15506300	1.48601400	-2.02416800
O	-8.33660800	2.00849900	0.13763500
²INT₁			
Fe	-3.51180888	0.14208129	0.04875650
O	-1.96182688	0.38614529	-0.47829150
S	-5.98168200	-0.40077800	0.66954800
H	-5.71303100	-1.27259900	1.70823700
N	-2.99077700	-0.17568300	1.93291500
C	-2.10921600	-1.19382600	3.82114700

C	-2.24186200	0.13419200	4.10814700
H	-1.72543600	-1.98268100	4.45055700
H	-1.99373400	0.65156700	5.02322000
N	-3.85843000	2.12358800	0.48749600
C	-3.54564800	2.75278400	1.67829600
C	-3.81223300	4.17118200	1.57567100
C	-4.28817700	4.39593600	0.31544500
H	-3.65234700	4.88502200	2.37032600
H	-4.59675600	5.33067000	-0.12912900
N	-4.40649500	0.48519100	-1.77671700
C	-4.79541400	1.70240100	-2.31892100
C	-4.60139100	-0.45437400	-2.77498500
C	-5.24830900	1.51462900	-3.68001500
C	-5.12566100	0.18488700	-3.96246200
H	-5.60906100	2.30612200	-4.32036200
H	-5.36692200	-0.33116800	-4.88008800
N	-3.56145100	-1.80597000	-0.32183700
C	-3.62494800	-3.86090100	-1.40341500
H	-3.79832900	-4.57807300	-2.19225000
C	-3.87813500	-2.44195500	-1.51849400
C	-2.57689000	-1.38205700	2.46614000
C	-2.78562100	0.76948800	2.92760900
C	-4.31573400	3.11585900	-0.35856100
C	-4.34516000	-1.81270200	-2.65854100
H	-4.53831000	-2.43297600	-3.52724500
C	-2.62001900	-2.60530000	1.81019400
H	-2.24736700	-3.47027800	2.34668600
C	-3.05161100	2.12407600	2.81280500
H	-2.84796600	2.74653400	3.67777300
C	-4.75349200	2.92042000	-1.66209700
H	-5.08954500	3.79419100	-2.21038000
C	-3.13991000	-4.08432400	-0.14745000
H	-2.83448400	-5.02024700	0.29670600
C	-3.08834000	-2.80557800	0.52488800
C	1.25826768	-0.42838573	-0.14636238
H	-1.12926847	-0.11667013	-0.29356703
C	4.23275368	-1.34869873	0.21444462
C	5.24206868	-0.91917573	1.31736462
H	3.95257268	-0.46052573	-0.35298538
H	5.49439968	-1.81188873	1.90342562
Cl	1.92192768	1.26593827	0.27467962
Cl	1.65830768	-0.85333073	-1.94553938
C	1.73352468	-1.52917173	0.79383362
O	0.85663468	-2.10226173	1.48117262
N	3.03708568	-1.91645273	0.84011862
H	3.20379468	-2.71732773	1.43907462

C	4.84347668	-2.37811273	-0.73831738
H	5.69074568	-1.94698173	-1.28338938
H	4.07836768	-2.69604573	-1.45337638
O	5.28527568	-3.49703273	0.09735762
H	5.45949568	-4.29019473	-0.44410538
O	4.52465868	0.04141727	2.13845462
H	5.03902468	0.25060127	2.94392962
C	6.51907968	-0.31898673	0.75269262
C	7.65221168	-1.12439373	0.53588762
C	6.57647068	1.05180527	0.44397162
C	8.82461668	-0.57610173	0.01685162
H	7.60308068	-2.18405073	0.76432462
C	7.74229868	1.61325227	-0.07662838
H	5.70499868	1.66916327	0.62800362
C	8.85204668	0.78894427	-0.28195338
H	9.70799568	-1.17701673	-0.15406738
H	7.80616368	2.66519827	-0.32183538
N	10.08173968	1.37179827	-0.82326638
O	10.09163968	2.61001027	-1.08094538
O	11.07304668	0.60700727	-1.00708338
⁴INT₁			
Fe	2.16125900	-1.09035900	-0.04739700
O	1.06271900	0.37152400	-0.03695700
S	3.64527200	-2.91158100	-0.12353200
H	3.23458500	-3.53570700	1.03821700
N	1.20064800	-1.94236700	1.50442700
C	0.48829600	-2.46385700	3.64488100
C	-0.33127800	-3.12619800	2.77381600
H	0.46074700	-2.46698400	4.72473700
H	-1.16247600	-3.77814600	2.99949500
N	0.90777200	-2.00593000	-1.32306700
C	-0.14697300	-2.84648700	-1.00139900
C	-0.79971800	-3.29354600	-2.21216900
C	-0.13194200	-2.73063900	-3.26130400
H	-1.65537400	-3.95214500	-2.23700100
H	-0.32939900	-2.83836700	-4.31767300
N	3.23779900	-0.38811900	-1.59068900
C	2.95174800	-0.54856400	-2.93769000
C	4.37129000	0.41029100	-1.52222300
C	3.93878600	0.14953700	-3.72868000
C	4.81373700	0.73592000	-2.85845900
H	3.94383800	0.18163900	-4.80822300
H	5.67619500	1.34575700	-3.08370700
N	3.40091300	-0.14642200	1.24270700
C	5.14470900	1.09205800	2.12802400
H	6.02668200	1.71493100	2.15176400

C	4.51452600	0.61529500	0.91827600
C	1.43868700	-1.71646600	2.85539500
C	0.10226400	-2.79001400	1.43782200
C	0.94262500	-1.93668000	-2.70784300
C	4.97089200	0.87332000	-0.36294400
H	5.85421400	1.49284500	-0.46720000
C	2.42492400	-0.89737200	3.38068700
H	2.49621000	-0.82658700	4.46027100
C	-0.52157700	-3.22033400	0.27743400
H	-1.37171900	-3.88518600	0.37955800
C	1.88267400	-1.25697400	-3.46170100
H	1.78497700	-1.29379400	-4.54067600
C	4.42144100	0.60550700	3.17968500
H	4.59583300	0.74765900	4.23613100
C	3.34088400	-0.18052500	2.62833800
C	-0.53618100	4.20089500	-0.50225200
H	1.44050900	1.22279600	0.29807200
C	-2.31860700	2.21795900	1.11775600
C	-2.13285200	0.79537000	0.47610600
H	-2.80649000	2.84343300	0.36886900
H	-1.58626000	0.17686900	1.19784800
Cl	0.53217700	4.57414800	-1.86238000
Cl	-2.00801600	5.21745300	-0.37658300
C	-0.07975100	3.29174900	0.54734900
O	1.16209400	3.06395200	0.65811900
N	-0.98604100	2.76051500	1.42754600
H	-0.54825500	2.29645800	2.21926000
C	-3.14802100	2.24303400	2.39487700
H	-4.16065200	1.87319500	2.20268200
H	-3.20573800	3.27170800	2.77024600
O	-2.45378200	1.38026500	3.35328400
H	-2.82737800	1.47958900	4.24981800
O	-1.36206400	0.98354400	-0.72104600
H	-0.41280800	0.65886900	-0.58264000
C	-3.45427400	0.12485600	0.14823700
C	-4.15848400	-0.58869800	1.13719400
C	-3.98434100	0.20541500	-1.15081900
C	-5.37552900	-1.20166800	0.84299600
H	-3.74153200	-0.66163400	2.13679000
C	-5.20257300	-0.39970500	-1.45883300
H	-3.41198400	0.72252400	-1.91029200
C	-5.88425300	-1.09470000	-0.45518300
H	-5.92850400	-1.75903200	1.58761700
H	-5.62630100	-0.34914300	-2.45324100
N	-7.15891200	-1.73686100	-0.77162700
O	-7.60505100	-1.63416300	-1.95166100

O	-7.75751400	-2.36543500	0.15090700
²TS-reb₁			
Fe	-2.77882300	-0.28575900	-0.57859400
O	-1.80458400	0.22751900	0.92683900
S	-4.04991600	-0.81827600	-2.51852600
H	-4.87820300	0.28719500	-2.54399100
N	-1.34274200	-1.45317300	-1.32883900
C	0.53189900	-2.18974200	-2.49015200
C	0.02323600	-3.26597500	-1.82438500
H	1.40699100	-2.13953800	-3.12010600
H	0.39184200	-4.28117700	-1.81090200
N	-3.51594000	-1.85730600	0.42302500
C	-3.02891300	-3.14915700	0.44510100
C	-3.84345800	-3.97551500	1.31272900
C	-4.82825300	-3.17444200	1.81289100
H	-3.67165500	-5.02518200	1.50066100
H	-5.62518200	-3.43662500	2.49331600
N	-4.27925000	0.90359700	0.10850500
C	-5.27873700	0.51846900	0.98534800
C	-4.49962800	2.24869600	-0.15275900
C	-6.14412000	1.64152200	1.27555100
C	-5.66270900	2.71009200	0.57257000
H	-7.00034100	1.60357400	1.93303000
H	-6.04563500	3.71963000	0.54210600
N	-2.08172300	1.30882700	-1.63114400
C	-1.77746500	3.42430500	-2.54147700
H	-1.96396900	4.46766700	-2.74984800
C	-2.59295700	2.60031100	-1.67574700
C	-0.32455800	-1.06006100	-2.18702700
C	-1.14146400	-2.80428100	-1.09758900
C	-4.62404600	-1.85234900	1.25406800
C	-3.71435400	3.03615100	-0.98643300
H	-3.99911100	4.07652700	-1.10289800
C	-0.14099600	0.22030800	-2.68811600
H	0.71217500	0.37488700	-3.34021500
C	-1.92435600	-3.59371300	-0.26910900
H	-1.65067300	-4.63876700	-0.16887100
C	-5.43493900	-0.75812700	1.51301200
H	-6.27101800	-0.91255500	2.18755900
C	-0.76979000	2.63241600	-3.01378600
H	0.02982900	2.89758700	-3.69001900
C	-0.96265200	1.31503500	-2.44420400
C	0.10120400	0.26920200	2.24254700
H	-1.98847700	1.15691900	1.18916700
C	2.90736900	1.25648600	1.05011400
C	3.49680900	0.95630100	-0.36267800

H	2.87721900	0.32208100	1.61254400
H	3.50020600	1.90037600	-0.92354900
Cl	0.84499200	-1.27931400	1.73959300
Cl	-0.75730600	0.21781800	3.80594000
C	0.41926900	1.58095900	1.67131900
O	-0.38239300	2.53485500	1.86329000
N	1.52973900	1.76312800	0.85959400
H	1.52165300	2.69636500	0.45173700
C	3.72035000	2.28499200	1.83968500
H	4.73131600	1.91036300	2.03605100
H	3.22252400	2.48330100	2.79713000
O	3.76403200	3.49007500	1.01405200
H	4.05793100	4.26425900	1.53085400
O	2.65824400	-0.01755900	-1.02852700
H	1.71621600	0.19949200	-0.86106600
C	4.90675400	0.40576200	-0.31763900
C	6.00652700	1.28339500	-0.28890300
C	5.12987200	-0.98148500	-0.30352200
C	7.30896500	0.78964400	-0.22979800
H	5.83314400	2.35451400	-0.31183400
C	6.42780000	-1.48894200	-0.24554200
H	4.27877400	-1.64735200	-0.36391500
C	7.50081900	-0.59452900	-0.20586900
H	8.16748400	1.44780200	-0.20983800
H	6.62126600	-2.55346900	-0.23554200
N	8.86522700	-1.12090800	-0.14449800
O	9.02082000	-2.37634600	-0.12953400
O	9.82275900	-0.29402200	-0.10655100
⁴TS-reb₁			
Fe	-2.73763000	-0.32224900	-0.63156600
O	-1.58774300	0.31462100	0.75851400
S	-4.11251500	-1.05894200	-2.43268700
H	-4.85186300	-2.00271800	-1.74610200
N	-1.27988200	-1.60169300	-1.17931100
C	0.59356200	-2.51579600	-2.18907700
C	0.04907000	-3.48547700	-1.39719000
H	1.47660600	-2.56812300	-2.80798000
H	0.39469300	-4.49692100	-1.24109800
N	-3.51664500	-1.73190600	0.57282000
C	-3.04945600	-3.02784800	0.74739400
C	-3.85440700	-3.70362600	1.73822600
C	-4.78796100	-2.80845400	2.18074900
H	-3.70227000	-4.72485600	2.05552800
H	-5.55285100	-2.95320600	2.92958600
N	-4.13647000	0.99008800	-0.00781300
C	-5.12298900	0.76171300	0.94452800

C	-4.37408000	2.26208400	-0.51654600
C	-5.96594000	1.92945400	1.05851800
C	-5.50916300	2.84890400	0.15683700
H	-6.80289200	2.01435600	1.73599200
H	-5.89636600	3.83620500	-0.04775600
N	-2.03488200	1.05113000	-1.91774300
C	-1.74514000	2.98963100	-3.14859400
H	-1.93701600	3.98625300	-3.51820200
C	-2.55438300	2.31544200	-2.16069800
C	-0.24768600	-1.34439500	-2.06581600
C	-1.12237300	-2.91409800	-0.76719800
C	-4.57301700	-1.57531400	1.45994000
C	-3.64660900	2.87843800	-1.52002000
H	-3.94177600	3.87920300	-1.81404800
C	-0.06300700	-0.16795000	-2.77469500
H	0.79567900	-0.10973500	-3.43301200
C	-1.94972000	-3.58669200	0.11594100
H	-1.70548400	-4.61663100	0.35068700
C	-5.31692200	-0.41971800	1.64006300
H	-6.12408700	-0.45010700	2.36326000
C	-0.72743400	2.14114400	-3.48574800
H	0.07568400	2.30394600	-4.18955400
C	-0.90662600	0.93106100	-2.71748400
C	0.01594800	0.41415500	2.25230200
H	-1.94560600	1.17623500	1.07778800
C	2.90348600	1.39869100	1.17026900
C	3.43708500	1.10808200	-0.26827200
H	2.85250000	0.45480700	1.71282400
H	3.46329900	2.06471100	-0.80675500
Cl	0.86487800	-1.11624100	1.86060500
Cl	-0.95282800	0.34434500	3.76060800
C	0.39100100	1.75120800	1.75878300
O	-0.43327900	2.69028100	1.92320700
N	1.54927000	1.97473700	1.03888900
H	1.57292500	2.92891000	0.68434600
C	3.78276800	2.37367300	1.95654500
H	4.78674500	1.95871900	2.09971100
H	3.33010900	2.55893800	2.93863700
O	3.83568800	3.60178500	1.16590900
H	4.18677300	4.34718100	1.68926500
O	2.54420900	0.18278600	-0.93186800
H	1.61378200	0.45633900	-0.78722800
C	4.82268500	0.49725600	-0.27931900
C	5.96034600	1.32545000	-0.26408000
C	4.98507500	-0.89839100	-0.30497000
C	7.24116300	0.77466300	-0.25777900

H	5.83400200	2.40338700	-0.25784500
C	6.26070000	-1.46256500	-0.30014200
H	4.10434300	-1.52551700	-0.35424100
C	7.37272700	-0.61661300	-0.27301100
H	8.12792400	1.39447900	-0.24949600
H	6.40742600	-2.53438900	-0.32154000
N	8.71406100	-1.20250500	-0.26738400
O	8.81502800	-2.46343200	-0.28878700
O	9.70748600	-0.41871000	-0.23855600
²P-OH₁			
Fe	-3.68739400	0.45556800	-0.19539900
S	-5.62994100	1.38787700	-1.11830400
H	-6.30286900	0.21908300	-1.42052600
N	-4.21914400	-1.46185100	-0.44512600
C	-4.70362900	-3.51263300	-1.40491700
C	-5.22248500	-3.52543900	-0.14137800
H	-4.72353700	-4.30084700	-2.14314200
H	-5.74948700	-4.32663000	0.35565700
N	-4.16086100	0.30942300	1.81565900
C	-4.81687700	-0.74442100	2.42883000
C	-5.11548500	-0.39490300	3.80235200
C	-4.66001200	0.87949800	4.00179000
H	-5.61498100	-1.04232900	4.50821300
H	-4.71610000	1.47394900	4.90202600
N	-2.85806000	2.25429000	0.15142300
C	-3.00837700	3.01994700	1.30228100
C	-2.14967100	3.03532100	-0.75730900
C	-2.41044500	4.32174000	1.09189600
C	-1.88670000	4.33179600	-0.16915100
H	-2.38451800	5.10794500	1.83210400
H	-1.34829400	5.12758100	-0.66252800
N	-2.47979500	0.29485000	-1.93383900
C	-1.52258900	1.00409700	-3.92241900
H	-1.01620300	1.64663800	-4.62782700
C	-1.86377500	1.37581700	-2.57329000
C	-4.05654800	-2.23234100	-1.59464200
C	-4.90820200	-2.25190900	0.46984000
C	-4.07633900	1.32469200	2.75301900
C	-1.69692400	2.63416100	-2.00873600
H	-1.17444300	3.37709400	-2.60171300
C	-3.33236900	-1.87948500	-2.72814700
H	-3.33077500	-2.58959000	-3.54825300
C	-5.18123300	-1.92439800	1.79266200
H	-5.70978800	-2.66567400	2.38236100
C	-3.56138900	2.59077500	2.50276700
H	-3.57857900	3.30532000	3.31875400

C	-1.98627000	-0.27098600	-4.12778700
H	-1.92667200	-0.86053700	-5.03095300
C	-2.61950000	-0.70097200	-2.90786700
C	0.57598200	-0.94317800	-0.08358800
C	3.64558900	-1.47094900	0.57435000
C	4.54371900	-0.74701000	1.61983700
H	3.35062900	-0.74360200	-0.18101300
H	4.80175100	-1.47781800	2.39657500
Cl	1.22708200	0.86425000	-0.05488900
Cl	1.27329600	-1.71395200	-1.75708800
C	1.11852500	-1.76930600	1.10841300
O	0.29159000	-2.26046000	1.89757800
N	2.45476400	-1.99713100	1.24733900
H	2.65666700	-2.63274900	2.01151700
C	4.38959500	-2.62358100	-0.10322000
H	5.23761900	-2.24809000	-0.68689600
H	3.69753000	-3.14812200	-0.76844600
O	4.85678300	-3.50008200	0.97374300
H	5.08738700	-4.38413800	0.63073000
O	3.71422000	0.31071000	2.17133600
H	4.13022300	0.68671700	2.97282800
C	5.82453200	-0.18795200	1.02136800
C	7.00888000	-0.94780000	1.03105000
C	5.83444000	1.09918100	0.45521700
C	8.18471000	-0.43741900	0.48219600
H	6.99642700	-1.94514900	1.45812400
C	7.00330200	1.62193400	-0.09775700
H	4.92290700	1.68489800	0.46779600
C	8.16417600	0.84407100	-0.07558900
H	9.10642500	-1.00408900	0.48187100
H	7.03122900	2.60983900	-0.53831600
N	9.39631300	1.38707800	-0.65095900
O	9.36165900	2.55122900	-1.14471400
O	10.43465400	0.66421800	-0.62692200
O	-0.75681700	-0.97080300	-0.10288400
H	-1.23468700	-0.45075800	-0.82108000
⁴P-OH₁			
Fe	-3.56839400	-0.18751500	-0.03475100
S	-5.98708300	0.45067000	-0.64407400
H	-5.71009800	1.29107600	-1.70633700
N	-3.00464100	0.15600400	-1.93954200
C	-2.13029900	1.15903000	-3.83904800
C	-2.27455800	-0.16948400	-4.11869700
H	-1.74589600	1.94213300	-4.47524700
H	-2.03753200	-0.69288900	-5.03328300
N	-3.88247800	-2.12449500	-0.47637500

C	-3.58562200	-2.76331400	-1.66693500
C	-3.87467300	-4.17646300	-1.55786800
C	-4.34871000	-4.38909100	-0.29477800
H	-3.73075300	-4.89546200	-2.35092500
H	-4.67101000	-5.31706600	0.15419600
N	-4.39444000	-0.47302200	1.78478000
C	-4.79485500	-1.68219000	2.33548800
C	-4.56198700	0.47263000	2.78267200
C	-5.22888900	-1.48379500	3.70121000
C	-5.08194400	-0.15540500	3.97817000
H	-5.59406100	-2.26782200	4.34818900
H	-5.30391600	0.36686900	4.89715100
N	-3.53574600	1.80561100	0.31413400
C	-3.54493600	3.86149000	1.39506900
H	-3.69367900	4.58216100	2.18575400
C	-3.82243700	2.44723400	1.51469700
C	-2.58488900	1.35709100	-2.48108000
C	-2.81343800	-0.79487400	-2.93094900
C	-4.35175600	-3.10702800	0.37533300
C	-4.28605000	1.82651800	2.66094100
H	-4.45826500	2.45048600	3.53139800
C	-2.60607900	2.58352900	-1.82982600
H	-2.22702600	3.44093500	-2.37388600
C	-3.08992600	-2.14673100	-2.80702800
H	-2.89761000	-2.77589900	-3.66970000
C	-4.77690100	-2.90229700	1.68150700
H	-5.12112400	-3.76985600	2.23452500
C	-3.07365000	4.07528100	0.13217900
H	-2.75678700	5.00504200	-0.31686200
C	-3.05470200	2.79505900	-0.53936700
C	0.95567500	0.24237600	0.31222900
C	3.93346900	1.14373800	-0.06605900
C	4.93944900	0.69808400	-1.16560100
H	3.65028700	0.26297600	0.51129200
H	5.19571000	1.58360200	-1.76083100
Cl	1.61466800	-1.45961600	-0.08483000
Cl	1.35816900	0.69184000	2.10509800
C	1.43408100	1.32878700	-0.64291800
O	0.55865400	1.89729300	-1.33596500
N	2.73932700	1.70953800	-0.69638800
H	2.90864700	2.50178200	-1.30596100
C	4.54984100	2.18056000	0.87499300
H	5.39563800	1.75136100	1.42389400
H	3.78680600	2.50943900	1.58732400
O	4.99595700	3.28850100	0.02711400
H	5.17475200	4.08640600	0.56005300

O	4.21645800	-0.26711200	-1.97637100
H	4.72902100	-0.48690900	-2.78017300
C	6.21402300	0.09710300	-0.59630400
C	7.35124500	0.89897100	-0.38803300
C	6.26502200	-1.27103200	-0.27492800
C	8.52148400	0.34979200	0.13493500
H	7.30704500	1.95666400	-0.62639200
C	7.42865900	-1.83334100	0.24960200
H	5.39028400	-1.88569800	-0.45233400
C	8.54261800	-1.01258500	0.44621000
H	9.40793700	0.94795100	0.29948200
H	7.48769200	-2.88330200	0.50434900
N	9.77007900	-1.59642200	0.99146300
O	9.77447500	-2.83237500	1.25995300
O	10.76515100	-0.83470600	1.16764500
O	-0.46888584	0.12644687	0.26654696
H	-0.76591528	-0.45406650	0.97108776

C-H hydroxylation through Path C

²RC₂

Fe	1.51629200	-1.36657800	-0.24527400
O	0.74559900	-0.05842000	0.40681700
S	2.53808300	-3.61842200	-0.98533000
H	1.50235000	-4.04678700	-1.79447500
N	0.39105400	-1.37043900	-1.91598600
C	-1.42747900	-1.53514300	-3.34941500
C	-0.45275700	-0.85033100	-4.01555200
H	-2.42566900	-1.77978500	-3.67712600
H	-0.48585400	-0.43701000	-5.01284800
N	2.92597400	-0.30068700	-1.19801400
C	2.87824300	0.17632800	-2.49587400
C	4.04978700	0.98000200	-2.77261500
C	4.80065800	0.99661900	-1.63164800
H	4.25277700	1.46678700	-3.71519000
H	5.73283600	1.50929200	-1.44923600
N	2.75992100	-1.60035600	1.32436700
C	3.96630400	-0.94509700	1.52625300
C	2.52902500	-2.33681000	2.47494400
C	4.50246200	-1.28716200	2.82558300
C	3.61880800	-2.14950100	3.40840600
H	5.43535400	-0.91337900	3.22128300
H	3.68322700	-2.62205300	4.37754400
N	0.23253400	-2.68417800	0.59701700
C	-0.85657400	-4.03360000	2.14192400
H	-1.01737500	-4.60144400	3.04667000
C	0.34061100	-3.27611100	1.85287100

C	-0.89363800	-1.86965300	-2.04734100
C	0.67468400	-0.73378200	-3.11508400
C	4.10314900	0.18566900	-0.65739200
C	1.40798100	-3.11771400	2.71903300
H	1.35875300	-3.63443700	3.67168600
C	-1.56185000	-2.62589000	-1.09280700
H	-2.57781500	-2.92393500	-1.32202900
C	1.84239600	-0.04199700	-3.39430100
H	1.93871700	0.39638000	-4.38218000
C	4.57993300	-0.10128900	0.61458800
H	5.52058800	0.35259800	0.90734600
C	-1.70219700	-3.87567500	1.08098800
H	-2.69127400	-4.28785700	0.94498900
C	-1.02912900	-3.03083600	0.11950400
C	-5.95080900	0.03141300	-0.37730700
H	-6.35930000	-0.32653100	-1.31552900
C	-2.39875600	1.25717800	0.47103300
C	-2.17456300	2.74711200	0.09387600
H	-1.90146900	0.63157100	-0.27336100
H	-2.80433500	3.35752000	0.75351200
Cl	-6.33170600	-1.29451500	0.89812900
Cl	-6.86932400	1.60424200	0.05352400
C	-4.43937600	0.21591600	-0.50792700
O	-3.87895200	-0.38323400	-1.45300500
N	-3.83541700	0.96185700	0.43745600
H	-4.37978200	1.36986800	1.18828800
C	-1.86815800	0.91496500	1.85855000
H	-0.79309600	1.09744700	1.91451200
H	-2.05884300	-0.14392900	2.06722300
O	-2.61739300	1.77123600	2.78908900
H	-2.41576800	1.53807400	3.71508300
O	-2.63997600	2.85009900	-1.28349800
H	-2.69130300	3.78948900	-1.55155400
C	-0.73102500	3.19710900	0.23260000
C	-0.29745200	3.82895300	1.41236300
C	0.18662600	2.97011600	-0.80605600
C	1.03345600	4.21287300	1.56506300
H	-1.00453500	3.99463000	2.21849900
C	1.52142000	3.34744900	-0.66812000
H	-0.15375800	2.48603200	-1.71301600
C	1.92756200	3.96164100	0.51973400
H	1.38817100	4.69400500	2.46682800
H	2.24716700	3.15737200	-1.44741600
N	3.32990300	4.34011900	0.68362600
O	4.13289900	4.10035500	-0.26637200
O	3.68044600	4.88693700	1.77075500

⁴RC₂

Fe	1.92563800	-1.16520700	-0.24201000
O	1.17980400	-0.40131800	1.02314200
S	2.98694100	-2.59228700	-2.09029500
H	1.94212100	-2.56525300	-2.99526500
N	0.84318400	-0.19286900	-1.63903300
C	-0.90979700	0.48338600	-3.00520800
C	0.06476300	1.43751300	-3.09503600
H	-1.88014300	0.45594900	-3.47748100
H	0.06175100	2.34512700	-3.68082800
N	3.36584500	0.23456200	-0.38644000
C	3.31178500	1.40933200	-1.11595600
C	4.48156100	2.21932100	-0.84449300
C	5.24788200	1.52116600	0.04367000
H	4.65927200	3.19731800	-1.26608100
H	6.19397900	1.80508500	0.48035600
N	3.13340600	-2.27990900	0.92574000
C	4.36984200	-1.90797900	1.43522100
C	2.85594400	-3.52360800	1.47067800
C	4.87731800	-2.94608400	2.30601800
C	3.94369400	-3.94155300	2.32874300
H	5.82535000	-2.90355700	2.82189600
H	3.97431200	-4.87770700	2.86665900
N	0.60796600	-2.69542400	-0.31396600
C	-0.54071200	-4.65070100	0.19095700
H	-0.73818100	-5.61732400	0.63073100
C	0.66519700	-3.88332200	0.40923300
C	-0.41720900	-0.53405900	-2.10203800
C	1.14881800	1.02301300	-2.23099000
C	4.55112800	0.28266800	0.32229600
C	1.70530800	-4.26275800	1.24002000
H	1.61622300	-5.21775100	1.74680100
C	-1.11146900	-1.69235000	-1.77172800
H	-2.11007200	-1.80160000	-2.17965700
C	2.29509200	1.76641700	-1.98925100
H	2.39479300	2.71775000	-2.50036400
C	5.02221300	-0.71682000	1.16337400
H	5.98122600	-0.55256500	1.64327100
C	-1.33814900	-3.92342900	-0.64553300
H	-2.31828700	-4.17314300	-1.02443600
C	-0.62819100	-2.70325900	-0.95862200
C	-6.04830300	-0.85219600	-0.39770100
H	-6.54059700	-0.87716200	-1.36330400
C	-2.79544600	0.93188500	0.60466400
C	-2.95244500	2.44764700	0.91059300
H	-2.37573800	0.82403200	-0.39853000

H	-3.36926900	2.54994800	1.91963900
Cl	-5.84786900	-2.64309300	0.13113300
Cl	-7.19986000	0.03007100	0.78242200
C	-4.67581600	-0.19819600	-0.53203500
O	-4.15202600	-0.21263000	-1.67098200
N	-4.10907000	0.28410400	0.59088800
H	-4.59777100	0.23183900	1.47587500
C	-1.89746200	0.22309800	1.61334500
H	-0.87037200	0.59324900	1.57199700
H	-1.87843800	-0.84822700	1.38710600
O	-2.50525600	0.46586800	2.92817400
H	-2.04586900	-0.05227800	3.61642200
O	-3.89648200	2.94049500	-0.08301300
H	-4.18834000	3.84485200	0.14871100
C	-1.62474400	3.18116400	0.82694800
C	-0.80009500	3.30985800	1.95916700
C	-1.19091900	3.69697400	-0.40620300
C	0.45540800	3.90867500	1.85834000
H	-1.13467500	2.90878900	2.91025200
C	0.06156700	4.29540100	-0.52205100
H	-1.84132400	3.61023300	-1.26769500
C	0.87567500	4.37922500	0.61060400
H	1.11254100	3.99914000	2.71306200
H	0.41914500	4.68362400	-1.46613100
N	2.21389300	4.94832200	0.47714600
O	2.64934000	5.18162800	-0.69252900
O	2.88223500	5.16831900	1.52658600
²TS-H₂			
Fe	0.22442800	-1.80996000	0.20017800
O	0.35259800	-0.10591700	-0.32554700
S	0.16802200	-4.27198300	0.50698400
H	-1.00561300	-4.36099400	1.23277200
N	-1.67861800	-2.09342100	-0.38919200
C	-3.99967300	-2.23721100	-0.44741700
C	-3.54810400	-2.47502500	-1.71257900
H	-5.01871900	-2.22325300	-0.08959900
H	-4.12456400	-2.69111000	-2.59990700
N	0.88762700	-2.31720500	-1.64892700
C	0.10549900	-2.53663000	-2.76625000
C	0.94823200	-2.77328000	-3.92351700
C	2.24172300	-2.69709500	-3.49804900
H	0.58042900	-2.97376700	-4.91906600
H	3.14639200	-2.82256500	-4.07476400
N	2.14297700	-1.73900700	0.83661100
C	3.28510500	-1.90281300	0.08215200
C	2.57072800	-1.42865900	2.11490200

C	4.46106000	-1.69083100	0.90222500
C	4.01889800	-1.39798300	2.16037400
H	5.47896600	-1.75681800	0.54729600
H	4.60337200	-1.18035400	3.04233100
N	-0.43762200	-1.46900300	2.07062200
C	-0.48722400	-0.99250000	4.34136200
H	-0.11939100	-0.78197000	5.33523400
C	0.35030400	-1.21370200	3.18401100
C	-2.83763800	-1.98499700	0.37660900
C	-2.10474100	-2.37877700	-1.67965700
C	2.20331900	-2.40526600	-2.07792500
C	1.74006600	-1.18856100	3.19985600
H	2.21808000	-0.97218800	4.15011100
C	-2.86832600	-1.66619600	1.72285400
H	-3.84098000	-1.60049800	2.19871500
C	-1.28160600	-2.55562400	-2.78023300
H	-1.76541500	-2.74601200	-3.73229700
C	3.31457400	-2.22109400	-1.27296000
H	4.29023100	-2.32120500	-1.73736400
C	-1.78565400	-1.12396000	3.92860100
H	-2.68782700	-1.04045000	4.51697600
C	-1.74940200	-1.42719200	2.51607900
C	-4.57724900	1.88317400	-0.86755900
H	-5.09814000	1.30653800	-1.62327600
C	-0.91825800	2.01643400	0.25178200
C	-0.20209800	3.04974000	-0.63867800
H	-0.38471000	0.70495300	-0.15971300
H	-0.54104600	4.02958200	-0.26042900
Cl	-5.40897800	1.48317000	0.77531900
Cl	-4.84213900	3.68750300	-1.27943100
C	-3.09368200	1.51860600	-0.87514900
O	-2.69911700	0.76135600	-1.77740700
N	-2.34606500	2.05341500	0.12996700
H	-2.82262400	2.55597100	0.87471800
C	-0.52358400	2.07621300	1.70708400
H	0.56300800	2.03330400	1.81247400
H	-0.97304400	1.24132700	2.25114500
O	-1.05274600	3.35755900	2.22352900
H	-0.95264200	3.40289700	3.19508100
O	-0.68784200	2.86420700	-1.99402600
H	-0.40367800	3.61566500	-2.55268400
C	1.31416300	3.01463100	-0.56905800
C	2.00056300	3.89179900	0.28905600
C	2.04107400	2.11985100	-1.37331200
C	3.39355000	3.87072700	0.36449600
H	1.43756000	4.58469400	0.90720300

C	3.43269800	2.08961700	-1.30962100
H	1.50340600	1.43283500	-2.01231100
C	4.09057000	2.96381000	-0.43832000
H	3.94010500	4.53496200	1.02068300
H	4.01020200	1.39733000	-1.90695700
N	5.55029300	2.92162100	-0.35654700
O	6.16667800	2.08191500	-1.07624100
O	6.12951300	3.72367000	0.43375200
⁴TS- H₂			
Fe	0.23959400	-1.72489000	0.32751600
O	0.08931300	-0.26274900	-0.64722800
S	0.28925700	-4.00582200	1.04855800
H	-1.06701000	-4.23724600	1.12660900
N	-1.65853600	-2.19025300	-0.32350000
C	-3.96748700	-2.32517000	-0.51025900
C	-3.44066300	-2.78212500	-1.68280400
H	-5.00588400	-2.23494900	-0.22810500
H	-3.96237400	-3.14341100	-2.55668800
N	1.00314000	-2.48907700	-1.41044600
C	0.27480400	-2.93855600	-2.50186800
C	1.18002700	-3.30929400	-3.57213900
C	2.44872800	-3.08326500	-3.12433600
H	0.86643000	-3.69386200	-4.53149000
H	3.38330400	-3.24638700	-3.64079800
N	2.07949700	-1.50700100	1.01877200
C	3.27500900	-1.76378800	0.35058100
C	2.44635700	-1.03201300	2.27356500
C	4.39623400	-1.44813100	1.20733000
C	3.88640000	-0.99865800	2.39056000
H	5.43218700	-1.55864500	0.92237800
H	4.42169600	-0.67115000	3.26962300
N	-0.52781900	-1.11604900	2.04539800
C	-0.73350800	-0.31865700	4.21883600
H	-0.43268500	0.03525900	5.19414700
C	0.18142600	-0.68675000	3.16541000
C	-2.85038400	-1.94521600	0.33061800
C	-1.99845900	-2.68574100	-1.56912600
C	2.33248900	-2.57236000	-1.77298500
C	1.56347200	-0.63897100	3.26618300
H	1.98528300	-0.28405800	4.20024600
C	-2.94840300	-1.41483400	1.60906300
H	-3.94219200	-1.27616400	2.01890900
C	-1.10584000	-3.03678100	-2.57142700
H	-1.52818300	-3.41510000	-3.49624000
C	3.39473900	-2.24101700	-0.94480100
H	4.39864900	-2.37320700	-1.33462300

C	-1.99864000	-0.53698400	3.74987500
H	-2.93786400	-0.39357600	4.26400100
C	-1.87689600	-1.04174000	2.40266000
C	-4.60640700	1.51361300	-1.00668100
H	-5.09336600	0.98346200	-1.81726800
C	-0.92782800	1.97912100	0.00750500
C	-0.17318600	3.05905200	-0.80389300
H	-0.34750800	0.82421700	-0.35152200
H	-0.49162600	4.02113500	-0.36981900
Cl	-5.19904700	1.13945500	0.62999900
Cl	-5.01229000	3.63914400	-1.12362200
C	-3.08620400	1.43100600	-1.18771200
O	-2.67970200	0.88685900	-2.22826200
N	-2.35388800	2.00343600	-0.19878100
H	-2.83930700	2.59277100	0.47584100
C	-0.62661700	2.04364900	1.48819400
H	0.45210900	1.97453000	1.66454200
H	-1.13766700	1.22741300	2.00665400
O	-1.14347900	3.34541900	1.96258900
H	-1.17954400	3.37176600	2.93901900
O	-0.63918000	2.96700500	-2.17782800
H	-0.22085900	3.66872200	-2.71671900
C	1.33616100	2.97395300	-0.72911700
C	2.06344300	3.87571400	0.06772300
C	2.02208300	2.00106300	-1.47973300
C	3.45536400	3.80420600	0.13697400
H	1.53343700	4.62790300	0.64379800
C	3.41150200	1.92172500	-1.42273300
H	1.45201600	1.31025700	-2.08796700
C	4.10977800	2.82006300	-0.60862900
H	4.03293200	4.48596600	0.74722800
H	3.95561600	1.17356800	-1.98139500
N	5.56613500	2.71809600	-0.52621300
O	6.14098000	1.80189900	-1.18599800
O	6.18493000	3.54433500	0.20688100
² INT ₂			
Fe	-2.00890700	-0.85937200	0.03068500
O	-0.28265000	-0.34392000	0.05964700
S	-4.25712000	-1.54207800	-0.07724900
H	-4.33854300	-2.15374100	1.15845200
N	-1.72249900	-2.14365200	1.55986100
C	-1.21023100	-4.02986600	2.80283500
C	-1.46038700	-3.01901400	3.68670900
H	-0.93498300	-5.05265700	3.01467700
H	-1.43306200	-3.05018300	4.76600700
N	-2.46487200	0.59245700	1.32934400

C	-2.36680800	0.53349200	2.70987500
C	-2.69941300	1.82496600	3.27690700
C	-3.01515500	2.65212300	2.23925500
H	-2.68666100	2.04984400	4.33317300
H	-3.29168300	3.69530000	2.26651100
N	-2.47078200	0.35080300	-1.50769800
C	-2.94312800	1.64901600	-1.41907600
C	-2.33700700	0.07160400	-2.86054800
C	-3.13589400	2.18756000	-2.74820500
C	-2.75758800	1.21925300	-3.63509800
H	-3.50997000	3.17932600	-2.95671100
H	-2.76226900	1.26030500	-4.71469300
N	-1.51595100	-2.32737100	-1.28067800
C	-0.98745800	-3.45994000	-3.22715400
H	-0.86329500	-3.64623500	-4.28428800
C	-1.46389700	-2.21715300	-2.66218000
C	-1.35499900	-3.48040100	1.47257200
C	-1.77015900	-1.83860300	2.91068400
C	-2.87730900	1.87761500	1.02187000
C	-1.84769800	-1.10635600	-3.40118400
H	-1.78203700	-1.17444000	-4.48165700
C	-1.08406400	-4.17189100	0.30395500
H	-0.78354500	-5.20989400	0.39307400
C	-2.05115400	-0.59229500	3.45005700
H	-2.03247400	-0.49624100	4.52974600
C	-3.13044500	2.36659900	-0.24747700
H	-3.46098600	3.39505500	-0.32964400
C	-0.79086200	-4.32960300	-2.18426100
H	-0.46716100	-5.35958800	-2.22469500
C	-1.13575500	-3.62515800	-0.97031500
C	5.14253500	-1.04558300	1.22343300
H	6.03810700	-0.67316500	1.70664300
C	2.97962600	0.18968600	-1.62496900
C	3.13951600	1.63116200	-2.06896500
H	0.37614200	-1.01441100	-0.24771700
H	2.72902700	1.66804700	-3.08495100
Cl	3.86361000	-1.28805900	2.58289000
Cl	5.57987500	-2.72335500	0.48995500
C	4.68030800	-0.06533300	0.18327600
O	5.26440700	1.06235900	0.12676800
N	3.64076400	-0.45521700	-0.61227400
H	3.25822700	-1.39244700	-0.45240700
C	1.91966700	-0.63512200	-2.30240400
H	2.25350500	-0.95386300	-3.30316300
H	0.99877800	-0.05040700	-2.41377800
O	1.66304200	-1.80800100	-1.46877900

H	1.16503600	-2.50210100	-1.94729500
O	4.50070000	2.07036100	-2.22191600
H	4.99362700	1.90994400	-1.37556900
C	2.27047500	2.56265800	-1.21233900
C	1.02521500	2.97947200	-1.71298600
C	2.67671500	2.99762400	0.06283600
C	0.17838400	3.78322000	-0.95354000
H	0.70836800	2.67027000	-2.70421900
C	1.84204700	3.80489900	0.83300000
H	3.64228600	2.70025000	0.45558700
C	0.59478100	4.17689900	0.31944200
H	-0.78633200	4.09676300	-1.32580200
H	2.13358200	4.13917100	1.81983900
N	-0.30285200	4.98340500	1.13947500
O	0.10557900	5.38057400	2.26815100
O	-1.46148300	5.24161600	0.68743500
⁴INT₂			
Fe	2.00763100	-0.86045600	-0.03097200
O	0.28148900	-0.34457800	-0.06034000
S	4.25552100	-1.54407400	0.07604800
H	4.33620100	-2.15638400	-1.15937200
N	1.72013200	-2.14507800	-1.55982200
C	1.20633700	-4.03128100	-2.80217400
C	1.45678200	-3.02077600	-3.68637000
H	0.93043100	-5.05396200	-3.01369100
H	1.42909400	-3.05218900	-4.76565200
N	2.46371100	0.59084800	-1.33019400
C	2.36496100	0.53161000	-2.71066900
C	2.69785100	1.82283200	-3.27813800
C	3.01444800	2.65007100	-2.24081400
H	2.68472300	2.04747200	-4.33445100
H	3.29146700	3.69311000	-2.26838600
N	2.47065200	0.34978700	1.50686400
C	2.94371600	1.64771900	1.41774900
C	2.33756200	0.07087800	2.85986600
C	3.13754900	2.18638000	2.74667300
C	2.75920700	1.21844800	3.63395300
H	3.51228100	3.17797700	2.95480100
H	2.76454800	1.25969900	4.71353700
N	1.51453400	-2.32795000	1.28088700
C	0.98631300	-3.45984500	3.22781000
H	0.86248900	-3.64585300	4.28503400
C	1.46325000	-2.21747600	2.66237900
C	1.35186400	-3.48156900	-1.47209800
C	1.76746900	-1.84036100	-2.91071300
C	2.87686500	1.87586400	-1.02319800

C	1.84803000	-1.10674500	3.40099400
H	1.78299800	-1.17464000	4.48151600
C	1.08086200	-4.17256900	-0.30320000
H	0.77961100	-5.21039300	-0.39194100
C	2.04869400	-0.59425200	-3.45046200
H	2.02962900	-0.49844800	-4.53016800
C	3.13087000	2.36497400	0.24593500
H	3.46203100	3.39325500	0.32774800
C	0.78854500	-4.32955100	2.18515900
H	0.46429600	-5.35935100	2.22594900
C	1.13334600	-3.62555000	0.97091000
C	-5.14194900	-1.04178500	-1.22351100
H	-6.03703200	-0.66832100	-1.70681800
C	-2.97806500	0.19051700	1.62544400
C	-3.13658000	1.63212300	2.06951900
H	-0.37736100	-1.01474000	0.24763600
H	-2.72584100	1.66863000	3.08541100
Cl	-3.86285300	-1.28490100	-2.58266100
Cl	-5.58116300	-2.71951100	-0.49090500
C	-4.67914400	-0.06250300	-0.18274600
O	-5.26230600	1.06567000	-0.12581100
N	-3.64012800	-0.45365600	0.61288100
H	-3.25858800	-1.39124000	0.45276500
C	-1.92124900	-0.63676500	2.30481100
H	-2.25900300	-0.95733100	3.30372600
H	-1.00023300	-0.05328900	2.42075600
O	-1.66347300	-1.80834600	1.46978600
H	-1.16581800	-2.50304200	1.94783400
O	-4.49745700	2.07227500	2.22285600
H	-4.99059700	1.91268500	1.37647400
C	-2.26723000	2.56326300	1.21284600
C	-1.02204200	2.98009900	1.71363300
C	-2.67331000	2.99813300	-0.06239700
C	-0.17517900	3.78389200	0.95428800
H	-0.70529200	2.67088900	2.70489300
C	-1.83859600	3.80545300	-0.83247800
H	-3.63873900	2.70056600	-0.45532700
C	-0.59145200	4.17755800	-0.31875300
H	0.78947700	4.09749400	1.32666700
H	-2.13005200	4.13969500	-1.81934900
N	0.30620700	4.98415700	-1.13866900
O	-0.10261900	5.38237000	-2.26685800
O	1.46520200	5.24139600	-0.68708300
²TS-reb₂			
Fe	0.31191900	-1.89991400	0.19482300
O	0.11035500	-0.11411000	0.06507400

S	0.63193100	-4.22641900	0.32429600
H	0.15809600	-4.42125900	1.60695500
N	0.12748800	-1.84288200	2.20306200
C	0.58588600	-1.65456900	4.46571500
C	-0.77016700	-1.75276000	4.33484600
H	1.16599800	-1.54860200	5.37069000
H	-1.52083600	-1.74563000	5.11140700
N	-1.66648000	-2.13649000	0.01527800
C	-2.60710600	-2.06789900	1.02991500
C	-3.93730900	-2.19816400	0.46984000
C	-3.79391900	-2.36390600	-0.87647600
H	-4.84924300	-2.16417200	1.04746700
H	-4.55986500	-2.47108100	-1.62965000
N	0.53624800	-2.14195300	-1.78888800
C	-0.46922500	-2.40277700	-2.70395800
C	1.71341500	-2.03611700	-2.51634600
C	0.09468500	-2.48934800	-4.03372400
C	1.43658500	-2.25807000	-3.91920600
H	-0.47646300	-2.69787500	-4.92664700
H	2.18296000	-2.24156700	-4.70015600
N	2.31428700	-1.62920900	0.38163600
C	4.54523600	-1.26128500	-0.10643200
H	5.44508800	-1.15391200	-0.69498300
C	3.23555300	-1.54150800	-0.65128800
C	1.14790300	-1.69167800	3.13334000
C	-1.05725200	-1.85992200	2.92146400
C	-2.37252600	-2.33467200	-1.15878900
C	2.96234300	-1.73345800	-1.99882000
H	3.79165800	-1.66491800	-2.69445200
C	2.49052500	-1.51814400	2.84265800
H	3.17180200	-1.38785300	3.67608000
C	-2.33125900	-1.94600900	2.38044700
H	-3.17069100	-1.92707000	3.06623100
C	-1.82353200	-2.48939400	-2.41938900
H	-2.50624000	-2.65083000	-3.24496100
C	4.41523200	-1.21969400	1.25884800
H	5.18633600	-1.06359800	1.99933600
C	3.02362000	-1.46463200	1.56270200
C	2.43531100	4.02408200	0.84812000
H	2.51920100	5.10208100	0.77659700
C	0.62782900	1.38366000	-1.17145500
C	-0.45924800	1.83679800	-2.12722100
H	0.85960300	0.43347100	0.40688100
H	-0.57621100	1.01455200	-2.84297700
Cl	1.81601200	3.65064100	2.58578800
Cl	4.17537700	3.33103800	0.65773500

C	1.49456500	3.51567300	-0.20681600
O	0.84416700	4.37072200	-0.88649700
N	1.39016900	2.16015000	-0.33810700
H	1.96981600	1.58638200	0.28243500
C	1.82847700	1.10118700	-2.03252800
H	1.54818200	0.45472600	-2.87257700
O	-0.11381900	2.96943100	-2.94395500
H	0.17089200	3.71966400	-2.35991000
C	-1.80230400	1.97462000	-1.39654800
C	-2.73480700	0.92714100	-1.48743900
C	-2.11975100	3.10988700	-0.62800700
C	-3.94622100	0.98260700	-0.80241100
H	-2.51307400	0.05504700	-2.09474800
C	-3.32923300	3.18153200	0.06014800
H	-1.41907100	3.93437700	-0.56277700
C	-4.22318600	2.10851900	-0.02491300
H	-4.66264600	0.17550800	-0.85625300
H	-3.58467900	4.04176100	0.66457600
N	-5.47058200	2.15739000	0.73024900
O	-5.73737000	3.20488600	1.38606800
O	-6.22937500	1.13907700	0.70490100
O	2.37175200	2.31528100	-2.55762600
H	2.89103700	2.12136300	-3.34142400
H	2.55963300	0.60983100	-1.42517200
⁴TS-reb₂			
Fe	0.31191900	-1.89991400	0.19482300
O	0.11035500	-0.11411000	0.06507400
S	0.63193100	-4.22641900	0.32429600
H	0.15809600	-4.42125900	1.60695500
N	0.12748800	-1.84288200	2.20306200
C	0.58588600	-1.65456900	4.46571500
C	-0.77016700	-1.75276000	4.33484600
H	1.16599800	-1.54860200	5.37069000
H	-1.52083600	-1.74563000	5.11140700
N	-1.66648000	-2.13649000	0.01527800
C	-2.60710600	-2.06789900	1.02991500
C	-3.93730900	-2.19816400	0.46984000
C	-3.79391900	-2.36390600	-0.87647600
H	-4.84924300	-2.16417200	1.04746700
H	-4.55986500	-2.47108100	-1.62965000
N	0.53624800	-2.14195300	-1.78888800
C	-0.46922500	-2.40277700	-2.70395800
C	1.71341500	-2.03611700	-2.51634600
C	0.09468500	-2.48934800	-4.03372400
C	1.43658500	-2.25807000	-3.91920600
H	-0.47646300	-2.69787500	-4.92664700

H	2.18296000	-2.24156700	-4.70015600
N	2.31428700	-1.62920900	0.38163600
C	4.54523600	-1.26128500	-0.10643200
H	5.44508800	-1.15391200	-0.69498300
C	3.23555300	-1.54150800	-0.65128800
C	1.14790300	-1.69167800	3.13334000
C	-1.05725200	-1.85992200	2.92146400
C	-2.37252600	-2.33467200	-1.15878900
C	2.96234300	-1.73345800	-1.99882000
H	3.79165800	-1.66491800	-2.69445200
C	2.49052500	-1.51814400	2.84265800
H	3.17180200	-1.38785300	3.67608000
C	-2.33125900	-1.94600900	2.38044700
H	-3.17069100	-1.92707000	3.06623100
C	-1.82353200	-2.48939400	-2.41938900
H	-2.50624000	-2.65083000	-3.24496100
C	4.41523200	-1.21969400	1.25884800
H	5.18633600	-1.06359800	1.99933600
C	3.02362000	-1.46463200	1.56270200
C	2.43531100	4.02408200	0.84812000
H	2.51920100	5.10208100	0.77659700
C	0.62782900	1.38366000	-1.17145500
C	-0.45924800	1.83679800	-2.12722100
H	0.85960300	0.43347100	0.40688100
H	-0.57621100	1.01455200	-2.84297700
Cl	1.81601200	3.65064100	2.58578800
Cl	4.17537700	3.33103800	0.65773500
C	1.49456500	3.51567300	-0.20681600
O	0.84416700	4.37072200	-0.88649700
N	1.39016900	2.16015000	-0.33810700
H	1.96981600	1.58638200	0.28243500
C	1.82847700	1.10118700	-2.03252800
H	1.54818200	0.45472600	-2.87257700
O	-0.11381900	2.96943100	-2.94395500
H	0.17089200	3.71966400	-2.35991000
C	-1.80230400	1.97462000	-1.39654800
C	-2.73480700	0.92714100	-1.48743900
C	-2.11975100	3.10988700	-0.62800700
C	-3.94622100	0.98260700	-0.80241100
H	-2.51307400	0.05504700	-2.09474800
C	-3.32923300	3.18153200	0.06014800
H	-1.41907100	3.93437700	-0.56277700
C	-4.22318600	2.10851900	-0.02491300
H	-4.66264600	0.17550800	-0.85625300
H	-3.58467900	4.04176100	0.66457600
N	-5.47058200	2.15739000	0.73024900

O	-5.73737000	3.20488600	1.38606800
O	-6.22937500	1.13907700	0.70490100
O	2.37175200	2.31528100	-2.55762600
H	2.89103700	2.12136300	-3.34142400
H	2.55963300	0.60983100	-1.42517200
²P-OH₂			
Fe	2.02587700	-0.87125100	0.60124100
O	0.09505000	-0.07215100	-0.89601500
S	3.62735000	-1.89676300	2.00186200
H	3.42010600	-1.14203600	3.14120800
N	1.37194600	0.42187500	2.00402100
C	1.26549000	2.22047800	3.45564200
C	0.34361500	1.30398100	3.87967700
H	1.48689500	3.18752200	3.88269500
H	-0.33089800	1.37939500	4.71997200
N	0.40151300	-2.14339300	1.07101400
C	-0.42846900	-2.03009700	2.17648500
C	-1.21199900	-3.24056100	2.31410300
C	-0.81980400	-4.09235300	1.31344200
H	-1.94662100	-3.41956600	3.08580600
H	-1.16985400	-5.09726500	1.12502800
N	2.52093300	-2.08301800	-0.92347100
C	2.00410800	-3.34761100	-1.17288400
C	3.51995400	-1.85598000	-1.86025600
C	2.71760700	-3.93652900	-2.29047000
C	3.64339600	-3.02438500	-2.71118200
H	2.51781900	-4.91834900	-2.69441900
H	4.34607600	-3.11570400	-3.52657900
N	3.25414600	0.62298600	-0.18787100
C	4.93161600	1.67839500	-1.37733500
H	5.69365100	1.83589300	-2.12675100
C	4.13433900	0.47326700	-1.24375600
C	1.91122400	1.67769500	2.27823700
C	0.39799400	0.17703200	2.97174000
C	0.20705700	-3.41305600	0.54900200
C	4.25515200	-0.68208800	-2.01204700
H	4.99547000	-0.67195200	-2.80537500
C	2.87581300	2.34243400	1.52268300
H	3.16963400	3.32723600	1.87066800
C	-0.43093800	-0.94077400	3.04562300
H	-1.13369800	-0.96943500	3.87187900
C	0.94471700	-3.95568600	-0.50170800
H	0.68484700	-4.96094600	-0.81795700
C	4.54186000	2.53331400	-0.38163000
H	4.92488900	3.52005600	-0.16547500
C	3.50092800	1.86196100	0.37432600

C	-1.89627100	4.07403600	0.18239900
H	-2.51112100	4.89851800	-0.15995900
C	-0.51136800	0.95757700	-1.70155100
C	-1.64286300	0.32789000	-2.59123900
H	-1.11603300	-0.45167200	-3.14835800
Cl	-2.74039400	3.36905100	1.69553500
Cl	-0.23275700	4.77910900	0.63432000
C	-1.81279900	3.02324700	-0.91852700
O	-2.61453600	3.17417500	-1.88014100
N	-0.94642600	2.00886800	-0.74352100
H	-0.34111000	2.04088200	0.07252900
C	0.63870400	1.49957600	-2.58193200
H	0.97260600	0.68705400	-3.24005700
O	-2.10313900	1.25202700	-3.60439400
H	-2.49007700	2.05346800	-3.15394700
C	-2.76612100	-0.33978200	-1.80616300
C	-2.59116500	-1.66678700	-1.36566800
C	-3.97593500	0.31743000	-1.51942100
C	-3.58225000	-2.31701000	-0.62942100
H	-1.68303900	-2.20686000	-1.61529900
C	-4.97848900	-0.32314400	-0.79201800
H	-4.14100200	1.33095900	-1.86124800
C	-4.76409200	-1.63069200	-0.34976200
H	-3.45203400	-3.33102100	-0.27776600
H	-5.91342400	0.17106800	-0.56339200
N	-5.81025200	-2.30336300	0.42451400
O	-6.88166500	-1.67212800	0.65201900
O	-5.58639400	-3.48079300	0.82964900
O	0.25614300	2.67834500	-3.31153300
H	-0.46096100	2.42867100	-3.93689700
H	1.46626300	1.78119800	-1.93211200
H	-0.54800200	-0.60925700	-0.38158800
⁴P-OH₂			
Fe	2.02587700	-0.87125100	0.60124100
O	0.09505000	-0.07215100	-0.89601500
S	3.62735000	-1.89676300	2.00186200
H	3.42010600	-1.14203600	3.14120800
N	1.37194600	0.42187500	2.00402100
C	1.26549000	2.22047800	3.45564200
C	0.34361500	1.30398100	3.87967700
H	1.48689500	3.18752200	3.88269500
H	-0.33089800	1.37939500	4.71997200
N	0.40151300	-2.14339300	1.07101400
C	-0.42846900	-2.03009700	2.17648500
C	-1.21199900	-3.24056100	2.31410300
C	-0.81980400	-4.09235300	1.31344200

H	-1.94662100	-3.41956600	3.08580600
H	-1.16985400	-5.09726500	1.12502800
N	2.52093300	-2.08301800	-0.92347100
C	2.00410800	-3.34761100	-1.17288400
C	3.51995400	-1.85598000	-1.86025600
C	2.71760700	-3.93652900	-2.29047000
C	3.64339600	-3.02438500	-2.71118200
H	2.51781900	-4.91834900	-2.69441900
H	4.34607600	-3.11570400	-3.52657900
N	3.25414600	0.62298600	-0.18787100
C	4.93161600	1.67839500	-1.37733500
H	5.69365100	1.83589300	-2.12675100
C	4.13433900	0.47326700	-1.24375600
C	1.91122400	1.67769500	2.27823700
C	0.39799400	0.17703200	2.97174000
C	0.20705700	-3.41305600	0.54900200
C	4.25515200	-0.68208800	-2.01204700
H	4.99547000	-0.67195200	-2.80537500
C	2.87581300	2.34243400	1.52268300
H	3.16963400	3.32723600	1.87066800
C	-0.43093800	-0.94077400	3.04562300
H	-1.13369800	-0.96943500	3.87187900
C	0.94471700	-3.95568600	-0.50170800
H	0.68484700	-4.96094600	-0.81795700
C	4.54186000	2.53331400	-0.38163000
H	4.92488900	3.52005600	-0.16547500
C	3.50092800	1.86196100	0.37432600
C	-1.89627100	4.07403600	0.18239900
H	-2.51112100	4.89851800	-0.15995900
C	-0.51136800	0.95757700	-1.70155100
C	-1.64286300	0.32789000	-2.59123900
H	-1.11603300	-0.45167200	-3.14835800
Cl	-2.74039400	3.36905100	1.69553500
Cl	-0.23275700	4.77910900	0.63432000
C	-1.81279900	3.02324700	-0.91852700
O	-2.61453600	3.17417500	-1.88014100
N	-0.94642600	2.00886800	-0.74352100
H	-0.34111000	2.04088200	0.07252900
C	0.63870400	1.49957600	-2.58193200
H	0.97260600	0.68705400	-3.24005700
O	-2.10313900	1.25202700	-3.60439400
H	-2.49007700	2.05346800	-3.15394700
C	-2.76612100	-0.33978200	-1.80616300
C	-2.59116500	-1.66678700	-1.36566800
C	-3.97593500	0.31743000	-1.51942100
C	-3.58225000	-2.31701000	-0.62942100

H	-1.68303900	-2.20686000	-1.61529900
C	-4.97848900	-0.32314400	-0.79201800
H	-4.14100200	1.33095900	-1.86124800
C	-4.76409200	-1.63069200	-0.34976200
H	-3.45203400	-3.33102100	-0.27776600
H	-5.91342400	0.17106800	-0.56339200
N	-5.81025200	-2.30336300	0.42451400
O	-6.88166500	-1.67212800	0.65201900
O	-5.58639400	-3.48079300	0.82964900
O	0.25614300	2.67834500	-3.31153300
H	-0.46096100	2.42867100	-3.93689700
H	1.46626300	1.78119800	-1.93211200
H	-0.54800200	-0.60925700	-0.38158800

C-H hydroxylation through Path D

${}^2\text{RC}_3$

Fe	-2.33279800	0.76456800	-0.21806900
O	-1.06821300	0.12672400	0.64457900
S	-4.46657100	1.39345300	-1.48390600
H	-5.16448900	1.96600600	-0.43655900
N	-2.65077400	2.28005800	1.07445800
C	-3.29085200	3.49916700	2.94115600
C	-2.42837900	4.28210200	2.22703600
H	-3.79669400	3.73066300	3.86696000
H	-2.08907800	5.28276100	2.45099600
N	-1.19939500	1.97816400	-1.35807100
C	-0.78318700	3.26233200	-1.04431400
C	0.08116400	3.77094100	-2.08507000
C	0.17787000	2.79400300	-3.03641300
H	0.53754600	4.74982100	-2.08123600
H	0.72687300	2.81631800	-3.96644000
N	-2.25013400	-0.64786900	-1.65266700
C	-1.52805600	-0.59694500	-2.83952300
C	-2.79861200	-1.91749400	-1.59913900
C	-1.64265500	-1.85727900	-3.54129100
C	-2.41541300	-2.67437200	-2.77085300
H	-1.17234800	-2.07555000	-4.48846200
H	-2.70284000	-3.69814900	-2.95513900
N	-3.70502500	-0.34251300	0.76853100
C	-4.94415100	-2.15494300	1.52502400
H	-5.36283300	-3.15016300	1.54197200
C	-4.05371800	-1.66178100	0.49807200
C	-3.42313200	2.25160100	2.22244800
C	-2.02870500	3.52014100	1.06541500
C	-0.62251300	1.67957200	-2.57899600
C	-3.61546800	-2.39763900	-0.58765100

H	-3.94106800	-3.42843200	-0.65932500
C	-4.21383400	1.18436400	2.63401000
H	-4.76481000	1.30157400	3.56101400
C	-1.16139500	3.97493400	0.08458800
H	-0.75624500	4.97454000	0.20165200
C	-0.78496200	0.48486000	-3.27470400
H	-0.28061500	0.39207100	-4.23102700
C	-5.12785100	-1.14331800	2.42230300
H	-5.72699000	-1.14572800	3.32094100
C	-4.34259200	-0.01852000	1.96492500
C	1.49012600	-4.52694000	0.28665200
H	1.01027500	-5.47323400	0.06600100
C	1.93871200	-1.51526300	0.95284700
C	2.03801600	-0.28977100	0.00467700
H	2.76472600	-2.19455700	0.74012300
H	1.20548300	0.38056500	0.25444600
Cl	2.75101500	-4.27151100	-1.07148700
Cl	2.35043000	-4.77604800	1.94198100
C	0.39883700	-3.45865900	0.33241000
O	-0.75190100	-3.87263500	0.03732800
N	0.65569200	-2.18690800	0.69910200
H	-0.15095400	-1.55385300	0.66293100
C	1.98379000	-1.13481600	2.43992600
O	1.84377300	-0.83567700	-1.33908100
H	1.63389500	-0.10852000	-1.95879100
C	3.34688600	0.47357900	0.06503800
C	3.40017800	1.75244500	0.64323200
C	4.51005300	-0.07095000	-0.50747500
C	4.59164400	2.47392500	0.67411800
H	2.50219800	2.18101500	1.07680800
C	5.71068400	0.63494600	-0.48288400
H	4.46108200	-1.04430800	-0.98142700
C	5.73542000	1.90124800	0.11090400
H	4.65218800	3.45913500	1.11703700
H	6.61768800	0.22976900	-0.91159700
N	6.98834100	2.65251000	0.13463900
O	8.01445800	2.12448400	-0.38594800
O	6.98953200	3.79874900	0.67461800
O	3.31495700	-0.63377700	2.73296500
H	3.41846700	-0.46980200	3.69021800
H	1.21207600	-0.37968300	2.65041800
H	1.76058800	-2.03362200	3.02592600
⁴ RC ₃			
Fe	-2.37028300	0.70010800	-0.22740200
O	-1.04744200	0.13009400	0.59698900
S	-4.50895100	1.63934400	-1.23521400

H	-4.03878100	2.89105100	-1.58630700
N	-1.29020200	1.97907900	-1.36393700
C	-0.04505700	3.80876500	-2.06030700
C	0.09483700	2.84006100	-3.01513300
H	0.38474400	4.79951100	-2.04353100
H	0.65994300	2.88334500	-3.93476800
N	-2.22396500	-0.69492500	-1.67045500
C	-1.49568300	-0.60965200	-2.84634100
C	-1.57555700	-1.86034000	-3.57031800
C	-2.34794400	-2.70206400	-2.82490100
H	-1.08819200	-2.05474700	-4.51407600
H	-2.61755600	-3.72682100	-3.02978900
N	-3.66382300	-0.47104500	0.77372900
C	-3.99871700	-1.78392100	0.46916600
C	-4.29540700	-0.18569300	1.97291100
C	-4.86240900	-2.32284700	1.49657600
C	-5.04562300	-1.33808000	2.42339600
H	-5.26459900	-3.32497200	1.49288800
H	-5.63085900	-1.37106400	3.33043100
N	-2.75686700	2.20567600	1.06188300
C	-3.44972600	3.39073900	2.93612000
H	-3.96310200	3.59660800	3.86377100
C	-3.51940400	2.13453500	2.22451600
C	-0.91055800	3.27071400	-1.03594300
C	-0.67902700	1.69998600	-2.57739000
C	-2.75356400	-1.96923400	-1.64585000
C	-4.22254000	1.02209500	2.65097800
H	-4.76638900	1.10290800	3.58589400
C	-1.32612300	3.96582500	0.09393600
H	-0.95298700	4.97643800	0.22193000
C	-0.78659500	0.50180600	-3.27230500
H	-0.26874800	0.42818700	-4.22320300
C	-3.57256800	-2.48005300	-0.64763400
H	-3.89431900	-3.50975200	-0.74886300
C	-2.63377100	4.21766000	2.21935900
H	-2.34669400	5.23441000	2.44399900
C	-2.19122200	3.48027600	1.05754900
C	1.55012200	-4.50652300	0.25478700
H	1.07648100	-5.45550300	0.03230500
C	1.97919000	-1.49239100	0.92393900
C	2.07266500	-0.26118800	-0.01713300
H	2.81035700	-2.16488700	0.70953100
H	1.23028600	0.39827800	0.22828800
Cl	2.81252800	-4.24191700	-1.10005700
Cl	2.40761300	-4.75167800	1.91194900
C	0.45253400	-3.44479800	0.29804500

O	-0.69536400	-3.86584600	0.00169300
N	0.70126900	-2.17066800	0.66191400
H	-0.10832500	-1.54219600	0.61933100
C	2.01890700	-1.12040800	2.41347800
O	1.89718800	-0.80240400	-1.36530600
H	1.67374100	-0.07621100	-1.98130100
C	3.37152900	0.51746300	0.06133900
C	3.40441000	1.78952600	0.65575100
C	4.54608100	-0.00644900	-0.50693100
C	4.58717000	2.52407800	0.70727200
H	2.49745600	2.20251000	1.08589900
C	5.73823700	0.71270400	-0.46186500
H	4.51273600	-0.97442000	-0.99306500
C	5.74277000	1.97145400	0.14824600
H	4.63216600	3.50426400	1.16302000
H	6.65391200	0.32318900	-0.88664000
N	6.98690000	2.73626100	0.19414800
O	8.02393200	2.22643300	-0.32288000
O	6.96986000	3.87528200	0.74886400
O	3.35087200	-0.62660200	2.71477100
H	3.45069200	-0.46683100	3.67313300
H	1.24921500	-0.36352200	2.62547300
H	1.78973400	-2.02154700	2.99345600
²TS-H₃			
Fe	-2.33033628	-0.20910169	0.12012723
O	-0.94901628	0.53806631	-0.41146677
S	-4.58317800	-1.44543400	0.79019300
H	-4.04544400	-2.68755400	1.07761000
N	-2.93103000	1.27265800	1.41767700
C	-2.89826100	2.68877700	3.25557900
C	-3.62703300	3.30827300	2.28041700
H	-2.67016600	3.04317600	4.24999600
H	-4.11293600	4.27212800	2.31607300
N	-3.68906200	0.61165200	-1.24472600
C	-4.35017200	1.83094600	-1.14833200
C	-5.06819600	2.09958400	-2.37554700
C	-4.83780200	1.04826600	-3.21381900
H	-5.66498300	2.98171600	-2.55465800
H	-5.20695800	0.89756000	-4.21744600
N	-2.23844000	-1.82663000	-1.05665600
C	-2.71657000	-1.98364300	-2.35275200
C	-1.43245600	-2.93711500	-0.81323300
C	-2.22328700	-3.22243500	-2.91349600
C	-1.43059000	-3.80598900	-1.96900600
H	-2.45660900	-3.57937100	-3.90568900
H	-0.88155300	-4.73350800	-2.03248400

N	-1.47809600	-1.17921200	1.59850600
C	-0.14148500	-2.68919700	2.74583500
H	0.45167400	-3.57556800	2.91530700
C	-0.79493100	-2.38031200	1.49292100
C	-2.47095400	1.41540500	2.71610300
C	-3.64567200	2.41855300	1.13860400
C	-3.97793400	0.12150100	-2.50935300
C	-0.74764200	-3.18715200	0.36159700
H	-0.12970200	-4.07725400	0.41535500
C	-1.71565500	0.48044700	3.40785400
H	-1.44938000	0.71503700	4.43314700
C	-4.31637900	2.67459200	-0.05256700
H	-4.86134600	3.60961800	-0.12577000
C	-3.51479800	-1.07652300	-3.02895200
H	-3.80811300	-1.32827100	-4.04217000
C	-0.43197100	-1.66680300	3.61021800
H	-0.12988700	-1.55627400	4.64143500
C	-1.25546200	-0.72259600	2.89167300
C	3.33336187	-2.72913942	-2.74811002
H	3.42121725	-3.49977301	-3.48520248
C	2.18991066	-0.75387710	-0.58269761
C	1.62691584	0.68799775	-0.69521513
H	3.24612025	-0.73267745	-0.85769906
H	0.38895839	0.61931724	-0.53633045
Cl	4.21893088	-1.30438695	-3.28050832
C	1.86422235	-2.37258999	-2.55874920
O	1.06866368	-2.87601425	-3.39653838
N	1.44616784	-1.57640240	-1.55370526
H	0.44722218	-1.39379020	-1.59441165
C	2.05668580	-1.39086945	0.81441880
O	1.89826809	1.10338825	-2.05461070
H	1.30589816	1.87848635	-2.25608213
C	2.18432483	1.67606627	0.31090686
C	1.41181531	2.10024895	1.40263891
C	3.47279930	2.20817985	0.12945031
C	1.91735851	3.01935715	2.31994094
H	0.40706532	1.71154266	1.53409155
C	3.99355804	3.12843119	1.03500975
H	4.04832635	1.90631713	-0.73777047
C	3.20720262	3.51912956	2.12486375
H	1.33825864	3.35427238	3.17013277
H	4.98257848	3.55004542	0.91416660
N	3.74394040	4.48647727	3.07858381
O	4.91169398	4.93648161	2.88370746
O	3.01734758	4.83110790	4.05760406
O	2.98974144	-0.77975180	1.74509683

H	3.71297991	-1.39729640	1.96587152
H	1.04194874	-1.24135951	1.20536242
H	2.23223978	-2.46607653	0.71740679
Cl	4.00037294	-3.29817896	-1.22203983
⁴TS- H₃			
Fe	-2.47397	-0.21779	0.13379
O	-1.09265	0.52938	-0.3978
S	-4.58318	-1.44543	0.79019
H	-4.04544	-2.68755	1.07761
N	-2.93103	1.27266	1.41768
C	-2.89826	2.68878	3.25558
C	-3.62703	3.30827	2.28042
H	-2.67017	3.04318	4.25
H	-4.11294	4.27213	2.31607
N	-3.68906	0.61165	-1.24473
C	-4.35017	1.83095	-1.14833
C	-5.0682	2.09958	-2.37555
C	-4.8378	1.04827	-3.21382
H	-5.66498	2.98172	-2.55466
H	-5.20696	0.89756	-4.21745
N	-2.23844	-1.82663	-1.05666
C	-2.71657	-1.98364	-2.35275
C	-1.43246	-2.93712	-0.81323
C	-2.22329	-3.22243	-2.9135
C	-1.43059	-3.80599	-1.96901
H	-2.45661	-3.57937	-3.90569
H	-0.88155	-4.73351	-2.03248
N	-1.4781	-1.17921	1.59851
C	-0.14149	-2.6892	2.74584
H	0.45167	-3.57557	2.91531
C	-0.79493	-2.38031	1.49292
C	-2.47095	1.41541	2.7161
C	-3.64567	2.41855	1.1386
C	-3.97793	0.1215	-2.50935
C	-0.74764	-3.18715	0.3616
H	-0.1297	-4.07725	0.41536
C	-1.71566	0.48045	3.40785
H	-1.44938	0.71504	4.43315
C	-4.31638	2.67459	-0.05257
H	-4.86135	3.60962	-0.12577
C	-3.5148	-1.07652	-3.02895
H	-3.80811	-1.32827	-4.04217
C	-0.43197	-1.6668	3.61022
H	-0.12989	-1.55627	4.64144
C	-1.25546	-0.7226	2.89167
C	2.40794	-2.07913	-4.57532

H	2.60934	-3.05907	-4.99229
C	1.30851	0.21027	-2.71843
C	-0.0355	0.98632	-2.72173
H	1.84335	0.44564	-3.6405
H	-0.57494	0.81521	-1.48873
Cl	1.88146	-1.00577	-6.00396
Cl	4.05652	-1.48893	-3.87723
C	1.3304	-2.23996	-3.51024
O	0.80656	-3.38358	-3.43299
N	0.96982	-1.22412	-2.69977
H	0.20495	-1.47625	-2.07985
C	2.22891	0.51994	-1.52159
O	-0.65885	0.52034	-3.94175
H	-1.64128	0.65576	-3.84815
C	-0.29888	2.47735	-2.6397
C	-0.78407	3.05555	-1.45697
C	-0.09655	3.28718	-3.77083
C	-1.04046	4.42332	-1.38465
H	-0.96565	2.43116	-0.58802
C	-0.34872	4.65526	-3.7173
H	0.24021	2.82731	-4.69253
C	-0.81444	5.20739	-2.51853
H	-1.41017	4.88739	-0.48005
H	-0.19962	5.29642	-4.5759
N	-1.0847	6.64133	-2.45371
O	-0.88254	7.33744	-3.49231
O	-1.50856	7.12374	-1.36155
O	2.80792	1.84576	-1.6526
H	3.75942	1.78868	-1.86367
H	1.65735	0.49132	-0.5849
H	3.00137	-0.25307	-1.47616

²INT₃

Fe	2.22181400	-0.61877000	0.20170000
O	0.74188200	0.27624800	-0.42305300
S	4.16652100	-1.66621200	1.00546500
H	3.87005300	-2.95397900	0.60336900
N	3.12886200	-0.29807200	-1.57751500
C	3.89883100	-0.56076500	-3.74535600
C	4.43793400	0.59815200	-3.26391800
H	4.03079400	-1.00766900	-4.71968400
H	5.09783500	1.28988800	-3.76631200
N	3.05928700	1.06177700	0.92383900
C	3.89748700	1.93515700	0.24438300
C	4.24362000	3.04200000	1.10573900
C	3.60708600	2.84160000	2.29801500
H	4.88544000	3.86152400	0.81781400

H	3.62585700	3.46408300	3.18049400
N	1.29163200	-0.92222900	1.96121200
C	1.34636300	-0.10164700	3.07864300
C	0.51524700	-2.01578100	2.31602600
C	0.55787800	-0.68017700	4.14385900
C	0.04662400	-1.85820000	3.67450700
H	0.44169400	-0.24253500	5.12493000
H	-0.57780300	-2.57237000	4.19115800
N	1.54788800	-2.39360800	-0.46084000
C	0.36525900	-4.38010700	-0.64368500
H	-0.29761100	-5.18631700	-0.36659700
C	0.71481200	-3.27377800	0.21942500
C	3.09283100	-1.12901900	-2.68850100
C	3.96772300	0.75793400	-1.90668400
C	2.86346100	1.60814300	2.18399200
C	0.24174900	-3.10921900	1.51099400
H	-0.39727200	-3.88689900	1.91334000
C	2.42234500	-2.33765800	-2.77234900
H	2.46741900	-2.87359000	-3.71357400
C	4.32371600	1.79851400	-1.06652500
H	4.98247700	2.56267400	-1.46274000
C	2.06707200	1.07618200	3.18497700
H	2.01822100	1.61329900	4.12564400
C	0.97442900	-4.15885800	-1.84704600
H	0.92674800	-4.76378400	-2.74038400
C	1.70381300	-2.91670900	-1.73925300
C	-1.72255400	4.07411300	-1.70038600
H	-1.19162000	4.52215500	-2.53214300
C	-2.46315200	2.14815600	0.69210800
C	-3.70430500	1.35871900	0.31579900
H	-2.79096500	3.18613300	0.76145400
H	0.89765300	0.80362900	-1.24467200
Cl	-3.44987400	3.72891000	-2.31610000
Cl	-1.73655700	5.37484600	-0.34787300
C	-0.97125800	2.81422300	-1.29427400
O	0.03861100	2.54697500	-2.00355000
N	-1.33507800	2.03969900	-0.24769100
H	-0.64970100	1.27813900	-0.08275200
C	-1.92138100	1.73464100	2.07648400
O	-4.80667500	2.17879700	0.38283800
H	-5.62907300	1.76104600	0.06130400
C	-3.82496100	-0.02980700	0.05855800
C	-2.68763200	-0.85971200	-0.21046900
C	-5.11059200	-0.67127300	0.06628000
C	-2.82881400	-2.21527800	-0.44056200
H	-1.69441100	-0.43834700	-0.27461600

C	-5.24876800	-2.02701100	-0.15906100
H	-6.00569000	-0.11020800	0.31773300
C	-4.10376800	-2.80528700	-0.40736600
H	-1.96717100	-2.83156100	-0.65430800
H	-6.21671000	-2.50971600	-0.12751200
N	-4.23647200	-4.22317700	-0.60858500
O	-5.40678500	-4.72672300	-0.62887100
O	-3.17519000	-4.91889400	-0.75021600
O	-3.02632300	1.84755100	3.00453500
H	-2.78190800	1.47549600	3.87375300
H	-1.53387300	0.70837200	2.03597300
H	-1.09612400	2.40823900	2.34170900
⁴INT₃			
Fe	2.22194600	-0.61912200	0.20161800
O	0.74256300	0.27726200	-0.42288400
S	4.16588600	-1.66835200	1.00521300
H	3.86754300	-2.95614200	0.60457200
N	3.12828700	-0.30073900	-1.57836800
C	3.89699600	-0.56609100	-3.74634000
C	4.43757300	0.59265200	-3.26612000
H	4.02803600	-1.01395200	-4.72035400
H	5.09798800	1.28325500	-3.76939800
N	3.06173000	1.06098300	0.92204000
C	3.90041400	1.93300100	0.24141500
C	4.24818200	3.04015700	1.10170800
C	3.61216400	2.84131300	2.29451900
H	4.89067700	3.85879800	0.81277900
H	3.63211000	3.46444700	3.17651300
N	1.29242000	-0.92024600	1.96191700
C	1.34880000	-0.09895300	3.07875700
C	0.51503900	-2.01265300	2.31799000
C	0.56040000	-0.67587400	4.14490400
C	0.04749100	-1.85362800	3.67668700
H	0.44539200	-0.23743800	5.12575900
H	-0.57737400	-2.56676200	4.19424400
N	1.54566800	-2.39370700	-0.45919300
C	0.36081700	-4.37908700	-0.63984800
H	-0.30281100	-5.18435000	-0.36182500
C	0.71196800	-3.27242200	0.22218300
C	3.09088400	-1.13258400	-2.68863800
C	3.96816000	0.75406600	-1.90881000
C	2.86719500	1.60854100	2.18187400
C	0.23977400	-3.10633000	1.51388300
H	-0.39990600	-3.88298500	1.91715900
C	2.41907100	-2.34058200	-2.77116600
H	2.46312200	-2.87732500	-3.71197700

C	4.32571700	1.79491900	-1.06964300
H	4.98505500	2.55808600	-1.46681500
C	2.07086000	1.07816900	3.18375400
H	2.02317500	1.61603800	4.12405000
C	0.96966500	-4.15948600	-1.84367900
H	0.92090800	-4.76510000	-2.73649300
C	1.70043400	-2.91803400	-1.73725300
C	-1.72270700	4.07446600	-1.70099000
H	-1.19225100	4.52239600	-2.53311000
C	-2.46251600	2.14873800	0.69179200
C	-3.70403400	1.35935400	0.31651000
H	-2.79020000	3.18675700	0.76113700
H	0.89888000	0.80462000	-1.24439000
Cl	-3.45033900	3.72891800	-2.31569600
Cl	-1.73616600	5.37548700	-0.34874500
C	-0.97108900	2.81477800	-1.29489600
O	0.03901700	2.54789300	-2.00396900
N	-1.33499200	2.03999900	-0.24855000
H	-0.64956500	1.27846800	-0.08364700
C	-1.91987800	1.73538000	2.07591300
O	-4.80626900	2.17953200	0.38482000
H	-5.62907700	1.76180800	0.06429900
C	-3.82516300	-0.02907100	0.05905000
C	-2.68830300	-0.85904400	-0.21175500
C	-5.11086300	-0.67040700	0.06841400
C	-2.82994500	-2.21454000	-0.44194900
H	-1.69514000	-0.43771600	-0.27716100
C	-5.24948900	-2.02608000	-0.15700200
H	-6.00553500	-0.10930700	0.32130000
C	-4.10491900	-2.80443700	-0.40706300
H	-1.96868300	-2.83086800	-0.65709200
H	-6.21743300	-2.50869500	-0.12415600
N	-4.23805200	-4.22225100	-0.60832300
O	-5.40844900	-4.72567500	-0.62716400
O	-3.17701700	-4.91809700	-0.75133900
O	-3.02419400	1.84807800	3.00470300
H	-2.77913300	1.47598600	3.87372200
H	-1.53219000	0.70918100	2.03510900
H	-1.09456500	2.40912700	2.34058100
²TS-reb₃			
Fe	-0.07669600	2.04809900	0.19535500
O	-0.08530200	0.16594100	-0.46073700
S	-0.12778400	4.38174800	0.85981800
H	1.03682100	4.40089000	1.60303300
N	1.54407400	1.73299800	1.34591800
C	2.91980900	1.19447300	3.13028000

C	3.73159300	1.48868000	2.06879900
H	3.20585700	0.90169600	4.12995300
H	4.81120600	1.48223300	2.03046800
N	1.12889700	2.48795100	-1.37849700
C	2.51820700	2.49269700	-1.38404600
C	2.99580600	2.94661400	-2.67042400
C	1.89748400	3.24311300	-3.42893500
H	4.03842500	3.03716600	-2.93811000
H	1.86508900	3.62365100	-4.43941000
N	-1.68724200	2.47724400	-0.92675300
C	-1.69584000	2.94179300	-2.23551600
C	-3.01663000	2.34025100	-0.55263100
C	-3.06080900	3.10869500	-2.68035800
C	-3.87222300	2.73243800	-1.64760300
H	-3.34494800	3.45639300	-3.66266900
H	-4.95085100	2.70164700	-1.61826000
N	-1.26959300	1.52230200	1.72987900
C	-3.13752500	1.13870500	3.04477400
H	-4.18065900	1.05765500	3.31287900
C	-2.65760000	1.52787800	1.73751700
C	1.55504900	1.33775200	2.67830200
C	2.87501600	1.81921600	0.95341000
C	0.73173600	2.97062700	-2.61997800
C	-3.47091900	1.89045800	0.67689300
H	-4.54259600	1.82023000	0.81692100
C	0.43586200	1.08589100	3.45827000
H	0.59877900	0.79291900	4.48939400
C	3.33031800	2.16536600	-0.30991600
H	4.40330500	2.20368400	-0.46155700
C	-0.57830700	3.17730000	-3.02150100
H	-0.74276200	3.55138600	-4.02581900
C	-2.04055400	0.92688700	3.83171700
H	-2.00799400	0.63771700	4.87202200
C	-0.87383900	1.17595700	3.01401300
C	-4.06042800	-3.17470300	-0.57272800
H	-5.11520600	-3.08811200	-0.80653600
C	-1.09853600	-2.47788500	0.07884500
C	0.07215900	-2.29938400	-0.87012300
H	-1.45399400	-3.50447900	-0.08177100
H	0.29712400	0.24615700	-1.36079200
Cl	-3.34493900	-4.34619200	-1.84619800
Cl	-3.99279700	-3.96270400	1.14039700
C	-3.45324800	-1.77166600	-0.62111800
O	-4.25244000	-0.86658000	-0.96417100
N	-2.16145400	-1.54400600	-0.30630000
H	-1.78502900	-0.59363700	-0.42704300

C	-0.79929900	-2.31023900	1.58090100
O	-0.37864100	-2.40518100	-2.16437800
H	0.32552700	-2.25883600	-2.82829500
C	1.49191100	-2.44902100	-0.64205800
C	2.16328000	-1.89858600	0.48165600
C	2.27427300	-3.13725800	-1.61705800
C	3.53799500	-2.01761000	0.61576300
H	1.61252400	-1.33949400	1.21863300
C	3.64898900	-3.26416800	-1.48175300
H	1.79045200	-3.64055800	-2.44848400
C	4.27454200	-2.69265600	-0.36734500
H	4.05317100	-1.57918200	1.45894300
H	4.24289900	-3.80405400	-2.20719500
N	5.71620600	-2.79938400	-0.23173600
O	6.35934000	-3.41976800	-1.13433400
O	6.26510800	-2.26327200	0.77976800
O	0.13305100	-3.30754200	2.07354500
H	-0.32572000	-4.15867900	2.22165700
H	-0.35249000	-1.33621200	1.76662800
H	-1.75356300	-2.35568300	2.11427400
⁴TS-reb₃			
Fe	-0.07669600	2.04809900	0.19535500
O	-0.08530200	0.16594100	-0.46073700
S	-0.12778400	4.38174800	0.85981800
H	1.03682100	4.40089000	1.60303300
N	1.54407400	1.73299800	1.34591800
C	2.91980900	1.19447300	3.13028000
C	3.73159300	1.48868000	2.06879900
H	3.20585700	0.90169600	4.12995300
H	4.81120600	1.48223300	2.03046800
N	1.12889700	2.48795100	-1.37849700
C	2.51820700	2.49269700	-1.38404600
C	2.99580600	2.94661400	-2.67042400
C	1.89748400	3.24311300	-3.42893500
H	4.03842500	3.03716600	-2.93811000
H	1.86508900	3.62365100	-4.43941000
N	-1.68724200	2.47724400	-0.92675300
C	-1.69584000	2.94179300	-2.23551600
C	-3.01663000	2.34025100	-0.55263100
C	-3.06080900	3.10869500	-2.68035800
C	-3.87222300	2.73243800	-1.64760300
H	-3.34494800	3.45639300	-3.66266900
H	-4.95085100	2.70164700	-1.61826000
N	-1.26959300	1.52230200	1.72987900
C	-3.13752500	1.13870500	3.04477400
H	-4.18065900	1.05765500	3.31287900

C	-2.65760000	1.52787800	1.73751700
C	1.55504900	1.33775200	2.67830200
C	2.87501600	1.81921600	0.95341000
C	0.73173600	2.97062700	-2.61997800
C	-3.47091900	1.89045800	0.67689300
H	-4.54259600	1.82023000	0.81692100
C	0.43586200	1.08589100	3.45827000
H	0.59877900	0.79291900	4.48939400
C	3.33031800	2.16536600	-0.30991600
H	4.40330500	2.20368400	-0.46155700
C	-0.57830700	3.17730000	-3.02150100
H	-0.74276200	3.55138600	-4.02581900
C	-2.04055400	0.92688700	3.83171700
H	-2.00799400	0.63771700	4.87202200
C	-0.87383900	1.17595700	3.01401300
C	-4.06042800	-3.17470300	-0.57272800
H	-5.11520600	-3.08811200	-0.80653600
C	-1.09853600	-2.47788500	0.07884500
C	0.07215900	-2.29938400	-0.87012300
H	-1.45399400	-3.50447900	-0.08177100
H	0.29712400	0.24615700	-1.36079200
Cl	-3.34493900	-4.34619200	-1.84619800
Cl	-3.99279700	-3.96270400	1.14039700
C	-3.45324800	-1.77166600	-0.62111800
O	-4.25244000	-0.86658000	-0.96417100
N	-2.16145400	-1.54400600	-0.30630000
H	-1.78502900	-0.59363700	-0.42704300
C	-0.79929900	-2.31023900	1.58090100
O	-0.37864100	-2.40518100	-2.16437800
H	0.32552700	-2.25883600	-2.82829500
C	1.49191100	-2.44902100	-0.64205800
C	2.16328000	-1.89858600	0.48165600
C	2.27427300	-3.13725800	-1.61705800
C	3.53799500	-2.01761000	0.61576300
H	1.61252400	-1.33949400	1.21863300
C	3.64898900	-3.26416800	-1.48175300
H	1.79045200	-3.64055800	-2.44848400
C	4.27454200	-2.69265600	-0.36734500
H	4.05317100	-1.57918200	1.45894300
H	4.24289900	-3.80405400	-2.20719500
N	5.71620600	-2.79938400	-0.23173600
O	6.35934000	-3.41976800	-1.13433400
O	6.26510800	-2.26327200	0.77976800
O	0.13305100	-3.30754200	2.07354500
H	-0.32572000	-4.15867900	2.22165700
H	-0.35249000	-1.33621200	1.76662800

H	-1.75356300	-2.35568300	2.11427400
² P-OH ₃			
Fe	-2.70170900	-0.27105700	-0.22603800
O	0.51213700	0.13652400	0.38334000
S	-4.66094100	-1.19973800	-1.00323400
H	-5.35914000	-1.18470200	0.18926200
N	-3.59025800	0.92224900	1.09319700
C	-4.65059200	1.81247400	3.04798000
C	-4.84230000	2.65920300	2.01053700
H	-4.99578600	1.91707700	4.06616600
H	-5.36482500	3.60393200	2.03780400
N	-2.67082100	1.21276200	-1.56871900
C	-3.38292800	2.40668300	-1.47984100
C	-3.22404700	3.17081900	-2.69783100
C	-2.41264000	2.44446400	-3.52368300
H	-3.67197400	4.13728100	-2.87626800
H	-2.06949500	2.69614100	-4.51632200
N	-1.49246000	-1.33256500	-1.43187500
C	-1.11119900	-1.03506400	-2.74502100
C	-1.09282300	-2.66030000	-1.22529000
C	-0.45584300	-2.17245600	-3.34001700
C	-0.43362600	-3.16741600	-2.40239500
H	-0.05285300	-2.19110500	-4.34196400
H	0.01074000	-4.14830300	-2.47161400
N	-2.39597400	-1.59259200	1.25108600
C	-1.88218200	-3.56809300	2.36984800
H	-1.49466500	-4.56458700	2.52371400
C	-1.82642100	-2.85644400	1.11311400
C	-3.87640100	0.69102400	2.46001600
C	-4.19019800	2.13871900	0.82242000
C	-2.08718600	1.21641700	-2.83244100
C	-1.24029200	-3.35955700	-0.04015600
H	-0.81955000	-4.35744100	0.00049500
C	-3.49843700	-0.45185700	3.15048100
H	-3.76988600	-0.52455000	4.19775100
C	-4.11600000	2.82356700	-0.37979200
H	-4.63279300	3.77578700	-0.44985600
C	-1.35424900	0.17227400	-3.38075900
H	-0.99459200	0.28979800	-4.39743800
C	-2.49198900	-2.74478100	3.27356400
H	-2.70888900	-2.93645400	4.31418700
C	-2.82580500	-1.52272900	2.58018000
C	4.12176900	-3.42440500	-0.29949800
H	4.30574200	-4.44065500	-0.62806400
C	2.69334100	-0.85972200	0.78943200
C	1.90074900	0.20082900	-0.03901500

H	3.73266600	-0.84655400	0.46441400
H	-0.03553700	-0.37605600	-0.26171800
Cl	4.75919100	-2.32692500	-1.67114800
Cl	5.14610300	-3.19421900	1.25607300
C	2.62514500	-3.28821500	-0.03922000
O	1.93063000	-4.29357600	-0.32686700
N	2.09841100	-2.17427200	0.52138600
H	1.09416200	-2.22564600	0.66502900
C	2.64453900	-0.60413800	2.30077900
O	2.01135300	-0.23757200	-1.40781500
H	1.69350200	0.46128500	-2.01704600
C	2.42135800	1.62996400	0.10724100
C	1.66623500	2.61203500	0.76565800
C	3.65807800	1.97117800	-0.46542200
C	2.14219800	3.91654300	0.87072700
H	0.71460600	2.33164100	1.18122900
C	4.14429400	3.27360800	-0.37384600
H	4.23772100	1.21625500	-0.98466000
C	3.37852000	4.22931100	0.29930900
H	1.57751200	4.68897100	1.37520300
H	5.09413900	3.55716200	-0.80663400
N	3.87884600	5.60165000	0.39978100
O	4.98821500	5.87829100	-0.14194900
O	3.17361700	6.44987500	1.02035000
O	3.48229900	0.55070900	2.57270600
H	3.31445900	0.89851700	3.46968500
H	1.60374200	-0.44000000	2.60787900
H	3.03385900	-1.49333900	2.80932500
⁴P-OH₃			
Fe	-2.23725000	-1.06841900	0.03908500
O	0.35654400	-0.00249300	-0.44504300
S	-4.17681700	-2.41168800	0.18600700
H	-4.91712400	-1.63049800	1.05318100
N	-2.89103300	0.36034100	1.30218900
C	-3.55328900	1.46105100	3.22555100
C	-4.05837600	2.16128400	2.16454500
H	-3.65280300	1.68574600	4.27759200
H	-4.65005200	3.06495100	2.18567100
N	-2.77818600	0.12303400	-1.58485900
C	-3.50128200	1.30043700	-1.52364200
C	-3.81187700	1.74447300	-2.86997800
C	-3.29050500	0.81646300	-3.73049800
H	-4.36627100	2.63912500	-3.11389400
H	-3.33907200	0.81060200	-4.80983500
N	-1.25928700	-2.31731900	-1.24560300
C	-1.42047500	-2.34990900	-2.63232100

C	-0.52681900	-3.45534000	-0.89916700
C	-0.77152000	-3.53303700	-3.15551300
C	-0.21986200	-4.20403200	-2.09830900
H	-0.73411800	-3.79892000	-4.20186400
H	0.35955200	-5.11504300	-2.11720700
N	-1.18023000	-1.95395600	1.62696600
C	0.00756200	-3.47729500	2.90119200
H	0.62803100	-4.32938800	3.13789600
C	-0.39872900	-3.09377900	1.56122200
C	-2.81332700	0.33552300	2.69216200
C	-3.64236800	1.48004700	0.95518400
C	-2.65063100	-0.20521800	-2.92202500
C	-0.10355600	-3.78797600	0.38622000
H	0.52164800	-4.66906600	0.47698600
C	-2.08066700	-0.57459000	3.45153000
H	-2.11148600	-0.44305500	4.52855600
C	-3.90757000	1.91690000	-0.34196000
H	-4.49116800	2.82702500	-0.43688300
C	-2.04018800	-1.36481900	-3.39845500
H	-2.04696200	-1.51869500	-4.47280000
C	-0.55586200	-2.57764600	3.76561300
H	-0.48435500	-2.55846100	4.84358100
C	-1.30890200	-1.62904700	2.96523800
C	5.05493300	-1.91338100	-0.24009200
H	5.63366500	-2.81231400	-0.41858800
C	2.65671900	0.02990400	0.38949300
C	1.63398200	0.66144400	-0.60792900
H	3.64857200	0.40777400	0.14540100
H	0.27725600	-0.78711300	-1.03114300
Cl	5.39731700	-0.78592000	-1.68646700
Cl	5.73694300	-1.17477900	1.34737600
C	3.59229600	-2.32753600	-0.09864600
O	3.34818600	-3.56943800	-0.25571100
N	2.62034500	-1.42690200	0.22481200
H	1.70711400	-1.85187100	0.35440000
C	2.35548700	0.36638900	1.85668600
O	2.15935800	0.36582700	-1.91716700
H	1.68209200	0.88856500	-2.59556800
C	1.41314500	2.15502000	-0.43588900
C	0.23061500	2.64872200	0.13634300
C	2.40144200	3.04924600	-0.88127600
C	0.03746700	4.02308600	0.27129000
H	-0.53250800	1.95504600	0.46365900
C	2.21875000	4.42439800	-0.75329100
H	3.31290800	2.66623200	-1.32562000
C	1.03570900	4.89236800	-0.17488000

H	-0.86683600	4.42572400	0.70765700
H	2.96745900	5.13054400	-1.08638900
N	0.83441500	6.33586600	-0.03713500
O	1.74304700	7.10896300	-0.45841800
O	-0.23950600	6.74062800	0.49716800
O	2.77666400	1.73896100	2.07360500
H	2.48490400	2.05858300	2.94898300
H	1.28522600	0.22871500	2.06060400
H	2.92913100	-0.32232400	2.48739900

C-H hydroxylation through Path E

²RC₄

Fe	-3.40159000	-0.21916700	-0.08675100
O	-2.05815700	-0.49923800	0.84187500
S	-5.27659700	0.06403800	-1.80432300
H	-5.93326600	-1.13244300	-1.58349600
N	-4.58247400	-1.44183400	0.99858400
C	-5.56039100	-3.33737700	1.91076900
C	-5.91189400	-2.28275900	2.70460700
H	-5.83030000	-4.37757500	2.01866600
H	-6.52748500	-2.28730100	3.59203100
N	-4.03647300	1.35276700	0.99295300
C	-4.83316100	1.31526900	2.12427000
C	-4.99003100	2.64768700	2.66483300
C	-4.28790600	3.49187200	1.85273600
H	-5.56751400	2.88898500	3.54500700
H	-4.17415100	4.56270200	1.93490800
N	-2.44697500	1.03486300	-1.34590900
C	-2.32066100	2.41179100	-1.21339700
C	-1.69338000	0.68999400	-2.45610600
C	-1.47977100	2.93423200	-2.26829300
C	-1.08858000	1.87173400	-3.03106600
H	-1.22935400	3.97724100	-2.39292000
H	-0.45410600	1.87142200	-3.90472500
N	-3.00802900	-1.75160900	-1.34938500
C	-2.03712300	-3.05230500	-3.01143100
H	-1.44651300	-3.29599300	-3.88211600
C	-2.17005900	-1.72237500	-2.46048400
C	-4.72891300	-2.81026400	0.85166600
C	-5.29783100	-1.10330400	2.13701000
C	-3.69481200	2.67993600	0.81291800
C	-1.55043300	-0.59276400	-2.96351200
H	-0.91424700	-0.71679000	-3.83284500
C	-4.16877000	-3.57441100	-0.16527800
H	-4.36823200	-4.64063200	-0.15418000

C	-5.41618200	0.17562000	2.65802600
H	-6.01604000	0.29545200	3.55392300
C	-2.90255900	3.17428400	-0.21570300
H	-2.71996900	4.24336800	-0.23418600
C	-2.77956600	-3.89009300	-2.23088500
H	-2.91694300	-4.95630900	-2.33500600
C	-3.37402400	-3.08643900	-1.18635700
C	3.95988800	2.93875200	-0.79478600
H	4.42667400	3.88424100	-1.04560800
C	2.66135100	0.57971200	0.82992800
C	3.19646700	-0.64174400	1.62364200
H	2.90629300	0.44663400	-0.22445200
Cl	5.05235000	1.61421300	-1.54455100
Cl	2.28211200	2.95446800	-1.63567700
C	3.87309000	2.85269800	0.72573600
O	4.37077300	3.81942800	1.34923400
N	3.29704100	1.79619300	1.34832300
H	3.32741600	1.83825700	2.36282300
C	1.13152400	0.65562800	0.96830000
O	3.13474900	-0.22413600	3.02634200
H	3.17215000	-0.99525300	3.62330300
C	4.59055100	-1.08065800	1.22657100
C	4.75134100	-1.95443100	0.13533400
C	5.72668000	-0.62534200	1.91576500
C	6.02008400	-2.36193700	-0.27080300
H	3.87608200	-2.31498800	-0.39658100
C	7.00383300	-1.02563400	1.52234600
H	5.60090700	0.03766300	2.76266500
C	7.13261900	-1.88981700	0.43247900
H	6.16282700	-3.03438300	-1.10620100
H	7.89057800	-0.68230500	2.03859000
N	8.46847300	-2.32010200	0.01893100
O	9.46353300	-1.89166100	0.67264000
O	8.56381100	-3.10158300	-0.97229400
O	0.61947200	-0.58152500	0.42937200
H	-0.36010800	-0.64654900	0.57961000
H	0.86886100	0.77805600	2.02791800
H	0.76402800	1.52472300	0.41089100
H	2.48076400	-1.44964300	1.43572200
⁴RC₄			
Fe	-3.31765300	-0.24715300	-0.13676900
O	-2.19256500	-0.26628400	1.08225500
S	-4.99511600	-0.48829800	-2.03731600
H	-6.14350100	-0.62351800	-1.27977200
N	-4.77580700	0.48443800	1.05264600
C	-6.43997000	0.65852700	2.65914800

C	-6.05750900	1.93012600	2.33788000
H	-7.19183600	0.34283100	3.36735000
H	-6.43384100	2.86314100	2.73076200
N	-2.84263400	1.62791500	-0.70345500
C	-3.35380100	2.80596000	-0.18603900
C	-2.69330300	3.94126100	-0.79225400
C	-1.78408300	3.44461500	-1.68213400
H	-2.90980600	4.97353300	-0.56012300
H	-1.10653700	3.98808200	-2.32382900
N	-2.05645900	-0.97991400	-1.52471000
C	-1.19675100	-0.25224600	-2.33799900
C	-1.78602000	-2.31377700	-1.78630200
C	-0.38395900	-1.15126700	-3.12666300
C	-0.74351200	-2.42174200	-2.78320400
H	0.36124900	-0.83405500	-3.84094400
H	-0.35475000	-3.35489600	-3.16320900
N	-3.99376500	-2.11594300	0.21327300
C	-4.14940700	-4.43217200	0.30093900
H	-3.93169300	-5.46477100	0.07123400
C	-3.46443400	-3.30220700	-0.28551300
C	-5.63736700	-0.23864400	1.85825500
C	-5.01719100	1.81926700	1.34008600
C	-1.88175400	2.00205000	-1.62275300
C	-2.42926900	-3.39263000	-1.19901600
H	-2.10859500	-4.38582900	-1.49403500
C	-5.73399900	-1.62494100	1.88889800
H	-6.45927300	-2.05889800	2.56883700
C	-4.36247200	2.89553600	0.76153600
H	-4.66246400	3.88920000	1.07699300
C	-1.11934400	1.12808700	-2.38853200
H	-0.39812600	1.56316900	-3.07144400
C	-5.08273700	-3.93604600	1.16428400
H	-5.77991300	-4.48171000	1.78297500
C	-4.98032300	-2.49469600	1.12274200
C	3.83583800	3.04100200	-0.66543300
H	4.31908000	3.96826300	-0.95081600
C	2.58718800	0.72019700	1.05409900
C	3.15055200	-0.51065100	1.81492100
H	2.75553900	0.57844700	-0.01411400
Cl	4.81251700	1.67613200	-1.49504200
Cl	2.10070000	3.13217600	-1.38140900
C	3.85245600	2.95767100	0.85774500
O	4.42604000	3.90757600	1.44021400
N	3.28472600	1.92296200	1.52221500
H	3.38688700	1.96463600	2.53215300
C	1.07238900	0.82944000	1.29807500

O	3.21603200	-0.08001500	3.21330700
H	3.26773500	-0.84685600	3.81455700
C	4.49392200	-0.99244800	1.30815900
C	4.53675500	-1.88331200	0.21966000
C	5.69660100	-0.55988100	1.89063700
C	5.75447000	-2.33106200	-0.28755400
H	3.60930000	-2.22483900	-0.23010200
C	6.92408400	-1.00063100	1.39514600
H	5.66151300	0.11650000	2.73554400
C	6.93546600	-1.88146400	0.31106800
H	5.80727300	-3.01731400	-1.12226200
H	7.86091300	-0.67617900	1.82848900
N	8.21880900	-2.35378200	-0.20957000
O	9.27751000	-1.94624900	0.35061300
O	8.20718200	-3.14841500	-1.19485200
O	0.50558900	-0.41050700	0.82466400
H	-0.47860800	-0.42706600	0.95955300
H	0.88726000	0.97991700	2.37051800
H	0.68085500	1.69281900	0.74799400
H	2.39998700	-1.29921000	1.69468100
²TS-H₄			
Fe	-2.40644900	-0.78931000	0.21847700
O	-1.17420800	0.07992000	-0.71239300
S	-4.21596300	-1.73401900	1.44848600
H	-4.98080200	-2.14746900	0.37619200
N	-2.92040200	-1.91541400	-1.37654100
C	-3.84716500	-2.62831300	-3.37600300
C	-2.97758200	-3.59816300	-2.96673000
H	-4.46027000	-2.60893400	-4.26493200
H	-2.73968600	-4.53370500	-3.45130200
N	-1.17054600	-2.24852900	0.85950400
C	-0.91356100	-3.45474200	0.21678700
C	-0.02506800	-4.25812100	1.02645600
C	0.22845300	-3.55367600	2.17013600
H	0.32880700	-5.24174700	0.75373500
H	0.83148700	-3.84724100	3.01722100
N	-2.00686400	0.25539200	1.88775200
C	-1.18528300	-0.11556700	2.94150200
C	-2.47088700	1.52908000	2.18172600
C	-1.12626800	0.95628900	3.91192100
C	-1.91132200	1.97108100	3.43904900
H	-0.55841900	0.92094900	4.83030100
H	-2.10281200	2.93521600	3.88507000
N	-3.67773700	0.65147000	-0.40879300
C	-4.83919800	2.64690300	-0.56953500
H	-5.17850200	3.63742600	-0.30502800

C	-3.90023800	1.86739200	0.21115900
C	-3.80492700	-1.57199400	-2.38805800
C	-2.39711800	-3.15054800	-1.71924600
C	-0.49187700	-2.30467400	2.07122100
C	-3.33314200	2.28347000	1.40336700
H	-3.58137500	3.27647900	1.75850500
C	-4.52439800	-0.39061100	-2.47006000
H	-5.17910000	-0.26046600	-3.32441300
C	-1.45916300	-3.86385100	-0.98878300
H	-1.15569700	-4.83155700	-1.37298500
C	-0.48904800	-1.31192700	3.03883200
H	0.09415200	-1.48373200	3.93705100
C	-5.18451100	1.89182600	-1.65200000
H	-5.86278800	2.13987000	-2.45499500
C	-4.45334900	0.64444000	-1.55172800
C	0.23927679	4.46571526	-0.81250855
H	-0.47563371	5.18621463	-0.43238486
C	1.84080100	1.28017000	0.13841500
C	3.05631700	1.18654300	1.12297400
H	2.19836100	1.68571500	-0.80774700
Cl	1.80937682	5.44100095	-1.11952382
Cl	-0.47103726	3.83698280	-2.41857010
C	0.37621200	3.37645900	0.24829400
O	-0.41480200	4.08010100	0.91622600
N	0.84533400	2.18679500	0.71035800
H	0.48542600	1.95627500	1.63222700
C	1.25031000	-0.09879300	-0.12251400
O	3.47734500	2.56133700	1.32504200
H	4.24767200	2.59801400	1.92802500
C	4.42335136	0.53916273	1.22536467
C	4.62009011	-0.58801312	2.04057227
C	5.51117029	1.07333456	0.51156022
C	5.87398989	-1.19058159	2.13533523
H	3.78880226	-0.99717461	2.60717842
C	6.77118168	0.48293861	0.59663006
H	5.36230014	1.95303613	-0.10416981
C	6.93321259	-0.64445358	1.40786121
H	6.04565751	-2.05821847	2.75872995
H	7.61973409	0.87403608	0.05096769
N	8.25414408	-1.27083049	1.50370492
O	9.20616824	-0.75636848	0.85012052
O	8.37421581	-2.29604696	2.23587420
O	1.93829200	-0.73079400	-1.16153900
H	1.63416600	-1.65158600	-1.29863300
H	1.10329300	-0.72663500	0.76232100
H	2.67968600	0.76499300	2.06971900

H	-0.13258400	0.00314100	-0.45896800
⁴ TS- H ₄			
Fe	-2.46251000	-0.74203400	0.19552200
O	-1.17852000	0.00043200	-0.76682100
S	-4.04588300	-1.71063100	1.72084600
H	-4.55871800	-2.68795000	0.88777300
N	-3.19895800	-1.81596900	-1.30408100
C	-4.38202800	-2.46030500	-3.19402100
C	-3.49639100	-3.46095100	-2.91483500
H	-5.09570700	-2.40394900	-4.00279100
H	-3.34563800	-4.38913000	-3.44646200
N	-1.25761700	-2.31402100	0.73101600
C	-1.07885500	-3.48638000	0.01679100
C	-0.14134800	-4.34741600	0.70881400
C	0.21938600	-3.70312000	1.85963400
H	0.16629400	-5.32408900	0.36412000
H	0.88617800	-4.04738700	2.63697700
N	-1.82690500	0.23696600	1.85963200
C	-0.96398500	-0.22170800	2.84399700
C	-2.13206400	1.54365300	2.18783100
C	-0.73057400	0.82805800	3.81308900
C	-1.44203300	1.92224200	3.39883900
H	-0.10327500	0.72974100	4.68723700
H	-1.51032600	2.89404400	3.86247200
N	-3.65254700	0.77654600	-0.28439100
C	-4.65601000	2.86766600	-0.33086800
H	-4.87383400	3.88589600	-0.04438400
C	-3.69782800	2.01418800	0.34386900
C	-4.18413400	-1.42573400	-2.20292400
C	-2.75398000	-3.06140600	-1.73896100
C	-0.47861800	-2.43491100	1.87494700
C	-2.98501400	2.37585500	1.47377100
H	-3.11351100	3.38465000	1.84698600
C	-4.83547500	-0.20269400	-2.19928800
H	-5.58043400	-0.02862000	-2.96797400
C	-1.75872600	-3.82169100	-1.14732000
H	-1.52284000	-4.77566500	-1.60683100
C	-0.35315500	-1.47007300	2.86334700
H	0.28820100	-1.69898600	3.70834000
C	-5.19906700	2.13761100	-1.34678300
H	-5.95117500	2.43735600	-2.06165300
C	-4.56767000	0.83281000	-1.31593000
C	0.43149795	3.87296281	-0.89807419
H	-0.23018298	4.72309906	-1.01784885
C	1.75991035	1.27696365	0.26861297
C	2.94866146	1.22584351	1.28157968

H	2.10894920	1.75228618	-0.64796258
Cl	2.09667798	4.31163313	-1.26186505
Cl	0.28962459	2.85435616	-2.28919332
C	0.08130006	3.21726642	0.43399505
O	-0.81541155	3.78591446	1.10256277
N	0.68482119	2.08000811	0.86276533
H	0.30349133	1.74719928	1.74405465
C	1.26985400	-0.12897300	-0.07334500
O	3.26462439	2.61397126	1.57256750
H	4.00646065	2.66770978	2.20882844
C	4.16484792	0.48572214	0.75946102
C	4.47327723	-0.80445908	1.22079721
C	5.00699111	1.10007575	-0.18496418
C	5.59108909	-1.48633454	0.74147423
H	3.83718451	-1.27868916	1.96194194
C	6.12808360	0.43243051	-0.67363519
H	4.77949758	2.10347014	-0.52613623
C	6.40300115	-0.85547399	-0.20347780
H	5.84597281	-2.47996762	1.08564790
H	6.78445982	0.88489657	-1.40503480
N	7.57965298	-1.56404238	-0.71133307
O	8.31142984	-0.97447371	-1.55733481
O	7.80477690	-2.73193527	-0.27835741
O	2.64226531	-0.46702498	-0.10091627
H	2.76618881	-1.43179226	-0.20575085
H	1.17426300	-0.69372800	0.86437900
H	2.58360558	0.72307596	2.19250262
H	-0.02299700	-0.06064200	-0.43953100
²INT₄			
Fe	-2.70560700	-0.64749100	0.22568100
O	-1.47206200	0.07372100	-0.87269700
S	-4.33735000	-1.54386100	1.72094000
H	-5.42035900	-1.42665400	0.87275500
N	-3.62970800	-1.58211500	-1.29754400
C	-4.94326700	-2.02392200	-3.15264800
C	-4.16467500	-3.12505300	-2.93964100
H	-5.67794600	-1.86150100	-3.92763300
H	-4.13606900	-4.04578800	-3.50364500
N	-1.58913600	-2.29945700	0.58296700
C	-1.61525200	-3.47763100	-0.15112600
C	-0.70473500	-4.43515000	0.43425900
C	-0.14833200	-3.84418700	1.53454200
H	-0.53887000	-5.43258500	0.05391000
H	0.56196200	-4.26379800	2.23232700
N	-1.86802500	0.22322700	1.84488900
C	-0.92385300	-0.31646200	2.70429000

C	-2.10306500	1.51856700	2.28020000
C	-0.54926700	0.67181600	3.69339300
C	-1.27170600	1.80341400	3.42682600
H	0.15908100	0.50231100	4.49170600
H	-1.25564500	2.74928300	3.94694200
N	-3.88154600	0.95521800	-0.06113400
C	-4.76151600	3.09232800	0.07938500
H	-4.91083000	4.09694300	0.44640700
C	-3.82423900	2.14680000	0.64545900
C	-4.60468800	-1.05705200	-2.13094900
C	-3.34121200	-2.84846200	-1.78265900
C	-0.70568300	-2.51388500	1.63273700
C	-2.99919300	2.41558800	1.72301300
H	-3.05260600	3.40444900	2.16219000
C	-5.17106900	0.20178200	-2.02016600
H	-5.92678600	0.48117400	-2.74542700
C	-2.41000200	-3.72868200	-1.25781900
H	-2.31025100	-4.69640900	-1.73683100
C	-0.39048300	-1.59470500	2.62193800
H	0.31920800	-1.89644900	3.38464500
C	-5.37893500	2.46987100	-0.96690700
H	-6.13562700	2.86302300	-1.62983800
C	-4.82160300	1.13725700	-1.05955400
C	1.07618400	3.63360800	-1.31317600
H	0.47827500	4.51105700	-1.53071700
C	2.23281200	1.10287100	0.10223000
C	3.38403600	1.01918200	1.15554500
H	2.65423600	1.51903600	-0.81322100
Cl	2.86223500	4.20843300	-1.42195700
Cl	0.69917500	2.39599700	-2.65666900
C	0.69941200	3.16273900	0.08789400
O	-0.10324100	3.89119300	0.71434900
N	1.19158600	2.00939900	0.61210100
H	0.85210700	1.83063600	1.55322800
C	1.66197400	-0.24845800	-0.21769900
O	3.78142000	2.39344100	1.40466900
H	4.52331500	2.42597600	2.04237300
C	4.54831600	0.17545800	0.67283200
C	4.71478900	-1.14435400	1.12364300
C	5.47064100	0.71355000	-0.24275500
C	5.77467400	-1.92647100	0.66525600
H	4.01429700	-1.56274600	1.83983700
C	6.53585100	-0.05477800	-0.70926500
H	5.34751200	1.73639900	-0.57982700
C	6.67103100	-1.36740900	-0.24809400
H	5.92113900	-2.94417500	1.00186900

H	7.25333400	0.33897800	-1.41687800
N	7.78895800	-2.18169500	-0.73186500
O	8.59507700	-1.65853500	-1.55298300
O	7.88164500	-3.37256100	-0.31488600
O	2.21918000	-0.85321200	-1.33590100
H	1.84758800	-1.74078300	-1.50603100
H	1.25127900	-0.88750700	0.56146900
H	2.96897500	0.57203400	2.07386800
H	-0.51064800	-0.02511200	-0.67176700
⁴ INT ₄			
Fe	-2.47144600	-0.69897200	0.31488800
O	-1.05409600	-0.03057700	-0.66542700
S	-4.43209000	-1.48248600	1.49910600
H	-4.71284800	-0.33944900	2.22308400
N	-3.10564800	-1.89777800	-1.18115300
C	-4.19832000	-2.67761800	-3.07568100
C	-3.47365300	-3.72164100	-2.57583700
H	-4.83924600	-2.66310000	-3.94503700
H	-3.40142600	-4.72989800	-2.95659900
N	-1.35206300	-2.23130800	1.01672600
C	-1.25181300	-3.51356000	0.51433300
C	-0.32482500	-4.28999800	1.30707300
C	0.13893400	-3.46516700	2.29443600
H	-0.06984700	-5.32316300	1.12235600
H	0.84844500	-3.69001700	3.07698900
N	-1.89578200	0.47387000	1.85896500
C	-0.96276900	0.14416300	2.82796700
C	-2.25941400	1.78009800	2.10981300
C	-0.74087800	1.27459900	3.70666500
C	-1.54506400	2.28706000	3.26179100
H	-0.05869700	1.27797200	4.54399200
H	-1.64917000	3.28532800	3.66014900
N	-3.68380800	0.77525900	-0.31563800
C	-4.74985200	2.82476600	-0.57521800
H	-5.03489900	3.84460800	-0.36379000
C	-3.83442200	2.04577400	0.23045400
C	-3.97526300	-1.54668400	-2.19923400
C	-2.79082500	-3.23635800	-1.39612500
C	-0.51054400	-2.18512900	2.11378000
C	-3.16968600	2.51182100	1.35037400
H	-3.34881000	3.53983900	1.64407100
C	-4.58372600	-0.30458100	-2.34038400
H	-5.23402000	-0.16838700	-3.19841900
C	-1.93539600	-3.98538600	-0.60444500
H	-1.77420900	-5.02110000	-0.88533400
C	-0.32433700	-1.08364400	2.94289900

H	0.38808200	-1.19335100	3.75331400
C	-5.13629900	2.03664500	-1.61928300
H	-5.80701000	2.28084500	-2.42987200
C	-4.46540900	0.76222800	-1.46392100
C	1.57804700	4.33133600	-0.60673500
H	1.11260500	5.30575100	-0.51498200
C	2.02831000	1.26541000	-0.90100700
C	2.23318100	0.14281700	0.17264800
H	2.84525200	1.98001000	-0.78925600
Cl	2.83324100	4.23103300	0.78384500
Cl	2.44569900	4.35130900	-2.27759700
C	0.47668600	3.27421600	-0.50617400
O	-0.67442800	3.74569900	-0.32063900
N	0.73911000	1.95135500	-0.59201300
H	-0.09284300	1.30154900	-0.59588400
C	2.05542500	0.75141100	-2.30075600
O	2.13470400	0.71911300	1.49979900
H	1.33979000	1.29026300	1.53660700
C	3.58995600	-0.51762300	0.05940200
C	3.78168500	-1.59821000	-0.82071500
C	4.67231600	-0.05402100	0.82708900
C	5.03136700	-2.20243100	-0.94415800
H	2.94653500	-1.96065800	-1.40912300
C	5.92841500	-0.64942800	0.71405200
H	4.50842400	0.75985200	1.52117400
C	6.09164800	-1.71679700	-0.17336000
H	5.19750300	-3.03611900	-1.61336500
H	6.77284700	-0.30725600	1.29765900
N	7.40413500	-2.34959500	-0.29499700
O	8.35230300	-1.90445400	0.41543400
O	7.53041500	-3.31365400	-1.10673700
O	1.24185600	-0.36233400	-2.56426500
H	1.21030800	-0.57301300	-3.51627000
H	2.30190000	1.39950700	-3.13467700
H	1.44060900	-0.60077800	0.03298000
H	-0.68871700	-0.65335900	-1.32576900
²TS-reb₄			
Fe	-2.35255000	-0.74432000	0.30429500
O	-0.91904800	-0.04322100	-0.78595600
S	-4.20153900	-1.54719700	1.61437100
H	-3.69099700	-2.79402400	1.91950700
N	-1.25729000	-2.34468100	0.84487600
C	-0.20901300	-4.40935300	0.84012100
C	0.21797600	-3.74204200	1.95573700
H	0.06123500	-5.40196900	0.51018800
H	0.91052500	-4.07860000	2.71334200

N	-1.61750600	0.28450200	1.86974900
C	-0.73806700	-0.17915800	2.83638100
C	-0.46135100	0.87549400	3.78704300
C	-1.18569200	1.96857600	3.39907100
H	0.20197000	0.77608600	4.63338800
H	-1.23819600	2.93950200	3.86916000
N	-3.54839300	0.79731000	-0.16721800
C	-3.59199500	2.03155300	0.46668300
C	-4.46909000	0.85759600	-1.20492500
C	-4.56601400	2.87572700	-0.18357100
C	-5.11190000	2.15145700	-1.20594200
H	-4.78535800	3.89105500	0.11097300
H	-5.86987100	2.45619900	-1.91247500
N	-3.03573300	-1.75654300	-1.31314000
C	-4.27388800	-2.38803700	-3.16589000
H	-4.99980700	-2.32186300	-3.96308500
C	-4.03395500	-1.34943000	-2.19019400
C	-1.12659500	-3.53715900	0.14360100
C	-0.42513900	-2.44848000	1.95315600
C	-1.92322600	1.59376400	2.21290800
C	-4.70445400	-0.13849200	-2.14035200
H	-5.46044400	0.05008300	-2.89423800
C	-1.77350500	-3.86031600	-1.03980000
H	-1.58403700	-4.84092900	-1.46223300
C	-0.19005000	-1.45083000	2.88676300
H	0.49441200	-1.67124300	3.69774600
C	-2.82651500	2.41229600	1.55667900
H	-2.94872000	3.42335700	1.92482900
C	-3.43495100	-3.42543200	-2.86817100
H	-3.34148100	-4.37633700	-3.37222300
C	-2.67504600	-3.04045100	-1.70004000
C	1.65786000	4.46477700	-0.57589100
H	1.26325100	5.47265300	-0.51911100
C	1.79412600	1.31106200	-0.73242400
C	2.09172000	0.34360200	0.46073800
H	2.66851500	1.95388600	-0.88154600
Cl	2.92189500	4.33543600	0.80542800
Cl	2.50033300	4.34399500	-2.24351100
C	0.48065000	3.50469400	-0.40224600
O	-0.63163400	4.06347300	-0.23876000
N	0.62986200	2.15756300	-0.39484400
H	-0.23526600	1.58904400	-0.38949700
C	1.49777900	0.52418700	-1.96290900
O	2.29391600	1.10238500	1.67654500
H	1.53263800	1.70435600	1.81302500
C	3.34575900	-0.47043800	0.23078100

C	3.26098000	-1.82693800	-0.12861700
C	4.61169700	0.12697900	0.37286000
C	4.41416200	-2.57389500	-0.37132200
H	2.28924400	-2.30620800	-0.19760100
C	5.77248400	-0.60679700	0.13535700
H	4.67538300	1.16027900	0.69173200
C	5.65620700	-1.94879000	-0.24117800
H	4.36925700	-3.61915500	-0.64674100
H	6.75479400	-0.16500300	0.23823900
N	6.87001700	-2.72567400	-0.49696400
O	7.98769300	-2.14866500	-0.36399400
O	6.74140700	-3.93710700	-0.84175900
O	1.23294200	1.24008000	-3.10136300
H	1.09594600	0.67986900	-3.88950900
H	1.61954000	-0.54829000	-2.02892400
H	-1.21005400	-0.07230700	-1.72229600
H	1.22595800	-0.32054100	0.56180400
⁴TS-reb₄			
Fe	-2.35255000	-0.74432000	0.30429500
O	-0.91904800	-0.04322100	-0.78595600
S	-4.20153900	-1.54719700	1.61437100
H	-3.69099700	-2.79402400	1.91950700
N	-1.25729000	-2.34468100	0.84487600
C	-0.20901300	-4.40935300	0.84012100
C	0.21797600	-3.74204200	1.95573700
H	0.06123500	-5.40196900	0.51018800
H	0.91052500	-4.07860000	2.71334200
N	-1.61750600	0.28450200	1.86974900
C	-0.73806700	-0.17915800	2.83638100
C	-0.46135100	0.87549400	3.78704300
C	-1.18569200	1.96857600	3.39907100
H	0.20197000	0.77608600	4.63338800
H	-1.23819600	2.93950200	3.86916000
N	-3.54839300	0.79731000	-0.16721800
C	-3.59199500	2.03155300	0.46668300
C	-4.46909000	0.85759600	-1.20492500
C	-4.56601400	2.87572700	-0.18357100
C	-5.11190000	2.15145700	-1.20594200
H	-4.78535800	3.89105500	0.11097300
H	-5.86987100	2.45619900	-1.91247500
N	-3.03573300	-1.75654300	-1.31314000
C	-4.27388800	-2.38803700	-3.16589000
H	-4.99980700	-2.32186300	-3.96308500
C	-4.03395500	-1.34943000	-2.19019400
C	-1.12659500	-3.53715900	0.14360100
C	-0.42513900	-2.44848000	1.95315600

C	-1.92322600	1.59376400	2.21290800
C	-4.70445400	-0.13849200	-2.14035200
H	-5.46044400	0.05008300	-2.89423800
C	-1.77350500	-3.86031600	-1.03980000
H	-1.58403700	-4.84092900	-1.46223300
C	-0.19005000	-1.45083000	2.88676300
H	0.49441200	-1.67124300	3.69774600
C	-2.82651500	2.41229600	1.55667900
H	-2.94872000	3.42335700	1.92482900
C	-3.43495100	-3.42543200	-2.86817100
H	-3.34148100	-4.37633700	-3.37222300
C	-2.67504600	-3.04045100	-1.70004000
C	1.65786000	4.46477700	-0.57589100
H	1.26325100	5.47265300	-0.51911100
C	1.79412600	1.31106200	-0.73242400
C	2.09172000	0.34360200	0.46073800
H	2.66851500	1.95388600	-0.88154600
Cl	2.92189500	4.33543600	0.80542800
Cl	2.50033300	4.34399500	-2.24351100
C	0.48065000	3.50469400	-0.40224600
O	-0.63163400	4.06347300	-0.23876000
N	0.62986200	2.15756300	-0.39484400
H	-0.23526600	1.58904400	-0.38949700
C	1.49777900	0.52418700	-1.96290900
O	2.29391600	1.10238500	1.67654500
H	1.53263800	1.70435600	1.81302500
C	3.34575900	-0.47043800	0.23078100
C	3.26098000	-1.82693800	-0.12861700
C	4.61169700	0.12697900	0.37286000
C	4.41416200	-2.57389500	-0.37132200
H	2.28924400	-2.30620800	-0.19760100
C	5.77248400	-0.60679700	0.13535700
H	4.67538300	1.16027900	0.69173200
C	5.65620700	-1.94879000	-0.24117800
H	4.36925700	-3.61915500	-0.64674100
H	6.75479400	-0.16500300	0.23823900
N	6.87001700	-2.72567400	-0.49696400
O	7.98769300	-2.14866500	-0.36399400
O	6.74140700	-3.93710700	-0.84175900
O	1.23294200	1.24008000	-3.10136300
H	1.09594600	0.67986900	-3.88950900
H	1.61954000	-0.54829000	-2.02892400
H	-1.21005400	-0.07230700	-1.72229600
H	1.22595800	-0.32054100	0.56180400
²P-OH₄			
Fe	2.06448200	1.10518400	0.21729000

O	0.60309300	-0.21537300	-0.51874200
S	3.65655600	2.53418000	1.02878800
H	4.71581300	2.10090900	0.25430400
N	2.62913700	1.39827000	-1.69321500
C	3.74381600	1.30485200	-3.72793600
C	2.83987800	2.32517200	-3.81014200
H	4.43842000	0.96292700	-4.48133900
H	2.65032700	2.98591700	-4.64358900
N	0.71725000	2.61015400	0.09904900
C	0.52118900	3.43391800	-1.00201900
C	-0.43666600	4.47052300	-0.67433000
C	-0.79940400	4.28700800	0.63036100
H	-0.76495100	5.24043900	-1.35752800
H	-1.48449000	4.87605500	1.22284800
N	1.38955300	0.72865400	2.08623700
C	0.49839500	1.47810000	2.84327100
C	1.83262400	-0.29455100	2.91354800
C	0.36630000	0.89937400	4.16345500
C	1.18244100	-0.19674900	4.20488000
H	-0.26196600	1.29555200	4.94826500
H	1.35339400	-0.87311600	5.02990700
N	3.29726300	-0.48405300	0.29030800
C	4.47001500	-2.32842800	1.07106200
H	4.77256800	-3.11665000	1.74440900
C	3.46001000	-1.33471100	1.37394200
C	3.61154400	0.72540500	-2.40806700
C	2.14858300	2.38810000	-2.53819100
C	-0.07800500	3.12954900	1.11390500
C	2.77449700	-1.25896500	2.57773400
H	3.00941600	-2.00649100	3.32747100
C	4.34684700	-0.35177300	-1.93436600
H	5.08548000	-0.78872700	-2.59751900
C	1.16583200	3.31685100	-2.22630800
H	0.90240800	4.03567700	-2.99515900
C	-0.18227100	2.60324000	2.39445500
H	-0.83648800	3.11009400	3.09611700
C	4.92618800	-2.06811700	-0.18895700
H	5.68027700	-2.59890800	-0.75155700
C	4.19248400	-0.91949900	-0.67768500
C	-0.06444500	-4.25674800	-0.92828200
H	0.55550300	-5.14087800	-1.02197300
C	-1.32855600	-1.61559600	0.18139000
C	-2.52016900	-1.50713700	1.17633600
H	-1.68158100	-2.10112200	-0.72845700
Cl	-1.81980100	-4.82589600	-1.15735700
Cl	0.45599600	-3.14041100	-2.36684300

C	0.24786300	-3.61972200	0.42324600
O	1.06288400	-4.24418600	1.13799200
N	-0.27303300	-2.42049500	0.78982500
H	0.12137700	-2.06983000	1.65800500
C	-0.80361300	-0.20990400	-0.19987600
O	-2.91035800	-2.88419400	1.42597500
H	-3.64469700	-2.91938200	2.07152000
C	-3.68877100	-0.68311500	0.66952800
C	-3.90164600	0.62095200	1.14598500
C	-4.57916600	-1.22955900	-0.27155700
C	-4.97314500	1.38297300	0.68037500
H	-3.22613200	1.04523200	1.88282900
C	-5.65526800	-0.48178100	-0.74442700
H	-4.42425000	-2.24263200	-0.62401900
C	-5.83481900	0.81806600	-0.26191400
H	-5.15391700	2.38951200	1.03339300
H	-6.34851400	-0.88091700	-1.47286600
N	-6.96407900	1.61105800	-0.75439800
O	-7.74124500	1.08001700	-1.59853400
O	-7.10371100	2.78757600	-0.31052800
O	-1.58229900	0.22764800	-1.30686800
H	-1.40782600	1.17446900	-1.48900600
H	-0.85649500	0.48320400	0.63970700
H	-2.13559800	-1.05002600	2.10262600
H	0.85026200	-0.84913400	-1.22267500
⁴P-OH₄			
Fe	2.67918800	0.01480100	0.38662500
O	-0.10725800	-0.22900000	-1.54413400
S	4.70651600	-0.33005200	1.52660000
H	4.77713900	-1.70671800	1.42207500
N	3.40273200	0.25348300	-1.55773300
C	4.34714000	-0.19369300	-3.62309500
C	4.48646700	1.14814000	-3.39641800
H	4.67183300	-0.76009800	-4.48385900
H	4.94699500	1.88643700	-4.03666200
N	2.71737000	2.02135600	0.62690800
C	3.37260900	2.93172500	-0.19281500
C	3.34197200	4.24113500	0.42894100
C	2.65992000	4.11846200	1.60653700
H	3.77539500	5.13296700	0.00048500
H	2.42901100	4.89055300	2.32584300
N	1.34406800	-0.11976100	2.00027300
C	1.02153100	0.90436900	2.87591900
C	0.80079000	-1.28292000	2.52185200
C	0.20870000	0.37598800	3.95408700
C	0.07258100	-0.97271800	3.73566400

H	-0.17299700	0.95592700	4.78235200
H	-0.44678000	-1.69749100	4.34594500
N	2.28417000	-1.92719900	-0.04661700
C	1.77317800	-4.17513100	0.21858800
H	1.33698500	-5.06436200	0.64772800
C	1.66332400	-2.85438800	0.79883300
C	3.67978000	-0.75512100	-2.46356000
C	3.90693400	1.42463700	-2.09522100
C	2.25800600	2.73125500	1.73177200
C	0.96719500	-2.55228000	1.96714000
H	0.48294700	-3.38306600	2.46846200
C	3.40439000	-2.10403400	-2.25270300
H	3.70103200	-2.79766100	-3.03264000
C	3.90680700	2.65752700	-1.44938500
H	4.36249400	3.48961400	-1.97624400
C	1.46584700	2.21961400	2.75482700
H	1.16222200	2.91560200	3.53012000
C	2.45959700	-4.05098500	-0.95805700
H	2.70890800	-4.82873500	-1.66494400
C	2.77851600	-2.65099100	-1.13549000
C	-3.82321800	-3.70629700	-0.09814200
H	-4.03276900	-4.73061700	0.18749700
C	-2.24362500	-0.99303400	-0.51845000
C	-2.07270100	0.10941500	0.57213100
H	-3.30097300	-1.09945700	-0.76333600
Cl	-5.04143500	-2.65994500	0.86550000
Cl	-4.18619400	-3.59959700	-1.92735400
C	-2.36599600	-3.43558500	0.26419600
O	-1.76598700	-4.38563900	0.82664500
N	-1.74272300	-2.26200400	-0.00145500
H	-0.78807400	-2.25478900	0.34337200
C	-1.48910900	-0.58387100	-1.80067600
O	-2.70232900	-0.40507300	1.77550200
H	-2.21445500	-0.09795100	2.56607700
C	-2.67613800	1.44630900	0.17358900
C	-1.87557800	2.44792500	-0.40624900
C	-4.04285500	1.69340600	0.39435000
C	-2.42974700	3.67528300	-0.77121200
H	-0.81933500	2.26122900	-0.57206000
C	-4.60917800	2.91516600	0.03304200
H	-4.64463700	0.92838000	0.87025000
C	-3.79207300	3.89021700	-0.54727800
H	-1.83112300	4.45977000	-1.21482200
H	-5.65833600	3.12508600	0.19416900
N	-4.37812100	5.17797800	-0.92390300
O	-5.61172700	5.35811600	-0.70933200

O	-3.62164700	6.04804700	-1.44608800
O	-1.58223600	-1.66328700	-2.72631200
H	-1.25145000	-1.38526900	-3.60451400
H	-1.91899800	0.33704000	-2.20124300
H	-0.99737300	0.23985100	0.73097000
H	0.43550800	-1.01746500	-1.32021000