

Supporting Information

Water Biocatalytic Effect Attenuates Cytochrome P450-Mediated Carcinogenicity of Diethylnitrosamine: A Computational Insight

Emadeldin M. Kamel^{1,2}, Al Mokhtar Lamsabhi^{2,3,*}

¹Chemistry Department, Faculty of Science, Beni-Suef University, Beni-Suef 62514, Egypt.

²Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, Campus de Excelencia UAM-CSIC Cantoblanco, 28049 Madrid, Spain.

³ Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid, Spain.

*E-mail: mokhtar.lamsabhi@uam.es

Table of Contents

Table S1. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the α -position (Path A) in the water-free system.....	S3
Table S2. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the β -position (Path B) in the water-free system.....	S3
Table S3. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the α -position (Path A) in the one-water system.....	S4
Table S4. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the β -position (Path B) in the one-water system.....	S4
Table S5. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the α -position (Path A) in the two-water system.....	S5

Table S6. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the β -position (Path B) in the two-water system.....	S5
Cartesian coordinates of all structures represented in this study.....	S6

Table S1. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the α -position (Path A) in the water-free system.

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1+Bulk Polarity		UB3LYP/BS2//BS1+ZPE+B Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
² RC _{α}	-1928.89654530	0.00	-1928.46082030	0.00	-1929.32200330	0.00	-1928.88627830	0.00	-1929.33913994	0.00	-1928.90341494	0.00
⁴ RC _{α}	-1928.89644987	0.06	-1928.46067787	0.09	-1929.32183450	0.11	-1928.88606250	0.14	-1929.33902770	0.07	-1928.90325570	0.10
² TS-H _{α}	-1928.867005	18.54	-1928.436875	15.03	-1929.293886	17.64	-1928.863756	14.13	-1929.309796	18.41	-1928.879666	14.90
⁴ TS- H _{α}	-1928.867085	18.49	-1928.4372	14.82	-1929.29679	15.82	-1928.866905	12.16	-1929.31089	17.73	-1928.881005	14.06
² INT _{α}	-1928.893625	1.83	-1928.460854	-0.02	-1929.330515	-5.34	-1928.897744	-7.19	-1929.346178	-4.42	-1928.913407	-6.27
⁴ INT _{α}	-1928.893494	1.91	-1928.460629	0.12	-1929.33042	-5.28	-1928.897555	-7.08	-1929.346144	-4.40	-1928.913279	-6.19
⁴ TS-reb _{α}	-1928.884005	7.87	-1928.454508	3.96	-1929.321035	0.61	-1928.891538	-3.30	-1929.338619	0.33	-1928.909122	-3.58
² P-OH _{α}	-1928.976021	-49.87	-1928.537479	-48.10	-1929.409966	-55.20	-1928.971424	-53.43	-1929.42433	-53.46	-1928.985788	-51.69
⁴ P-OH _{α}	-1928.973888	-48.53	-1928.536627	-47.57	-1929.409144	-54.68	-1928.971883	-53.72	-1929.427037	-55.16	-1928.989776	-54.19
² P-NO	-1928.90319363	-4.17	-1928.47268063	-7.44	-1929.33895020	-10.63	-1928.90843720	-13.90	-1929.35330880	-8.89	-1928.92279580	-12.16
⁴ P-NO	-1928.90327761	-4.22	-1928.47230861	-7.21	-1929.34166940	-12.34	-1928.91070040	-15.33	-1929.35429700	-9.58	-1928.92332800	-12.50

Table S2. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the β -position (Path B) in the water-free system.

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1+Bulk Polarity		UB3LYP/BS2//BS1+ZPE+B Bulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
² RC _{β}	-1928.89492311	1.02	-1928.45908711	1.09	-1929.31854160	2.17	-1928.88270560	2.24	-1929.33475180	2.75	-1928.89891580	2.82
⁴ RC _{β}	-1928.89483856	1.07	-1928.45896556	1.16	-1929.31840270	2.26	-1928.88252970	2.35	-1929.33467020	2.80	-1928.89879720	2.90
² TS-H _{β}	-1928.85481094	26.19	-1928.42644294	21.57	-1929.28469360	23.41	-1928.85632560	18.80	-1929.30230173	23.12	-1928.87393373	18.50
⁴ TS- H _{β}	-1928.85301060	27.32	-1928.42495960	22.50	-1929.28277940	24.61	-1928.85472840	19.80	-1929.30065840	24.15	-1928.87260740	19.33
² INT _{β}	-1928.86401068	20.42	-1928.43152468	18.38	-1929.29991730	13.86	-1928.86743130	11.83	-1929.31575329	14.68	-1928.88326730	12.64
⁴ INT _{β}	-1928.86376144	20.57	-1928.43152544	18.38	-1929.29958110	14.07	-1928.86734510	11.88	-1929.31543960	14.87	-1928.88320360	12.68
² TS-reb _{β}	-1928.861059	22.27	-1928.430481	19.04	-1929.296722	15.86	-1928.866144	12.63	-1929.313529	16.07	-1928.882951	12.84
⁴ TS-reb _{β}	-1928.85867	23.77	-1928.426718	21.40	-1929.297488	15.38	-1928.865536	13.02	-1929.313836	15.88	-1928.881884	13.51
² P-OH _{β}	-1928.97014519	-46.18	-1928.53022019	-43.55	-1929.40465200	-51.86	-1928.96472700	-49.23	-1929.42051814	-51.07	-1928.98059310	-48.43
⁴ P-OH _{β}	-1928.95021609	-33.68	-1928.51310909	-32.81	-1929.38575680	-40.01	-1928.94864980	-39.14	-1929.40118383	-38.93	-1928.96407680	-38.07

Table S3. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the α -position (Path A) in the one-water system.

	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 _{α}	-2005.319444	0.00	-2004.85926131	0.00	-2005.789649	0.00	-2005.32946570	0.00	-2005.80982	0.00	-2005.34963687	0.00
⁴ RC _{α}	-2005.319244	0.13	-2004.85905762	0.13	-2005.789319	0.21	-2005.32913310	0.21	-2005.809548	0.17	-2005.34936206	0.17
² TS-H _{α}	-2005.295266	15.17	-2004.841051	11.43	-2005.767855	13.68	-2005.31364	9.93	-2005.784859	15.66	-2005.330644	11.92
⁴ TS-H _{α}	-2005.29384	16.07	-2004.839484	12.41	-2005.767913	13.64	-2005.313557	9.98	-2005.783244	16.68	-2005.328888	13.02
² INT _{α}	-2005.323073	-2.28	-2004.865748	-4.07	-2005.805498	-9.95	-2005.348173	-11.74	-2005.821571	-7.37	-2005.364246	-9.17
⁴ INT _{α}	-2005.323025	-2.25	-2004.865484	-3.90	-2005.80554	-9.97	-2005.347999	-11.63	-2005.821653	-7.43	-2005.364112	-9.08
⁴ TS-reb _{α}	-2005.315523	2.46	-2004.860686	-0.89	-2005.799761	-6.35	-2005.340794	-7.11	-2005.818117	-5.21	-2005.35915	-5.97
² P-OH _{α}	-2005.401508	-51.50	-2004.937839	-49.31	-2005.879177	-56.18	-2005.415508	-53.99	-2005.894309	-53.02	-2005.43064	-50.83
⁴ P-OH _{α}	-2005.397212	-48.80	-2004.934766	-47.38	-2005.877457	-55.10	-2005.415011	-53.68	-2005.896042	-54.11	-2005.433596	-52.69
² P-NO ₁	-2005.32906699	-6.04	-2004.87282899	-8.51	-2005.81050780	-13.09	-2005.35426980	-15.56	-2005.82777202	-11.27	-2005.37153402	-13.74
⁴ P-NO ₁	-2005.32985317	-6.53	-2004.87483217	-9.77	-2005.81404800	-15.31	-2005.35902700	-18.55	-2005.82666245	-10.57	-2005.37164145	-13.81
² P-NO ₂	-2005.33859	-12.01	-2004.881634	-14.04	-2005.809835	-12.67	-2005.352879	-14.69	-2005.829871	-12.58	-2005.372915	-14.61
⁴ P-NO ₂	-2005.339011	-12.28	-2004.881971	-14.25	-2005.818022	-17.80	-2005.360982	-19.78	-2005.832188	-14.04	-2005.375148	-16.01

Table S4. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the β -position (Path B) in the one-water system.

	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 _{β}	-2005.31556254	2.44	-2004.85607354	2.00	-2005.78663320	1.89	-2005.32714420	1.46	-2005.80573134	2.57	-2005.34624234	2.13
⁴ RC _{β}	-2005.31538298	2.55	-2004.85581598	2.16	-2005.78642330	2.02	-2005.32685630	1.64	-2005.80555856	2.67	-2005.34599156	2.29
² TS-H _{β}	-2005.27908389	25.33	-2004.82581089	20.99	-2005.75469170	21.94	-2005.30141870	17.60	-2005.77464786	22.07	-2005.32137486	17.73
⁴ TS-H _{β}	-2005.27725657	26.47	-2004.82424457	21.97	-2005.75278510	23.13	-2005.29977310	18.63	-2005.77318773	22.99	-2005.32017573	18.49
² INT _{β}	-2005.28779483	19.86	-2004.83254183	16.77	-2005.76968960	12.52	-2005.31443660	9.43	-2005.79064036	12.04	-2005.33538736	8.94
⁴ INT _{β}	-2005.28653295	20.65	-2004.83278195	16.62	-2005.76746275	13.92	-2005.31371175	9.89	-2005.78209330	17.40	-2005.32834230	13.36
² TS-reb _{β}	-2005.289138	19.02	-2004.833369	16.25	-2005.770056	12.29	-2005.314287	9.53	-2005.789623	12.67	-2005.333854	9.90
⁴ TS-reb _{β}	-2005.283663	22.45	-2004.825966	20.89	-2005.766424	14.57	-2005.308727	13.01	-2005.78542	15.31	-2005.327723	13.75
² P-OH _{β}	-2005.40116506	-51.28	-2004.93577006	-48.01	-2005.87985040	-56.60	-2005.41445540	-53.33	-2005.89818457	-55.45	-2005.43278957	-52.18
⁴ P-OH _{β}	-2005.38458539	-40.88	-2004.92100139	-38.74	-2005.86644170	-48.19	-2005.40285770	-46.05	-2005.89050833	-50.63	-2005.42692433	-48.50

Table S5. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the α -position (Path A) in the two-water system.

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1+Bulk Polarity		UB3LYP/BS2//BS1+ZPE+B ulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
² RC _{α}	-2081.74543185	0.00	-2081.26129285	0.00	-2082.26148920	0.00	-2081.77735020	0.00	-2082.28081165	0.00	-2081.79667265	0.00
⁴ RC _{α}	-2081.74513139	0.19	-2081.26093739	0.22	-2082.26117300	0.20	-2081.77697900	0.23	-2082.28048985	0.20	-2081.79629585	0.24
² TS-H _{α}	-2081.721471	15.04	-2081.240865	12.82	-2082.235755	16.15	-2081.755149	13.93	-2082.255028	16.18	-2081.774422	13.96
⁴ TS-H _{α}	-2081.72142	15.07	-2081.241754	12.26	-2082.237007	15.36	-2081.757341	12.56	-2082.256227	15.43	-2081.776561	12.62
² INT _{α}	-2081.75253	-4.45	-2081.269008	-4.84	-2082.27816	-10.46	-2081.794638	-10.85	-2082.295012	-8.91	-2081.81149	-9.30
⁴ INT _{α}	-2081.751885	-4.05	-2081.268455	-4.49	-2082.277191	-9.85	-2081.793761	-10.30	-2082.294519	-8.60	-2081.811089	-9.05
⁴ TS-reb _{α}	-2081.739618	3.65	-2081.259477	1.14	-2082.261883	-0.25	-2081.781742	-2.76	-2082.279176	1.03	-2081.799035	-1.48
² P-OH _{α}	-2081.826901	-51.12	-2081.33758	-47.87	-2082.349045	-54.94	-2081.859724	-51.69	-2082.367018	-54.10	-2081.877697	-50.84
⁴ P-OH _{α}	-2081.824725	-49.76	-2081.336105	-46.95	-2082.346033	-53.05	-2081.857413	-50.24	-2082.366907	-54.03	-2081.878287	-51.21
² P-NO ₁	-2081.761737	-10.23	-2081.278977	-11.10	-2082.286774	-15.87	-2081.804014	-16.73	-2082.306365	-16.04	-2081.823605	-16.90
⁴ P-NO ₁	-2081.758468	-8.18	-2081.286595	-15.88	-2082.283724	-13.95	-2081.811851	-21.65	-2082.299662	-11.83	-2081.827789	-19.53
² P-NO ₂	-2081.764728	-12.11	-2081.293831	-20.42	-2082.27954	-11.33	-2081.808643	-19.64	-2082.298785	-11.28	-2081.827888	-19.59
⁴ P-NO ₂	-2081.764828	-12.12	-2081.293226	-20.04	-2082.28963	-17.66	-2081.818128	-25.59	-2082.30463	-14.95	-2081.833128	-22.88

Table S6. Relative energies (RE) (in kcal/mol) and atomic energies (AE) (in a.u.) at the B3LYP level of theory for DEN catalyzed biotransformation by P450 (Cpd I) at the β -position (Path B) in the two-water system.

	UB3LYP/BS1		UB3LYP/BS1+ZPE		UB3LYP/BS2//BS1		UB3LYP/BS2//BS1+ZPE		UB3LYP/BS2//BS1+Bulk Polarity		UB3LYP/BS2//BS1+ZPE+B ulk Polarity	
	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE	AE	RE
² RC _{β}	-2081.74159432	2.41	-2081.25644632	3.04	-2082.25582490	3.55	-2081.77067690	4.19	-2082.27728362	2.21	-2081.79213562	2.85
⁴ RC _{β}	-2081.74139987	2.53	-2081.25617587	3.21	-2082.25563020	3.68	-2081.77040620	4.36	-2082.27708881	2.34	-2081.79186481	3.02
² TS-H _{β}	-2081.70491047	25.43	-2081.22694947	21.55	-2082.22468680	23.09	-2081.74672580	19.22	-2082.24774317	20.75	-2081.76978217	16.87
⁴ TS-H _{β}	-2081.70275660	26.78	-2081.22476860	22.92	-2082.22272280	24.33	-2081.74473480	20.47	-2082.24594242	21.88	-2081.76795442	18.02
² INT _{β}	-2081.72107627	15.28	-2081.23998227	13.37	-2082.24505610	10.31	-2081.76396210	8.40	-2082.26638501	9.05	-2081.78529101	7.14
⁴ INT _{β}	-2081.72073706	15.50	-2081.23900606	13.99	-2082.24417940	10.86	-2081.76244840	9.35	-2082.26610785	9.23	-2081.78437685	7.72
² TS-reb _{β}	-2081.711777	21.12	-2081.233816	17.24	-2082.232056	18.47	-2081.754095	14.59	-2082.25510785	16.13	-2081.77614685	12.88
⁴ TS-reb _{β}	-2081.714777	19.24	-2081.228358	20.67	-2082.229056	20.35	-2081.751095	16.48	-2082.25210785	18.01	-2081.77414685	14.14
² P-OH _{β}	-2081.81896671	-46.14	-2081.32913471	-42.57	-2082.34230300	-50.71	-2081.85247100	-47.14	-2082.36431210	-52.40	-2081.87448010	-48.82
⁴ P-OH _{β}	-2081.81100690	-41.15	-2081.32292490	-38.67	-2082.31822090	-35.60	-2081.83013890	-33.13	-2082.34389293	-39.58	-2081.85581093	-37.11

Cartesian coordinates of all structures presented in this study.

Water-free system

²RC_α

Fe	0.92613900	0.03130500	0.23050400
O	-0.37932200	0.01042600	-0.74154600
S	2.73757900	0.10972700	2.05051100
H	2.83895300	-1.22001600	2.27565400
N	1.50847900	-1.83478400	-0.26550300
C	1.63840700	-4.13666700	-0.41557600
C	2.40060000	-3.62634300	-1.42112600
H	1.45828200	-5.17387000	-0.16368300
H	2.97763300	-4.15700100	-2.16748500
N	2.16478400	0.78657500	-1.16086800
C	2.88183200	0.08352300	-2.09223500
C	3.57732500	0.98531800	-2.97823700
C	3.27166100	2.24624500	-2.56756800
H	4.21454600	0.67675000	-3.79698900
H	3.60474000	3.19062300	-2.97839700
N	0.56710400	1.89649800	0.91949500
C	1.00519300	3.07539100	0.36738900
C	-0.26785500	2.25180000	1.94740700
C	0.44159200	4.20032300	1.07405400
C	-0.35339000	3.68878300	2.05174200
H	0.63830400	5.23799700	0.83721900
H	-0.94495400	4.21826000	2.78738700
N	-0.07578700	-0.72229500	1.82185300
C	-1.50962100	-0.92192900	3.62634900
H	-2.15677000	-0.61436500	4.43763500
C	-0.82980700	-0.01627800	2.73296600
C	1.08492600	-3.00993200	0.29566300
C	2.30947700	-2.19027800	-1.32055100
C	2.38937100	2.10790200	-1.43418000
C	-0.93298200	1.36457700	2.78443800
H	-1.57171500	1.78843400	3.55312000
C	0.24770900	-3.11620100	1.40259900
H	-0.00774400	-4.11678000	1.73801600
C	2.95188200	-1.30165700	-2.17218400
H	3.56159900	-1.72421500	-2.96503800
C	1.85624400	3.17793400	-0.72235000
H	2.12323000	4.17699300	-1.05316500
C	-1.17185900	-2.18291900	3.24322500
H	-1.48596600	-3.12523300	3.67339200
C	-0.28923000	-2.05292500	2.10991000
N	-4.14989500	0.31663000	-1.70754000
C	-3.79743400	-0.01979100	-0.32492300
C	-4.27864200	-1.40993400	0.10707500
H	-4.26277100	0.74177200	0.31014900
H	-2.71021700	0.06019900	-0.24593200
H	-3.99419700	-1.58806900	1.15085200
H	-5.36616300	-1.48002900	0.02567700
H	-3.82677000	-2.19602600	-0.50688700

C	-3.16484700	0.32335800	-2.78647700
C	-2.68729300	-1.07403600	-3.18910600
H	-2.30650300	0.92836300	-2.47123300
H	-3.65592000	0.82377100	-3.62582200
H	-1.99093600	-0.99503200	-4.03197500
H	-2.15462600	-1.56091800	-2.36656900
H	-3.53047400	-1.70370700	-3.49348200
N	-5.37324100	0.74392800	-2.02823600
O	-6.17843900	0.77196200	-1.09445100
⁴RC_α			
Fe	-0.91969500	-0.03173900	0.23707100
O	0.36089200	-0.00956500	-0.77010900
S	-2.73902600	-0.12033800	2.03390400
H	-2.83941100	1.20753500	2.27017500
N	-1.49830900	1.83997300	-0.25036400
C	-1.62095400	4.14298700	-0.39024900
C	-2.38726000	3.63955000	-1.39610900
H	-1.43673500	5.17845100	-0.13421600
H	-2.96407400	4.17540800	-2.13892300
N	-2.16496500	-0.77651200	-1.16224500
C	-2.87956800	-0.06530800	-2.08850500
C	-3.57321600	-0.95933600	-2.98434800
C	-3.26792800	-2.22375700	-2.58444800
H	-4.20827400	-0.64356800	-3.80204000
H	-3.59930300	-3.16458500	-3.00469200
N	-0.56351900	-1.90151400	0.90856600
C	-1.00660100	-3.07573500	0.34897000
C	0.26636000	-2.26685400	1.93681800
C	-0.44889900	-4.20688300	1.05028600
C	0.34593200	-3.70458100	2.03288500
H	-0.64968400	-5.24231100	0.80711300
H	0.93328300	-4.24085500	2.76696400
N	0.08362300	0.70819700	1.82512900
C	1.50222400	0.89319000	3.64354600
H	2.14254700	0.57893900	4.45766100
C	0.82858900	-0.00522000	2.73872900
C	-1.07054500	3.01098700	0.31505300
C	-2.30093200	2.20258100	-1.30208700
C	-2.38833000	-2.09473100	-1.44749400
C	0.93061100	-1.38626400	2.78157700
H	1.56474000	-1.81577500	3.55091600
C	-0.23452600	3.10718700	1.42385800
H	0.02324000	4.10437900	1.76745100
C	-2.94802100	1.32071100	-2.15710500
H	-3.55811800	1.75011200	-2.94601200
C	-1.85696500	-3.16999600	-0.74185000
H	-2.12506400	-4.16669700	-1.07885000
C	1.16920100	2.15727000	3.26664200
H	1.48092800	3.09610600	3.70603200
C	0.29521700	2.03708100	2.12586800
N	4.14176700	-0.30971100	-1.71094100

C	3.77862900	0.02485200	-0.33072700
C	4.25879400	1.41331400	0.10781600
H	4.23711400	-0.73875600	0.30686000
H	2.69061800	-0.05349400	-0.26078900
H	3.96741200	1.58952900	1.15000200
H	5.34698500	1.48176500	0.03432600
H	3.81264100	2.20151800	-0.50761700
C	3.16550700	-0.31325200	-2.79785400
C	2.69221200	1.08543500	-3.20096400
H	2.30425100	-0.91858300	-2.49119100
H	3.66312700	-0.81194500	-3.63435600
H	2.00274100	1.00899300	-4.04968800
H	2.15316500	1.57087300	-2.38169900
H	3.53829600	1.71524700	-3.49683200
N	5.36688500	-0.73919900	-2.02213300
O	6.16416900	-0.77039400	-1.08174500
²TS-H_a			
Fe	-0.77693000	0.04222800	-0.35625400
O	0.03395200	0.11330600	1.15027100
S	-2.04694700	0.25299900	-2.34267000
H	-3.21649800	-0.23123800	-1.86919300
N	-1.86234700	1.59951200	0.37412100
C	-3.43258900	2.85652800	1.50040400
C	-2.55693100	3.72621600	0.92875400
H	-4.30453000	3.07414800	2.10403500
H	-2.55798800	4.80815100	0.96506300
N	0.48876600	1.33219100	-1.24186100
C	0.43672700	2.70262200	-1.17502100
C	1.55700500	3.27149600	-1.88329100
C	2.29022300	2.23090200	-2.36592400
H	1.74508100	4.33298400	-1.98228400
H	3.20564600	2.25802300	-2.94269800
N	0.26129800	-1.49128300	-1.11002300
C	1.40971300	-1.42404600	-1.86269900
C	-0.05882300	-2.82688700	-1.01990100
C	1.84265700	-2.75008800	-2.22430100
C	0.93184800	-3.61847300	-1.70557500
H	2.72852500	-2.96723400	-2.80684700
H	0.91161400	-4.69845200	-1.77754700
N	-2.16277500	-1.23843000	0.36584100
C	-3.26871200	-3.16804000	0.97393400
H	-3.48342700	-4.22679400	1.04393500
C	-2.14298300	-2.60530600	0.27034000
C	-2.99322100	1.52739200	1.14324200
C	-1.57842900	2.93063800	0.22425200
C	1.61550300	1.02331000	-1.95901300
C	-1.16957500	-3.35252800	-0.37940500
H	-1.28648300	-4.43163800	-0.38507000
C	-3.64893500	0.35869400	1.50041800
H	-4.54267800	0.45133000	2.10941500
C	-0.51761200	3.45124800	-0.50136500

H	-0.42017500	4.53166000	-0.53935200
C	2.05659000	-0.26020300	-2.24869600
H	2.97010700	-0.36075900	-2.82491100
C	-3.95857500	-2.12347900	1.50969800
H	-4.85836900	-2.14607700	2.11127500
C	-3.25799500	-0.92104600	1.13101500
N	3.19730100	-0.37896000	1.48963400
C	2.09784300	-1.24050400	1.74464000
C	1.79169300	-1.54609900	3.20209800
H	2.20625400	-2.12709800	1.11745300
H	1.07547400	-0.65783600	1.33273700
H	0.89182400	-2.16558800	3.25749700
H	2.62186100	-2.09400200	3.66733800
H	1.60504600	-0.63735600	3.78214900
C	3.30457800	0.96286800	2.07750200
C	4.34085800	1.04688600	3.20181000
H	2.30395800	1.23497600	2.42112600
H	3.58294600	1.63357600	1.25947000
H	4.38724400	2.07342300	3.58194700
H	4.08453100	0.38564100	4.03595000
H	5.33160600	0.77374700	2.82945600
N	4.04268100	-0.77352800	0.50287400
O	4.92481800	0.03436700	0.23632600
⁴TS-H_a			
Fe	0.83305900	-0.08640000	-0.30888400
O	-0.07375300	-0.02431100	1.15959300
S	1.85383100	-0.05337700	-2.47730000
H	2.54236200	1.10267500	-2.34597500
N	1.88945700	-1.63640000	0.36200200
C	3.50643900	-2.93084500	1.38832200
C	2.58170300	-3.78212900	0.87111900
H	4.40918200	-3.16588500	1.93763000
H	2.56540400	-4.86404200	0.90499900
N	-0.47222800	-1.33862300	-1.20198800
C	-0.46466300	-2.70588700	-1.13205900
C	-1.60848200	-3.24715500	-1.82509000
C	-2.31551900	-2.18660000	-2.30346200
H	-1.82945200	-4.30283500	-1.91807700
H	-3.23948400	-2.18922400	-2.86694800
N	-0.21679100	1.50693400	-1.06416900
C	-1.37623100	1.45832100	-1.79503000
C	0.07789900	2.83626400	-0.90240400
C	-1.83211800	2.79484700	-2.09497700
C	-0.92965100	3.65072700	-1.54143800
H	-2.72839600	3.02744500	-2.65517200
H	-0.92778500	4.73322400	-1.55926600
N	2.22998200	1.18464200	0.38334700
C	3.34222600	3.10348300	1.02581900
H	3.54793100	4.16076000	1.13536100
C	2.18952200	2.55826800	0.35125600
C	3.07028000	-1.59318700	1.05963200

C	1.58040300	-2.96604800	0.22326800
C	-1.60204900	-0.99707100	-1.90752900
C	1.19366900	3.32867500	-0.23681700
H	1.30470900	4.40748500	-0.18163700
C	3.76591800	-0.43989100	1.38806100
H	4.69202500	-0.55507100	1.94280200
C	0.48968100	-3.46985200	-0.46936700
H	0.37272000	-4.54881800	-0.49991400
C	-2.02791000	0.29495600	-2.18330500
H	-2.95336900	0.40396600	-2.73916500
C	4.07333700	2.04552100	1.47309400
H	5.00271600	2.05354600	2.02813600
C	3.36424900	0.85391000	1.07666300
N	-3.25296400	0.36821400	1.42643400
C	-2.18959400	1.27617800	1.65739900
C	-1.87866500	1.62279500	3.10141400
H	-2.31501000	2.13626800	0.99898300
H	-1.06977600	0.66230100	1.25371200
H	-0.99790300	2.27096400	3.13423000
H	-2.71831700	2.15508400	3.57036200
H	-1.65594700	0.73386100	3.69981400
C	-3.31207000	-0.95603200	2.06059500
C	-4.35388200	-1.03969200	3.17941900
H	-2.30493300	-1.17721000	2.42069000
H	-3.55912400	-1.66487700	1.26505200
H	-4.36432500	-2.05253200	3.59747900
H	-4.13091000	-0.33834300	3.99016200
H	-5.35087300	-0.81908200	2.78923600
N	-4.10718300	0.69053800	0.42544100
O	-4.94763900	-0.16990100	0.17294400
² INT _α			
Fe	3.10523300	-0.91214900	0.06525600
O	1.84361100	0.12722900	-0.32135500
S	5.11526200	-2.08184400	0.45642100
H	5.94884800	-1.02777400	0.32155800
N	3.62305700	0.31630500	1.61982600
C	4.42737000	2.07865800	2.86371800
C	3.82845800	1.21973700	3.72723400
H	4.92253300	3.01788000	3.07348500
H	3.72172400	1.30242300	4.80118700
N	2.17311300	-2.14105200	1.31821900
C	2.06909400	-1.99092000	2.68388800
C	1.31217200	-3.08628300	3.23336300
C	0.96619700	-3.89504800	2.19719800
H	1.08637300	-3.19792600	4.28584700
H	0.39655900	-4.81517000	2.21275800
N	2.68396600	-2.16136800	-1.46843700
C	1.95742100	-3.31662700	-1.41486400
C	3.07995300	-2.00918000	-2.77152000
C	1.88063100	-3.91307400	-2.72594400
C	2.57870600	-3.10441800	-3.56424200

H	1.35815100	-4.83514800	-2.94544100
H	2.75164300	-3.21179600	-4.62732100
N	4.14794300	0.30274000	-1.19428400
C	5.09771400	1.19653900	-3.08936300
H	5.38812100	1.27346300	-4.12984400
C	4.33854200	0.09623900	-2.53944600
C	4.29696100	1.49985000	1.54056900
C	3.31851000	0.11651500	2.93862100
C	1.51270000	-3.30035900	1.00161800
C	3.85240500	-0.97557600	-3.27099700
H	4.08327800	-1.00311300	-4.33190000
C	4.81758000	2.06132900	0.38058600
H	5.33944500	3.00976400	0.46587400
C	2.59827100	-0.95796400	3.43766300
H	2.42084300	-0.99390100	4.50849700
C	1.39621600	-3.85359500	-0.26764100
H	0.85161300	-4.78781100	-0.36600600
C	5.34297200	2.06257400	-2.06818600
H	5.87950400	3.00247600	-2.08811000
C	4.74841800	1.49483100	-0.88201200
N	-0.46230060	1.81291164	-1.75129557
C	0.87943003	1.30230343	-2.06742560
C	1.52926296	2.63145764	-2.31605446
H	0.86481302	0.62958875	-2.95919735
H	1.41768400	0.61944623	-1.04052702
H	2.60523569	2.50124250	-2.58642673
H	1.02162346	3.16883414	-3.15367391
H	1.47403466	3.27487524	-1.40444156
C	-1.52325977	1.60561343	-0.75515649
C	-2.89709463	2.20690066	-0.71294935
H	-1.03228662	1.88763743	0.20787177
H	-1.67010842	0.49818017	-0.76058767
H	-3.46079195	1.84305855	0.18015690
H	-2.83908158	3.32124838	-0.65871541
H	-3.47698086	1.93179920	-1.62734838
N	-1.31946844	1.57305307	-2.83191166
O	-1.54826153	2.49111494	-3.49753759
⁴INT_{α}			
Fe	-0.89854100	0.00660100	-0.33263100
S	-2.16455400	-0.20858600	-2.24882700
H	-1.28182900	0.32264200	-3.12367000
N	0.00379500	-1.77249500	-0.74239100
C	1.46709000	-3.36707900	-1.53647200
C	0.43287900	-4.02768400	-0.94585800
H	2.34660800	-3.77650000	-2.01599400
H	0.28569700	-5.09515600	-0.84209900
N	-2.41712200	-0.97650500	0.54461800
C	-2.56431200	-2.33863500	0.65914800
C	-3.76258000	-2.63909900	1.40100900
C	-4.32142600	-1.44756100	1.75116900
H	-4.10881300	-3.63951200	1.62722600

H	-5.22290200	-1.26671400	2.32254700
N	-1.73351000	1.75886700	0.14770300
C	-2.87910600	1.94759800	0.87934900
C	-1.30294900	3.00734600	-0.22645100
C	-3.15861600	3.35762800	1.00016100
C	-2.18557200	4.01360000	0.31145600
H	-4.00369000	3.77145800	1.53539800
H	-2.06277800	5.07914500	0.16491300
N	0.53362300	0.96176700	-1.37616100
C	1.86288100	2.61712000	-2.27241900
H	2.18911300	3.61500000	-2.53671300
C	0.66010500	2.31914600	-1.53620000
C	1.18129900	-1.95875600	-1.42577400
C	-0.48259900	-3.02576500	-0.45988100
C	-3.47108200	-0.41352300	1.21855500
C	-0.19858100	3.27885900	-1.01828500
H	0.02342500	4.31932100	-1.23264100
C	1.96087600	-0.95339200	-1.97783100
H	2.89125200	-1.24343000	-2.45289300
C	-1.67890000	-3.29720200	0.18851300
H	-1.93642900	-4.33883800	0.35097600
C	-3.69033900	0.94603200	1.38805700
H	-4.57115600	1.24689100	1.94586800
C	2.47852400	1.42810700	-2.52338000
H	3.41736600	1.24520100	-3.02909900
C	1.64777200	0.39765500	-1.95391900
N	3.64378200	0.01499500	1.36128200
C	3.34111200	-0.99760600	2.17170200
C	2.53847100	-0.87353700	3.42408400
H	3.79234000	-1.93556900	1.86741700
H	2.11438400	-1.84792100	3.68769600
H	3.15701000	-0.55471200	4.27824300
H	1.71368400	-0.15889000	3.32950500
C	3.20372700	1.40460900	1.52870700
C	3.98666200	2.15311300	2.60936500
H	2.12729200	1.40181400	1.72259200
H	3.36583300	1.86601800	0.55174700
H	3.65704400	3.19747800	2.64155600
H	3.83220700	1.72284900	3.60408500
H	5.05899100	2.13743400	2.38887600
N	4.44193600	-0.16458200	0.19605700
O	4.79789900	-1.33951500	0.03491800
O	0.06713000	0.07730900	1.18845900
H	0.59049000	-0.74476100	1.21048500
⁴TS-reb_a			
Fe	-0.75729200	-0.05369400	-0.27385400
N	-1.79577300	1.80943900	0.12432900
N	0.64161300	0.95915700	-1.28023600
N	0.27112500	-1.87855200	-0.65822900
N	-2.27456100	-1.05752900	0.54052700
C	-0.25835300	3.26812000	-1.05789300

C	2.12136100	-0.93488800	-1.90664100
C	-1.39328200	-3.36640800	0.29081500
C	-3.74832400	0.83909500	1.18812000
C	-1.44176000	3.03275400	-0.34429000
C	0.68489600	2.32438500	-1.47388800
C	1.76329400	0.42699700	-1.85026700
C	1.38640800	-2.01879300	-1.41430400
C	-0.20185400	-3.12730100	-0.39156300
C	-2.32598300	-2.41463500	0.73476000
C	-3.39004000	-0.51530500	1.13673800
C	-3.03210700	1.92727700	0.68288900
C	-3.47007900	3.30940100	0.61174600
C	-2.48082800	3.99748900	-0.03057300
C	1.88624500	2.65698700	-2.20415800
C	2.55310900	1.48836800	-2.43445300
C	1.67429700	-3.43036900	-1.61064900
C	0.68758600	-4.12057600	-0.97102100
C	-3.52539900	-2.74685300	1.46719100
C	-4.18129400	-1.57634300	1.71467200
H	-0.06112500	4.29526000	-1.35419400
H	2.16857600	3.65878900	-2.50352400
H	3.48550500	1.34304900	-2.96611400
H	3.02184700	-1.16335700	-2.46923000
H	2.51333900	-3.82819900	-2.16806200
H	0.55419100	-5.19372100	-0.91153600
H	-1.64912900	-4.40449800	0.48670100
H	-3.81709000	-3.75041300	1.75063600
H	-5.11598600	-1.43154100	2.24192300
H	-4.70633300	1.05527500	1.65415400
H	-4.41490300	3.68928400	0.98075400
H	-2.45921600	5.05009500	-0.28522900
O	0.09590500	0.15110100	1.38998100
S	-1.86675400	-0.19448500	-2.41049400
H	-2.94168800	-0.91178200	-2.01527000
H	4.05323600	1.39703600	0.05849100
C	3.82819500	1.46297900	1.12765900
H	3.09955900	2.27281500	1.25046000
N	3.21235500	0.20109200	1.49153100
C	2.33889100	-0.04307800	2.38673800
N	3.73633100	-1.21771500	0.49216700
H	-0.31132800	0.96461300	1.73321600
H	2.02940500	-1.08895500	2.44190700
O	3.29108200	-2.19193500	0.96588700
C	1.88975500	0.88748200	3.47255500
H	1.86554000	1.92918600	3.14112100
H	0.89830400	0.59347900	3.81806700
H	2.58929200	0.81470400	4.31730600
C	5.10648300	1.73898700	1.92578300
H	5.82988700	0.92815200	1.79263400
H	5.56771500	2.67032600	1.58023300
H	4.89723900	1.83903900	2.99628300

²P-OH_a

Fe	-0.84575800	-0.15538800	0.45644700
O	1.06914300	-0.03748700	-0.98734900
S	-2.56229800	-0.49915600	1.84127800
H	-2.63457700	-1.84393900	1.71347100
N	0.05466500	1.11599300	1.73351200
C	1.26762000	1.94024900	3.52222000
C	0.60328200	2.99240000	2.97151000
H	1.93890300	1.93552400	4.37149100
H	0.61269400	4.03113700	3.27651700
N	-1.75428400	1.41075900	-0.40710100
C	-1.74756700	2.72287600	0.00406700
C	-2.63665300	3.51001900	-0.81535200
C	-3.19193200	2.65798600	-1.71950000
H	-2.80406800	4.57315600	-0.69757000
H	-3.91036500	2.87655700	-2.49942500
N	-1.56561400	-1.39634100	-0.94658300
C	-2.46400900	-1.06371900	-1.93100100
C	-1.34845800	-2.74812300	-1.07800900
C	-2.81323000	-2.23081400	-2.70554100
C	-2.12056000	-3.27574500	-2.17686700
H	-3.50070700	-2.23093800	-3.54197600
H	-2.12045300	-4.31282600	-2.48773700
N	0.25874200	-1.69229600	1.18318300
C	1.03526700	-3.81506500	1.67791200
H	1.17723200	-4.88437100	1.58543300
C	0.21517800	-3.01869100	0.80291700
C	0.91424100	0.77288100	2.75065000
C	-0.15669900	2.46879900	1.86312300
C	-2.64214200	1.35013100	-1.45316000
C	-0.52149200	-3.51237700	-0.26514900
H	-0.45845900	-4.57652900	-0.47061900
C	1.38789500	-0.50484600	3.01606300
H	2.06163400	-0.61924300	3.85938100
C	-0.99587300	3.22628500	1.05719600
H	-1.08102300	4.28640900	1.27529300
C	-2.96937500	0.20684300	-2.16857000
H	-3.68226700	0.31464000	-2.98042200
C	1.56591500	-2.96628700	2.60277100
H	2.23392200	-3.19706200	3.42275800
C	1.07312000	-1.64837600	2.29576200
N	3.29799900	0.35283700	-1.66662400
C	2.12199200	0.93730100	-1.01950300
C	1.59615100	2.16930400	-1.73479200
H	2.44075700	1.17835900	-0.00471600
H	1.37314600	-0.80189400	-0.46102500
H	0.75686700	2.57895500	-1.16939300
H	2.38138000	2.92801500	-1.80253800
H	1.24138300	1.92605100	-2.74106800
C	3.31347600	-0.02046400	-3.08532200
C	3.97476500	1.02213500	-3.99026900

H	2.27832700	-0.21318100	-3.38282700
H	3.85604100	-0.96767200	-3.15295000
H	3.98633600	0.66227000	-5.02553100
H	3.44284800	1.97809200	-3.96913700
H	5.00895600	1.19632300	-3.67600200
N	4.35148600	-0.10962200	-0.95596200
O	4.32105000	0.08789000	0.25242500
⁴P-OH_a			
Fe	-1.18993500	0.00709200	-0.45462400
O	1.68483400	0.56620600	1.61067300
S	-2.54377500	-0.11835100	-2.44475500
H	-3.34862300	0.91739000	-2.11522500
N	-0.42076400	-1.83907800	-0.64830300
C	0.81210200	-3.64424700	-1.40617500
C	-0.23174000	-4.14395000	-0.68761300
H	1.60923600	-4.18049800	-1.90402900
H	-0.47210500	-5.17822700	-0.47748300
N	-2.53384200	-0.71612900	0.86279300
C	-2.82079500	-2.04223800	1.09854700
C	-3.96808400	-2.16234000	1.96081200
C	-4.38163200	-0.89692100	2.24353000
H	-4.38802100	-3.10140000	2.29773700
H	-5.21276300	-0.57981200	2.86037700
N	-1.67939500	1.87042600	0.11747700
C	-2.74885800	2.24510400	0.90300100
C	-1.10871900	3.04893300	-0.31741500
C	-2.85712700	3.67824300	0.95070800
C	-1.84127300	4.17676300	0.19179300
H	-3.61380100	4.21932400	1.50431100
H	-1.59143400	5.21143300	-0.00520100
N	0.51238700	0.75174900	-1.28071000
C	1.95382500	2.19650100	-2.37369200
H	2.37450900	3.13351200	-2.71560800
C	0.77916900	2.08100700	-1.55423500
C	0.68739100	-2.21203500	-1.38012900
C	-0.99091000	-3.01729300	-0.21575900
C	-3.48917900	-0.00318900	1.55083700
C	0.02637000	3.15433900	-1.10634600
H	0.35498500	4.15071000	-1.38386500
C	1.57809200	-1.34548800	-1.99495900
H	2.41749100	-1.78001900	-2.52575100
C	-2.11412300	-3.11933900	0.59004600
H	-2.45367600	-4.11543300	0.85505500
C	-3.59910100	1.37773800	1.57132500
H	-4.40401000	1.81172400	2.15573000
C	2.39452500	0.92949400	-2.61792400
H	3.25220900	0.61266300	-3.19687900
C	1.48664700	0.03589600	-1.95358300
N	3.90397000	0.01194900	0.98574800
C	2.66479900	-0.44500700	1.66373800
C	2.90392500	-0.79791200	3.12533200

H	2.36665200	-1.33483700	1.10419300
H	1.35150400	0.63359500	0.69598500
H	1.98033000	-1.19497800	3.55789400
H	3.69053300	-1.55379400	3.20781900
H	3.19583400	0.08888300	3.69734200
C	4.44408100	1.36143800	1.17535100
C	5.64836700	1.40587100	2.11990700
H	3.62135200	1.97644500	1.54647900
H	4.72629500	1.73915300	0.18777700
H	6.02255400	2.43301700	2.20175400
H	5.38615100	1.05869200	3.12455700
H	6.45664600	0.77416500	1.73755600
N	4.55257700	-0.73731900	0.08888700
O	4.14089500	-1.89018800	-0.05792800
²P-NO			
Fe	1.08869800	-0.02766300	0.22451000
O	-0.33595900	-0.02666300	-0.91830600
S	2.92040300	0.10031600	1.78610700
H	2.26534300	-0.29719500	2.90042900
N	2.16757000	-1.18419000	-1.03777600
C	3.03185200	-3.03134200	-2.12131000
C	3.60638500	-1.93163800	-2.68318300
H	3.19042800	-4.07410100	-2.36520900
H	4.33241400	-1.88378800	-3.48470500
N	1.91875600	1.60389100	-0.62641700
C	2.85496000	1.65067600	-1.63263600
C	3.18275100	3.02040600	-1.95003600
C	2.42945800	3.80181600	-1.12972300
H	3.89676000	3.32550300	-2.70436300
H	2.39957600	4.88226400	-1.06868900
N	0.09152800	1.12982400	1.54291700
C	0.06875300	2.50101900	1.56056400
C	-0.75222700	0.72495600	2.54979500
C	-0.80071000	2.97449400	2.61405700
C	-1.30644700	1.87225700	3.23077700
H	-0.98315900	4.01725000	2.84105300
H	-1.99267000	1.82215300	4.06664800
N	0.32880200	-1.66469500	1.13864600
C	-0.89394000	-3.08077500	2.49393500
H	-1.57052000	-3.38529700	3.28224300
C	-0.55034600	-1.71208200	2.18118600
C	2.14116200	-2.55121200	-1.09064500
C	3.05873100	-0.78703600	-1.99500300
C	1.64967700	2.90912400	-0.30369900
C	-1.05186000	-0.59616700	2.85134000
H	-1.74267900	-0.77609600	3.66993300
C	1.39083400	-3.37691000	-0.25717100
H	1.47606900	-4.44721300	-0.42208500
C	3.39109500	0.53921200	-2.26940700
H	4.12132200	0.71793900	-3.05312000
C	0.77492900	3.32663700	0.69403600

H	0.65825800	4.39800100	0.82935900
C	-0.20766600	-3.86123300	1.61473800
H	-0.20260400	-4.94065600	1.53189400
C	0.55125500	-2.96395200	0.77236000
N	-4.51988300	0.02174000	-1.45593900
C	-4.30061100	1.24842600	-1.23216500
C	-3.02714700	1.95654300	-0.85996000
H	-5.19150900	1.88920800	-1.32523600
H	0.02280600	0.14729800	-1.80547400
H	-2.87030200	2.79560800	-1.55078300
H	-3.14028400	2.39642100	0.14047600
H	-2.14143300	1.31440700	-0.86102200
C	-3.54832200	-1.06074700	-1.39298900
C	-3.89621500	-2.00864800	-0.24001200
H	-2.51628000	-0.70369100	-1.28869500
H	-3.62797100	-1.60432800	-2.34325000
H	-3.21393300	-2.86518300	-0.24196200
H	-3.79296500	-1.49808900	0.72371900
H	-4.92461100	-2.37406300	-0.32860600
N	-6.63287700	-0.31193600	-2.01309200
O	-7.13154600	0.74071800	-1.93481800
⁴P-NO			
Fe	-1.14794100	-0.00240500	0.25268800
O	0.12139600	-0.05914000	-1.02216200
S	-2.84400900	0.00832000	1.81485300
H	-2.49525400	1.13549400	2.47429200
N	-2.27157600	1.16739200	-0.97791100
C	-3.26316500	2.99282000	-1.97728900
C	-3.85944000	1.88049900	-2.48918500
H	-3.46321300	4.03172600	-2.20642900
H	-4.64992900	1.81734200	-3.22602900
N	-2.08186400	-1.63547300	-0.46118100
C	-3.06859700	-1.67217800	-1.41673200
C	-3.43239400	-3.03935100	-1.69171600
C	-2.64359800	-3.82450900	-0.90737900
H	-4.18890000	-3.34082300	-2.40486100
H	-2.61820200	-4.90469800	-0.84229100
N	0.02508000	-1.15581700	1.39706900
C	0.02466100	-2.52661400	1.45117800
C	0.96257100	-0.73231900	2.30417500
C	1.01375700	-2.98168400	2.39826700
C	1.59429300	-1.87024800	2.92713500
H	1.21455100	-4.02119900	2.62396700
H	2.37302500	-1.80599500	3.67626300
N	-0.35527700	1.64872300	1.08509100
C	0.98210700	3.05740100	2.32552300
H	1.73386900	3.36036800	3.04290000
C	0.63512100	1.68910900	2.03507000
C	-2.28510600	2.54055800	-1.01997600
C	-3.24742600	0.74401500	-1.84800500
C	-1.79545800	-2.94045400	-0.14863100

C	1.25092300	0.58789800	2.61278300
H	2.01903100	0.77520900	3.35599000
C	-1.50972000	3.37842800	-0.23173400
H	-1.61574500	4.44805100	-0.38127400
C	-3.61883900	-0.57481200	-2.06309800
H	-4.40147000	-0.76351200	-2.79071600
C	-0.81663500	-3.36555400	0.73806500
H	-0.70406000	-4.43464400	0.88592600
C	0.20929600	3.84056000	1.52308400
H	0.19349000	4.92023600	1.44662600
C	-0.61463100	2.95430400	0.74003700
N	4.64592200	0.04688900	-1.47122200
C	4.40272400	-1.19453100	-1.37532200
C	3.09762200	-1.93663700	-1.23534600
H	5.29428700	-1.83790500	-1.40086700
H	-0.21836500	0.42377300	-1.79750400
H	3.01182100	-2.66885500	-2.04956400
H	3.10625600	-2.51213700	-0.29984600
H	2.21124500	-1.29908700	-1.23965900
C	3.62910100	1.08789400	-1.44346200
C	3.95406100	2.09633600	-0.33657400
H	2.60718100	0.70729100	-1.31432900
H	3.67373800	1.59816100	-2.41541000
H	3.24586200	2.93211400	-0.36059700
H	3.88415200	1.62187900	0.64852300
H	4.96990600	2.48596900	-0.45664000
N	7.12576000	0.32841300	-1.69128200
O	7.49655900	-0.77658600	-1.59848500
² RC _β			
Fe	-1.28323600	0.02293100	0.03711100
O	-0.45980800	0.02934300	-1.36619700
S	-2.41014600	-0.32724400	2.32431300
H	-1.47615200	0.28325800	3.08819000
N	-0.34102700	1.65298600	0.75923000
C	1.26948000	3.05319100	1.64447100
C	0.28754900	3.84518900	1.13280600
H	2.18435100	3.34502600	2.14378700
H	0.22700300	4.92597700	1.12345400
N	-2.78493600	1.18636800	-0.62749400
C	-2.83050300	2.55513900	-0.61813100
C	-4.03211200	3.02371100	-1.26491500
C	-4.71465900	1.91644700	-1.66560300
H	-4.30322500	4.06495500	-1.38353800
H	-5.66398500	1.85721000	-2.18237100
N	-2.36228400	-1.62267300	-0.42537100
C	-3.56443500	-1.65890600	-1.08872800
C	-1.98861300	-2.93010700	-0.25464300
C	-3.96200700	-3.02455400	-1.33180100
C	-2.98135600	-3.81412100	-0.81679600
H	-4.87522700	-3.32082800	-1.83180100
H	-2.92112400	-4.89484200	-0.80387500

N	0.07007500	-1.15456300	0.97308000
C	1.33313900	-2.99156800	1.59149000
H	1.60591700	-4.03252300	1.70968900
C	0.12545200	-2.53060400	0.95050100
C	0.86633700	1.68864000	1.40431600
C	-0.70796400	2.96169200	0.57651200
C	-3.92603200	0.77777600	-1.26124100
C	-0.82496700	-3.35715200	0.37376400
H	-0.65193500	-4.42773600	0.42650000
C	1.60898500	0.57494100	1.78655200
H	2.57070200	0.74914700	2.25594700
C	-1.86796100	3.38589300	-0.05772100
H	-2.03483800	4.45673200	-0.12557100
C	-4.29469200	-0.54639000	-1.47761900
H	-5.23298700	-0.72261400	-1.99492800
C	2.02076200	-1.88545600	1.98454600
H	2.98172800	-1.81885500	2.47683000
C	1.23150300	-0.74363700	1.58929900
N	5.27596100	-0.22262800	-1.03334300
C	3.87447800	-0.47311400	-1.39242400
C	3.10759600	0.80643200	-1.74012200
H	3.41391700	-0.97060300	-0.53678300
H	3.88092700	-1.16911900	-2.23818500
H	2.05837000	0.56726900	-1.94309200
H	3.13744400	1.50522400	-0.89960300
H	3.53176700	1.30108400	-2.62179000
C	6.30673600	-0.23309700	-2.07327500
C	7.70424500	0.12237300	-1.57501800
H	5.99793500	0.47145800	-2.85745200
H	6.31228600	-1.23159700	-2.53287100
H	8.39462300	0.09132800	-2.42496200
H	7.73190000	1.12451600	-1.13937000
H	8.05239800	-0.58222100	-0.81591900
N	5.64907600	0.04239900	0.21270400
O	4.73616500	0.06539900	1.04680200
⁴ RC _β			
Fe	-1.27608000	0.01737000	0.04234200
O	-0.47160200	0.05984300	-1.37343300
S	-2.42407300	-0.31592300	2.30868400
H	-1.48529800	0.27350500	3.08315700
N	-0.33361100	1.64736500	0.76855500
C	1.27738100	3.04550900	1.65649100
C	0.29368300	3.83866200	1.15016400
H	2.19291700	3.33601300	2.15535200
H	0.23228100	4.91943500	1.14519900
N	-2.77866600	1.18826600	-0.62485200
C	-2.82246900	2.55643700	-0.61054000
C	-4.01801400	3.02927000	-1.26619700
C	-4.69775700	1.92440000	-1.67792200
H	-4.28664000	4.07130300	-1.38353200
H	-5.64210300	1.86813600	-2.20405900

N	-2.35570900	-1.62254000	-0.43125600
C	-3.55634900	-1.65440100	-1.09867700
C	-1.98930600	-2.93134000	-0.25658900
C	-3.95838300	-3.01876400	-1.34151900
C	-2.98344400	-3.81194100	-0.82123400
H	-4.87102400	-3.31182500	-1.84446200
H	-2.92811800	-4.89288600	-0.80620200
N	0.07168800	-1.15925900	0.97198300
C	1.32124800	-2.99988600	1.60775800
H	1.58811900	-4.04163500	1.73213300
C	0.11984200	-2.53610400	0.95760700
C	0.87406400	1.68170300	1.41215500
C	-0.70230900	2.95669000	0.59185000
C	-3.91379900	0.78337000	-1.27007800
C	-0.82990000	-3.36109900	0.37779300
H	-0.66102000	-4.43211300	0.43488600
C	1.61370400	0.56552100	1.79293000
H	2.57496100	0.73582400	2.26461700
C	-1.86222600	3.38365000	-0.04053800
H	-2.02884400	4.45488700	-0.10288200
C	-4.28236200	-0.54031000	-1.49076600
H	-5.21795300	-0.71494700	-2.01351300
C	2.01203700	-1.89542100	1.99970000
H	2.97045300	-1.83139900	2.49727900
C	1.23081900	-0.75142400	1.59573900
N	5.26568700	-0.22214100	-1.04005800
C	3.86279800	-0.46773800	-1.39673700
C	3.09948600	0.81480800	-1.74134900
H	3.40262700	-0.96460900	-0.54054500
H	3.86518300	-1.16280200	-2.24332400
H	2.04916000	0.57970600	-1.94344400
H	3.13275900	1.51235200	-0.89987900
H	3.52403600	1.30950800	-2.62280300
C	6.29369400	-0.22956100	-2.08274300
C	7.69322200	0.12071000	-1.58646900
H	5.98425600	0.47944000	-2.86264100
H	6.29603900	-1.22580600	-2.54724900
H	8.38127100	0.09253700	-2.43839800
H	7.72401700	1.12062900	-1.14594400
H	8.04201100	-0.58832300	-0.83180900
N	5.64275000	0.03560200	0.20641300
O	4.73225600	0.05624900	1.04315200
²TS-H_β			
Fe	-0.99617700	-0.02892300	0.23191000
O	-0.05640100	-0.07607000	-1.25400800
S	-2.58841600	0.26539300	2.06967000
H	-3.59979700	-0.48633200	1.57942700
N	0.37991200	-0.92394900	1.38337400
C	1.67360300	-2.54408900	2.40555200
C	2.14525100	-1.33585500	2.81890400
H	2.02654100	-3.53253900	2.67090100

H	2.97391000	-1.12203500	3.48068000
N	-0.29820400	1.76142700	0.83319500
C	0.72821000	2.01376800	1.71183900
C	0.93119200	3.43525700	1.85283100
C	0.01967000	4.04134200	1.04411800
H	1.67915300	3.89103600	2.48877900
H	-0.13952800	5.09993500	0.88291500
N	-2.49238100	0.88238400	-0.80124700
C	-2.62991400	2.23261200	-1.00216700
C	-3.48667400	0.28717100	-1.54004800
C	-3.75443800	2.49746600	-1.87060100
C	-4.28908600	1.29123500	-2.19981400
H	-4.07776300	3.48429000	-2.17658000
H	-5.14073100	1.08131800	-2.83434800
N	-1.80460400	-1.81918700	-0.25611500
C	-3.07649800	-3.48391000	-1.23023300
H	-3.86293700	-3.93459900	-1.82214100
C	-2.87835700	-2.06234800	-1.06669300
C	0.56727600	-2.27563500	1.51710000
C	1.32675000	-0.33498500	2.17899000
C	-0.74847900	2.99040200	0.41940900
C	-3.67164300	-1.08210100	-1.66025800
H	-4.49492900	-1.42017900	-2.28280800
C	-0.20860000	-3.26022800	0.91401300
H	0.06420400	-4.29234100	1.11488000
C	1.48468200	1.03766600	2.34678800
H	2.28252600	1.36949700	3.00336400
C	-1.81106500	3.20900600	-0.45116400
H	-2.04065600	4.24179600	-0.69670300
C	-2.09836000	-4.09738000	-0.50933000
H	-1.91486000	-5.15705000	-0.38506800
C	-1.30975300	-3.04681000	0.09176700
N	4.59381000	-0.32025000	-1.25070100
C	3.13438400	-0.54249800	-1.19363500
C	2.33893000	0.73817900	-1.27217900
H	2.93610900	-1.05445400	-0.24843900
H	0.99357900	0.33398400	-1.17427400
H	2.46450100	1.40980300	-0.42580400
H	2.34337000	1.24287700	-2.23918400
C	5.37972800	-0.55332900	-2.45827800
C	5.10749800	0.45571100	-3.57732700
H	5.18299900	-1.57448100	-2.81089200
H	6.42492700	-0.50306900	-2.14104900
H	5.75284300	0.23879100	-4.43606000
H	4.06852700	0.41062600	-3.92062800
H	5.31485400	1.47568800	-3.23790500
N	5.27830100	0.05659500	-0.16899500
O	4.60033900	0.25031300	0.84053800
H	2.88323000	-1.21380400	-2.01977300
⁴ TS-H _β			
Fe	-1.02384200	0.01379700	0.19007800

O	-0.06576300	0.03662200	-1.28463400
S	-2.41623600	-0.24034700	2.21367900
H	-3.59517900	-0.51059700	1.60891300
N	0.34225700	-0.98776800	1.28789700
C	1.62430700	-2.69040100	2.18530900
C	2.12922200	-1.51974400	2.66051700
H	1.95941400	-3.69998100	2.38639600
H	2.97370300	-1.36370000	3.31849000
N	-0.25494500	1.75100000	0.88157600
C	0.79964500	1.92434400	1.73375200
C	1.05640500	3.32856200	1.94467000
C	0.13411400	4.00503200	1.20481300
H	1.84053300	3.72556600	2.57634000
H	0.00104400	5.07487400	1.10648900
N	-2.49836000	1.01569700	-0.76527400
C	-2.60965700	2.37612000	-0.87595100
C	-3.52379900	0.49389000	-1.49883400
C	-3.74285200	2.72233300	-1.70289600
C	-4.31397800	1.54903600	-2.08992400
H	-4.04806900	3.73304700	-1.94220700
H	-5.18487200	1.39494700	-2.71418800
N	-1.89800100	-1.72310400	-0.33519100
C	-3.27624600	-3.30295100	-1.31692800
H	-4.10508400	-3.70240300	-1.88738700
C	-3.02011100	-1.89644300	-1.11390000
C	0.50675300	-2.34856700	1.33620600
C	1.32548600	-0.46319900	2.09424500
C	-0.68182900	3.00876900	0.55223900
C	-3.77636900	-0.86870800	-1.65619100
H	-4.63098900	-1.14859200	-2.26524200
C	-0.30089300	-3.27641100	0.68756400
H	-0.04729800	-4.32498300	0.81349000
C	1.53749900	0.89067200	2.30956400
H	2.36559300	1.16676400	2.95414500
C	-1.76849100	3.30088300	-0.26852300
H	-1.98717400	4.35130700	-0.43814400
C	-2.28785100	-3.97823800	-0.67164800
H	-2.13826200	-5.04801400	-0.59976000
C	-1.43112400	-2.98612500	-0.06472100
N	4.63376600	-0.31616900	-1.20769600
C	3.17257900	-0.53629200	-1.16255600
C	2.37590700	0.74042500	-1.28210200
H	2.96679000	-1.02716500	-0.20776900
H	1.01618200	0.36118000	-1.18436800
H	2.50870100	1.44206600	-0.46144500
H	2.38272200	1.21287800	-2.26553800
C	5.43300700	-0.57878500	-2.40038900
C	5.17066600	0.40041600	-3.54794600
H	5.24150600	-1.60906900	-2.72860500
H	6.47477200	-0.51856800	-2.07378000
H	5.82458000	0.16191700	-4.39440900
H	4.13510000	0.34519900	-3.89978000

H	5.37345700	1.42920000	-3.23331600
N	5.30576800	0.08585700	-0.12867900
O	4.61723400	0.30376500	0.86953400
H	2.93300900	-1.22843100	-1.97507100
² INT _β			
Fe	-1.17254600	0.03155400	-0.20513100
O	-0.11782500	0.08919200	1.23860600
S	-2.60206700	-0.11121900	-2.02579900
H	-1.98755400	0.79000500	-2.82393200
N	0.03814300	-1.36949000	-1.02905300
C	1.71501900	-2.39986000	-2.23003300
C	0.94550100	-3.38376600	-1.68572900
H	2.59696600	-2.49376400	-2.85007800
H	1.06147500	-4.45665300	-1.77259100
N	-2.32877300	-1.42655600	0.56328900
C	-2.14730000	-2.78106800	0.42846500
C	-3.16154600	-3.48668800	1.17095200
C	-3.94246200	-2.54425700	1.76761700
H	-3.24335900	-4.56476300	1.22543700
H	-4.79950200	-2.68755700	2.41322400
N	-2.33336400	1.42389900	0.66321000
C	-3.41043300	1.19826200	1.47987100
C	-2.22399600	2.78358300	0.53128300
C	-3.98115400	2.45565500	1.90054200
C	-3.24755600	3.43790900	1.31107400
H	-4.83854000	2.55202500	2.55438500
H	-3.37491400	4.51076000	1.37979800
N	-0.12259500	1.47725100	-1.13530400
C	0.69294400	3.53721500	-1.76871800
H	0.75994200	4.61522100	-1.84226200
C	-0.31249700	2.83120900	-1.01487300
C	1.12961900	-1.14426700	-1.83237800
C	-0.10760600	-2.73321900	-0.94697000
C	-3.41102500	-1.25888300	1.38934000
C	-1.29250200	3.44866100	-0.25040000
H	-1.32399200	4.53342000	-0.25697900
C	1.59102800	0.09878400	-2.24008300
H	2.48753600	0.12465800	-2.84940300
C	-1.12176900	-3.39786100	-0.27326600
H	-1.10968900	-4.48284700	-0.29253600
C	-3.91831300	-0.04380500	1.82660100
H	-4.78388300	-0.06829300	2.48065700
C	1.50772600	2.59600400	-2.32099700
H	2.38291700	2.73844200	-2.94187100
C	0.99929000	1.31059400	-1.91243100
N	4.74905400	0.15705300	1.25697900
C	3.26536700	0.09918100	1.27985200
C	2.75379700	-1.28895500	1.48017500
H	2.93465200	0.49939500	0.31809600
H	2.93554800	0.76883500	2.07873700
H	0.57624500	-0.59720900	1.15583500

H	2.78304400	-1.99092700	0.65385000
H	2.58085900	-1.67570000	2.48013700
C	5.49318000	0.43342800	2.48794800
C	7.00835200	0.45328300	2.30886800
H	5.21273700	-0.32638900	3.23016600
H	5.14610000	1.39996600	2.87841200
H	7.46946200	0.67367100	3.27772200
H	7.38421700	-0.50977000	1.95435300
H	7.31806300	1.21855600	1.59274600
N	5.42751700	-0.08039500	0.14161500
O	4.74271300	-0.36558300	-0.84399800
⁴INT_β			
Fe	-1.18210700	0.04096300	-0.20548900
O	-0.11548300	0.08455200	1.23083300
S	-2.58512000	-0.13160200	-2.03760400
H	-1.86366400	0.61064200	-2.90680900
N	-0.09344100	-1.52166200	-0.92198300
C	1.48618200	-2.77772300	-2.03587800
C	0.62891700	-3.64907700	-1.43408200
H	2.35474500	-2.99354100	-2.64448200
H	0.64648000	-4.73142700	-1.44851500
N	-2.46339900	-1.25314100	0.65101500
C	-2.40088400	-2.62537500	0.61063300
C	-3.47419400	-3.18624400	1.39257600
C	-4.16993200	-2.14029600	1.91771100
H	-3.65012900	-4.24669400	1.52069400
H	-5.03675400	-2.16316900	2.56575500
N	-2.21175700	1.58187500	0.55141700
C	-3.30690400	1.51103200	1.37420900
C	-1.98063000	2.91559200	0.32843600
C	-3.76252700	2.84036000	1.70310800
C	-2.94282800	3.71009100	1.05364300
H	-4.60867600	3.05800600	2.34230400
H	-2.97341500	4.79220300	1.04833300
N	0.00161200	1.31736900	-1.22070500
C	1.00908800	3.24670700	-1.97715900
H	1.17534300	4.30673100	-2.12111500
C	-0.06454700	2.68735000	-1.19485100
C	1.01707700	-1.45004500	-1.72627200
C	-0.36197900	-2.85688300	-0.74924500
C	-3.52710500	-0.93572300	1.45561800
C	-0.99083400	3.44060600	-0.48642300
H	-0.92525600	4.52091900	-0.56624200
C	1.59326700	-0.28244900	-2.20614800
H	2.49526600	-0.37576500	-2.80041100
C	-1.43397100	-3.37836900	-0.03856400
H	-1.52008200	-4.45874500	0.01777900
C	-3.92515600	0.34750100	1.80289300
H	-4.79019500	0.44667900	2.45054900
C	1.74098300	2.20024100	-2.45045800
H	2.63366600	2.21994100	-3.06220700

C	1.11215500	0.99685900	-1.96649600
N	4.75102700	0.14997100	1.25082200
C	3.26911900	0.05736500	1.29739800
C	2.79302900	-1.33444900	1.55013500
H	2.91662300	0.41855200	0.32803400
H	2.93416000	0.74562200	2.07803900
H	0.52956800	-0.64836800	1.17233800
H	2.82998100	-2.06342300	0.74794400
H	2.62638800	-1.68877700	2.56289900
C	5.50613500	0.47148900	2.46385600
C	7.01704500	0.53209800	2.25945300
H	5.25995100	-0.28141600	3.22509000
H	5.13710000	1.43505800	2.84120800
H	7.48676700	0.78691200	3.21565400
H	7.41600500	-0.42667100	1.91896300
H	7.29213600	1.29069100	1.52231800
N	5.42002500	-0.10236000	0.13334400
O	4.72963200	-0.42976100	-0.83529300
²TS-reb_p			
Fe	-1.13829	0.02636	0.27863
N	-0.91954	-1.95154	0.51941
N	0.19445	0.36501	1.72913
N	-1.34965	2.00232	0.01922
N	-2.46437	-0.31451	-1.17851
C	0.99474	-1.93031	2.05374
C	-0.07681	2.79011	1.95887
C	-2.71009	1.97935	-2.01833
C	-2.74846	-2.73841	-0.90839
C	0.05734	-2.57182	1.2553
C	1.02143	-0.56383	2.30284
C	0.45914	1.5644	2.33616
C	-0.88223	2.98961	0.84556
C	-1.99049	2.62169	-1.01965
C	-2.96597	0.61474	-2.05656
C	-3.06549	-1.51335	-1.48337
C	-1.71188	-2.94126	-0.00636
C	-1.22434	-4.2298	0.42164
C	-0.11577	-4.00264	1.17887
C	1.84836	0.07394	3.30048
C	1.4814	1.38448	3.34008
C	-1.25427	4.28085	0.31691
C	-1.91585	4.05457	-0.85089
C	-3.90067	-0.02096	-2.95164
C	-3.9824	-1.32921	-2.58008
H	1.70227	-2.55228	2.59206
H	2.58956	-0.43726	3.90132
H	1.87203	2.17539	3.96759
H	0.22884	3.66628	2.52141
H	-1.01039	5.22787	0.78117
H	-2.34471	4.77657	-1.53398
H	-3.18691	2.59893	-2.7709

H	-4.43705	0.48902	-3.74157
H	-4.58411	-2.11655	-3.01566
H	-3.28952	-3.61165	-1.25763
H	-1.66929	-5.17719	0.14579
H	0.52592	-4.72444	1.66744
O	0.38049	0.02541	-1.03795
S	-2.82477	0.0598	1.92618
H	-3.70719	-0.74191	1.29015
H	5.00259	1.80681	-2.07149
C	5.45598	1.22052	-1.26048
H	5.33724	1.81105	-0.34057
N	4.67837	-0.00959	-1.11035
C	3.21374	0.06125	-0.88828
N	5.31252	-1.17552	-1.20945
H	0.1154	-0.60252	-1.73208
H	3.02188	0.94829	-0.27823
O	4.59819	-2.17712	-1.12619
C	2.43899	0.10582	-2.15986
H	2.35049	-0.79554	-2.75905
H	2.16434	1.05062	-2.61138
C	6.93723	0.99303	-1.54889
H	7.08323	0.43005	-2.47453
H	7.42625	1.96811	-1.65145
H	7.42446	0.44094	-0.74137
H	2.95293	-0.82942	-0.31287
⁴TS-reb_β			
Fe	-1.10393000	0.04765800	0.29404300
S	-2.77591800	0.31332300	1.91525500
H	-2.71222000	-0.92313000	2.45711200
N	-1.51327500	1.95845800	-0.18851000
C	-1.43827200	4.25710700	-0.31645600
C	-2.37939000	3.83521100	-1.20570600
H	-1.12330200	5.26926100	-0.09676700
H	-2.99721400	4.42909400	-1.86709300
N	-2.45767300	-0.58759900	-1.07313900
C	-3.24265300	0.20305400	-1.87844700
C	-4.13075800	-0.62158300	-2.65902200
C	-3.89378100	-1.91275100	-2.29702600
H	-4.84629700	-0.24311900	-3.37779900
H	-4.37404300	-2.81346500	-2.65749100
N	-0.81280600	-1.85812900	0.88360700
C	-1.41813200	-2.98075400	0.37447600
C	0.11261900	-2.29791700	1.79815600
C	-0.88619500	-4.15830700	1.01382600
C	0.06211300	-3.73542100	1.89476000
H	-1.19966500	-5.17086500	0.79412500
H	0.68863500	-4.32923000	2.54792800
N	0.32452000	0.66852400	1.57650600
C	1.98521300	0.70435900	3.17399800
H	2.69434600	0.32569800	3.89913800
C	1.08552600	-0.11838400	2.40094500

C	-0.89340800	3.07759600	0.30811800
C	-2.41367900	2.39615800	-1.12731000
C	-2.85943300	-1.88374100	-1.29322200
C	0.99515500	-1.49849700	2.51101100
H	1.66603200	-1.99183100	3.20699600
C	0.13127100	3.09172500	1.24393200
H	0.52159900	4.05906500	1.54366700
C	-3.22212000	1.58921800	-1.91644000
H	-3.89563200	2.08155100	-2.61048600
C	-2.37596400	-3.00233700	-0.63046700
H	-2.77663500	-3.96859300	-0.91950800
C	1.74115300	1.99573400	2.81838300
H	2.20762600	2.89859700	3.19174100
C	0.69271000	1.96486800	1.82639000
C	2.35256800	-0.06970000	-2.25604000
C	3.12525100	-0.30053500	-1.00399200
H	2.15925300	0.93945600	-2.60183100
H	2.20741000	-0.88866200	-2.95114600
H	2.94061800	-1.30673000	-0.62107700
H	2.85458000	0.42895800	-0.23731400
O	0.20799500	-0.08176300	-0.98092100
H	-0.22809700	-0.42412200	-1.78229400
N	4.59135600	-0.18537600	-1.20507500
C	5.28821400	1.05367100	-0.85775600
C	6.78971700	1.01970400	-1.12800600
H	5.09937400	1.25984900	0.20511500
H	4.82453500	1.87359300	-1.42372900
H	7.21844100	1.98492500	-0.83689800
H	7.28302300	0.23073600	-0.55480400
H	7.00303100	0.84731700	-2.18596700
N	5.29146900	-1.19043400	-1.71851900
O	4.62825200	-2.18193500	-2.03152200
²P-OH_β			
Fe	0.98189500	0.00353800	-0.41935600
S	2.30249500	-0.01749800	-2.22168100
H	3.40298100	0.52280000	-1.65028700
N	2.41430700	-0.70424800	0.82092100
C	4.26924400	-0.86845800	2.19180400
C	3.89630700	-2.13775100	1.86620100
H	5.09201700	-0.54796400	2.81833000
H	4.35031500	-3.07198400	2.17167100
N	0.34386500	-1.87933200	-0.78873300
C	0.95928000	-3.03598700	-0.37555600
C	0.28409300	-4.18625600	-0.92907700
C	-0.73995500	-3.71340700	-1.69026900
H	0.57202700	-5.21443800	-0.74979200
H	-1.46637800	-4.27222100	-2.26663000
N	-0.57851500	0.69638000	-1.48606100
C	-1.49584600	-0.02712400	-2.20951800
C	-0.84733500	2.01808300	-1.74744600
C	-2.37975600	0.86087800	-2.92607300

C	-1.97749900	2.12997100	-2.63865900
H	-3.18858300	0.53894400	-3.57002300
H	-2.39007900	3.06517900	-2.99579800
N	1.51910500	1.87132200	0.08648500
C	1.63481500	4.17851400	0.15635400
H	1.37469200	5.20724900	-0.05869100
C	0.94708500	3.02727700	-0.38177500
C	3.34798800	0.02002900	1.52948400
C	2.74417500	-2.02901600	1.00605300
C	-0.69062000	-2.27381300	-1.60383500
C	-0.14679400	3.10220900	-1.23357600
H	-0.48271800	4.09305800	-1.52408100
C	3.40663700	1.40639300	1.58302100
H	4.18957200	1.85320800	2.18797800
C	2.06817500	-3.11159600	0.45800600
H	2.44273400	-4.10236400	0.69665300
C	-1.56036600	-1.41443100	-2.26268800
H	-2.33204500	-1.85875000	-2.88398600
C	2.62793900	3.70457800	0.95584300
H	3.35383400	4.26212000	1.53404200
C	2.54918800	2.26344800	0.90503600
N	-3.91643000	0.24215000	1.61541300
C	-2.52094600	0.67542400	1.62018600
C	-1.55526300	-0.51138900	1.58607900
H	-2.34872700	1.26024600	2.52792700
H	-2.35705700	1.30827800	0.74479400
H	-1.63940600	-1.07734200	2.51707300
H	-1.77254400	-1.17004100	0.74058700
C	-4.70627500	0.30683200	0.38182400
C	-6.12156100	-0.24388500	0.52477100
H	-4.15964100	-0.24679800	-0.39236600
H	-4.73758900	1.35454200	0.05152000
H	-6.62238800	-0.17094400	-0.44669900
H	-6.11419300	-1.29221200	0.83533700
H	-6.70187700	0.31877400	1.25978900
N	-4.51396400	-0.16267300	2.73664500
O	-3.78556200	-0.18831200	3.73088900
O	-0.22335800	0.01725200	1.44714700
H	0.40237000	-0.49121100	1.98869700
⁴P-OH_β			
Fe	1.01347300	0.04502500	-0.46079000
S	2.42241800	0.05977400	-2.28280100
H	2.94380100	1.29557000	-2.10933800
N	2.40589200	-0.79255100	0.91311500
C	4.27308800	-1.00457000	2.23829600
C	3.89014700	-2.26358100	1.87288700
H	5.11320100	-0.71746400	2.85833200
H	4.35588500	-3.20480800	2.13704500
N	0.38482000	-1.83384900	-0.91380300
C	0.98720600	-3.01131500	-0.53513800
C	0.32319700	-4.11718000	-1.18987500

C	-0.67164300	-3.59148900	-1.95791200
H	0.59112000	-5.15853700	-1.06304500
H	-1.38074200	-4.11662600	-2.58542800
N	-0.66815700	0.83115300	-1.44536500
C	-1.53952900	0.13138200	-2.23117800
C	-0.93414300	2.16036700	-1.62167200
C	-2.43074800	1.05421400	-2.90365200
C	-2.05697900	2.31181700	-2.52354100
H	-3.22055000	0.77206300	-3.58893400
H	-2.48210800	3.25716500	-2.83727000
N	1.54050500	1.89224900	0.14323900
C	1.65707500	4.17817200	0.35490800
H	1.39804200	5.22073100	0.21975600
C	0.94725400	3.06912400	-0.24550700
C	3.34701700	-0.08555900	1.61267900
C	2.72823400	-2.11852700	1.02302600
C	-0.63161300	-2.15614200	-1.78386000
C	-0.18670800	3.19559400	-1.05257500
H	-0.51247200	4.20967800	-1.26647700
C	3.41246200	1.30948500	1.65231800
H	4.19818400	1.74506200	2.26310300
C	2.05286400	-3.14629100	0.35955200
H	2.40465300	-4.15852000	0.53735900
C	-1.52115600	-1.25890300	-2.38149200
H	-2.26552200	-1.69066000	-3.04471100
C	2.66230000	3.65117100	1.10813400
H	3.39058200	4.17573600	1.71368400
C	2.58130400	2.21174500	0.98152400
N	-3.95058400	0.11180100	1.64303500
C	-2.56259600	0.56453000	1.70071000
C	-1.57367500	-0.59998200	1.61289400
H	-2.41677100	1.09600300	2.64496800
H	-2.39359800	1.25200300	0.86815700
H	-1.66416400	-1.22168000	2.50809700
H	-1.77469600	-1.21246700	0.72721500
C	-4.71207100	0.22106200	0.39523000
C	-6.12561500	-0.34581100	0.48191500
H	-4.14392200	-0.29548900	-0.38925300
H	-4.74493800	1.28129800	0.10785600
H	-6.60514100	-0.23526900	-0.49680900
H	-6.11651900	-1.40620800	0.74807100
H	-6.72703500	0.18069200	1.22678400
N	-4.56704400	-0.35988600	2.72736000
O	-3.86260600	-0.42435700	3.73690800
O	-0.25729900	-0.03456500	1.52539100
H	0.39090000	-0.62222900	1.94868700

One-water system

²RC_α

Fe	1.32987100	0.04923300	-0.06573600
O	0.62290600	-0.02335300	1.40467800

S	2.26306600	-0.15755300	-2.42951200
H	1.30599500	0.55492100	-3.06593000
N	0.34433100	1.72256500	-0.60481100
C	-1.32721800	3.17595100	-1.26469200
C	-0.31541400	3.93253200	-0.75776700
H	-2.27795000	3.49410200	-1.67221200
H	-0.25805800	5.00947300	-0.66473800
N	2.88571200	1.16718200	0.54732900
C	2.93155400	2.53272100	0.63797700
C	4.18392200	2.95725900	1.21318300
C	4.89727600	1.82636400	1.46945900
H	4.46522800	3.98799500	1.38664200
H	5.88682900	1.73367700	1.89820700
N	2.42670300	-1.62408500	0.21007400
C	3.68029900	-1.70318600	0.76638400
C	2.02692200	-2.91805000	-0.00010000
C	4.08194900	-3.08180000	0.90138600
C	3.05269700	-3.83663400	0.43008600
H	5.03104300	-3.41015800	1.30522400
H	2.98060400	-4.91460100	0.36372400
N	-0.09685400	-1.06332800	-0.97038600
C	-1.40079500	-2.85398600	-1.63786000
H	-1.68576300	-3.88459900	-1.80625400
C	-0.16031600	-2.43893300	-1.03091400
C	-0.90358700	1.80044900	-1.16280700
C	0.71982600	3.01683400	-0.34495100
C	4.07514300	0.71748400	1.05202900
C	0.81632500	-3.30254500	-0.56496000
H	0.63019200	-4.36718600	-0.66725100
C	-1.66862900	0.71724200	-1.58755200
H	-2.65251500	0.93110500	-1.99240900
C	1.92491700	3.39873700	0.22724800
H	2.09600100	4.46198900	0.36565200
C	4.45224000	-0.61795800	1.15182300
H	5.43036500	-0.82774600	1.57397500
C	-2.09819800	-1.72362200	-1.93045600
H	-3.08087300	-1.62502800	-2.37252400
C	-1.28648100	-0.61122300	-1.50066500
N	-4.73041000	-0.16961400	0.43470200
C	-4.31839600	0.96517100	1.27167500
C	-5.49923300	1.79307000	1.78993700
H	-3.67688500	1.59461900	0.64773800
H	-3.70983400	0.55274000	2.08016800
H	-5.12538500	2.63876800	2.37852600
H	-6.08375400	2.18680900	0.95430400
H	-6.15951600	1.19924400	2.43031000
C	-4.71608600	-1.54652000	0.93482100
C	-5.82293800	-1.83234800	1.95340900
H	-3.72956700	-1.73197600	1.37311200
H	-4.83636000	-2.18008500	0.05193800
H	-5.77932400	-2.88469000	2.25669600
H	-5.70747900	-1.22354700	2.85651000

H	-6.81315200	-1.63706000	1.52761600
N	-5.01472500	-0.01775200	-0.85114400
O	-4.96669000	1.14778000	-1.27279100
O	-1.80930700	-0.98093800	2.44919300
H	-1.04138900	-0.59869300	1.97355200
H	-1.42739000	-1.27400600	3.28957900
⁴ RC _α			
Fe	1.15005100	-0.04820600	0.17857500
O	-0.24858500	0.02229200	-0.66373200
S	3.35229700	-0.42453600	1.38364700
H	4.16929600	0.10758800	0.44662500
N	1.97463600	1.49580700	-0.82230100
C	2.97769900	2.76903400	-2.46852800
C	2.47489400	3.63328300	-1.54570500
H	3.51646300	2.99177100	-3.38041000
H	2.51192400	4.71485300	-1.54192900
N	0.50657000	1.22562300	1.60683500
C	0.58232600	2.59375400	1.58185300
C	-0.07427000	3.15458600	2.73665000
C	-0.54575600	2.10383900	3.46476600
H	-0.14897500	4.21290300	2.95108000
H	-1.08739200	2.12031200	4.40173500
N	0.56850900	-1.60706200	1.32111900
C	-0.12369800	-1.54897800	2.50802500
C	0.66847900	-2.93802100	1.01212200
C	-0.45682500	-2.87831100	2.95911300
C	0.03092700	-3.74070400	2.02766700
H	-0.99566500	-3.10245100	3.87062700
H	-0.02264800	-4.82152700	2.01400900
N	2.05052800	-1.33237800	-1.08721600
C	2.63501600	-3.26292700	-2.22033800
H	2.71212100	-4.32128000	-2.43323700
C	1.95971100	-2.70705500	-1.07366000
C	2.65796800	1.44029800	-2.00684500
C	1.84725200	2.83010900	-0.52577700
C	-0.17531500	0.90791400	2.74932000
C	1.30369100	-3.45472000	-0.11078700
H	1.29939800	-4.53318500	-0.23375100
C	3.01942300	0.27059700	-2.66956400
H	3.56446300	0.37575800	-3.60254300
C	1.20881000	3.34464700	0.59303800
H	1.18820900	4.42469400	0.70066900
C	-0.46709700	-0.38500200	3.17654200
H	-1.01349600	-0.48909600	4.10895700
C	3.12243600	-2.21628500	-2.93814000
H	3.68259600	-2.23574300	-3.86405900
C	2.74387300	-1.01491300	-2.23567100
N	-4.58198600	-0.46870800	-0.87806600
C	-4.55843800	0.41671400	-2.04821800
C	-5.83328500	1.25532200	-2.19681000
H	-4.43663200	-0.22545700	-2.92703300

H	-3.67872500	1.05820300	-1.94581100
H	-5.76125500	1.87773200	-3.09617300
H	-6.70815200	0.60784400	-2.29215800
H	-5.97669300	1.91827000	-1.33688000
C	-3.75526000	-0.22316600	0.29952800
C	-4.18159600	1.01524400	1.09252200
H	-2.70993400	-0.12399900	-0.01585900
H	-3.84210700	-1.12538600	0.91150400
H	-3.53421100	1.13224300	1.97001400
H	-4.09089400	1.92147500	0.48468900
H	-5.21805100	0.92874400	1.43580100
N	-5.25572700	-1.62127500	-0.88799600
O	-5.89475800	-1.84451700	-1.91855200
O	-1.74888700	2.37631200	-1.14331200
H	-1.20398900	1.56290300	-1.13190500
H	-1.81942800	2.60046000	-0.20373900
²TS-H_a			
Fe	0.85421500	0.11294400	-0.37222100
O	0.06846700	-0.16192600	1.17491700
S	2.04375500	0.11532100	-2.48893500
H	3.29357000	-0.08493200	-2.01381200
N	1.77735200	-1.68485500	-0.11848400
C	3.23025100	-3.35518300	0.55305300
C	2.19438000	-3.95796600	-0.08958500
H	4.10266600	-3.81142200	1.00328300
H	2.03771500	-5.01255700	-0.27610800
N	-0.60000400	-0.77155400	-1.44320200
C	-0.75444400	-2.12082600	-1.64986300
C	-1.95272100	-2.37419500	-2.41393700
C	-2.52029200	-1.16428800	-2.67083900
H	-2.29781000	-3.35704400	-2.70818100
H	-3.43140900	-0.94501500	-3.21175300
N	0.00344200	1.89440000	-0.72158400
C	-1.13699200	2.15587000	-1.43270300
C	0.46758900	3.11497200	-0.29934000
C	-1.41579300	3.57155600	-1.44317800
C	-0.41826000	4.16860000	-0.73609000
H	-2.26720100	4.02806200	-1.93070400
H	-0.27455800	5.22124700	-0.52839400
N	2.41648400	1.00372100	0.54848200
C	3.75407200	2.59684600	1.55225800
H	4.08525700	3.57507100	1.87670600
C	2.54421900	2.34134200	0.80858700
C	2.95776300	-1.93652000	0.53829000
C	1.29311800	-2.90745000	-0.50347100
C	-1.67161300	-0.17212100	-2.05727800
C	1.63996300	3.32369700	0.41588900
H	1.87859700	4.34900100	0.68348000
C	3.76622800	-0.96521600	1.11084300
H	4.67468000	-1.30032000	1.60282500
C	0.10969500	-3.11173700	-1.20155300

H	-0.15682600	-4.13861400	-1.43226200
C	-1.92260200	1.19330300	-2.05955700
H	-2.81659700	1.53459900	-2.57089800
C	4.35428600	1.38958000	1.74483900
H	5.28041200	1.17066200	2.26083500
C	3.50690700	0.40343300	1.11927400
N	-3.27606100	0.26938000	1.26364200
C	-2.14132900	0.84072400	1.89363500
C	-1.96378600	0.55756600	3.37542200
H	-2.10187700	1.89855300	1.62765100
H	-1.05752200	0.36085800	1.37816300
H	-1.06031300	1.06501900	3.72642700
H	-2.81931000	0.93060900	3.95429100
H	-1.84200200	-0.51285100	3.56461300
C	-3.66369400	-1.14264400	1.41308700
C	-4.87136700	-1.32810500	2.33792700
H	-2.79087000	-1.68655100	1.78166900
H	-3.90552500	-1.49947000	0.40790200
H	-5.12972700	-2.39169300	2.38744600
H	-4.65233200	-0.98588100	3.35467700
H	-5.73862700	-0.78001900	1.96061600
N	-3.92691600	1.07594700	0.39096300
O	-4.86163500	0.54278300	-0.20296400
O	-0.75678800	-2.54045600	2.32313900
H	-0.38268400	-1.76145700	1.84762600
H	-0.21128300	-2.60744300	3.12089500
⁴TS-H_a			
Fe	0.89736700	0.04475800	-0.36176400
O	0.00801800	-0.13092300	1.12542300
S	1.88977000	0.42160300	-2.52131900
H	2.58883000	1.53702800	-2.21213600
N	1.86011400	-1.67498800	-0.04687200
C	3.41589600	-3.24772900	0.62384400
C	2.40855300	-3.91946500	0.00556000
H	4.31961000	-3.64425800	1.06877300
H	2.31031200	-4.98395300	-0.16415800
N	-0.50968300	-0.92056000	-1.44418600
C	-0.60624500	-2.27479600	-1.62464200
C	-1.79269100	-2.59470000	-2.38002700
C	-2.41734600	-1.41475100	-2.64820500
H	-2.09514200	-3.59660400	-2.65647400
H	-3.34147400	-1.24520900	-3.18511100
N	-0.04591800	1.81452200	-0.77580700
C	-1.20427800	1.99208200	-1.49022800
C	0.33067200	3.06085500	-0.34587600
C	-1.56991300	3.38818700	-1.50844100
C	-0.61853000	4.05206700	-0.79674900
H	-2.44766600	3.78682000	-2.00001500
H	-0.54774600	5.11249100	-0.59052800
N	2.38387500	1.05275900	0.52885400
C	3.62903600	2.72981400	1.51355000

H	3.90154000	3.72726200	1.83432000
C	2.42797600	2.40244500	0.78544000
C	3.06672000	-1.84696400	0.58321200
C	1.44760300	-2.92908700	-0.42044600
C	-1.61175700	-0.37432400	-2.05785700
C	1.47447100	3.33461500	0.39385600
H	1.65191500	4.36962900	0.67045500
C	3.84938500	-0.82636900	1.10292300
H	4.78584400	-1.10542100	1.57622700
C	0.30020100	-3.21437900	-1.14620000
H	0.09750200	-4.25767300	-1.36690700
C	-1.93848600	0.97494200	-2.08463400
H	-2.85715700	1.25299400	-2.59016700
C	4.30936500	1.56428200	1.69553800
H	5.25454500	1.40598000	2.19894500
C	3.51876200	0.52344200	1.08735400
N	-3.31189600	0.27691300	1.24604400
C	-2.19604600	0.92007000	1.83629100
C	-1.98530400	0.70676400	3.32512700
H	-2.19490600	1.96425600	1.51920600
H	-1.08255500	0.42952200	1.31941000
H	-1.09867700	1.26494100	3.64093900
H	-2.84636600	1.06924000	3.90314500
H	-1.81747800	-0.34882100	3.55843000
C	-3.63834700	-1.14264100	1.45888800
C	-4.83522000	-1.33805000	2.39553600
H	-2.74401300	-1.63303300	1.84951700
H	-3.86602500	-1.55408100	0.47141900
H	-5.04798800	-2.40841200	2.49228500
H	-4.62821900	-0.94297200	3.39551700
H	-5.72569800	-0.84393100	1.99837200
N	-4.00288300	1.01589000	0.34455400
O	-4.91302600	0.41512000	-0.22269300
O	-0.70020800	-2.44117900	2.47631300
H	-0.35959900	-1.69763700	1.92735900
H	-0.13766600	-2.42124700	3.26480900
²INT_α			
Fe	1.25290000	0.01122900	-0.22618800
S	2.31246300	0.31726600	-2.24361200
H	1.26986000	0.01529500	-3.04881300
N	0.40676100	1.85681100	-0.40654400
C	-1.05377100	3.56525500	-0.91602200
C	0.08173500	4.13820600	-0.42681000
H	-1.96051300	4.04412100	-1.26240100
H	0.30006100	5.18903500	-0.28502100
N	2.90522700	0.86363300	0.54475800
C	3.14487800	2.20818900	0.71309200
C	4.42794200	2.39929700	1.33805100
C	4.94663900	1.16028400	1.56724200
H	4.85513700	3.36449200	1.57834200
H	5.88917600	0.89856800	2.03083000

N	2.04021500	-1.80239100	0.04084500
C	3.24064500	-2.09445400	0.64248300
C	1.52465300	-2.99898000	-0.39417500
C	3.46545400	-3.51895000	0.62246700
C	2.40767400	-4.07775500	-0.02577800
H	4.33632400	-4.00760300	1.04040800
H	2.22565900	-5.12154900	-0.24754800
N	-0.32610100	-0.79772300	-1.15270300
C	-1.81037600	-2.31638800	-2.04804700
H	-2.20395000	-3.27447000	-2.36270200
C	-0.52679700	-2.12949100	-1.42393600
C	-0.83391500	2.14119000	-0.92208900
C	0.99359400	3.06606000	-0.11794800
C	3.98762900	0.20682600	1.07320700
C	0.34003000	-3.16102200	-1.09263600
H	0.05218900	-4.16906100	-1.37229900
C	-1.72838200	1.21190300	-1.43577000
H	-2.69589500	1.57086000	-1.77012300
C	2.27058200	3.23760500	0.39644700
H	2.60403700	4.25305600	0.58436600
C	4.14582700	-1.17083900	1.13761300
H	5.05951700	-1.55077600	1.58291700
C	-2.40198800	-1.09105700	-2.11863000
H	-3.38467100	-0.82885300	-2.48686800
C	-1.47355000	-0.14602100	-1.55180300
N	-4.62964600	0.13998900	0.58583700
C	-4.15669200	1.09822700	1.36719000
C	-3.60227600	0.88130300	2.73539300
H	-4.21713500	2.08207300	0.91445600
H	-3.05632900	1.77528600	3.05281700
H	-4.39705200	0.71092200	3.47802700
H	-2.92246200	0.01934100	2.77319300
C	-4.72006100	-1.28299900	0.93783500
C	-5.93281800	-1.59032800	1.81952100
H	-3.78005900	-1.58643600	1.40749300
H	-4.80766600	-1.80123700	-0.01987400
H	-5.98681500	-2.66902800	2.00319200
H	-5.87143400	-1.08805100	2.79049300
H	-6.85880000	-1.27752500	1.32615400
N	-5.12164600	0.40862600	-0.73066500
O	-5.03650600	1.61231000	-1.03434700
O	0.46507800	-0.11403000	1.41706600
H	0.13053300	0.77518200	1.63082200
O	-1.60613700	-1.78909400	2.15486800
H	-1.20000200	-2.23485000	2.91299200
H	-0.87756700	-1.22945200	1.79503900
⁴ INT _a			
Fe	1.25842100	0.01362400	-0.22190100
S	2.31680000	0.30276700	-2.24360100
H	1.30034400	-0.09280500	-3.04152100
N	0.39259500	1.84559800	-0.41202000

C	-1.08735300	3.53343900	-0.93458900
C	0.04109000	4.12293900	-0.44895500
H	-1.99966700	3.99885900	-1.28460400
H	0.24725800	5.17717500	-0.31449800
N	2.90358900	0.88957800	0.53738700
C	3.12819800	2.23738900	0.69831900
C	4.41113900	2.44659700	1.31751200
C	4.94545200	1.21488000	1.55017000
H	4.82774700	3.41791000	1.55160600
H	5.89280400	0.96658400	2.01131300
N	2.06791400	-1.79301300	0.05685900
C	3.27502400	-2.06571300	0.65316700
C	1.56325500	-2.99820700	-0.36479900
C	3.51627200	-3.48749500	0.64365200
C	2.46051100	-4.06387900	0.00723900
H	4.39527300	-3.96261800	1.06014700
H	2.28895900	-5.11152000	-0.20451700
N	-0.31153200	-0.82181100	-1.14020000
C	-1.78308300	-2.36425900	-2.01574600
H	-2.16838200	-3.32941400	-2.31880800
C	-0.50005100	-2.15891000	-1.39605700
C	-0.85104200	2.11212500	-0.93105000
C	0.96552100	3.06391100	-0.13261100
C	3.99610400	0.24761400	1.06467000
C	0.37678500	-3.17871100	-1.05636900
H	0.09759300	-4.19216100	-1.32502000
C	-1.73511900	1.17030200	-1.43838200
H	-2.70645800	1.51693800	-1.77465200
C	2.24096600	3.25470100	0.37808400
H	2.56258500	4.27524500	0.55868500
C	4.17148800	-1.12730800	1.13678500
H	5.09197800	-1.49293800	1.58002500
C	-2.38634700	-1.14546700	-2.09821500
H	-3.37260300	-0.89605100	-2.46605400
C	-1.46607500	-0.18576000	-1.54342000
N	-4.65061400	0.14101100	0.57108400
C	-4.19304100	1.10579400	1.35474400
C	-3.65082100	0.89650900	2.72910700
H	-4.25331500	2.08727600	0.89715200
H	-3.12242700	1.79867800	3.05293900
H	-4.45031000	0.71265800	3.46337000
H	-2.95754200	0.04559500	2.77428600
C	-4.73654900	-1.28058700	0.92953100
C	-5.95690900	-1.59102900	1.79957400
H	-3.79956600	-1.57604100	1.41021200
H	-4.81102000	-1.80430800	-0.02630100
H	-6.00673200	-2.66919300	1.98765200
H	-5.90923800	-1.08395000	2.76878900
H	-6.87919700	-1.28589000	1.29462500
N	-5.12622300	0.39952200	-0.75146700
O	-5.04411400	1.60272700	-1.06092500
O	0.47884400	-0.11737300	1.42613300

H	0.14248900	0.77073900	1.64180000
O	-1.62165700	-1.76223200	2.16079100
H	-1.22142900	-2.21893700	2.91548200
H	-0.88407600	-1.21474700	1.80126900
⁴TS-reb_a			
Fe	-0.87078300	0.11611000	-0.40727100
N	-1.22114500	2.08466300	0.04318000
N	0.63072200	0.65756000	-1.62233500
N	-0.51332400	-1.83797500	-0.82391400
N	-2.48718700	-0.40431700	0.66702600
C	0.54491500	3.10053900	-1.31953000
C	1.37573700	-1.56805600	-2.35980100
C	-2.35734400	-2.85231700	0.43181700
C	-3.22852300	1.82312100	1.42160000
C	-0.53637900	3.16548000	-0.45183800
C	1.07608900	1.93415100	-1.85835300
C	1.45163400	-0.18160600	-2.33342000
C	0.45486100	-2.33111600	-1.65633900
C	-1.23648000	-2.91662500	-0.38487600
C	-2.93057800	-1.68090200	0.91382200
C	-3.32511100	0.43887200	1.36115100
C	-2.25541800	2.58708800	0.78944000
C	-2.19904100	4.02895500	0.80052600
C	-1.13243300	4.38731300	0.03192400
C	2.20630500	1.89952900	-2.75339700
C	2.43896800	0.58954100	-3.04690000
C	0.36354100	-3.77074900	-1.72031900
C	-0.68348300	-4.13484600	-0.93017800
C	-4.08929700	-1.64118200	1.76887200
C	-4.33365100	-0.32998500	2.04551400
H	0.99933600	4.03869500	-1.62283900
H	2.73957400	2.77417400	-3.10403600
H	3.20492700	0.16646600	-3.68409500
H	2.09641700	-2.09500800	-2.97618800
H	1.02114200	-4.40362800	-2.30234500
H	-1.06876400	-5.12791700	-0.73613800
H	-2.83400300	-3.78836400	0.70568200
H	-4.62896700	-2.51443400	2.11241700
H	-5.11709800	0.09457100	2.66028700
H	-3.98219600	2.34904300	1.99920500
H	-2.89884600	4.66926800	1.32259700
H	-0.78019300	5.38244700	-0.20884100
O	0.31032900	0.01582100	1.12738100
S	-2.26709200	0.33361700	-2.41294300
H	-3.43419800	-0.04069600	-1.84231800
H	4.50736400	1.38828200	0.29144100
C	4.28539400	1.17765900	1.34328200
H	3.60398900	1.95861700	1.70036000
N	3.60082400	-0.10203500	1.35310700
C	2.75326200	-0.55926600	2.19272200
N	3.99729000	-1.07629100	-0.03249100

H	0.09863900	0.81596900	1.63769800
H	2.35358300	-1.54990400	1.96629700
O	3.43182600	-2.11478600	0.02993300
C	2.35682700	0.07673700	3.48884700
H	2.29840000	1.16755200	3.41929900
H	1.40223800	-0.33750200	3.81510000
H	3.10693800	-0.16970000	4.25386400
C	5.58000900	1.15463400	2.16226900
H	6.25153000	0.37135200	1.79697700
H	6.09412600	2.11771000	2.07444500
H	5.38084000	0.96992300	3.22311600
O	0.13715800	-2.14504600	2.78880700
H	-0.14587600	-2.89611800	2.24723100
H	0.08134800	-1.37849800	2.16492400
²P-OH_a			
Fe	1.06001200	-0.14441800	0.03791000
O	-1.35427500	0.11449300	0.15479100
S	3.26151900	-0.48737100	0.14668100
H	3.40657300	-0.32546700	1.48190800
N	0.75528600	-1.77065800	-1.11002400
C	0.51750300	-3.97271700	-1.77816600
C	0.65109700	-3.22559900	-2.90714000
H	0.38021000	-5.04282700	-1.68902200
H	0.65162200	-3.55430900	-3.93866200
N	1.24638600	0.95747100	-1.63227500
C	1.25757000	0.51927700	-2.93567200
C	1.53956700	1.61449900	-3.83142800
C	1.71306100	2.71955100	-3.05605400
H	1.59801200	1.52980300	-4.90916500
H	1.94127100	3.73165900	-3.36551800
N	1.11993900	1.51197600	1.16935400
C	1.38959400	2.78546100	0.72689500
C	0.98079000	1.60793900	2.53489700
C	1.40190700	3.70678900	1.83756600
C	1.14494600	2.97555000	2.95945400
H	1.59019900	4.76990500	1.75476400
H	1.07443100	3.31558100	3.98483700
N	0.65817200	-1.22339000	1.69212900
C	0.42241300	-1.89046600	3.89564900
H	0.34237200	-1.80457700	4.97184400
C	0.60980900	-0.77992700	2.99630500
C	0.58933800	-3.05998700	-0.66236400
C	0.81269300	-1.85652000	-2.48163600
C	1.53066500	2.30142900	-1.68697400
C	0.74048500	0.54277300	3.39326300
H	0.66726200	0.75932200	4.45443400
C	0.48887500	-3.44846500	0.66601600
H	0.35725100	-4.50692300	0.86699700
C	1.03503300	-0.78992100	-3.34080100
H	1.06736700	-0.99958500	-4.40551300
C	1.59565600	3.15532100	-0.59575800

H	1.81244800	4.20088200	-0.79256200
C	0.37092000	-3.01380900	3.12831000
H	0.23489100	-4.04021400	3.44413700
C	0.51896000	-2.59188500	1.75766300
N	-3.69677800	-0.02682100	-0.13671200
C	-2.39889400	0.08426700	-0.83035400
C	-2.27238300	1.31461300	-1.70671100
H	-2.29254100	-0.83529100	-1.41361600
H	-1.43176700	-0.73461500	0.63964400
H	-1.31943000	1.25848700	-2.23590900
H	-3.07679200	1.35126600	-2.44568400
H	-2.27979500	2.22329900	-1.09953000
C	-4.70664300	1.03619200	-0.00009300
C	-5.72306300	1.07085900	-1.14364100
H	-4.17918200	1.98451500	0.12398900
H	-5.21905200	0.82814800	0.94217400
H	-6.46862100	1.84962100	-0.94733900
H	-5.25765300	1.28951400	-2.10966400
H	-6.24348000	0.11058600	-1.22274500
N	-3.96195700	-1.14157000	0.54451500
O	-3.05070700	-1.98029400	0.54876600
O	-2.11321800	2.64253600	1.36847500
H	-1.34956800	3.22402200	1.50442700
H	-1.71176700	1.77573700	1.17268200
⁴P-OH_a			
Fe	1.19484500	0.01406800	-0.60166400
O	-1.73377800	-0.75123400	1.38377900
S	2.43778000	0.15043400	-2.51417200
H	3.26763400	-0.89107400	-2.27728600
N	-0.09134000	1.47722400	-1.18521900
C	-1.67690900	2.62609500	-2.40913000
C	-0.90784200	3.55350700	-1.77689200
H	-2.53740700	2.78715600	-3.04459800
H	-1.00335200	4.63148100	-1.79979600
N	2.15266500	1.41678100	0.61968600
C	1.95689300	2.77308600	0.62220900
C	2.92620700	3.40607800	1.48617000
C	3.71950400	2.41430100	1.98465600
H	2.99127400	4.47085700	1.67096500
H	4.55951700	2.50566200	2.66152100
N	2.24610400	-1.44310500	0.28076600
C	3.34598700	-1.29091800	1.09422700
C	2.05739400	-2.79840700	0.11495400
C	3.89567200	-2.58838900	1.40891300
C	3.10349500	-3.51649300	0.80444100
H	4.76112000	-2.75312900	2.03780200
H	3.19115800	-4.59497200	0.83512600
N	-0.26127700	-1.39059600	-1.19135900
C	-1.11782300	-3.39771800	-1.93240200
H	-1.22323500	-4.46776800	-2.05967400
C	-0.08496300	-2.75564900	-1.15826700

C	-1.17075800	1.32746800	-2.03266900
C	0.08033100	2.83399900	-1.00780400
C	3.23701500	1.17232800	1.42620400
C	0.98979700	-3.40065200	-0.54759000
H	0.99558800	-4.48600200	-0.58665900
C	-1.75076900	0.11889800	-2.41161200
H	-2.61507600	0.17964600	-3.06527500
C	1.00754100	3.43160700	-0.15783600
H	0.98329600	4.51553800	-0.09603000
C	3.80571200	-0.08563100	1.62182400
H	4.66999200	-0.13962300	2.27696300
C	-1.88877100	-2.40611800	-2.47080600
H	-2.74388600	-2.50593700	-3.12717300
C	-1.33242800	-1.15422700	-2.02442900
N	-3.96076900	-0.07629700	0.98176600
C	-2.61845100	0.35859700	1.41856900
C	-2.62568200	0.92583400	2.83187700
H	-2.32875300	1.12287500	0.69485000
H	-1.39290600	-0.88322100	0.47590600
H	-1.60568700	1.18381900	3.13074400
H	-3.25682400	1.81854100	2.87260000
H	-3.00423000	0.18948700	3.54841100
C	-4.59389700	-1.29410400	1.50059300
C	-5.76241500	-1.01094900	2.44762100
H	-3.80577800	-1.86639500	1.99420800
H	-4.93695600	-1.88258600	0.64343100
H	-6.20960500	-1.95375300	2.78292600
H	-5.43608800	-0.45430400	3.33224500
H	-6.53307300	-0.42515600	1.93715000
N	-4.65886500	0.57266400	0.05390600
O	-4.15483800	1.60491300	-0.34918300
O	0.48742900	-0.56589200	3.18632300
H	1.06223900	0.10147900	2.78310400
H	-0.26459300	-0.62958900	2.56746100
²P-NO₁			
Fe	-1.11772600	0.10686700	0.27329300
O	0.37407800	-0.12950800	-0.85105900
S	-2.97071100	0.46086700	1.67953900
H	-2.51250300	-0.17574000	2.78114000
N	-1.44947500	1.95485800	-0.48817200
C	-1.40244100	4.24494000	-0.79490900
C	-2.22002200	3.73095500	-1.75406600
H	-1.13919400	5.28002600	-0.61754800
H	-2.76560200	4.25582200	-2.52793700
N	-2.33230200	-0.65140900	-1.15814100
C	-3.00650200	0.02204200	-2.13898300
C	-3.77313000	-0.89743900	-2.94641700
C	-3.55533500	-2.13891800	-2.43084600
H	-4.39273000	-0.61434900	-3.78783900
H	-3.95830700	-3.08746700	-2.76215800
N	-0.81029500	-1.73399800	1.04763500

C	-1.34877500	-2.90170700	0.58191500
C	-0.03839200	-2.07719900	2.12217000
C	-0.90315800	-4.01769200	1.38531900
C	-0.08542500	-3.50490400	2.34394500
H	-1.18499500	-5.04944100	1.21903200
H	0.44023700	-4.02676000	3.13352600
N	0.04981900	0.87714400	1.72715100
C	1.44225700	1.12806200	3.55589400
H	2.03640600	0.84796500	4.41664200
C	0.70786500	0.20280600	2.72397800
C	-0.93147400	3.12848100	-0.00792800
C	-2.24439400	2.30134300	-1.55297400
C	-2.65658900	-1.97079600	-1.31253700
C	0.67603000	-1.17533300	2.90763600
H	1.24497400	-1.58028000	3.73965800
C	-0.08501700	3.24384500	1.09118700
H	0.24311200	4.24503600	1.35577900
C	-2.96875900	1.40233100	-2.32768500
H	-3.55839700	1.80974300	-3.14366500
C	-2.20495800	-3.01386600	-0.50823900
H	-2.55038800	-4.01199200	-0.76021100
C	1.22389500	2.37012000	3.04386700
H	1.60308000	3.32090300	3.39667700
C	0.35716800	2.20227400	1.89931800
N	4.45421800	-0.03295400	-1.23516700
C	4.46074100	-1.23112600	-0.82089400
C	3.45633900	-1.92216100	0.04101000
H	5.31351800	-1.81934700	-1.19085200
H	0.14525300	0.36169200	-1.65817800
H	2.69859500	-2.39741300	-0.60879300
H	3.94418300	-2.70315200	0.63267600
H	2.92498400	-1.23182700	0.70011900
C	3.48589700	1.02033000	-0.96631300
C	3.94266400	1.90441000	0.19883700
H	2.48816200	0.59748100	-0.78517000
H	3.43494800	1.62122900	-1.88259000
H	3.23112100	2.72507300	0.33296400
H	3.98034100	1.33741700	1.13470600
H	4.93468700	2.32698600	0.00711300
N	5.90850800	0.42726700	-2.40862700
O	6.59074800	-0.51812100	-2.52577900
O	0.96670300	-2.62627500	-1.79255800
H	0.69483600	-1.74843600	-1.41196100
H	1.12948800	-2.43550800	-2.72864300
⁴P-NO₁			
Fe	-1.32062000	0.00587400	0.18009500
O	-0.70907500	-0.01769600	-1.53284300
S	-2.20022100	0.02408100	2.30549800
H	-1.28393400	0.83189100	2.88347700
N	-2.47231500	1.61199400	-0.31621700
C	-3.25196300	3.76716400	-0.56415800

C	-4.27023100	2.92877300	-0.90466100
H	-3.24263000	4.84961500	-0.55709300
H	-5.26998400	3.18083700	-1.23454200
N	-2.85715400	-1.21734400	-0.24180300
C	-4.10481700	-0.85407000	-0.69114300
C	-4.90038700	-2.03129300	-0.92716500
C	-4.11725100	-3.10564500	-0.63105700
H	-5.92282900	-2.01868300	-1.28253600
H	-4.36330800	-4.15794800	-0.69309400
N	-0.15324700	-1.56982900	0.57422900
C	-0.50714400	-2.89412700	0.49721500
C	1.13946800	-1.54131000	1.03696700
C	0.60428100	-3.72367400	0.89177000
C	1.62356300	-2.88626500	1.22586600
H	0.58376800	-4.80577800	0.91299600
H	2.61583200	-3.13397700	1.58005200
N	0.14421800	1.25309600	0.76615300
C	2.20019300	2.07094400	1.42157400
H	3.23562500	2.04826000	1.73615000
C	1.40561400	0.89419300	1.17745800
C	-2.13796100	2.93847800	-0.17979300
C	-3.78277300	1.58437900	-0.72997000
C	-2.83926000	-2.59001600	-0.21325000
C	1.87684200	-0.40258700	1.31808700
H	2.89602900	-0.53079400	1.66436600
C	-0.92366500	3.41895300	0.28759800
H	-0.78917100	4.49518300	0.32283900
C	-4.54494100	0.44141000	-0.91884800
H	-5.56649500	0.56994600	-1.26154600
C	-1.75218000	-3.37947700	0.13120900
H	-1.88790900	-4.45591100	0.11452400
C	1.41034300	3.14395600	1.13750200
H	1.65921000	4.19637800	1.18647200
C	0.13326600	2.62810600	0.71403300
N	5.04723500	0.02979400	-0.79145300
C	4.93434200	-1.23386200	-0.81803700
C	4.53566000	-2.09214100	-1.99025900
H	5.13647800	-1.74355900	0.13362500
H	-1.09657200	0.75380500	-1.98335000
H	5.16302900	-1.87772000	-2.86519600
H	4.62395100	-3.15530600	-1.74939200
H	3.49723100	-1.86422100	-2.27102200
C	4.79955800	0.83196600	-1.99142800
C	4.89918200	2.32279500	-1.67642300
H	3.81090100	0.58888500	-2.40401500
H	5.54052400	0.56315500	-2.76070300
H	4.74315600	2.91730500	-2.58397600
H	4.13995600	2.61194100	-0.94225000
H	5.88271400	2.57036300	-1.26284200
N	5.58360600	0.64780700	1.51778400
O	5.49647800	-0.38953100	2.05577800
O	1.66774200	-0.61420100	-2.84801000

H	1.25735300	-1.10285400	-3.57647300
H	0.91073600	-0.40591500	-2.25568900
²P-NO₂			
Fe	1.07506	0.06565	0.30074
O	0.0421	-0.06359	-1.13057
S	2.5337	0.21122	2.11287
H	1.78455	-0.46729	3.01032
N	-0.43678	-0.40892	1.5533
C	-2.26426	-0.27166	2.95135
C	-2.0029	-1.59476	2.75867
H	-3.04428	0.1825	3.54918
H	-2.52311	-2.45131	3.16847
N	1.52321	-1.89665	0.10523
C	0.8323	-2.95418	0.63315
C	1.46154	-4.19569	0.24722
C	2.5457	-3.86791	-0.50749
H	1.11262	-5.17877	0.53736
H	3.26986	-4.52561	-0.97119
N	2.67891	0.55203	-0.80992
C	3.57325	-0.31871	-1.37756
C	3.03977	1.80698	-1.22452
C	4.54358	0.41336	-2.15506
C	4.21025	1.72964	-2.06439
H	5.35986	-0.04064	-2.70224
H	4.69716	2.58305	-2.51871
N	0.6242	2.0235	0.51041
C	0.67004	4.32217	0.33772
H	0.99536	5.30142	0.01075
C	1.27633	3.07913	-0.07467
C	-1.28718	0.46301	2.18652
C	-0.8618	-1.67381	1.88139
C	2.57741	-2.42683	-0.58906
C	2.38911	2.9883	-0.89612
H	2.79687	3.91235	-1.29286
C	-1.24949	1.84946	2.08725
H	-1.97826	2.41358	2.66071
C	-0.28488	-2.86136	1.45282
H	-0.72545	-3.78777	1.80801
C	3.54217	-1.70147	-1.2729
H	4.32313	-2.25902	-1.77989
C	-0.33757	4.00479	1.19429
H	-1.01609	4.66809	1.71528
C	-0.35665	2.56532	1.30102
N	-3.45278	-1.23072	-1.49609
C	-2.52282	-2.0882	-1.67248
C	-2.60799	-3.57305	-1.91108
H	-1.50634	-1.68302	-1.65359
H	-2.82954	0.45441	-1.26591
H	-2.24775	-3.79348	-2.92487
H	-1.92694	-4.08532	-1.22101
H	-3.60984	-3.99332	-1.80385

C	-4.87131	-1.57203	-1.47312
C	-5.56699	-0.83694	-0.32419
H	-5.05682	-2.65174	-1.39481
H	-5.30196	-1.24128	-2.42822
H	-6.63912	-1.06315	-0.31655
H	-5.14389	-1.13868	0.64061
H	-5.44139	0.24593	-0.42833
N	-4.47588	2.93049	-1.10607
O	-4.53749	3.49563	-2.11606
O	-2.33332	1.30916	-1.12112
H	-0.7046	0.5975	-1.14291
H	-2.41674	1.48406	-0.16953
⁴P-NO₂			
Fe	0.85404	0.11253	0.5086
O	-0.24509	-0.14613	-0.86244
S	2.25534	0.52753	2.32005
H	3.308	-0.21848	1.91786
N	2.19912	-1.19326	-0.23131
C	3.30913	-3.13908	-0.77045
C	3.8811	-2.13607	-1.49233
H	3.56053	-4.192	-0.75993
H	4.70032	-2.19396	-2.19767
N	1.72874	1.60625	-0.53434
C	2.77067	1.48971	-1.41534
C	3.09938	2.78387	-1.96441
C	2.25288	3.68072	-1.38971
H	3.88484	2.96288	-2.68759
H	2.19705	4.75111	-1.54225
N	-0.37265	1.44377	1.39204
C	-0.40593	2.79812	1.17096
C	-1.38884	1.16597	2.27179
C	-1.46071	3.39491	1.95143
C	-2.07127	2.38336	2.63163
H	-1.69096	4.45279	1.96492
H	-2.90553	2.43925	3.31949
N	-0.03252	-1.38521	1.53281
C	-1.41961	-2.56695	2.9444
H	-2.22101	-2.7498	3.64881
C	-1.09152	-1.27277	2.39729
C	2.2488	-2.54481	0.0047
C	3.17533	-0.92416	-1.15847
C	1.4023	2.93565	-0.49194
C	-1.73422	-0.09382	2.74137
H	-2.5606	-0.15857	3.44189
C	1.39311	-3.2559	0.83401
H	1.55869	-4.32425	0.92764
C	3.44687	0.3168	-1.71718
H	4.25559	0.37447	-2.43855
C	0.41589	3.50148	0.30135
H	0.27176	4.57516	0.23456
C	-0.53576	-3.4545	2.41464

H	-0.46048	-4.52008	2.58939
C	0.33318	-2.70681	1.53887
N	-3.98366	-0.39488	-1.29734
C	-3.46521	0.76773	-1.19381
C	-4.11933	2.11982	-1.0827
H	-2.37111	0.78847	-1.16817
H	-2.70675	-1.71625	-1.28872
H	-3.80176	2.58626	-0.14118
H	-3.75146	2.76672	-1.88942
H	-5.21029	2.10267	-1.11584
C	-5.42059	-0.63659	-1.35079
C	-5.75909	-1.51364	-2.55995
H	-6.02076	0.28282	-1.37586
H	-5.6904	-1.17234	-0.43078
H	-6.82525	-1.76595	-2.56578
H	-5.52419	-0.99479	-3.49594
H	-5.18189	-2.44386	-2.5333
N	-0.29226	-0.67438	-3.54639
O	0.79773	-0.5995	-3.93111
O	-1.88027	-2.27008	-1.28734
H	-0.76782	-0.9944	-0.79958
H	-1.58286	-2.25265	-2.21185
²RC_β			
Fe	1.22200500	0.05887400	-0.19872900
O	0.43612700	0.00146000	1.23221600
S	2.26927300	-0.16132900	-2.51751000
H	1.32649200	0.51632700	-3.21080100
N	0.24938400	1.71359700	-0.81582700
C	-1.40050400	3.14103500	-1.57573000
C	-0.40636400	3.91569000	-1.06078400
H	-2.33437400	3.44878300	-2.02802000
H	-0.35257400	4.99515400	-1.00087400
N	2.73768700	1.19967200	0.46689000
C	2.77417600	2.56810300	0.52343600
C	3.99352300	3.01423400	1.15155800
C	4.69677500	1.89469000	1.47333500
H	4.25990100	4.05061300	1.31432100
H	5.66112700	1.81705400	1.95834400
N	2.32650900	-1.59661400	0.14503700
C	3.55369400	-1.65499700	0.75979000
C	1.95494900	-2.89871400	-0.07564200
C	3.96794800	-3.02612600	0.92193000
C	2.97283100	-3.79913600	0.40665300
H	4.90108600	-3.33807100	1.37301300
H	2.91995900	-4.87846300	0.34348500
N	-0.15708000	-1.08326200	-1.14171700
C	-1.43010600	-2.89831500	-1.80320800
H	-1.70059600	-3.93445700	-1.96176000
C	-0.20347200	-2.45947300	-1.18384900
C	-0.98124700	1.77027400	-1.41488800
C	0.61290100	3.01507000	-0.58190900

C	3.90323200	0.77122800	1.04050000
C	0.77185800	-3.30479800	-0.68171600
H	0.60435700	-4.37303100	-0.78002100
C	-1.73198400	0.67097000	-1.82058300
H	-2.71053700	0.85986700	-2.24734100
C	1.79002000	3.41763600	0.03474600
H	1.95213200	4.48504200	0.14996500
C	4.29020500	-0.55694800	1.17664600
H	5.24377100	-0.75003600	1.65769500
C	-2.13763800	-1.77989600	-2.11818000
H	-3.11598700	-1.69620800	-2.57190600
C	-1.34150100	-0.65270500	-1.69665100
N	-5.34000800	-0.27651900	1.03052300
C	-3.93361500	-0.52058100	1.37452300
C	-3.17695100	0.75856200	1.74534600
H	-3.47368800	-0.99453200	0.50511100
H	-3.92765700	-1.23474400	2.20487300
H	-2.12491900	0.52461200	1.93913700
H	-3.21630800	1.47439000	0.91982500
H	-3.60079800	1.23081000	2.63915700
C	-6.36587400	-0.33567100	2.07413100
C	-7.77120700	0.01133200	1.59230200
H	-6.06498100	0.34967400	2.87808700
H	-6.35254200	-1.34771700	2.50265300
H	-8.45707200	-0.05701600	2.44365600
H	-7.81765400	1.02558100	1.18739800
H	-8.11105100	-0.67586400	0.81369600
N	-5.72240200	0.02214400	-0.20441700
O	-4.81310100	0.08382200	-1.04103200
O	1.89692000	-0.67957200	3.58501000
H	1.81809400	-1.62852000	3.40860600
H	1.36521700	-0.28626900	2.86531100
⁴ RC _β			
Fe	1.21704300	0.05418200	-0.20499000
O	0.45323400	0.02679300	1.24044500
S	2.27715200	-0.14272200	-2.50322500
H	1.33920000	0.53820200	-3.19979000
N	0.25429300	1.71976900	-0.81309800
C	-1.38711400	3.16159700	-1.56428400
C	-0.38438200	3.92745700	-1.05293200
H	-2.32033200	3.47746800	-2.01230100
H	-0.32171700	5.00637800	-0.99180000
N	2.74198000	1.18763600	0.47086700
C	2.78699800	2.55500500	0.52931800
C	4.00447900	2.99233600	1.16811400
C	4.69690600	1.86754500	1.49492400
H	4.27635900	4.02664000	1.33495500
H	5.65622100	1.78248200	1.98859500
N	2.31089600	-1.60633500	0.13866600
C	3.53614700	-1.67295100	0.75768400
C	1.93739700	-2.90541600	-0.09457900

C	3.94527000	-3.04664500	0.91072200
C	2.95046700	-3.81270900	0.38446900
H	4.87559900	-3.36493400	1.36318500
H	2.89497600	-4.89131300	0.31207100
N	-0.16644900	-1.07185900	-1.14573900
C	-1.43891000	-2.87627800	-1.83761200
H	-1.71041200	-3.90984500	-2.01050900
C	-0.21465600	-2.44780800	-1.20689600
C	-0.97743100	1.78741500	-1.40766000
C	0.62970800	3.01807400	-0.57905200
C	3.89902000	0.75030600	1.05286000
C	0.75515200	-3.30172000	-0.70905400
H	0.58453700	-4.36827100	-0.81939900
C	-1.73389200	0.69335200	-1.81713200
H	-2.71169100	0.88793200	-2.24303600
C	1.81071700	3.41141200	0.03615800
H	1.98055300	4.47766600	0.15116800
C	4.27604500	-0.58141500	1.18549400
H	5.22551500	-0.78314700	1.67109800
C	-2.14292600	-1.75272100	-2.14172600
H	-3.11895000	-1.66162400	-2.59898400
C	-1.34678700	-0.63217000	-1.70343600
N	-5.33348200	-0.27719200	1.03505400
C	-3.92528800	-0.51591400	1.37529400
C	-3.17386800	0.76526900	1.74972600
H	-3.46494700	-0.98427300	0.50304200
H	-3.91433600	-1.23328300	2.20281100
H	-2.12085400	0.53529600	1.94308300
H	-3.21627700	1.48337600	0.92635600
H	-3.59953800	1.23310300	2.64498600
C	-6.35730700	-0.34758900	2.07997900
C	-7.76582000	-0.00889900	1.60151900
H	-6.06021700	0.33676200	2.88621100
H	-6.33605100	-1.36118200	2.50446800
H	-8.44994600	-0.08583900	2.45353500
H	-7.82036200	1.00662000	1.20086400
H	-8.10168600	-0.69541500	0.82057200
N	-5.71951000	0.02596100	-0.19768700
O	-4.81192500	0.09687000	-1.03539000
O	1.89414800	-0.70460200	3.59328200
H	1.80897000	-1.64910500	3.39719900
H	1.37055500	-0.29242600	2.87844400
²TS-H_β			
Fe	-1.02484400	0.11192900	-0.31790900
O	-0.05770300	-0.11818800	1.14986000
S	-2.45302200	0.82228400	-2.15314100
H	-3.64741900	0.69913600	-1.53136600
N	0.31608800	1.34581200	-1.17086500
C	1.56415300	3.22412900	-1.67732000
C	2.08346500	2.19468400	-2.40000900
H	1.88452600	4.25782300	-1.65123900

H	2.92696600	2.19997500	-3.07728300
N	-0.23354800	-1.41800600	-1.34929500
C	0.80683700	-1.38513700	-2.24034100
C	1.06542400	-2.70343200	-2.76604400
C	0.16002600	-3.53779100	-2.18523300
H	1.83968700	-2.94027900	-3.48425200
H	0.03296900	-4.60283400	-2.33156000
N	-2.47077900	-1.09248800	0.42346100
C	-2.57300700	-2.44464600	0.23179100
C	-3.48610900	-0.75738900	1.27807900
C	-3.68937700	-2.97695300	0.97681200
C	-4.25850000	-1.92580100	1.62730000
H	-3.98225600	-4.01888500	0.99214800
H	-5.11543300	-1.92496800	2.28853100
N	-1.91092300	1.68385100	0.61504300
C	-3.25939200	2.98158700	1.97466100
H	-4.06981500	3.23076000	2.64761700
C	-3.00499300	1.66171500	1.44556900
C	0.45886500	2.68749500	-0.91840800
C	1.30014200	1.02756000	-2.07664000
C	-0.65177300	-2.72383900	-1.31212600
C	-3.74334400	0.52753100	1.75083200
H	-4.58446500	0.64764200	2.42714500
C	-0.34681600	3.43952100	-0.07037700
H	-0.10182100	4.49247100	0.03377400
C	1.52402400	-0.24316000	-2.58744600
H	2.34215900	-0.35987200	-3.29069500
C	-1.72881000	-3.20376400	-0.57280800
H	-1.93965900	-4.26703400	-0.64369100
C	-2.29472300	3.79688900	1.47089800
H	-2.14991100	4.85591500	1.64215900
C	-1.45462600	2.97760100	0.62728600
N	4.65450400	0.14747900	1.20764600
C	3.20845400	0.44401100	1.23364000
C	2.36091200	-0.78068600	0.98033700
H	3.03587300	1.19558300	0.45836600
H	1.06399000	-0.35923800	0.96637900
H	2.49219300	-1.22345000	-0.00548500
H	2.30029000	-1.51117000	1.78758700
C	5.44477600	-0.02591100	2.42351700
C	5.11007700	-1.30144800	3.20123800
H	5.30056300	0.85737000	3.05961000
H	6.48747100	-0.03647200	2.09443100
H	5.75964100	-1.37778700	4.08047900
H	4.07248800	-1.30535600	3.55013400
H	5.26664600	-2.18762400	2.57788800
N	5.31940000	0.05910000	0.05501600
O	4.63406500	0.19525900	-0.95970700
H	2.99025300	0.88229300	2.21165800
O	0.01132300	-2.49750200	2.65726800
H	-0.15379600	-3.09046100	1.90974400
H	-0.15563200	-1.61360200	2.26615400

⁴TS-H_β

Fe	1.03917700	-0.12327600	-0.28366600
O	0.05645300	0.19715000	1.15767300
S	2.42405600	-0.76893400	-2.19455500
H	3.61377600	-0.85239900	-1.55718500
N	-0.31829900	-1.35768200	-1.12549900
C	-1.57394300	-3.23419600	-1.62495200
C	-2.10164700	-2.20231400	-2.33724500
H	-1.89255800	-4.26843600	-1.59967700
H	-2.95292000	-2.20452300	-3.00469900
N	0.23931100	1.41241700	-1.33145100
C	-0.81852800	1.37928800	-2.19638100
C	-1.09332700	2.69766600	-2.71282700
C	-0.17793000	3.53320600	-2.14679800
H	-1.88379000	2.93514200	-3.41289900
H	-0.05821600	4.59950000	-2.29016400
N	2.48915000	1.08977700	0.43563600
C	2.58645600	2.44243800	0.23869000
C	3.52180500	0.75770500	1.26442400
C	3.71531200	2.97707300	0.96417400
C	4.29912600	1.92694000	1.60260900
H	4.00673200	4.01944300	0.97370200
H	5.16964100	1.92661900	2.24581800
N	1.93776600	-1.68563700	0.60637100
C	3.33777000	-2.99149300	1.90781300
H	4.16985100	-3.24345800	2.55268200
C	3.05906700	-1.66714600	1.40588300
C	-0.45892900	-2.69851700	-0.87869700
C	-1.31341100	-1.03591000	-2.01923000
C	0.65169900	2.71706800	-1.29300500
C	3.79523800	-0.53366700	1.71449400
H	4.65164000	-0.66020900	2.37018800
C	0.36780500	-3.45076200	-0.05092300
H	0.13259100	-4.50581800	0.05414800
C	-1.54457300	0.23443400	-2.52560600
H	-2.37770400	0.35127200	-3.21096600
C	1.73658000	3.19777900	-0.56120600
H	1.94553000	4.26134800	-0.63414600
C	2.36380100	-3.80740100	1.42318300
H	2.23181600	-4.86953900	1.58513700
C	1.49246600	-2.98550000	0.61646200
N	-4.68068300	-0.17408700	1.16689900
C	-3.22996400	-0.45061200	1.20306600
C	-2.39303200	0.78962900	0.99646100
H	-3.03918400	-1.17860700	0.40967700
H	-1.07612200	0.39211700	0.97880000
H	-2.53255300	1.26967900	0.02941600
H	-2.34260700	1.49168800	1.82949500
C	-5.48645100	-0.03982100	2.37746200
C	-5.17824800	1.22271700	3.18686600
H	-5.33582200	-0.93507300	2.99500200

H	-6.52576000	-0.03675100	2.03769100
H	-5.83753400	1.27070100	4.06090000
H	-4.14419600	1.23363000	3.54589300
H	-5.34085700	2.12008600	2.58133400
N	-5.33290100	-0.06089900	0.01049700
O	-4.63482900	-0.15930900	-1.00073200
H	-3.01968000	-0.91516800	2.17081200
O	-0.06543700	2.60856200	2.60119500
H	-0.01986500	3.17638100	1.81814500
H	0.12155000	1.72042700	2.22852400
²INT_β			
Fe	1.07942300	0.02722400	-0.37624000
O	0.00863900	-0.12272200	1.10596900
S	2.66708600	0.22120400	-2.17264700
H	2.91782100	-1.09419400	-2.36058400
N	-0.20221200	1.31103000	-1.25112000
C	-2.01300300	2.14933000	-2.41688800
C	-1.31592000	3.21702300	-1.93739300
H	-2.92548200	2.14042500	-2.99788400
H	-1.53217500	4.27149300	-2.05205200
N	2.07367900	1.60802000	0.39856400
C	1.81235100	2.94338200	0.21748800
C	2.75305000	3.74650700	0.96090400
C	3.57850400	2.87958500	1.60758300
H	2.76135500	4.82871300	0.98064500
H	4.40731300	3.10234000	2.26707600
N	2.42185700	-1.24810200	0.44401200
C	3.44337600	-0.91261100	1.29159500
C	2.45956900	-2.61784500	0.33258300
C	4.15273700	-2.09636500	1.71887200
C	3.54563800	-3.15576900	1.11810700
H	5.00161500	-2.09729600	2.39037500
H	3.79318200	-4.20699900	1.19269200
N	0.15833000	-1.54569600	-1.23245100
C	-0.47978700	-3.68104800	-1.84154100
H	-0.44520100	-4.76062600	-1.91317200
C	0.47723600	-2.87012300	-1.12696600
C	-1.29965500	0.96871300	-1.99309400
C	-0.19086600	2.68007800	-1.21032100
C	3.15115700	1.54856600	1.24608400
C	1.56046900	-3.37373300	-0.40659600
H	1.69830600	-4.45117800	-0.40696300
C	-1.67113100	-0.33217400	-2.32542600
H	-2.58458600	-0.44769800	-2.89908000
C	0.76249600	3.44569200	-0.54274900
H	0.66126900	4.52556900	-0.59918600
C	3.76833400	0.38218400	1.68084300
H	4.59988800	0.49381500	2.36989500
C	-1.39577100	-2.82328400	-2.36990800
H	-2.27018900	-3.05052300	-2.96589000
C	-0.98674000	-1.49390200	-1.98235300

N	-4.67545900	-0.20308200	1.25984400
C	-3.21479900	0.00565300	1.43532400
C	-2.86244700	1.44709100	1.59590800
H	-2.73612500	-0.41445700	0.54829700
H	-2.91281600	-0.58146600	2.30634000
H	-0.40126200	0.74766100	1.25631900
H	-2.91723500	2.10663800	0.73671900
H	-2.73040200	1.88513600	2.58017800
C	-5.52363700	-0.44475600	2.42944800
C	-7.00531800	-0.60690800	2.10387500
H	-5.38066500	0.39280500	3.12559200
H	-5.14662200	-1.34400500	2.93559500
H	-7.54905900	-0.78404500	3.03815700
H	-7.41233700	0.28849500	1.62725400
H	-7.17928100	-1.45207900	1.43316100
N	-5.24862600	-0.12501200	0.06844600
O	-4.49155500	0.14331000	-0.87056800
O	1.08427200	-0.84661400	3.57566700
H	1.31142000	-1.77564300	3.42533900
H	0.69400300	-0.57357300	2.71387200
⁴INT_β			
Fe	1.13058700	-0.01776400	-0.33730500
O	0.14299100	-0.16019100	1.18333500
S	2.45226600	0.29870500	-2.31685500
H	1.45012100	0.57008100	-3.18273700
N	0.30982800	1.79207400	-0.78354300
C	-1.08233100	3.46754700	-1.56722300
C	-0.08014200	4.06951800	-0.86909800
H	-1.91716900	3.92585800	-2.08169300
H	0.07903200	5.12590600	-0.69414600
N	2.65938400	0.88241300	0.59377300
C	2.81007500	2.23437300	0.80266800
C	4.01477700	2.49094300	1.55503100
C	4.58976200	1.28226300	1.80184500
H	4.36150100	3.47434200	1.84587200
H	5.50388600	1.06733400	2.34013300
N	1.96581600	-1.80420400	0.04890700
C	3.11022400	-2.06044700	0.74491000
C	1.47679600	-3.02569900	-0.32969100
C	3.35195000	-3.48341300	0.82548100
C	2.33386300	-4.08525400	0.15540700
H	4.19308000	-3.93996300	1.33080500
H	2.16327700	-5.14162900	-0.00795800
N	-0.34156500	-0.89558200	-1.41950700
C	-1.71566600	-2.50414200	-2.34361300
H	-2.07418400	-3.48999000	-2.61098900
C	-0.51354600	-2.24098500	-1.58962400
C	-0.83315500	2.04738500	-1.50711500
C	0.78098300	3.01620400	-0.38640400
C	3.73257000	0.28557100	1.20773400
C	0.33403300	-3.23010000	-1.09200400

H	0.07120000	-4.25947700	-1.31850300
C	-1.64024300	1.07461100	-2.08351700
H	-2.53837200	1.40676900	-2.59358700
C	1.93434800	3.21924800	0.36683700
H	2.18544900	4.24610800	0.61636600
C	3.94478300	-1.08463400	1.28242500
H	4.82738900	-1.42255900	1.81653800
C	-2.27742100	-1.29329400	-2.61826900
H	-3.19904600	-1.07440500	-3.14063500
C	-1.40904600	-0.29938300	-2.03643300
N	-4.83406900	-0.22336700	1.19989200
C	-3.35200300	-0.21496300	1.30164000
C	-2.81152200	1.13463400	1.63912500
H	-2.98708600	-0.55091200	0.32740800
H	-3.08224100	-0.95632000	2.05822200
H	-0.62659400	0.43648200	1.12895800
H	-2.83590500	1.91909200	0.89091500
H	-2.59039200	1.40473000	2.66673800
C	-5.64860100	-0.57249000	2.36684400
C	-7.15214700	-0.53268700	2.11132000
H	-5.38584300	0.11847900	3.17927500
H	-5.34687800	-1.57633800	2.69521200
H	-7.66843400	-0.81537900	3.03503900
H	-7.48437400	0.46611000	1.81739000
H	-7.44361700	-1.22957700	1.32141200
N	-5.44566200	0.13442200	0.08063600
O	-4.70195600	0.48238700	-0.84240300
O	1.47059800	-0.48737700	3.60114600
H	1.89145000	0.38410000	3.62063100
H	0.94299600	-0.45395200	2.77153800
²TS-reb_p			
Fe	-1.19638900	0.09773300	0.30478000
S	-3.00110300	0.45205300	1.75347500
H	-3.18361700	-0.83260000	2.13212700
N	-1.27600800	2.10098100	0.03180400
C	-0.86716700	4.35964000	0.21513000
C	-1.75842000	4.19274200	-0.80225900
H	-0.44064300	5.27981900	0.59383400
H	-2.21284900	4.94722100	-1.43170100
N	-2.43130400	-0.15633500	-1.27958200
C	-3.01086000	0.83367100	-2.04105400
C	-3.88734600	0.24535900	-3.02154400
C	-3.85126100	-1.10269200	-2.82922100
H	-4.45786300	0.80760100	-3.74977900
H	-4.38636900	-1.87540100	-3.36620300
N	-1.23317700	-1.86869800	0.65732500
C	-1.90565200	-2.82545600	-0.06775700
C	-0.52552200	-2.54640400	1.62327400
C	-1.64561400	-4.13056600	0.48220100
C	-0.79376600	-3.95735900	1.52866800
H	-2.05411600	-5.05277600	0.08972300

H	-0.35400200	-4.70804500	2.17217000
N	0.13524500	0.34615300	1.79773000
C	1.55741200	-0.04499700	3.56789800
H	2.10189400	-0.60412200	4.31808000
C	0.65671800	-0.63026100	2.60511600
C	-0.56411900	3.04704400	0.72568400
C	-1.99991800	2.77717900	-0.91805500
C	-2.95507700	-1.34509700	-1.72762400
C	0.34831300	-1.98088900	2.53723500
H	0.84015500	-2.64670800	3.23841800
C	0.33888600	2.79392400	1.74946000
H	0.82541000	3.64831700	2.20930200
C	-2.81357900	2.19659600	-1.88253300
H	-3.33431800	2.86093800	-2.56461400
C	-2.70631400	-2.59322000	-1.17551400
H	-3.18014200	-3.45179900	-1.63989200
C	1.55771700	1.29752700	3.34115200
H	2.09929200	2.07149500	3.87026100
C	0.65429000	1.53637800	2.24123400
C	2.45491500	0.62175500	-1.80003700
C	3.27617400	0.15747300	-0.64454100
H	2.15202500	1.65775700	-1.88819300
H	2.35662600	-0.02164200	-2.66604800
H	2.92304300	-0.81240400	-0.28224000
H	3.24234800	0.87015000	0.18262400
O	0.26588400	-0.02128600	-0.86761700
H	-0.13302900	-0.02891900	-1.75713500
N	4.70550300	-0.01126100	-1.01242900
C	5.67550300	1.03767000	-0.68530200
C	7.09401500	0.74879500	-1.16598900
H	5.66545800	1.17290400	0.40484600
H	5.31171700	1.97664500	-1.12448300
H	7.73763500	1.58507800	-0.87204600
H	7.48922700	-0.16868600	-0.72283900
H	7.13554200	0.64077200	-2.25272700
N	5.12295600	-1.06299900	-1.69414400
O	4.24950800	-1.88480300	-2.00155100
O	1.53843300	-2.63901200	-0.79737100
H	1.06693300	-1.78451300	-0.85358600
H	2.34433400	-2.51192700	-1.32613100
⁴TS-reb_β			
Fe	-1.19638900	0.09773300	0.30478000
S	-3.00110300	0.45205300	1.75347500
H	-3.18361700	-0.83260000	2.13212700
N	-1.27600800	2.10098100	0.03180400
C	-0.86716700	4.35964000	0.21513000
C	-1.75842000	4.19274200	-0.80225900
H	-0.44064300	5.27981900	0.59383400
H	-2.21284900	4.94722100	-1.43170100
N	-2.43130400	-0.15633500	-1.27958200
C	-3.01086000	0.83367100	-2.04105400

C	-3.88734600	0.24535900	-3.02154400
C	-3.85126100	-1.10269200	-2.82922100
H	-4.45786300	0.80760100	-3.74977900
H	-4.38636900	-1.87540100	-3.36620300
N	-1.23317700	-1.86869800	0.65732500
C	-1.90565200	-2.82545600	-0.06775700
C	-0.52552200	-2.54640400	1.62327400
C	-1.64561400	-4.13056600	0.48220100
C	-0.79376600	-3.95735900	1.52866800
H	-2.05411600	-5.05277600	0.08972300
H	-0.35400200	-4.70804500	2.17217000
N	0.13524500	0.34615300	1.79773000
C	1.55741200	-0.04499700	3.56789800
H	2.10189400	-0.60412200	4.31808000
C	0.65671800	-0.63026100	2.60511600
C	-0.56411900	3.04704400	0.72568400
C	-1.99991800	2.77717900	-0.91805500
C	-2.95507700	-1.34509700	-1.72762400
C	0.34831300	-1.98088900	2.53723500
H	0.84015500	-2.64670800	3.23841800
C	0.33888600	2.79392400	1.74946000
H	0.82541000	3.64831700	2.20930200
C	-2.81357900	2.19659600	-1.88253300
H	-3.33431800	2.86093800	-2.56461400
C	-2.70631400	-2.59322000	-1.17551400
H	-3.18014200	-3.45179900	-1.63989200
C	1.55771700	1.29752700	3.34115200
H	2.09929200	2.07149500	3.87026100
C	0.65429000	1.53637800	2.24123400
C	2.45491500	0.62175500	-1.80003700
C	3.27617400	0.15747300	-0.64454100
H	2.15202500	1.65775700	-1.88819300
H	2.35662600	-0.02164200	-2.66604800
H	2.92304300	-0.81240400	-0.28224000
H	3.24234800	0.87015000	0.18262400
O	0.26588400	-0.02128600	-0.86761700
H	-0.13302900	-0.02891900	-1.75713500
N	4.70550300	-0.01126100	-1.01242900
C	5.67550300	1.03767000	-0.68530200
C	7.09401500	0.74879500	-1.16598900
H	5.66545800	1.17290400	0.40484600
H	5.31171700	1.97664500	-1.12448300
H	7.73763500	1.58507800	-0.87204600
H	7.48922700	-0.16868600	-0.72283900
H	7.13554200	0.64077200	-2.25272700
N	5.12295600	-1.06299900	-1.69414400
O	4.24950800	-1.88480300	-2.00155100
O	1.53843300	-2.63901200	-0.79737100
H	1.06693300	-1.78451300	-0.85358600
H	2.34433400	-2.51192700	-1.32613100

²P-OH_β

Fe	-1.15602400	0.31452900	0.21389700
S	-3.18055500	1.04002100	0.84453100
H	-2.94749300	2.36776700	0.73343800
N	-1.97366300	-1.13905700	-0.92386600
C	-3.01228100	-2.22186900	-2.68001900
C	-2.97422800	-3.09618900	-1.63658100
H	-3.42340400	-2.37164100	-3.67057200
H	-3.34923800	-4.11104600	-1.59214700
N	-1.06913800	-0.99371200	1.74786000
C	-1.53690800	-2.28410300	1.78337600
C	-1.35844800	-2.84523200	3.10155000
C	-0.78902500	-1.87463900	3.86595800
H	-1.64130100	-3.85067000	3.38652400
H	-0.50608800	-1.91697800	4.91027700
N	-0.18593100	1.70388100	1.30545300
C	0.13578500	1.60272800	2.63771700
C	0.18658500	2.97079100	0.91989500
C	0.73803200	2.83087300	3.09846000
C	0.77258200	3.67815700	2.03235100
H	1.08188700	3.00629500	4.11021000
H	1.14809500	4.69295700	1.98909600
N	-1.10408400	1.56923900	-1.36101800
C	-0.80454500	3.41353100	-2.72112800
H	-0.49660000	4.40872400	-3.01667000
C	-0.59821300	2.84344100	-1.41037200
C	-2.39016900	-1.00080700	-2.22458500
C	-2.33219200	-2.40859700	-0.54204000
C	-0.61578600	-0.72073500	3.01390800
C	0.01102300	3.50421500	-0.35072700
H	0.35462000	4.52008300	-0.52171200
C	-2.22939400	0.13450700	-3.00862700
H	-2.60376300	0.09110800	-4.02710300
C	-2.12131200	-2.95435400	0.71766700
H	-2.45223600	-3.97445000	0.88614000
C	-0.05876100	0.48047900	3.43340000
H	0.25182300	0.54822200	4.47175400
C	-1.44583200	2.46832400	-3.46110800
H	-1.77218200	2.52520900	-4.49204000
C	-1.62718500	1.31923400	-2.60410800
N	4.39194200	-0.57088400	-0.86852000
C	3.01567100	-0.25314000	-1.24338100
C	2.04138600	-0.29064600	-0.04650300
H	2.70163300	-0.99784100	-1.97753800
H	3.00932100	0.73047400	-1.72099200
H	2.32102700	-1.09936400	0.63867500
H	2.04964900	0.64997400	0.50580000
C	5.33067100	0.50629700	-0.52884000
C	6.72754300	0.02329000	-0.15400400
H	4.89267000	1.07941800	0.29860300
H	5.37975300	1.18278700	-1.39234200
H	7.34292700	0.89832300	0.07992000
H	6.70649300	-0.63187000	0.72053000

H	7.19772200	-0.52474400	-0.97423400
N	4.83689100	-1.80729700	-0.82928800
O	4.02380400	-2.67953000	-1.10839900
O	0.72343100	-0.48445000	-0.53539000
H	0.62946100	-1.45761200	-0.70263200
O	1.17967700	-3.11829800	-0.91022300
H	2.15402700	-3.07430600	-1.01705700
H	0.83928700	-3.53922100	-1.71556000
⁴P-OH_β			
Fe	-1.50407600	-0.19713500	-0.35403400
S	-3.50364200	-0.56908600	-1.63972500
H	-4.34413200	-0.50521500	-0.58221800
N	-0.95043900	1.58625700	-1.16027000
C	-1.02419000	3.82324500	-1.75413500
C	-0.32178700	3.17383700	-2.72448900
H	-1.25704500	4.87772700	-1.68260700
H	0.13735300	3.58627300	-3.61367300
N	-0.27564900	-1.11089500	-1.66422300
C	0.31185700	-0.55886500	-2.78325100
C	0.95230300	-1.58001400	-3.56761100
C	0.74884900	-2.76151600	-2.91973800
H	1.48634400	-1.40076200	-4.49194600
H	1.08109000	-3.75194200	-3.20341000
N	-1.54411400	-1.88387600	0.74667800
C	-1.10958200	-3.13113100	0.35571500
C	-2.19158300	-2.07660800	1.94605800
C	-1.48204900	-4.12119600	1.33275500
C	-2.15150500	-3.46647900	2.32089000
H	-1.25206400	-5.17627500	1.25748000
H	-2.58587800	-3.87189500	3.22574200
N	-2.31306900	0.79646800	1.19317100
C	-3.47145100	1.27977500	3.13628200
H	-3.96234200	1.10849300	4.08566800
C	-2.85475000	0.25364300	2.33819800
C	-1.42335600	2.83298800	-0.79249500
C	-0.29065900	1.78406700	-2.35981300
C	-0.01441400	-2.46324300	-1.73820000
C	-2.80845200	-1.08548400	2.69288500
H	-3.28190600	-1.37659800	3.62494600
C	-2.17385200	3.09995200	0.34022100
H	-2.46126900	4.13030000	0.52198200
C	0.30619900	0.78810000	-3.11542400
H	0.80058200	1.08198500	-4.03561700
C	-0.40533000	-3.40998000	-0.80430200
H	-0.13084000	-4.44332900	-0.99067700
C	-3.29673000	2.45522300	2.47111100
H	-3.61255900	3.44884200	2.76162600
C	-2.57096900	2.14881100	1.26738100
N	4.72688400	-0.17556100	1.09257800
C	3.42256400	0.30769200	1.54391400
C	2.46040100	0.53586000	0.37265100

H	3.56336100	1.25430300	2.07238900
H	3.01009800	-0.42620700	2.24163200
H	2.96335300	1.13995900	-0.39260900
H	2.16528500	-0.42207300	-0.07603900
C	5.06796400	-1.59714300	1.20573000
C	6.45676500	-1.94915100	0.68240100
H	4.30407600	-2.16968300	0.66197600
H	4.97999200	-1.87914500	2.26385300
H	6.61149100	-3.02625900	0.80780300
H	6.56222400	-1.70216500	-0.37709100
H	7.23908300	-1.41789300	1.22987200
N	5.63432500	0.64952200	0.58315600
O	5.28764100	1.83303800	0.49759400
O	1.32926500	1.21923600	0.90686600
H	0.68811300	1.37949100	0.18977100
O	2.97100400	3.55891000	1.72339000
H	3.73709100	3.23177500	1.22302000
H	2.25643400	2.94400000	1.47777100
Two-water system			
²RC_α			
Fe	1.12943100	0.07865200	-0.26596700
O	0.32240100	-0.04271600	1.16201300
S	2.64284000	0.27049300	-2.28265800
H	2.66643500	-1.04002500	-2.61497500
N	0.32633600	-1.60092700	-1.03476700
C	-0.14766300	-3.82180400	-1.45972400
C	-1.17282800	-3.08875100	-1.97365700
H	-0.01784500	-4.89617800	-1.46006200
H	-2.06314100	-3.43118100	-2.48420500
N	-0.29919800	1.17048900	-1.16260700
C	-1.41049700	0.69616900	-1.80771100
C	-2.26642800	1.78420800	-2.21086900
C	-1.64937900	2.92947200	-1.80999500
H	-3.21689100	1.65810500	-2.71174300
H	-1.98038500	3.95304100	-1.92816800
N	2.09187100	1.77510600	0.25209600
C	1.65281800	3.06250500	0.06417300
C	3.25737000	1.87683300	0.96944600
C	2.56969100	3.99713600	0.66628600
C	3.56350100	3.26036700	1.23368300
H	2.45076700	5.07275500	0.64998800
H	4.43362400	3.60498000	1.77740100
N	2.71552600	-0.99797900	0.38136900
C	4.65039900	-1.61930800	1.48428700
H	5.57216300	-1.50911000	2.04090300
C	3.79979400	-0.52587600	1.08639600
C	0.77631900	-2.88544900	-0.87145700
C	-0.86892600	-1.70679200	-1.70127600
C	-0.42721100	2.53380700	-1.15507700
C	4.04503000	0.80721600	1.37510700
H	4.93980500	1.03657200	1.94566100

C	1.95613100	-3.24625500	-0.23026700
H	2.18395100	-4.30573600	-0.16919700
C	-1.68349900	-0.64220500	-2.06244900
H	-2.61564200	-0.87054800	-2.56683300
C	0.48530000	3.41984100	-0.59525000
H	0.25635700	4.47861600	-0.66381800
C	4.06825800	-2.75988000	1.02451500
H	4.41061300	-3.78150200	1.12756900
C	2.85666200	-2.36730700	0.34974800
N	-4.15554700	-0.30599500	0.66585500
C	-4.57327600	1.05950100	1.00617900
C	-6.01306600	1.13654600	1.52481000
H	-4.48186300	1.64811200	0.08849000
H	-3.84776700	1.43950100	1.73008100
H	-6.27307100	2.17893800	1.74277500
H	-6.70910000	0.75877300	0.77091600
H	-6.14201600	0.55409200	2.44289000
C	-3.26358000	-1.08264000	1.53052600
C	-3.92065800	-1.59299000	2.81302700
H	-2.40420600	-0.45237700	1.77505600
H	-2.90911200	-1.92148600	0.92867000
H	-3.17988400	-2.18235500	3.36300600
H	-4.25430900	-0.77123100	3.45689600
H	-4.78351300	-2.23043700	2.59095000
N	-4.42731200	-0.83774200	-0.51839700
O	-5.11037200	-0.13588900	-1.27770700
O	-1.41173200	1.90691900	2.22991900
H	-0.82359900	1.29000600	1.74563400
H	-1.15735400	1.77494400	3.15564000
O	-0.42557900	-2.49656700	2.38739900
H	-0.21419700	-1.68670400	1.87972100
H	0.04448700	-2.36309300	3.22390800
⁴RC_α			
Fe	1.14477800	0.07589700	-0.26173000
O	0.30554000	-0.03423900	1.14929300
S	2.62797200	0.26897700	-2.27762500
H	2.64445300	-1.03935100	-2.61874000
N	0.33062600	-1.60212100	-1.02768300
C	-0.15374400	-3.82117800	-1.45002600
C	-1.17472600	-3.08390600	-1.96620100
H	-0.02913400	-4.89616500	-1.44848300
H	-2.06633100	-3.42285100	-2.47682900
N	-0.28944500	1.17445100	-1.15666500
C	-1.40123600	0.70242000	-1.80088100
C	-2.25837000	1.79209000	-2.19854900
C	-1.64042000	2.93580300	-1.79455200
H	-3.21017400	1.66773500	-2.69733600
H	-1.97179400	3.95983500	-1.90756900
N	2.10611600	1.76995900	0.25891400
C	1.66946000	3.05862900	0.06949500
C	3.27502900	1.87043300	0.96994800

C	2.59136700	3.99162700	0.66638300
C	3.58587900	3.25339000	1.23080700
H	2.47524200	5.06753600	0.64863300
H	4.45928800	3.59677600	1.76999400
N	2.71943300	-1.00286100	0.38716800
C	4.66505900	-1.62856100	1.46922300
H	5.59221700	-1.52047900	2.01720800
C	3.81213800	-0.53335100	1.08210200
C	0.77438200	-2.88790100	-0.86316100
C	-0.86455200	-1.70270700	-1.69568700
C	-0.41639000	2.53684400	-1.14429900
C	4.06188300	0.79842600	1.37189700
H	4.96086500	1.02498400	1.93690100
C	1.95545200	-3.25083800	-0.22490200
H	2.18247400	-4.31054700	-0.16479000
C	-1.67496100	-0.63562200	-2.05875200
H	-2.60687200	-0.86176800	-2.56461400
C	0.50076400	3.41955300	-0.58577600
H	0.27505600	4.47915200	-0.65265300
C	4.07765100	-2.76743700	1.01213300
H	4.42033700	-3.78953400	1.10921300
C	2.86030500	-2.37288600	0.34932500
N	-4.17212800	-0.30251900	0.65769600
C	-4.59690200	1.06138200	0.99568000
C	-6.04215100	1.13391600	1.49947900
H	-4.49735900	1.65175300	0.07996900
H	-3.87992700	1.44212000	1.72761000
H	-6.30712500	2.17527800	1.71635500
H	-6.72932400	0.75552200	0.73781100
H	-6.17909800	0.54966700	2.41526100
C	-3.28564500	-1.07748300	1.52957900
C	-3.95329300	-1.59255500	2.80470800
H	-2.43120300	-0.44419800	1.78333700
H	-2.92234800	-1.91391000	0.92963500
H	-3.21599800	-2.18035700	3.36103000
H	-4.29614300	-0.77320400	3.44680800
H	-4.81165200	-2.23265200	2.57305800
N	-4.43046900	-0.83328900	-0.52989000
O	-5.10807500	-0.13237500	-1.29500600
O	-1.43664500	1.90691000	2.23011000
H	-0.84993400	1.29599300	1.73709600
H	-1.17682500	1.76671900	3.15309900
O	-0.44642400	-2.48163700	2.39071900
H	-0.23743700	-1.67526600	1.87690900
H	0.03098800	-2.34488500	3.22252500
²TS-H_a			
Fe	0.80321	0.18893	-0.52138
O	-0.00122	-0.28789	0.93352
S	2.13131	0.66048	-2.43993
H	1.62521	-0.30351	-3.24058
N	2.2822	1.11101	0.49468

C	3.5191	2.68997	1.63221
C	4.20747	1.51746	1.69733
H	3.78497	3.65323	2.04819
H	5.15459	1.31685	2.18142
N	1.81813	-1.56514	-0.3916
C	3.0205	-1.77647	0.2345
C	3.38704	-3.16997	0.14237
C	2.39203	-3.79431	-0.54335
H	4.29247	-3.59579	0.55555
H	2.30803	-4.8399	-0.80976
N	-0.55908	-0.69825	-1.70515
C	-0.63598	-2.03534	-2.01298
C	-1.65711	-0.1082	-2.28009
C	-1.80861	-2.28987	-2.8114
C	-2.43982	-1.09483	-2.98016
H	-2.09721	-3.26442	-3.18367
H	-3.35652	-0.88362	-3.51508
N	-0.14895	1.93858	-0.72405
C	-1.65913	3.5675	-1.35081
H	-2.52648	4.00639	-1.82623
C	-1.28811	2.17865	-1.45336
C	2.31898	2.42729	0.87837
C	3.42624	0.53397	0.98987
C	1.41899	-2.78332	-0.88031
C	-1.99744	1.23294	-2.17722
H	-2.90143	1.56046	-2.67924
C	1.35496	3.37929	0.57781
H	1.51683	4.38906	0.94113
C	3.77888	-0.80344	0.87018
H	4.72034	-1.11258	1.31359
C	0.27314	-3.01133	-1.62704
H	0.07703	-4.03005	-1.94506
C	-0.72708	4.16693	-0.56126
H	-0.66368	5.20461	-0.25978
C	0.22002	3.14703	-0.18404
N	-3.31751	0.11591	1.30598
C	-2.17699	0.65183	1.95694
C	-1.96752	0.25019	3.40934
H	-2.16589	1.73008	1.78221
H	-1.1633	0.24879	1.36678
H	-1.05512	0.72146	3.78547
H	-2.81162	0.58229	4.02776
H	-1.84558	-0.83066	3.51466
C	-3.70969	-1.30061	1.37859
C	-4.91513	-1.53227	2.29663
H	-2.83796	-1.86704	1.71618
H	-3.95576	-1.60083	0.35586
H	-5.17387	-2.59657	2.28757
H	-4.68982	-1.24831	3.32949
H	-5.78316	-0.96284	1.95427
N	-3.97069	0.97685	0.47935
O	-4.90803	0.4803	-0.1342

O	-0.8038	-2.80901	2.09092
H	-0.60006	-2.17524	1.379
H	-0.16252	-2.52045	2.77253
O	1.17421	-1.16818	3.32635
H	0.85822	-0.68857	2.5288
H	2.04149	-1.5056	3.05397
⁴TS-H_a			
Fe	0.82224700	0.14041000	-0.49706300
O	-0.02606700	-0.27779700	0.99561600
S	2.05944700	0.84859500	-2.47542500
H	3.22666300	0.21499800	-2.22011900
N	2.42710200	0.86669500	0.46363400
C	3.85328600	2.27800500	1.61500500
C	4.44486900	1.05331200	1.58275400
H	4.22123400	3.19150400	2.06413400
H	5.39653000	0.75335400	2.00235400
N	1.68102600	-1.68627900	-0.50967000
C	2.87806600	-2.05471300	0.03917900
C	3.10637800	-3.46930100	-0.14193600
C	2.02351600	-3.95332400	-0.80839300
H	3.98245100	-4.00397100	0.20202400
H	1.82393700	-4.96892800	-1.12453700
N	-0.69505600	-0.53885200	-1.64420400
C	-0.91112600	-1.83977600	-2.00785100
C	-1.74891800	0.17171600	-2.14558400
C	-2.14086600	-1.95546900	-2.75448600
C	-2.66181500	-0.69970900	-2.84359200
H	-2.53866100	-2.88085600	-3.15063700
H	-3.58150800	-0.37947000	-3.31472400
N	0.02769800	2.00099900	-0.59942200
C	-1.35708700	3.79836600	-1.05240300
H	-2.19612900	4.34457100	-1.46312400
C	-1.11444300	2.39024300	-1.25637500
C	2.59593300	2.15640200	0.91928200
C	3.54598700	0.17412700	0.87731200
C	1.14305600	-2.83182400	-1.03707300
C	-1.93879000	1.54350800	-1.98368100
H	-2.82732400	1.97621500	-2.43152400
C	1.69605800	3.19574200	0.73621600
H	1.95992300	4.15820900	1.16426800
C	3.75734100	-1.18340700	0.68114300
H	4.68192700	-1.60320800	1.06684700
C	-0.06252100	-2.90691200	-1.72378900
H	-0.36594400	-3.88608600	-2.08169800
C	-0.35006600	4.25623600	-0.26020400
H	-0.18444500	5.26073000	0.10753700
C	0.51300200	3.12879400	0.00607800
N	-3.35230000	0.15019900	1.22207900
C	-2.21314800	0.70856500	1.86106900
C	-2.01728000	0.36561600	3.32765300
H	-2.18864400	1.77664300	1.63644500

H	-1.13426100	0.25504400	1.29546700
H	-1.11354700	0.85907900	3.69681500
H	-2.86965300	0.71087900	3.92814200
H	-1.88759900	-0.70976500	3.47649200
C	-3.74202700	-1.26473700	1.34402000
C	-4.95774600	-1.46296100	2.25523400
H	-2.87410000	-1.81716300	1.71244400
H	-3.97609000	-1.60440500	0.33101100
H	-5.21674100	-2.52699000	2.28581200
H	-4.74593600	-1.13755300	3.27884200
H	-5.82128400	-0.90794100	1.87939200
N	-3.99235400	0.97098900	0.36025700
O	-4.92125400	0.45157700	-0.25660700
O	-0.82280200	-2.76169100	2.13158100
H	-0.62042100	-2.08563700	1.45635900
H	-0.20754200	-2.48507000	2.84007700
O	1.16938500	-1.10417700	3.36170300
H	0.81459800	-0.63887400	2.56921300
H	1.99613500	-1.49403400	3.03859300
²INT_a			
Fe	1.04213200	0.18899300	-0.41968900
S	2.34596400	0.72909900	-2.26924100
H	2.09913700	-0.36913700	-3.01886700
N	0.45542000	2.12549500	-0.28249000
C	-0.68916700	4.09946600	-0.63133600
C	0.34689600	4.38431200	0.20445800
H	-1.44496300	4.76903200	-1.02174900
H	0.62113800	5.33684100	0.63992100
N	2.62807200	0.63441100	0.75828500
C	2.95759700	1.83836700	1.31182800
C	4.18655600	1.73081200	2.06486500
C	4.59780600	0.43873400	1.95421900
H	4.65899000	2.54652900	2.59725100
H	5.47742000	-0.02831000	2.37853100
N	1.63554800	-1.73720700	-0.55551700
C	2.75369800	-2.27915200	0.01578900
C	1.00622100	-2.76614000	-1.20807600
C	2.83850600	-3.69096500	-0.28602100
C	1.74903200	-3.99314300	-1.04588200
H	3.63340800	-4.34779700	0.04414800
H	1.46299000	-4.94943100	-1.46472800
N	-0.53136000	-0.24357400	-1.60686800
C	-2.07602800	-1.33998500	-2.92829500
H	-2.55820900	-2.15924900	-3.44624900
C	-0.88228400	-1.45890200	-2.12529300
C	-0.60577600	2.68660300	-0.92839900
C	1.06423200	3.14669400	0.40742600
C	3.61796100	-0.23942100	1.13664300
C	-0.17306900	-2.64214600	-1.93398900
H	-0.56918600	-3.54050700	-2.39761200
C	-1.49672500	2.00763500	-1.76603700

H	-2.26914800	2.60003200	-2.24339300
C	2.22182100	3.01518500	1.16061200
H	2.60145100	3.90537100	1.65349500
C	3.67619400	-1.58403000	0.79888700
H	4.52049500	-2.15066300	1.18114200
C	-2.43421800	-0.02531900	-2.89652200
H	-3.27152500	0.45752800	-3.38363900
C	-1.46073000	0.64837300	-2.06642800
N	-4.04329400	-0.01380500	1.05164400
C	-3.26067400	0.53533100	1.88780000
C	-2.73044400	-0.07333000	3.14795400
H	-2.97376500	1.55798000	1.61325400
H	-1.95720800	0.56124900	3.58566300
H	-3.53773900	-0.19091400	3.88177700
H	-2.31464600	-1.06346100	2.92208400
C	-4.61286000	-1.35573700	1.04715800
C	-5.86826800	-1.45273000	1.92023600
H	-3.82903400	-2.06002100	1.34861500
H	-4.86557200	-1.56096300	0.00130600
H	-6.29302300	-2.45788500	1.83129500
H	-5.64141600	-1.27723400	2.97697100
H	-6.62835000	-0.73030500	1.60483000
N	-4.48323600	0.96198200	-0.38801100
O	-3.93178900	1.99916200	-0.33511900
O	-0.00197300	-0.25642000	1.10866200
H	0.01840500	0.53567300	1.66918500
O	-1.68792000	-2.51274900	1.32916700
H	-0.96414800	-2.81085000	1.92303600
H	-1.29672200	-1.67335900	1.00559700
O	0.71157100	-2.35270800	2.72556700
H	1.38816500	-2.84559000	2.23683000
H	0.59738000	-1.52639600	2.18599300
⁴INT_a			
Fe	1.26843600	0.13615800	-0.31867100
S	2.30398000	0.65280400	-2.29954900
H	1.24317800	0.46147100	-3.11458200
N	0.43981200	1.99007700	-0.27554400
C	-1.02466500	3.74918200	-0.54376900
C	0.12761300	4.26008700	-0.02697100
H	-1.93919400	4.26534700	-0.80551200
H	0.35588500	5.28708400	0.22800700
N	2.93912900	0.88289400	0.52157200
C	3.20034800	2.20092700	0.82007400
C	4.49678300	2.31313600	1.43507500
C	5.00387400	1.05151900	1.52677200
H	4.94031700	3.24382300	1.76487400
H	5.95099900	0.73385000	1.94347500
N	2.04667900	-1.70455800	-0.26649900
C	3.24964900	-2.07112300	0.29191300
C	1.51145600	-2.84448100	-0.81756700
C	3.45187400	-3.48880700	0.12957600

C	2.38015200	-3.96615300	-0.56371600
H	4.31778100	-4.02967400	0.48929600
H	2.18331300	-4.98015200	-0.88748100
N	-0.32824000	-0.55841000	-1.29473100
C	-1.83751700	-1.95576200	-2.33527200
H	-2.24385100	-2.86968700	-2.74902400
C	-0.54266700	-1.84969900	-1.71674900
C	-0.81319300	2.33437500	-0.71859600
C	1.04163200	3.15733800	0.13259500
C	4.02515800	0.16383500	0.95625800
C	0.31716700	-2.91842800	-1.51604200
H	0.01411900	-3.88747200	-1.89813900
C	-1.72665200	1.47450400	-1.31233900
H	-2.70125700	1.87150200	-1.57611500
C	2.33088900	3.26550100	0.63187900
H	2.67755900	4.25258800	0.91972100
C	4.16983600	-1.21386200	0.87221500
H	5.08292900	-1.64798800	1.26586400
C	-2.42366400	-0.72914500	-2.24937500
H	-3.41316600	-0.42305800	-2.56109600
C	-1.48045900	0.13960300	-1.59347400
N	-4.76562600	0.14852100	0.51245100
C	-4.31429600	0.94732100	1.46659900
C	-3.85106000	0.48684200	2.80836300
H	-4.30656000	1.99204100	1.17447100
H	-3.34839200	1.31119200	3.32323200
H	-4.68793600	0.16849300	3.44800300
H	-3.15383700	-0.35920400	2.72791800
C	-4.93082100	-1.30702000	0.62759100
C	-6.20519100	-1.69356400	1.38163000
H	-4.02973000	-1.72091400	1.08932200
H	-4.98127100	-1.66303600	-0.40416200
H	-6.31046700	-2.78400500	1.38393600
H	-6.18309000	-1.35811900	2.42335600
H	-7.08760600	-1.26257600	0.89745900
N	-5.15127000	0.64294600	-0.77250300
O	-4.99884900	1.87575700	-0.87415900
O	0.49742400	-0.16911000	1.32472900
H	0.29538200	0.69492900	1.72415600
O	-1.82090400	-1.88973100	1.64643700
H	-1.15811100	-2.36622800	2.19053900
H	-1.27388800	-1.16513900	1.29043600
O	0.67510200	-2.54333100	2.79624100
H	1.09516800	-3.13354000	2.15162600
H	0.79566800	-1.65223000	2.39941400
⁴TS-reb_a			
Fe	0.79883200	0.56569500	-0.39766400
N	1.98559200	-1.10317800	-0.93252200
N	-0.23090500	0.40026900	-2.16560300
N	-0.41603900	2.21970200	0.13586400
N	1.83973400	0.74724800	1.34882400

C	0.97098700	-1.53937900	-3.11119200
C	-1.79610700	2.28909900	-1.87263800
C	0.66612100	2.71693900	2.26565700
C	3.36541900	-1.17490600	1.08167400
C	1.89403000	-1.81391500	-2.08684500
C	0.00202400	-0.53077100	-3.14790500
C	-1.25761700	1.19741000	-2.58274500
C	-1.39147500	2.78518400	-0.62846700
C	-0.27001600	2.97699300	1.25579100
C	1.62489000	1.69122000	2.31439200
C	2.84670700	-0.07239100	1.78247800
C	2.97785100	-1.65321100	-0.17722100
C	3.54663900	-2.78495800	-0.88455200
C	2.87564100	-2.88457800	-2.07081300
C	-0.92844300	-0.31021500	-4.23641500
C	-1.70777500	0.75312500	-3.88692400
C	-1.91259200	3.95993100	0.05049600
C	-1.21625800	4.08010500	1.21686300
C	2.54386700	1.46520100	3.41271000
C	3.29569700	0.37492200	3.08680100
H	1.01295100	-2.18786500	-3.98259400
H	-0.96932900	-0.89712900	-5.14552100
H	-2.51020700	1.20787700	-4.45421100
H	-2.59989200	2.82536900	-2.37010700
H	-2.69951700	4.60198500	-0.32523000
H	-1.32185300	4.84099100	1.98023600
H	0.65794400	3.39486100	3.11542900
H	2.59487600	2.06503200	4.31274700
H	4.08222800	-0.09187300	3.66612800
H	4.16274900	-1.71960100	1.57989800
H	4.35145100	-3.41087300	-0.51988400
H	3.03005200	-3.60573800	-2.86399500
O	-0.46918900	-0.59404100	0.45130200
S	2.28244200	2.01044300	-1.49118000
H	3.27295700	2.00775400	-0.57088700
H	-3.84139500	-1.97622700	-0.81244400
C	-3.68800400	-2.40121100	0.18621500
H	-2.81570500	-3.06287700	0.13452600
N	-3.36323100	-1.27067800	1.04804700
C	-2.71104300	-1.25661000	2.14332500
N	-3.84648200	0.33469200	0.39843800
H	-1.25450900	-0.48521200	-0.10833700
H	-2.55256900	-0.25158600	2.54982500
O	-3.55319700	1.16559300	1.16839000
C	-2.20126700	-2.41454100	2.92197800
H	-2.50895000	-3.37519600	2.50627500
H	-1.09694600	-2.39338100	2.95844000
H	-2.55657200	-2.32824200	3.95684000
C	-4.95325000	-3.13768300	0.63674700
H	-5.80869500	-2.45576000	0.68044800
H	-5.18608300	-3.93531100	-0.07629400
H	-4.82375100	-3.59193900	1.62431400

O	0.92440000	-2.87933500	2.75944700
H	0.59709900	-3.18409000	1.88118800
H	1.23511600	-1.97967900	2.57283400
O	-0.28055000	-3.23894400	0.27307900
H	0.34344300	-3.46936100	-0.43279800
H	-0.29214100	-2.23423400	0.27575400
²P-OH_a			
Fe	-1.18204100	-0.27925600	0.27650500
O	1.09228700	0.40083100	-0.26754000
S	-3.17555800	-0.97562300	0.98803300
H	-2.74245000	-1.83690500	1.93723700
N	-1.72840700	1.65527400	0.30091200
C	-2.26649400	3.77540500	1.05491300
C	-2.67886300	3.69553300	-0.23915100
H	-2.34366700	4.61215900	1.73749000
H	-3.16811000	4.45142900	-0.84023500
N	-1.74349800	-0.37926400	-1.64841300
C	-2.37931600	0.58608100	-2.39270800
C	-2.72877600	0.06981200	-3.69383000
C	-2.30807900	-1.22368200	-3.72695500
H	-3.23267200	0.63626200	-4.46665700
H	-2.39272400	-1.94037100	-4.53399900
N	-0.40568800	-2.13140600	0.17515800
C	-0.51406800	-2.99613200	-0.88848300
C	0.27317700	-2.82051300	1.15439400
C	0.12871600	-4.25009300	-0.57952200
C	0.62039800	-4.13986800	0.68837900
H	0.18346700	-5.09717800	-1.25171700
H	1.16151700	-4.87645000	1.26870500
N	-0.40805400	-0.10096400	2.13250800
C	0.49666700	-0.57975300	4.20929100
H	1.00111400	-1.14385900	4.98329200
C	0.23376300	-1.06732000	2.87923900
C	-1.68152500	2.49805000	1.38655500
C	-2.35045300	2.36781100	-0.69776900
C	-1.69795700	-1.49686800	-2.44771200
C	0.57204800	-2.33150400	2.41998000
H	1.09734100	-2.99167300	3.10300700
C	-1.14928800	2.18722700	2.63007800
H	-1.18769200	2.95685400	3.39461600
C	-2.65168000	1.87731900	-1.96041100
H	-3.15750900	2.54385200	-2.65213700
C	-1.12536200	-2.71192900	-2.10240400
H	-1.14520400	-3.50217000	-2.84657800
C	-0.00054600	0.68597000	4.26945700
H	0.01395100	1.37632300	5.10308000
C	-0.56350300	0.97744400	2.97491000
N	3.17088200	1.42338500	-0.72719200
C	1.71608000	1.47565700	-0.98388900
C	1.35164100	1.35480400	-2.44906600
H	1.36130800	2.42077300	-0.56015400

H	1.25719900	0.59851600	0.68156400
H	0.27241000	1.48742200	-2.54677100
H	1.85334100	2.12345100	-3.04380500
H	1.61255600	0.36572000	-2.83561800
C	4.23041400	1.18584300	-1.72752200
C	4.82474100	2.48250200	-2.27821400
H	3.80148600	0.57067700	-2.51945400
H	4.98397800	0.57086400	-1.22836800
H	5.61755900	2.24769000	-2.99691400
H	4.07459800	3.09675500	-2.78933700
H	5.26174700	3.07714700	-1.46945900
N	3.60215700	1.57845700	0.51843700
O	2.71391600	1.74037200	1.37072000
O	2.73009400	-1.80056600	-1.05003000
H	2.34746500	-2.68042800	-0.90516100
H	2.05726700	-1.17885900	-0.70738600
O	5.22544100	-1.20534200	0.20690300
H	4.95648600	-0.53098100	0.84938300
H	4.38117100	-1.49789900	-0.19994000
⁴P-OH_a			
Fe	-1.48181300	-0.02501900	0.44947700
O	1.52702400	0.18232700	-1.38556200
S	-3.26105300	-0.18877800	2.07632600
H	-2.47264800	0.02346200	3.15477000
N	-2.04285400	1.71686800	-0.40830500
C	-2.46623700	3.96941600	-0.73015100
C	-3.24109700	3.28595600	-1.61551500
H	-2.38871200	5.03930100	-0.58497600
H	-3.93484000	3.67733300	-2.34857400
N	-2.47679300	-1.01589500	-0.98842800
C	-3.36622400	-0.48791000	-1.89744100
C	-4.01281400	-1.54012300	-2.63547500
C	-3.50896200	-2.71647000	-2.16862600
H	-4.75239400	-1.38281900	-3.41014600
H	-3.74843000	-3.72471000	-2.48152700
N	-0.51989100	-1.73742800	0.92624800
C	-0.83853200	-3.00662500	0.49638100
C	0.47058400	-1.89988400	1.86923400
C	-0.02201900	-3.98247400	1.17048500
C	0.79280100	-3.29467200	2.02263300
H	-0.08097500	-5.05149200	1.00938400
H	1.54477600	-3.67930700	2.69953000
N	-0.13784500	0.99132600	1.54723800
C	1.41719000	1.51793000	3.17948800
H	2.18586900	1.36309100	3.92550700
C	0.78767900	0.46571800	2.43030500
C	-1.72731800	2.98662800	0.02078100
C	-2.97897100	1.88508100	-1.40335200
C	-2.55209800	-2.38348600	-1.14744400
C	1.08547800	-0.87891500	2.57819500
H	1.88136300	-1.14849000	3.26267600

C	-0.83130400	3.29336700	1.03138200
H	-0.68441400	4.34021900	1.27619400
C	-3.60460800	0.86350500	-2.09831500
H	-4.33337100	1.13929800	-2.85370600
C	-1.79558600	-3.31652800	-0.45756600
H	-1.95151100	-4.36450100	-0.69278300
C	0.86848100	2.69004400	2.75457200
H	1.09822400	3.69742200	3.07636400
C	-0.09113000	2.35859800	1.73841200
N	3.85511200	0.63323700	-1.26815200
C	2.64430900	0.65847100	-2.12362500
C	2.76587100	-0.18908400	-3.37605400
H	2.48304100	1.71255600	-2.37432100
H	1.37353200	0.83402400	-0.67232200
H	1.86223100	-0.03983100	-3.97342900
H	3.63221700	0.10121500	-3.97688800
H	2.83520400	-1.25017700	-3.12127700
C	5.04554800	-0.21852800	-1.44387600
C	6.15573900	0.46841500	-2.24021300
H	4.72143900	-1.14817100	-1.91273700
H	5.38163900	-0.48018800	-0.43781200
H	7.02078000	-0.19927900	-2.31971400
H	5.83423200	0.72770600	-3.25512500
H	6.47618800	1.38643900	-1.73705200
N	3.87974800	1.41571400	-0.19556600
O	2.86813300	2.11256800	-0.02549900
O	2.69660000	-2.22763600	-0.50061500
H	2.11604900	-2.90651300	-0.12000500
H	2.10370000	-1.47410400	-0.70862700
O	4.25239400	-1.18072100	1.68034100
H	4.13568300	-0.22697100	1.54883300
H	3.72888900	-1.58421600	0.95429500
²P-NO₁			
Fe	-1.24773	-0.13612	-0.35922
O	-0.10837	0.09027	1.14655
S	-2.67507	-0.44032	-2.16623
H	-1.76404	-0.37078	-3.16342
N	-2.47843	-1.30508	0.74777
C	-3.44953	-3.15692	1.72944
C	-4.19403	-2.07618	2.09257
H	-3.59623	-4.19637	1.99399
H	-5.07741	-2.04439	2.71755
N	-2.33256	1.47735	0.22027
C	-3.44571	1.50299	1.01834
C	-3.92326	2.8566	1.17139
C	-3.08028	3.64898	0.45165
H	-4.79036	3.14547	1.75173
H	-3.11493	4.72273	0.31686
N	-0.01909	1.03708	-1.45542
C	-0.10724	2.40058	-1.58261
C	1.03535	0.6531	-2.23045

C	0.93185	2.88958	-2.46066
C	1.64109	1.80135	-2.86861
H	1.07853	3.92908	-2.72548
H	2.49123	1.75983	-3.53763
N	-0.17271	-1.74244	-0.93542
C	1.3693	-3.1356	-1.94499
H	2.20801	-3.42836	-2.56366
C	0.90031	-1.77769	-1.77918
C	-2.38547	-2.66235	0.88673
C	-3.57869	-0.92601	1.47371
C	-2.09486	2.77385	-0.14045
C	1.46814	-0.66498	-2.39558
H	2.28993	-0.83855	-3.07992
C	-1.41483	-3.46669	0.29052
H	-1.46828	-4.53215	0.49503
C	-4.03233	0.38344	1.60182
H	-4.91808	0.54554	2.20916
C	-1.05962	3.20436	-0.97119
H	-1.00129	4.27119	-1.16728
C	0.56315	-3.91995	-1.18038
H	0.59908	-4.99309	-1.04205
C	-0.40035	-3.03989	-0.55647
N	4.80696	0.16856	0.78632
C	4.13212	1.23373	0.65445
C	3.97061	2.37353	1.60315
H	3.6269	1.31924	-0.31762
H	-0.67149	-0.13351	1.90636
H	4.45131	3.25998	1.16619
H	2.90157	2.59736	1.70981
H	4.39947	2.17441	2.58618
C	5.58966	-0.3191	1.90916
C	4.88267	-1.47915	2.61722
H	5.78736	0.50193	2.60738
H	6.55158	-0.64475	1.49544
H	5.51399	-1.83982	3.43685
H	3.92004	-1.14295	3.01191
H	4.71515	-2.30847	1.92259
N	4.8035	-0.96278	-0.68091
O	4.21378	-0.43726	-1.54814
O	0.74538	2.47796	2.01497
H	0.37339	1.66839	1.56015
H	-0.03058	2.9877	2.29008
O	2.07242	0.12358	2.89869
H	1.4925	-0.1802	2.16823
H	1.72723	1.02442	3.03869
⁴P-NO₁			
Fe	-1.31902	-0.02378	-0.33617
O	-0.22544	0.09809	1.1241
S	-2.68045	-0.29186	-2.16834
H	-3.40185	0.84277	-2.03289
N	-0.5392	-1.78628	-0.89274

C	0.84301	-3.3869	-1.80788
C	-0.09844	-4.04112	-1.07397
H	1.6664	-3.80178	-2.37438
H	-0.20936	-5.1057	-0.91365
N	-2.67581	-0.99511	0.82569
C	-2.80059	-2.35553	0.97706
C	-3.92164	-2.6536	1.83139
C	-4.4887	-1.46299	2.17109
H	-4.22668	-3.65222	2.11652
H	-5.35591	-1.28129	2.79286
N	-2.21951	1.72258	0.09298
C	-3.30756	1.91445	0.91359
C	-1.80308	2.974	-0.29391
C	-3.60235	3.32013	1.01467
C	-2.67158	3.97585	0.26665
H	-4.41308	3.73566	1.59925
H	-2.5601	5.0411	0.1102
N	0.07872	0.94367	-1.3938
C	1.31362	2.5993	-2.4178
H	1.61145	3.59721	-2.71337
C	0.17699	2.3003	-1.58255
C	0.56898	-1.97932	-1.68236
C	-0.95076	-3.03681	-0.4926
C	-3.71662	-0.43203	1.52532
C	-0.69343	3.25268	-1.07823
H	-0.49023	4.29326	-1.30909
C	1.34329	-0.97931	-2.25043
H	2.2039	-1.27941	-2.83726
C	-1.99892	-3.31147	0.37206
H	-2.20705	-4.35349	0.59113
C	-4.01187	0.92162	1.57879
H	-4.85876	1.22796	2.18402
C	1.88961	1.40945	-2.74384
H	2.76202	1.22267	-3.35547
C	1.10355	0.37841	-2.11181
N	4.55337	0.30704	1.00253
C	4.1235	1.46872	0.70491
C	4.05684	2.67011	1.60958
H	3.73588	1.58843	-0.31313
H	-0.7062	-0.28481	1.88083
H	3.78044	3.5702	1.05366
H	3.29913	2.47423	2.38215
H	5.01257	2.84633	2.11815
C	5.09614	0.05016	2.34206
C	5.46059	-1.42329	2.50753
H	4.36227	0.35152	3.1012
H	5.98717	0.67832	2.49413
H	5.90016	-1.59954	3.49589
H	4.5699	-2.05209	2.41143
H	6.18368	-1.73172	1.74512
N	4.92488	-1.11632	-1.15613
O	4.79273	-0.34191	-2.01822

O	1.678	0.84659	3.1955
H	1.04849	1.0991	2.4978
H	1.97166	-0.03158	2.8721
O	2.13104	-1.4299	1.52775
H	1.32212	-1.00609	1.17097
H	2.86256	-1.04969	1.007
²P-NO₂			
Fe	-1.07509700	-0.06561700	0.30075000
O	-0.04208900	0.06340800	-1.13056100
S	-2.53382500	-0.21077500	2.11290900
H	-1.78454400	0.46793600	3.01008300
N	0.43699700	0.40785600	1.55342200
C	2.26431300	0.26932000	2.95156000
C	2.00389500	1.59260300	2.75885300
H	3.04399700	-0.18536500	3.54941900
H	2.52468300	2.44878600	3.16867800
N	-1.52228000	1.89699400	0.10580300
C	-0.83077700	2.95402700	0.63392400
C	-1.45948800	4.19596000	0.24846800
C	-2.54389900	3.86892700	-0.50620300
H	-1.11006000	5.17877600	0.53888000
H	-3.26780200	4.52712100	-0.96959700
N	-2.67906500	-0.55083600	-0.81023200
C	-3.57300900	0.32049300	-1.37757900
C	-3.04040100	-1.80547300	-1.22536900
C	-4.54355900	-0.41086100	-2.15547600
C	-4.21075000	-1.72730400	-2.06534600
H	-5.35961000	0.04370300	-2.70253600
H	-4.69796300	-2.58032800	-2.52007200
N	-0.62539300	-2.02370800	0.51009900
C	-0.67228800	-4.32230100	0.33667300
H	-0.99800400	-5.30129100	0.00929800
C	-1.27784400	-3.07883900	-0.07552300
C	1.28676300	-0.46466600	2.18667900
C	0.86283600	1.67246000	1.88158500
C	-2.57631200	2.42789000	-0.58821300
C	-2.39035600	-2.98720400	-0.89723900
H	-2.79846000	-3.91093700	-1.29438500
C	1.24812100	-1.85108200	2.08732200
H	1.97649100	-2.41574900	2.66074800
C	0.28654300	2.86041700	1.45330900
H	0.72770100	3.78650400	1.80859900
C	-3.54138200	1.70319500	-1.27232100
H	-4.32210700	2.26127600	-1.77910500
C	0.33522800	-4.00567400	1.19361700
H	1.01327000	-4.66946500	1.71460600
C	0.35500400	-2.56623800	1.30078900
N	3.45299600	1.23030000	-1.49563200
C	2.52306900	2.08775100	-1.67235200
C	2.60833700	3.57253200	-1.91137500
H	1.50658100	1.68257900	-1.65358500

H	2.82971000	-0.45487900	-1.26496500
H	2.25065200	3.79242800	-2.92619200
H	1.92540900	4.08488400	-1.22324800
H	3.60980100	3.99315400	-1.80182300
C	4.87152500	1.57173000	-1.47262400
C	5.56740900	0.83613800	-0.32414800
H	5.05690800	2.65142100	-1.39378400
H	5.30211000	1.24154100	-2.42794900
H	6.63947400	1.06267600	-0.31636000
H	5.14421700	1.13718900	0.64083400
H	5.44214000	-0.24669800	-0.42895000
N	4.47683300	-2.92963900	-1.10730900
O	4.53620200	-3.49573800	-2.11690800
O	2.33325700	-1.30948800	-1.12012800
H	0.70485100	-0.59740600	-1.14244700
H	2.41683500	-1.48444900	-0.16854700
O	-1.24584706	0.73994237	-3.43389216
H	-2.17209074	0.98483153	-3.49473588
H	-1.01793048	0.57375119	-2.51626777
⁴P-NO₂			
Fe	1.17085800	0.24509000	0.32751300
O	-0.10194800	-0.35035900	-0.76783000
S	2.90570900	1.00350400	1.67401800
H	2.52840000	0.40251100	2.82443800
N	0.13693500	-0.30930400	1.96812200
C	-1.31545300	-0.31755200	3.75754500
C	-0.80090900	-1.57424400	3.65095900
H	-2.03033300	0.06040000	4.47736000
H	-1.00407400	-2.44067100	4.26744900
N	2.02679900	-1.58397400	0.25058900
C	1.72745800	-2.66282600	1.04141900
C	2.52576500	-3.79784900	0.64483500
C	3.32349400	-3.38009100	-0.37841700
H	2.48030800	-4.77466700	1.10943700
H	4.06273700	-3.94515300	-0.93153100
N	2.32680000	0.85558900	-1.19858500
C	3.27230300	0.11177200	-1.85942100
C	2.26251100	2.06384500	-1.84241100
C	3.83948400	0.88602700	-2.93595700
C	3.20942100	2.09225500	-2.92980600
H	4.60815000	0.52873700	-3.60912400
H	3.35586700	2.93451900	-3.59372500
N	0.31029500	2.06805800	0.40974000
C	-0.26082700	4.25373500	-0.05034700
H	-0.27420400	5.20306600	-0.57004200
C	0.52927900	3.11405000	-0.45008600
C	-0.73501300	0.46368900	2.69394000
C	0.10324000	-1.56413400	2.52880800
C	3.00662100	-1.99305100	-0.61578100
C	1.42060900	3.11648100	-1.51103400
H	1.48577000	4.01843700	-2.11070800

C	-1.05798700	1.78960200	2.42820100
H	-1.75532000	2.28091300	3.09926000
C	0.82709800	-2.66621700	2.09802000
H	0.69686100	-3.59528100	2.64379100
C	3.60544200	-1.20635100	-1.58906400
H	4.37090800	-1.66635900	-2.20533000
C	-0.93603800	3.89135400	1.07282000
H	-1.62458300	4.47837100	1.66679100
C	-0.57045900	2.52423200	1.35690100
N	-3.94851700	-1.55537300	-1.16274200
C	-3.12652600	-2.53191000	-1.19789600
C	-3.28080500	-3.92115700	-1.74961200
H	-2.13064700	-2.32926500	-0.79992500
H	-3.16496400	-0.03721900	-0.70899300
H	-2.41476100	-4.10747600	-2.39463700
H	-3.22550300	-4.65173600	-0.93100200
H	-4.20333700	-4.08924600	-2.30845900
C	-5.31462800	-1.64039700	-1.67139400
C	-6.27546800	-0.93378500	-0.71156000
H	-5.64527400	-2.67344500	-1.84137000
H	-5.33475300	-1.12962000	-2.64389700
H	-7.29508400	-0.94345100	-1.11274100
H	-6.28741100	-1.43181700	0.26455100
H	-5.97126200	0.10728500	-0.55967000
N	-4.42932100	2.67643500	-0.31602800
O	-4.25159500	3.43468200	-1.17444000
O	-2.58114700	0.74574600	-0.48032700
H	-0.95576700	0.16672600	-0.70952100
H	-2.63172500	0.83082800	0.48499800
O	-0.05609000	-2.85025000	-2.09899400
H	0.57533100	-3.29846400	-1.51723600
H	-0.05536000	-1.92976900	-1.75870900
² RC _β			
Fe	-1.18096	0.07384	0.31964
O	-0.46787	-0.10235	-1.14989
S	-2.24723	0.63715	2.54798
H	-3.53838	0.50286	2.16926
N	-2.75504	-1.10466	-0.1183
C	-4.74313	-1.89034	-0.99262
C	-4.07467	-2.96486	-0.49174
H	-5.70738	-1.86179	-1.48305
H	-4.37398	-4.00481	-0.48515
N	-0.23257	-1.4982	1.14247
C	-0.65024	-2.80249	1.14565
C	0.3471	-3.64889	1.75054
C	1.37898	-2.83711	2.11244
H	0.25289	-4.71989	1.87515
H	2.30914	-3.0995	2.59961
N	0.25899	1.30122	1.02198
C	1.43931	0.92719	1.61655
C	0.33725	2.66113	0.86061

C	2.27818	2.07886	1.843
C	1.59139	3.15613	1.3744
H	3.26687	2.03379	2.27919
H	1.89036	4.19646	1.36633
N	-2.2656	1.69068	-0.23133
C	-2.86492	3.84995	-0.80185
H	-2.78482	4.92501	-0.89844
C	-1.85649	3.00448	-0.21267
C	-3.91089	-0.73844	-0.75456
C	-2.8345	-2.46574	0.04537
C	1.00353	-1.49872	1.73049
C	-0.64315	3.45631	0.28199
H	-0.44602	4.52208	0.21874
C	-4.25815	0.56329	-1.1018
H	-5.20305	0.70503	-1.61602
C	-1.8628	-3.25702	0.64032
H	-2.05955	-4.32268	0.70331
C	1.79112	-0.3724	1.94935
H	2.76711	-0.5192	2.39801
C	-3.88201	3.03664	-1.19393
H	-4.81	3.30287	-1.68291
C	-3.49838	1.6919	-0.84505
N	5.42799	-0.30994	-0.92993
C	4.03473	-0.63931	-1.25324
C	3.22179	0.57876	-1.70373
H	3.5962	-1.07525	-0.35328
H	4.06131	-1.40684	-2.03418
H	2.17659	0.29311	-1.86379
H	3.24201	1.3534	-0.93273
H	3.61471	1.00102	-2.63584
C	6.45473	-0.38169	-1.97235
C	7.84487	0.04759	-1.51329
H	6.12572	0.24708	-2.81085
H	6.48264	-1.41495	-2.34571
H	8.53261	-0.04006	-2.36129
H	7.85092	1.08352	-1.1648
H	8.21211	-0.58196	-0.69914
N	5.79587	0.08625	0.28219
O	4.88594	0.15411	1.11724
O	-0.7579	-2.41027	-2.72305
H	-0.12997	-2.20869	-3.43438
H	-0.57293	-1.71747	-2.05177
O	-2.15631	-0.03846	-3.58924
H	-1.60662	0.36671	-2.89759
H	-1.98813	-0.98717	-3.43054
⁴ RC _β			
Fe	1.18475900	0.08497200	-0.32162500
O	0.46749200	-0.13596900	1.14117100
S	2.23721200	0.63219800	-2.53644300
H	3.52975700	0.49387100	-2.16421200
N	2.75729100	-1.10191700	0.11244600

C	4.74225200	-1.89754400	0.98437800
C	4.07391200	-2.96680800	0.47219600
H	5.70523400	-1.87440100	1.47756900
H	4.37197600	-4.00703800	0.45759000
N	0.22962100	-1.48763400	-1.15056300
C	0.64792100	-2.79094200	-1.16284900
C	-0.35264500	-3.63485400	-1.76688200
C	-1.38663400	-2.82135500	-2.11890300
H	-0.25916700	-4.70525000	-1.89715900
H	-2.31947700	-3.08132400	-2.60224100
N	-0.25756100	1.31282400	-1.00964400
C	-1.43838700	0.94222100	-1.60693100
C	-0.33279100	2.67255800	-0.84697100
C	-2.27441400	2.09640400	-1.83100100
C	-1.58550800	3.17135800	-1.36013200
H	-3.26296400	2.05448900	-2.26784400
H	-1.88217400	4.21232000	-1.35033200
N	2.26550100	1.69061300	0.24492400
C	2.87621500	3.84815000	0.81102600
H	2.80097200	4.92362400	0.90676100
C	1.86281700	3.00674500	0.22493300
C	3.91164200	-0.74280900	0.75365800
C	2.83521400	-2.46166400	-0.06343200
C	-1.00833300	-1.48474000	-1.73224500
C	0.65023500	3.46364200	-0.26677500
H	0.45713100	4.53005200	-0.20206700
C	4.25945800	0.55726700	1.10797700
H	5.20465100	0.69654700	1.62233800
C	1.86325100	-3.24767800	-0.66511500
H	2.06064200	-4.31268800	-0.73708400
C	-1.79380900	-0.35512200	-1.94428300
H	-2.77096000	-0.49724700	-2.39196700
C	3.89070000	3.03083700	1.20134000
H	4.82120400	3.29363900	1.68740700
C	3.50136800	1.68740000	0.85412600
N	-5.43207500	-0.31413100	0.92764600
C	-4.03922500	-0.64878500	1.24723700
C	-3.22337900	0.56382600	1.70698700
H	-3.60205100	-1.07835700	0.34354400
H	-4.06682100	-1.42254700	2.02194600
H	-2.17882000	0.27424000	1.86418700
H	-3.24220100	1.34464700	0.94220600
H	-3.61473700	0.97949900	2.64269800
C	-6.45902300	-0.39631000	1.96910200
C	-7.84914000	0.03720900	1.51393800
H	-6.13036400	0.22415900	2.81390900
H	-6.48684900	-1.43324300	2.33210400
H	-8.53709600	-0.05917400	2.36081500
H	-7.85542500	1.07657600	1.17586000
H	-8.21594500	-0.58427600	0.69341300
N	-5.79934400	0.09575800	-0.28007800
O	-4.88914200	0.17171100	-1.11413100

O	0.77136200	-2.44709100	2.71329700
H	0.13913900	-2.25060100	3.42224600
H	0.58197100	-1.75705000	2.04070000
O	2.14949100	-0.06741900	3.58829600
H	1.59945700	0.33882900	2.89771000
H	1.98593300	-1.01619200	3.42478300
²TS-H_β			
Fe	1.07915600	0.09104200	-0.40168800
O	-0.13905800	-0.23105000	0.86577800
S	2.72540400	0.20732300	-2.14895900
H	3.70084000	-0.51163900	-1.54930400
N	-0.26550800	0.36472600	-1.87530600
C	-1.76575700	-0.03277300	-3.59078500
C	-1.72571800	1.31388600	-3.40036900
H	-2.35069800	-0.59476900	-4.30745200
H	-2.27479800	2.08627000	-3.92292400
N	1.12042800	2.07318700	-0.10519700
C	0.41904300	3.04153800	-0.77356800
C	0.73364700	4.34763100	-0.24891900
C	1.64301200	4.15738700	0.74659200
H	0.30792300	5.27618200	-0.60662400
H	2.12099000	4.89818600	1.37457400
N	2.51128700	-0.18832700	0.99906600
C	3.07020900	0.78209100	1.78390900
C	3.06402100	-1.37040300	1.41638000
C	4.00807800	0.20225600	2.71696700
C	4.00404100	-1.13837800	2.48833400
H	4.57695000	0.76139600	3.44830700
H	4.57118200	-1.91134600	2.99057100
N	1.12941000	-1.90437100	-0.78881200
C	1.53712500	-4.17602100	-0.65612700
H	1.98248700	-5.10197700	-0.31579600
C	1.86186700	-2.86795900	-0.14026100
C	-0.84601500	-0.61529400	-2.64201500
C	-0.78805000	1.55161500	-2.33000700
C	1.88330300	2.73597500	0.82163700
C	2.76702600	-2.62088200	0.88442100
H	3.27621600	-3.47783900	1.31502300
C	-0.58454300	-1.97693800	-2.54043100
H	-1.13739300	-2.63433200	-3.20508300
C	-0.46756400	2.80295100	-1.82019700
H	-0.95385500	3.66407800	-2.26833500
C	2.78182100	2.14010800	1.70094500
H	3.30647500	2.79743700	2.38762100
C	0.58722000	-3.99391200	-1.61527300
H	0.09711600	-4.73952500	-2.22826700
C	0.33647600	-2.57317500	-1.68787200
N	-4.69016200	-0.21360000	0.96691500
C	-3.36142600	-0.25075500	0.33053200
C	-2.42051400	0.81133800	0.85772700
H	-3.50394200	-0.12525000	-0.74837500

H	-1.20872900	0.32313100	0.72593600
H	-2.40374300	1.74886600	0.30365900
H	-2.44309600	0.95290600	1.94026300
C	-5.21019800	-1.32871000	1.76024200
C	-4.41547300	-1.58687600	3.04240500
H	-5.21617900	-2.22974200	1.13238600
H	-6.24803500	-1.06572000	1.98134400
H	-4.89738000	-2.39124500	3.61005600
H	-3.39048400	-1.90147500	2.82272500
H	-4.38991600	-0.69128600	3.67220000
N	-5.50692900	0.81168300	0.76517500
O	-5.03850600	1.72601200	0.08390100
H	-2.95446800	-1.24726800	0.52989600
O	-0.07036800	1.20454300	3.32921400
H	-0.12629000	2.07074700	2.90052000
H	0.00328900	0.59064700	2.56972100
O	-1.36933400	-2.68064900	1.45430500
H	-0.83635100	-1.86327400	1.33049900
H	-1.09396700	-3.24954200	0.72003500
⁴TS-H_β			
Fe	-1.07373400	0.04715000	0.39625100
O	0.10005300	-0.11463600	-0.94501600
S	-2.63284300	0.12657100	2.24358700
H	-3.57867400	-0.70052300	1.74306700
N	0.34323900	0.19667100	1.84034400
C	1.90771300	-0.34113800	3.45767300
C	1.88867100	1.01556100	3.35782100
H	2.51017100	-0.96082500	4.10925400
H	2.47719100	1.74099600	3.90412400
N	-1.09025600	2.06409200	0.25447700
C	-0.32849200	2.96302200	0.94851500
C	-0.61445500	4.30850200	0.51587900
C	-1.56614600	4.20850400	-0.45495900
H	-0.14215200	5.19910700	0.90981100
H	-2.03793700	5.00088400	-1.02156800
N	-2.56545200	-0.09167000	-0.95267900
C	-3.12764100	0.94550900	-1.64852900
C	-3.17976700	-1.22311100	-1.40975500
C	-4.12483300	0.45328200	-2.57069000
C	-4.15833500	-0.89815500	-2.42170300
H	-4.70724200	1.07411200	-3.23888900
H	-4.77574100	-1.62040000	-2.93988100
N	-1.16610300	-1.94055100	0.67499900
C	-1.67622300	-4.18593700	0.44716800
H	-2.17518900	-5.07427700	0.08197000
C	-1.97068000	-2.84270600	0.01426500
C	0.93460900	-0.83952300	2.51355900
C	0.91060300	1.34106400	2.34714200
C	-1.85653900	2.80302400	-0.60308900
C	-2.90564500	-2.51153400	-0.95638900
H	-3.46315600	-3.32706400	-1.40709600

C	0.62709100	-2.18481600	2.33624300
H	1.18665700	-2.90191800	2.92966000
C	0.59794100	2.62991000	1.93581000
H	1.12925600	3.44702100	2.41445800
C	-2.79978800	2.28579400	-1.49006800
H	-3.32777900	2.99867400	-2.11589200
C	-0.67323100	-4.09341900	1.36366000
H	-0.18510300	-4.89031700	1.91001000
C	-0.35731500	-2.69181900	1.49904700
N	4.68661200	-0.20968900	-0.99454700
C	3.32885500	-0.26351500	-0.42395900
C	2.42985400	0.84671200	-0.92407800
H	3.42660200	-0.20731200	0.66520700
H	1.17592600	0.38945300	-0.79098300
H	2.46828000	1.77519400	-0.35674300
H	2.44539000	1.00213900	-2.00491900
C	5.20093000	-1.25511700	-1.87951700
C	4.43449400	-1.36842500	-3.19955200
H	5.16876500	-2.21397200	-1.34430500
H	6.25043200	-0.99986600	-2.04888800
H	4.90911200	-2.12938900	-3.82966200
H	3.39569900	-1.67242900	-3.03535900
H	4.44888500	-0.41717500	-3.74201100
N	5.53761900	0.74582500	-0.63786200
O	5.07837200	1.59344900	0.13049100
H	2.91434200	-1.23593200	-0.70600100
O	-0.06061300	1.57308000	-3.23023700
H	0.18717500	2.36983300	-2.73923700
H	-0.10568500	0.88951100	-2.52958300
O	1.24777600	-2.54195600	-1.74121300
H	0.74851900	-1.71449200	-1.55657300
H	1.02450200	-3.11431000	-0.99215000
² INT _β			
Fe	-1.22520100	0.20519100	0.37630600
O	-0.22981100	-0.23453000	-1.12887100
S	-2.42284000	0.74123700	2.34271300
H	-2.84191900	-0.50203700	2.66978300
N	0.04312100	1.69663500	0.86611200
C	1.86262400	2.84711200	1.71498900
C	1.09158100	3.75408200	1.05739500
H	2.80613500	2.99627400	2.22213600
H	1.26217800	4.81464100	0.92439900
N	-2.31913900	1.53950000	-0.68177300
C	-2.11230900	2.88096000	-0.81923000
C	-3.12954600	3.47040400	-1.65451800
C	-3.95937900	2.45543500	-2.02585200
H	-3.18627700	4.51912400	-1.91609600
H	-4.83920600	2.49921100	-2.65473000
N	-2.50958800	-1.28273400	-0.09459200
C	-3.59296100	-1.17792500	-0.92560900
C	-2.44965400	-2.59496300	0.28046800

C	-4.23158700	-2.46283500	-1.08516000
C	-3.51805900	-3.34743900	-0.33143400
H	-5.10934700	-2.64771000	-1.69104600
H	-3.68848900	-4.40728600	-0.19288900
N	-0.18315400	-1.09513700	1.50507800
C	0.57309400	-3.00957800	2.56462800
H	0.59630100	-4.04569200	2.87610500
C	-0.43740500	-2.43010000	1.71198400
C	1.18871200	1.57418100	1.60269500
C	-0.03809500	3.02893800	0.52526700
C	-3.44530600	1.25720700	-1.40808300
C	-1.48793000	-3.13105500	1.13882000
H	-1.55624800	-4.19185700	1.36021100
C	1.63618100	0.39598600	2.19963400
H	2.58021200	0.44730000	2.73108600
C	-1.04885500	3.58338800	-0.24536700
H	-0.99952200	4.65129400	-0.43699600
C	-4.02916300	-0.00051400	-1.52880800
H	-4.91648700	-0.06992200	-2.15158600
C	1.45832500	-2.01849300	2.84930900
H	2.35863000	-2.06795600	3.44768500
C	0.98312400	-0.83000000	2.17916100
N	4.90057700	-0.19729900	-0.92669700
C	3.45958800	-0.44672000	-1.11524600
C	2.93047100	0.11033800	-2.38948500
H	2.98768500	0.01624900	-0.23823900
H	3.25874800	-1.52377800	-1.07188500
H	0.23734200	0.56038900	-1.43547700
H	3.18292500	1.11886000	-2.70384900
H	2.22833300	-0.47267700	-2.97324900
C	5.85775800	-0.80177700	-1.85855800
C	7.30905200	-0.39622400	-1.62109800
H	5.54382200	-0.52039400	-2.87099700
H	5.74989800	-1.89359200	-1.78946900
H	7.93158500	-0.87404700	-2.38544200
H	7.43904300	0.68717800	-1.69418300
H	7.66374900	-0.71022400	-0.63662100
N	5.38738600	0.46891600	0.11243900
O	4.56156600	0.91889300	0.91448800
O	-0.95316900	-1.94601500	-3.18406900
H	-1.67052300	-2.46199400	-2.78536600
H	-0.79780000	-1.22591100	-2.52675000
O	1.18046200	-2.67342600	-1.40600500
H	0.84148000	-1.82455300	-1.05792400
H	0.63004000	-2.75665500	-2.20968500
⁴INT_β			
Fe	1.16758300	0.17278800	-0.40213800
O	0.15392600	-0.24996900	1.09027400
S	2.38411200	0.68790400	-2.36978400
H	2.84656400	-0.55165500	-2.64932600
N	-0.05424700	1.70655900	-0.89336300

C	-1.82253300	2.92347700	-1.75637500
C	-1.03911400	3.79654000	-1.06756800
H	-2.74766700	3.11147500	-2.28420400
H	-1.18021400	4.85972800	-0.92149200
N	2.29656600	1.46418300	0.67087700
C	2.11843700	2.80706200	0.82997700
C	3.14485400	3.36004400	1.67891500
C	3.95100200	2.32114600	2.03585000
H	3.22324300	4.40272800	1.95835800
H	4.82853700	2.33465000	2.66925000
N	2.40782100	-1.35425400	0.06302400
C	3.49569600	-1.28780300	0.89215400
C	2.30630900	-2.66236700	-0.31767800
C	4.09551900	-2.59290300	1.04270600
C	3.35234700	-3.45088900	0.28774300
H	4.96900000	-2.80782700	1.64489000
H	3.48834100	-4.51502800	0.14435200
N	0.09903800	-1.08111900	-1.55549900
C	-0.71058300	-2.96672800	-2.62711000
H	-0.76590500	-4.00094400	-2.94100900
C	0.30875100	-2.42450900	-1.76064800
C	-1.18828900	1.62986500	-1.65264300
C	0.05966900	3.02983600	-0.52888400
C	3.41233300	1.14501700	1.39711700
C	1.32881000	-3.16332700	-1.17871100
H	1.36115300	-4.22549300	-1.40178200
C	-1.66099100	0.47257400	-2.27131200
H	-2.59343400	0.55718000	-2.81883500
C	1.07626800	3.54453600	0.26131700
H	1.05236700	4.61001500	0.47058400
C	3.96476100	-0.12818200	1.50472600
H	4.84883300	-0.22671800	2.12809100
C	-1.55490200	-1.94401300	-2.92522600
H	-2.44717900	-1.96139500	-3.53730800
C	-1.04876100	-0.77342100	-2.24719700
N	-4.67095400	-0.21011700	1.03175000
C	-3.20214700	-0.12798600	1.23032700
C	-2.80114500	1.09268800	1.99008400
H	-2.77990900	-0.10797400	0.22304100
H	-2.87719700	-1.04904800	1.72299900
H	-0.37453200	0.52821200	1.34212700
H	-2.88958700	2.06741900	1.52082800
H	-2.60431100	1.04912200	3.05676900
C	-5.49777600	-0.90720300	2.02094600
C	-6.99143600	-0.88707300	1.71192500
H	-5.30810700	-0.44094100	2.99684300
H	-5.13385100	-1.94086100	2.08846900
H	-7.51801900	-1.42354400	2.50869500
H	-7.37853500	0.13425800	1.66409600
H	-7.21219500	-1.37426200	0.75889700
N	-5.26186900	0.32830200	-0.02055700
O	-4.51879600	0.92949400	-0.80717700

O	0.98402400	-1.68462100	3.30903100
H	1.65715800	-2.26201200	2.91757300
H	0.77989900	-1.05133500	2.57921300
O	-1.18884200	-2.68233900	1.71109100
H	-0.85761000	-1.90595600	1.21826700
H	-0.62924900	-2.62243600	2.51075700
²TS-reb_β			
Fe	1.11290200	0.04883700	0.44077500
N	2.03751400	-1.58602900	-0.30378500
N	2.30825900	1.19734200	-0.72308500
N	0.16011000	1.68428500	1.15283400
N	-0.13832400	-1.10298300	1.53384900
C	3.71756300	-0.52841300	-1.74222000
C	1.41114300	3.39625000	-0.09228300
C	-1.39938700	0.63130600	2.72540900
C	0.73433500	-3.30447900	0.87273900
C	3.10285300	-1.63294500	-1.16536300
C	3.33945200	0.79345300	-1.53219600
C	2.28127400	2.56690700	-0.79100900
C	0.44905000	2.98407200	0.82479800
C	-0.81079000	1.73927700	2.12028500
C	-1.08764700	-0.69384600	2.43607000
C	-0.12851700	-2.47261400	1.58251400
C	1.74894900	-2.88542300	0.01759500
C	2.65570400	-3.78208700	-0.66627900
C	3.49771000	-3.00456600	-1.39759900
C	3.97423300	1.93983500	-2.14054100
C	3.31505700	3.03981300	-1.68431600
C	-0.37777900	3.88586400	1.59502200
C	-1.15441300	3.11377100	2.40435900
C	-1.71722900	-1.84000900	3.05168400
C	-1.12623400	-2.94464800	2.51732400
H	4.55606400	-0.71100400	-2.40730200
H	4.81370300	1.89101000	-2.82260700
H	3.50362600	4.08134900	-1.91268100
H	1.51857200	4.46592800	-0.24667000
H	-0.34562300	4.96582300	1.52295600
H	-1.89194100	3.42963700	3.13178500
H	-2.15709500	0.81578700	3.48160700
H	-2.49627400	-1.78920300	3.80238700
H	-1.32015200	-3.98669100	2.73955800
H	0.63302400	-4.37425100	1.03277500
H	2.63631700	-4.86139100	-0.58191500
H	4.31361700	-3.31120100	-2.03986700
O	-0.14778900	-0.04914400	-1.15711000
S	2.63488600	0.15055500	2.12822000
H	1.77977100	0.32056700	3.16227900
H	-5.06967000	0.34897000	0.88849000
C	-5.15148500	0.02361200	-0.15590300
H	-6.06457200	0.44947000	-0.57759600
N	-4.05175700	0.65136200	-0.89890300

C	-2.62615900	0.34624600	-0.66243400
N	-4.32412700	1.51833000	-1.80024300
H	0.48186000	0.17022100	-1.86507200
H	-2.48967100	-0.73164700	-0.71736500
O	-3.29714000	1.98716400	-2.36480100
C	-1.83013600	1.03183800	-1.74214800
H	-1.25220700	1.91557600	-1.52701100
H	-1.71268800	0.52923400	-2.68881400
C	-5.13845300	-1.50301100	-0.26121700
H	-4.31613500	-1.93787000	0.31583400
H	-6.07596000	-1.89233800	0.14908900
H	-5.03472400	-1.81476500	-1.30422800
H	-2.35432600	0.70055200	0.33340500
O	-1.10263900	-2.44773500	-1.86114200
H	-0.96817700	-3.03150900	-1.09903600
H	-0.64665000	-1.59712300	-1.59606200
O	-3.35271500	-1.48334800	-3.04938700
H	-3.34850800	-1.73122700	-3.98519100
H	-2.59984100	-1.98541100	-2.65131900
⁴TS-reb_β			
Fe	1.16304200	0.04060900	0.44144800
N	-0.28521500	-0.77194400	1.61086300
N	1.77466600	-1.80217100	-0.08980800
N	2.47595500	0.85631000	-0.89131900
N	0.52562800	1.88602100	0.94041200
C	0.19386700	-3.14821500	1.22686800
C	3.57189800	-1.19711000	-1.65800200
C	1.98201000	3.22815300	-0.52341900
C	-1.19529800	1.28423300	2.59235000
C	-0.51647200	-2.10718800	1.81619000
C	1.27191300	-2.99656600	0.35815500
C	2.80700200	-2.11008200	-0.94057700
C	3.41089900	0.18284500	-1.63360300
C	2.67869700	2.19056200	-1.13058400
C	0.99480700	3.07918800	0.44655400
C	-0.42803200	2.20105800	1.87673800
C	-1.12729300	-0.09775300	2.45776800
C	-1.94202100	-1.03621000	3.19532600
C	-1.56778100	-2.28330900	2.79195900
C	2.01530000	-4.09187500	-0.21760300
C	2.96897100	-3.54175800	-1.01899500
C	4.21590200	1.12018000	-2.38332300
C	3.75937600	2.36509900	-2.07462900
C	0.31991800	4.17699500	1.09322000
C	-0.55772900	3.63314100	1.98419200
H	-0.08686500	-4.16138500	1.49900000
H	1.82047700	-5.13918000	-0.02418600
H	3.71583800	-4.04508500	-1.61966000
H	4.35691800	-1.59728800	-2.29206500
H	5.02467900	0.84517700	-3.04849200
H	4.11800200	3.32187700	-2.43290300

H	2.25022300	4.24175700	-0.80563200
H	0.50703900	5.22340900	0.88718500
H	-1.23720300	4.14301000	2.65579200
H	-1.90420100	1.68336600	3.31185300
H	-2.68269700	-0.76326500	3.93688000
H	-1.93805600	-3.24130500	3.13513700
O	-0.25674500	0.00596000	-1.32978900
S	2.87013900	-0.00316800	2.25299500
H	2.75718400	1.29363600	2.62115200
H	-4.95961600	0.73553400	1.05655800
C	-5.13279900	0.23963600	0.09372300
H	-6.09090200	0.58219000	-0.30326400
N	-4.12149200	0.74293200	-0.84509400
C	-2.67209400	0.48088000	-0.72282600
N	-4.49431800	1.43986000	-1.84751900
H	0.38826100	0.24874400	-2.01495600
H	-2.51985700	-0.59134600	-0.62637600
O	-3.52732700	1.80272900	-2.58288500
C	-2.03798200	0.99672100	-1.98866300
H	-1.42887000	1.88574200	-1.97078000
H	-1.96777500	0.32991900	-2.83241400
C	-5.09062600	-1.28321200	0.24079400
H	-4.21741900	-1.60524200	0.81704100
H	-5.98542600	-1.60782400	0.78201600
H	-5.06038500	-1.76151600	-0.74228800
H	-2.29703000	0.98766600	0.16836500
O	-1.18740000	-2.38445100	-1.90158300
H	-1.02568700	-2.90940100	-1.10289800
H	-0.73785300	-1.49770700	-1.70474800
O	-3.65728500	-1.64352600	-2.71858000
H	-3.79475300	-1.97715600	-3.61686800
H	-2.79642900	-2.04470300	-2.42875900
²P-OH_β			
Fe	-1.24229200	0.13351900	0.40707800
S	-3.06901400	0.14301800	1.68548300
H	-2.45833500	0.05088500	2.88899000
N	-1.89834600	1.68337300	-0.71912500
C	-2.46618300	3.82817900	-1.37016000
C	-3.06778400	2.97272100	-2.24258700
H	-2.50123300	4.91027100	-1.35582800
H	-3.69793200	3.20760500	-3.09103000
N	-2.10166800	-1.12351000	-0.91162000
C	-2.88674900	-0.81128200	-1.99492300
C	-3.39242400	-2.01458600	-2.61260400
C	-2.91357200	-3.05827200	-1.88516100
H	-4.02714700	-2.03686800	-3.48920400
H	-3.06804100	-4.11801200	-2.04175000
N	-0.40336500	-1.40481600	1.38451100
C	-0.64244700	-2.73556300	1.14370000
C	0.43695000	-1.35899600	2.47238000
C	0.07687000	-3.55017500	2.09387900

C	0.75280200	-2.69498000	2.91505900
H	0.05431500	-4.63244400	2.11908400
H	1.39520500	-2.93218000	3.75372100
N	-0.23839800	1.40116800	1.60906200
C	1.01576800	2.29334600	3.33569400
H	1.66299300	2.31825500	4.20324600
C	0.56662300	1.08965200	2.68051100
C	-1.74665800	3.01857300	-0.41771200
C	-2.72099600	1.63790100	-1.82313500
C	-2.11245100	-2.49435200	-0.82392500
C	0.89857700	-0.19783400	3.08044500
H	1.55257700	-0.30598400	3.94012000
C	-1.00957400	3.52710100	0.64306700
H	-0.97706900	4.60693000	0.75254000
C	-3.17259900	0.47504900	-2.43309100
H	-3.81522900	0.57944000	-3.30169600
C	-1.43849700	-3.24676500	0.12585800
H	-1.52685000	-4.32642700	0.05939100
C	0.46798400	3.33750900	2.65480900
H	0.57317200	4.39763700	2.84833700
C	-0.31249900	2.77289200	1.57967900
N	4.18767600	0.50422000	-1.41890800
C	2.80733100	0.15434700	-1.76976600
C	1.82264600	0.53738700	-0.65541000
H	2.72164500	-0.91839200	-1.97281100
H	2.56879900	0.69020600	-2.69454200
H	2.05901400	-0.00944900	0.25511500
H	1.85060800	1.61083500	-0.43612300
C	4.83549200	1.65498800	-2.06239400
C	6.26222400	1.91454300	-1.59103300
H	4.20880300	2.53695500	-1.87305900
H	4.81967700	1.48083100	-3.14660400
H	6.64763800	2.79034000	-2.12391400
H	6.30145800	2.11427200	-0.51712300
H	6.91562500	1.06399400	-1.79925600
N	4.89696200	-0.19951900	-0.55387700
O	4.30651800	-1.15346400	-0.02871100
O	0.48950400	0.13578900	-1.01647400
O	2.61923300	-3.53246700	-0.11562000
H	3.26820900	-2.80541100	-0.12927400
H	2.12624400	-3.40577400	0.71164900
H	0.11943100	0.75126400	-1.67339300
O	1.20007800	-2.54724500	-2.33267900
H	1.60815100	-3.04123000	-1.58748100
H	0.63440600	-1.89295100	-1.89237300
⁴P-OH_β			
Fe	1.41734100	-0.13415200	0.40765000
S	3.50884300	-0.09214900	1.63217700
H	3.03248900	-0.68410000	2.75119400
N	1.85733800	-1.71374900	-0.79777200
C	2.30274900	-3.86947500	-1.50660300

C	2.87953400	-3.02424400	-2.40555800
H	2.29945300	-4.95210100	-1.50534900
H	3.44676400	-3.27013800	-3.29424600
N	2.11977000	1.10268200	-1.00895200
C	2.82883500	0.75911000	-2.13715800
C	3.27806300	1.94299000	-2.82313400
C	2.82887000	3.00922500	-2.10548700
H	3.85261900	1.94153100	-3.74047300
H	2.95417700	4.06380200	-2.31340500
N	0.55998700	1.43756100	1.34455600
C	0.74521700	2.76617700	1.04795500
C	-0.19536700	1.40623900	2.49210100
C	0.07591300	3.59265800	2.02197800
C	-0.51171400	2.74766100	2.91751800
H	0.06864800	4.67508400	2.01031800
H	-1.09533000	2.99538100	3.79516200
N	0.42569300	-1.38104200	1.63798900
C	-0.73726800	-2.22063400	3.44945300
H	-1.32313500	-2.22052700	4.35981700
C	-0.29682100	-1.03701700	2.76038500
C	1.67914300	-3.04713800	-0.50107700
C	2.60955500	-1.68389500	-1.95106500
C	2.10632600	2.47904800	-0.97905600
C	-0.59190100	0.25801600	3.16330000
H	-1.18133900	0.38113800	4.06627200
C	1.01545200	-3.53947000	0.61246600
H	0.94896200	-4.61738800	0.72182700
C	3.06431200	-0.53497900	-2.58086600
H	3.64788400	-0.65557500	-3.48791200
C	1.47010400	3.25967100	-0.02664200
H	1.53052200	4.33690800	-0.13996200
C	-0.28448300	-3.28793500	2.73186700
H	-0.42172700	-4.34261200	2.93418100
C	0.43281000	-2.75844800	1.60236500
N	-4.50595600	-0.46376200	-1.22807900
C	-3.15269500	-0.12968000	-1.68378900
C	-2.07875300	-0.53892700	-0.66192200
H	-3.06882700	0.94390800	-1.87926900
H	-2.99551500	-0.65362600	-2.63204000
H	-2.23638500	0.00240700	0.27077800
H	-2.12092000	-1.61397400	-0.44575700
C	-5.21583900	-1.60178900	-1.82717400
C	-6.59818700	-1.85913700	-1.23735000
H	-4.58137800	-2.48994700	-1.70390600
H	-5.29265200	-1.41432600	-2.90656900
H	-7.03400400	-2.72667300	-1.74440900
H	-6.54584400	-2.07083900	-0.16627200
H	-7.26172400	-1.00273400	-1.37864500
N	-5.13493800	0.23245200	-0.29801700
O	-4.49867100	1.17682600	0.19024500
O	-0.77980100	-0.16489800	-1.12731800
O	-2.63979800	3.41727700	0.03307000

H	-3.32112400	2.72000800	0.04132600
H	-2.11684600	3.26521300	0.83646300
H	-0.41734900	-0.85837700	-1.70175800
O	-1.37023900	2.50553300	-2.31754500
H	-1.72015700	2.96871600	-1.52630600
H	-0.90792900	1.73611100	-1.94553000