

Electronic Supporting Information

**Regioselectivity of aliphatic versus aromatic hydroxylation by a
nonheme iron(II)-superoxo complex**

*Reza Latifi,^{a,b} Laleh Tahsini,^{a,b} Wonwoo Nam^{*b} and Sam P. de Visser^{*a}*

Address:

- (a) The Manchester Interdisciplinary Biocenter and the School of Chemical Engineering and Analytical Science, 131 Princess Street, Manchester M1 7DN, United Kingdom.
- (b) Department of Chemistry and Nano Science, Department of Bioinspired Science, Centre for Biomimetic Systems, Ewha Womans University, Seoul 120-750, Korea.

Email: sam.devisser@manchester.ac.uk; wwnam@ewha.ac.kr

Table S1. Group spin densities and charges of UB3LYP/B1 optimized geometries for the reaction of ^{2,4,6}FeOO(14TMC) with ethylbenzene.

(a) Spin densities

	ρ_{Fe}	ρ_{O1}	ρ_{O2}	ρ_{TMC}	ρ_{SubH}	Total
² R	2.00	-0.30	-0.61	-0.08	0.00	1.00
⁴ R	3.69	-0.21	-0.64	0.16	0.00	3.00
⁶ R	3.69	0.47	0.67	0.17	0.00	5.00
² TS _{arom}	1.93	-0.08	-0.51	-0.07	-0.27	1.00
⁴ TS _{arom}	3.65	0.15	-0.31	0.15	-0.64	3.00
⁶ TS _{arom}	3.68	0.20	0.43	0.16	0.53	5.00
² Int _{arom}	1.94	0.11	-0.08	-0.07	-0.90	1.00
⁴ Int _{arom}	3.66	0.14	-0.06	0.14	-0.88	3.00
⁶ Int _{arom}	3.68	0.17	0.08	0.16	0.91	5.00
	ρ_{Fe}	ρ_{O1}	ρ_{OH}	ρ_{TMC}	$\rho_{\text{Sub.}}$	Total
² TS _{aliph}	1.90	0.01	-0.34	-0.08	-0.50	1.00
⁴ TS _{aliph}	3.64	0.05	-0.36	0.17	-0.50	3.00
⁶ TS _{aliph}	3.66	0.19	0.29	0.15	0.71	5.00
² Int _{aliph}	1.94	0.13	-0.02	-0.06	-0.98	1.00
⁴ Int _{aliph}	3.67	0.18	-0.03	0.16	-0.98	3.00
⁶ Int _{aliph}	3.68	0.18	0.01	0.16	0.98	5.00

(b) Charges

	Q_{Fe}	Q_{O1}	Q_{O2}	Q_{TMC}	Q_{SubH}	Total
² R	0.59	-0.36	-0.21	0.95	0.03	1.00
⁴ R	0.70	-0.39	-0.17	0.85	0.01	1.00
⁶ R	0.69	-0.37	-0.20	0.85	0.02	1.00
² TS _{arom}	0.59	-0.41	-0.24	0.91	0.15	1.00
⁴ TS _{arom}	0.67	-0.46	-0.29	0.78	0.30	1.00
⁶ TS _{arom}	0.67	-0.46	-0.28	0.78	0.29	1.00
² Int _{arom}	0.58	-0.46	-0.34	0.89	0.33	1.00
⁴ Int _{arom}	0.67	-0.49	-0.33	0.78	0.37	1.00
⁶ Int _{arom}	0.68	-0.49	-0.33	0.79	0.35	1.00
	Q_{Fe}	Q_{O1}	Q_{OH}	Q_{TMC}	$Q_{\text{Sub.}}$	Total
² TS _{aliph}	0.60	-0.43	-0.02	0.92	-0.08	1.00
⁴ TS _{aliph}	0.72	-0.44	-0.02	0.78	-0.05	1.00
⁶ TS _{aliph}	0.67	-0.48	-0.01	0.77	0.05	1.00
² Int _{aliph}	0.58	-0.47	-0.06	0.90	0.05	1.00
⁴ Int _{aliph}	0.68	-0.48	-0.05	0.80	0.05	1.00
⁶ Int _{aliph}	0.68	-0.48	-0.05	0.80	0.05	1.00

Table S2. Group spin densities and charges of UB3LYP/B2 single points on UB3LYP/B1 optimized geometries for the reaction of ^{2,4,6}FeOO(14TMC) with ethylbenzene.

(a) Spin densities

	ρ_{Fe}	ρ_{O1}	ρ_{O2}	ρ_{TMC}	ρ_{SubH}	Total
² R	2.01	-0.30	-0.62	-0.09	0.00	1.00
⁴ R	3.75	-0.21	-0.64	0.10	0.00	3.00
⁶ R	3.75	0.45	0.66	0.14	0.00	5.00
² TS _{arom}	1.94	-0.08	-0.49	-0.08	-0.30	1.00
⁴ TS _{arom}	3.73	0.14	-0.28	0.10	-0.68	3.00
⁶ TS _{arom}	3.75	0.17	0.40	0.12	0.57	5.00
² Int _{arom}	1.96	0.11	-0.06	-0.07	-0.94	1.00
⁴ Int _{arom}	3.71	0.14	-0.05	0.11	-0.91	3.00
⁶ Int _{arom}	3.74	0.15	0.06	0.12	0.94	5.00
	ρ_{Fe}	ρ_{O1}	ρ_{OH}	ρ_{TMC}	$\rho_{\text{Sub.}}$	Total
² TS _{aliph}	1.91	0.01	-0.32	-0.08	-0.52	1.00
⁴ TS _{aliph}	3.69	0.03	-0.35	0.14	-0.52	3.00
⁶ TS _{aliph}	3.72	0.17	0.28	0.11	0.71	5.00
² Int _{aliph}	1.95	0.12	-0.02	-0.06	-0.99	1.00
⁴ Int _{aliph}	3.74	0.16	-0.03	0.12	-0.99	3.00
⁶ Int _{aliph}	3.74	0.15	0.00	0.12	0.99	5.00

(b) Charges

	Q_{Fe}	Q_{O1}	Q_{O2}	Q_{TMC}	Q_{SubH}	Total
² R	0.54	-0.19	-0.12	0.80	-0.03	1.00
⁴ R	0.58	-0.27	-0.08	0.79	-0.01	1.00
⁶ R	0.59	-0.22	-0.07	0.73	-0.03	1.00
² TS _{arom}	0.52	-0.19	-0.07	0.87	-0.13	1.00
⁴ TS _{arom}	0.57	-0.21	-0.10	0.77	-0.03	1.00
⁶ TS _{arom}	0.63	-0.20	-0.03	0.61	-0.01	1.00
² Int _{arom}	0.49	-0.33	-0.04	0.84	0.04	1.00
⁴ Int _{arom}	0.71	-0.39	-0.01	0.61	0.08	1.00
⁶ Int _{arom}	0.69	-0.37	-0.01	0.62	0.07	1.00
	Q_{Fe}	Q_{O1}	Q_{OH}	Q_{TMC}	$Q_{\text{Sub.}}$	Total
² TS _{aliph}	0.52	-0.27	0.13	0.85	-0.23	1.00
⁴ TS _{aliph}	0.67	-0.26	0.15	0.67	-0.23	1.00
⁶ TS _{aliph}	0.62	-0.33	0.20	0.64	-0.13	1.00
² Int _{aliph}	0.58	-0.34	0.07	0.77	-0.08	1.00
⁴ Int _{aliph}	0.68	-0.34	0.11	0.62	-0.07	1.00
⁶ Int _{aliph}	0.72	-0.37	0.11	0.62	-0.08	1.00

Table S3. Group spin densities and charges of UB3LYP/B2 Solvent single points on UB3LYP/B1 optimized geometries for the reaction of ^{2,4,6}FeOO(14TMC) with ethylbenzene.

(a) Spin densities

	ρ_{Fe}	ρ_{O1}	ρ_{O2}	ρ_{TMC}	ρ_{SubH}	Total
² R	2.02	-0.33	-0.60	-0.09	0.00	1.00
⁴ R	3.77	-0.23	-0.63	0.10	0.00	3.00
⁶ R	3.77	0.44	0.63	0.15	0.00	5.00
² TS _{arom}	1.96	-0.11	-0.49	-0.08	-0.28	1.00
⁴ TS _{arom}	3.74	0.12	-0.29	0.11	-0.68	3.00
⁶ TS _{arom}	3.76	0.16	0.40	0.12	0.56	5.00
² Int _{arom}	1.97	0.10	-0.06	-0.07	-0.94	1.00
⁴ Int _{arom}	3.73	0.13	-0.05	0.11	-0.92	3.00
⁶ Int _{arom}	3.75	0.13	0.06	0.12	0.94	5.00
	ρ_{Fe}	ρ_{O1}	ρ_{OH}	ρ_{TMC}	$\rho_{\text{Sub.}}$	Total
² TS _{aliph}	1.93	-0.01	-0.32	-0.08	-0.51	1.00
⁴ TS _{aliph}	3.71	0.00	-0.35	0.14	-0.51	3.00
⁶ TS _{aliph}	3.74	0.15	0.28	0.12	0.71	5.00
² Int _{aliph}	1.96	0.11	-0.02	-0.06	-0.99	1.00
⁴ Int _{aliph}	3.75	0.15	-0.03	0.12	-0.99	3.00
⁶ Int _{aliph}	3.75	0.14	0.00	0.12	0.99	5.00

(b) Charges

	Q_{Fe}	Q_{O1}	Q_{O2}	Q_{TMC}	Q_{SubH}	Total
² R	0.59	-0.22	-0.18	0.84	-0.03	1.00
⁴ R	0.62	-0.31	-0.12	0.83	-0.01	1.00
⁶ R	0.64	-0.26	-0.13	0.78	-0.02	1.00
² TS _{arom}	0.56	-0.19	-0.11	0.90	-0.16	1.00
⁴ TS _{arom}	0.59	-0.21	-0.14	0.79	-0.03	1.00
⁶ TS _{arom}	0.66	-0.20	-0.04	0.62	-0.04	1.00
² Int _{arom}	0.53	-0.33	-0.04	0.85	0.00	1.00
⁴ Int _{arom}	0.74	-0.40	0.00	0.63	0.04	1.00
⁶ Int _{arom}	0.72	-0.39	-0.01	0.64	0.03	1.00
	Q_{Fe}	Q_{O1}	Q_{OH}	Q_{TMC}	$Q_{\text{Sub.}}$	Total
² TS _{aliph}	0.56	-0.30	0.12	0.87	-0.25	1.00
⁴ TS _{aliph}	0.72	-0.30	0.12	0.70	-0.24	1.00
⁶ TS _{aliph}	0.67	-0.39	0.17	0.68	-0.13	1.00
² Int _{aliph}	0.61	-0.35	0.05	0.77	-0.08	1.00
⁴ Int _{aliph}	0.71	-0.34	0.09	0.63	-0.08	1.00
⁶ Int _{aliph}	0.75	-0.38	0.09	0.62	-0.08	1.00

Table S4. Absolute energies, zero-point energies and free energies of UB3LYP/B1 and UB3LYP/B2 calculated energies on UB3LYP/B1 optimized geometries.

	E _{B1} (au)	ZPE	G (au)	E _{B2} (au)	E _{B2,Solvent} (au)
⁴ R	-1355.945925	401.468	-1355.368187	-1356.549113	-1356.624263
⁴ TS _{aliph}	-1355.914628	398.570	-1355.339448	-1356.507685	-1356.579639
⁴ Int _{aliph}	-1355.938986	399.978	-1355.366381	-1356.540099	-1356.606680
² R	-1355.940284	404.221	-1355.357526	-1356.537864	-1356.614965
² TS _{aliph}	-1355.906719	398.506	-1355.328926	-1356.499550	-1356.570138
² Int _{aliph}	-1355.923775	401.378	-1355.346253	-1356.521553	-1356.588138
⁴ TS _{arom}	-1355.918810	401.180	-1355.341229	-1356.515437	-1356.581921
⁴ Int _{arom}	-1355.927241	406.273	-1355.342916	-1356.528753	-1356.593370
² TS _{arom}	-1355.903854	402.785	-1355.318413	-1356.497360	-1356.568256
² Int _{arom}	-1355.908598	403.045	-1355.327380	-1356.506149	-1356.573242
⁶ R	-1355.952382	401.845	-1355.377206	-1356.553215	-1356.629595
⁶ TS _{aliph}	-1355.926652	397.747	-1355.354004	-1356.523343	-1356.591883
⁶ Int _{aliph}	-1355.938205	399.942	-1355.365957	-1356.539065	-1356.605334
⁶ TS _{arom}	-1355.915165	401.238	-1355.338372	-1356.511639	-1356.576803
⁶ Int _{arom}	-1355.924727	401.451	-1355.346965	-1356.525627	-1356.591307

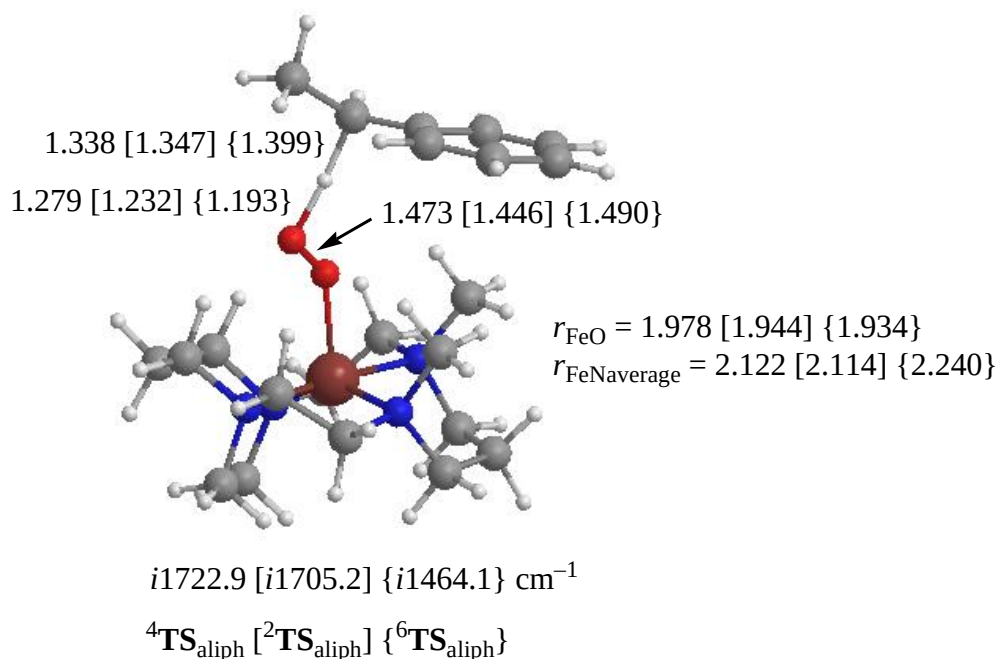


Figure S1. Optimized geometry of ${}^{4,2,6}\text{TS}_{\text{aliph}}$ as calculated with UB3LYP/B1 in Jaguar. Bond distances are in angstroms and the imaginary frequency in wave numbers.

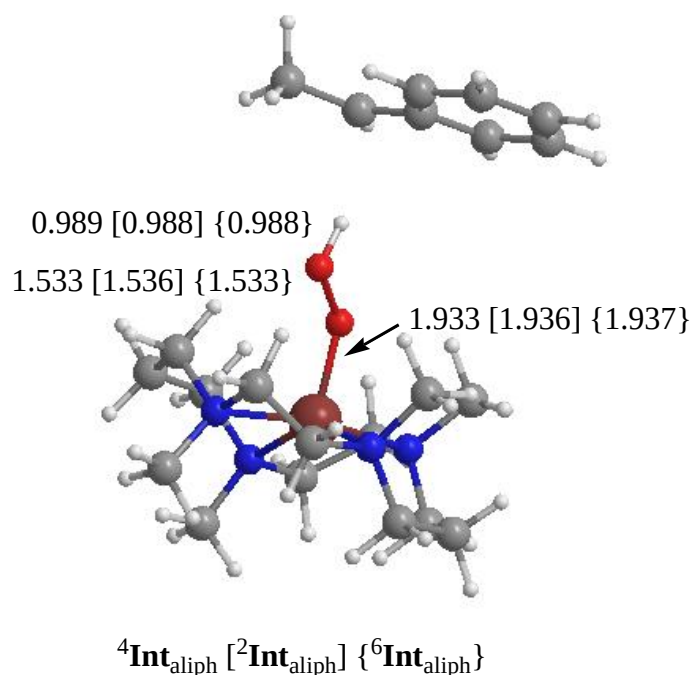


Figure S2. Optimized geometries of ${}^{4,2,6}\text{Int}_{\text{aliph}}$ as obtained at UB3LYP/B1 in Jaguar with bond lengths given in angstroms.

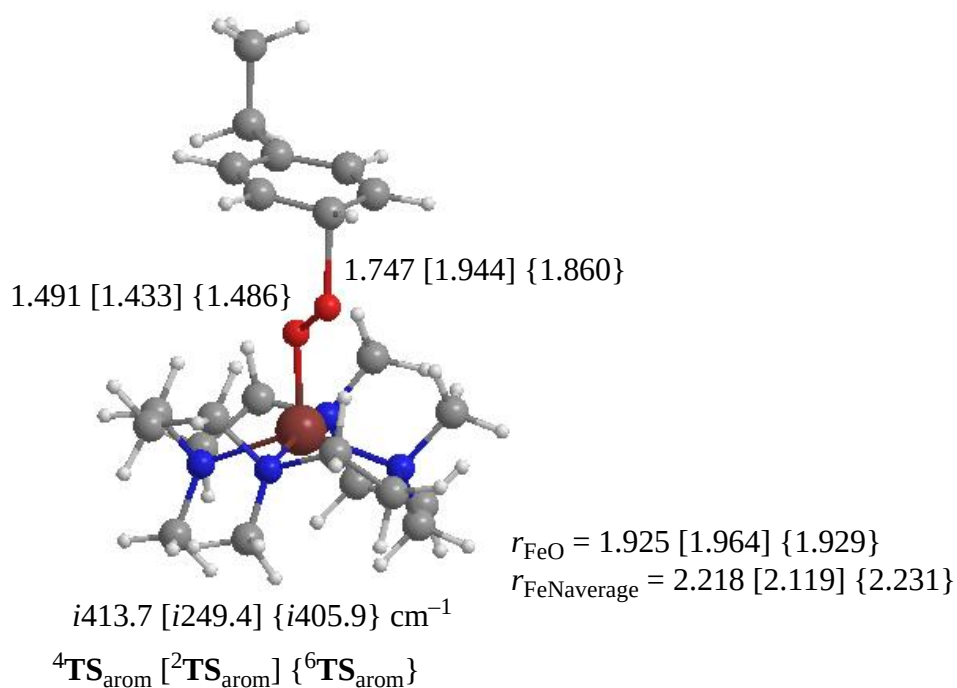


Figure S3. Optimized geometry of ${}^{4,2,6}\text{TS}_{\text{arom}}$ as calculated with UB3LYP/B1 in Jaguar. Bond distances are in angstroms and the imaginary frequency in wave numbers.

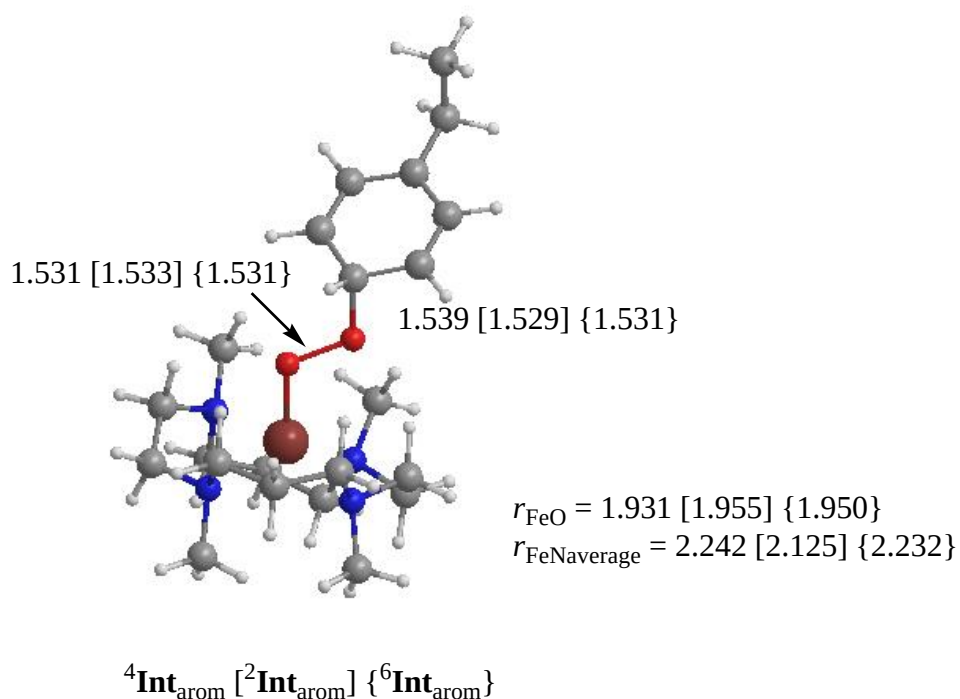


Figure S4. Optimized geometries of ${}^{4,2,6}\text{Int}_{\text{arom}}$ as obtained at UB3LYP/B1 in Jaguar with bond lengths given in angstroms.

Cartesian Coordinates:

⁴Re:

O	0.047577825	0.273990655	0.356042085
N	0.635648452	-0.207159560	3.314139992
C	3.051686723	-0.494826531	2.580467554
H	3.924107199	0.088942511	2.253703868
H	3.388510664	-1.115260073	3.416063805
C	1.959041674	0.461593700	3.048766865
H	2.307794639	0.989618441	3.951562159
H	1.754473615	1.215580661	2.281964023
C	0.648377832	-1.207929939	4.437496290
H	0.870735334	-0.696694296	5.389727594
H	1.470894465	-1.909197496	4.249585855
C	-0.668631949	-2.002153911	4.604185609
H	-1.494408288	-1.327162129	4.855762964
H	-0.534298843	-2.627095122	5.499778068
C	-1.095321812	-2.967824185	3.475001432
H	-0.278344109	-3.672926855	3.269432301
H	-1.949715150	-3.561238427	3.838535160
C	-0.350906332	0.898042626	3.553905737
H	0.014181128	1.571948386	4.342918704
H	-1.312623206	0.503694477	3.866020151
H	-0.487251996	1.458094881	2.626790315
O	-1.260832837	0.407197532	-0.098389282
N	-1.458414025	-2.326185547	2.154291449
C	-1.730973998	-3.353039244	1.071683380
H	-2.811860662	-3.525845159	0.990393986
H	-1.279348055	-4.303438317	1.370567058
C	-1.175111266	-2.889677358	-0.286473141
H	-1.517927328	-3.566559748	-1.084400200
H	-1.536808857	-1.880420565	-0.517437978
C	-2.659726157	-1.432613671	2.256811727
H	-3.556854895	-2.022352474	2.493895112
H	-2.795560593	-0.909330645	1.307056834
H	-2.522249125	-0.685041420	3.031535718
C	2.460320875	-1.735019092	-1.104365128
H	3.068384942	-2.647545642	-1.101567120
H	2.790027917	-1.183357045	-1.995484787
C	2.850546041	-0.839368798	0.098286510
H	3.926287404	-0.616724524	0.013820518
H	2.303563939	0.106736987	0.044628654
C	0.972516788	-2.078492692	-1.352650362
H	0.900921185	-2.661124937	-2.284453047
H	0.400051171	-1.160509702	-1.487876194
N	0.329020322	-2.853305022	-0.225673067
N	2.603872004	-1.427999899	1.480836473
C	3.338106840	-2.721261758	1.655846263
H	4.425041127	-2.565450028	1.598970420
H	3.098076266	-3.147003673	2.633778572
H	3.052928839	-3.437084309	0.893038046
C	0.855019626	-4.254557102	-0.185747848
H	1.910345853	-4.272027871	-0.446513831
H	0.742769584	-4.696419064	0.805389076
H	0.323886966	-4.882230488	-0.915051722
H	-2.668779955	5.050018105	0.128040783
C	-3.290404307	4.401119180	-0.473326900
C	-2.710608367	3.582330128	-1.452101358
C	-4.671336001	4.386158338	-0.264950684

C	-3.529765724	2.757225426	-2.227881856
H	-1.635635676	3.584648971	-1.602635257
C	-5.504493140	3.560464542	-1.033217788
H	-5.112562727	5.024736927	0.496521005
C	-4.910472390	2.746275299	-2.017694624
H	-3.090867607	2.120247956	-2.990749923
H	-5.539448417	2.101853182	-2.621433462
C	-7.010889477	3.573910983	-0.836392353
H	-7.251433389	3.828316863	0.213156115
H	-7.440886625	2.562384942	-1.012586308
C	-7.697914197	4.573266281	-1.786432665
H	-8.774512827	4.547780164	-1.625526084
H	-7.324765793	5.594012868	-1.619268044
H	-7.511069660	4.337416379	-2.835542396
Fe	0.368096138	-1.333783139	1.440813238

⁴TS_{aliph}:

O	0.002849830	-0.003592425	0.001224027
N	0.001162307	-0.003233490	2.753495992
C	2.529650094	-0.001410136	2.808479009
H	3.402786659	0.646264511	2.638400129
H	2.650260817	-0.435715897	3.806567543
C	1.260252853	0.835523719	2.751694490
H	1.254444720	1.539685446	3.599930760
H	1.220717467	1.418545913	1.827073732
C	-0.210335666	-0.776181761	4.035384240
H	-0.283245351	-0.072148160	4.881185753
H	0.675572070	-1.400610267	4.205628402
C	-1.470853620	-1.679225969	4.040016230
H	-2.376568909	-1.071383993	3.942164946
H	-1.529096979	-2.121826208	5.044566648
C	-1.515804865	-2.864794217	3.046880694
H	-0.675675116	-3.542525727	3.251699076
H	-2.443518383	-3.432703020	3.232920013
C	-1.112964646	0.989264372	2.531075752
H	-0.979663569	1.852875659	3.199795885
H	-2.086174059	0.554494362	2.741912911
H	-1.080860643	1.299510900	1.486670968
O	-0.449821404	-0.316844426	-1.364676949
N	-1.433309329	-2.486572936	1.587177250
C	-1.320095220	-3.701133868	0.690583015
H	-2.315897019	-4.039623767	0.372974910
H	-0.865750958	-4.521466433	1.253517064
C	-0.463379789	-3.334569534	-0.527515188
H	-0.398038059	-4.182431365	-1.227859013
H	-0.876553180	-2.471022943	-1.057261301
C	-2.642841993	-1.714922278	1.130073878
H	-3.534978397	-2.358909047	1.162706585
H	-2.481855661	-1.360046669	0.110284556
H	-2.822582900	-0.846702917	1.754140731
C	3.105805513	-1.768565237	-0.636369328
H	3.803335798	-2.565434251	-0.347961032
H	3.566580927	-1.294511311	-1.514489188
C	3.055538189	-0.676924401	0.458252765
H	4.076721846	-0.286441663	0.607114969
H	2.407541732	0.138102299	0.120032846
C	1.762271355	-2.353440465	-1.128722928

H	1.972486907	-3.131661374	-1.881475945
H	1.164937366	-1.570529523	-1.600638740
N	0.909009657	-2.952455892	-0.026625031
N	2.518632748	-1.137494972	1.809745190
C	3.401679749	-2.205428223	2.394855757
H	4.393046400	-1.791160453	2.635432855
H	2.952280954	-2.593177277	3.315119608
H	3.543282070	-3.031959167	1.706568564
C	1.568415420	-4.199635443	0.519252180
H	2.645808280	-4.159655707	0.369517689
H	1.373100407	-4.323494533	1.587622191
H	1.200835314	-5.088027585	-0.011207746
H	-6.225997814	-0.482249219	-1.825881023
C	-5.514191774	0.231662575	-1.417819403
C	-5.835069487	0.950087204	-0.248604544
C	-4.290127157	0.443781157	-2.068110966
C	-4.915765682	1.889208442	0.262561438
H	-6.791278768	0.793729739	0.243978688
C	-3.346755432	1.381166906	-1.564019232
H	-4.066579546	-0.110466244	-2.975631157
C	-3.687092559	2.094598282	-0.381683039
H	-5.167888690	2.468015160	1.148192531
H	-2.988826843	2.833572767	0.007904346
C	-2.029170523	1.590838682	-2.198682047
H	-1.237607553	0.629187916	-1.709827781
H	-1.490889236	2.460268444	-1.804421356
C	-1.858586355	1.416189329	-3.704652962
H	-0.803175601	1.507530915	-3.985018615
H	-2.213859420	0.440888284	-4.057963769
H	-2.420263402	2.189389611	-4.250778615
Fe	0.413816831	-1.430533485	1.307388925

⁴Int_{aliph}:

O	0.325733163	0.339668734	-0.710161018
N	-1.044231039	-2.088282777	-1.279767374
C	-2.872668111	-0.765889080	-2.462197595
H	-3.087685568	-0.270687361	-3.420399061
H	-3.677892248	-1.486754291	-2.295806859
C	-1.538914221	-1.498043898	-2.570869950
H	-1.634524931	-2.282489794	-3.340236080
H	-0.752283437	-0.810983681	-2.895215954
C	-1.901399680	-3.174948286	-0.699937392
H	-1.895387904	-4.054783139	-1.365522138
H	-2.933180615	-2.806406371	-0.662116899
C	-1.475944540	-3.632317186	0.716893838
H	-0.457810254	-4.033879780	0.697230520
H	-2.112741897	-4.492867922	0.963824473
C	-1.633383531	-2.645373726	1.896563346
H	-2.674838612	-2.302434306	1.948592057
H	-1.426674009	-3.194366579	2.829558954
C	0.357800682	-2.549831480	-1.537990001
H	0.391455068	-3.191941937	-2.430726492
H	0.740346187	-3.123508808	-0.697552742
H	0.983589370	-1.667345200	-1.670310082
O	1.163552646	1.261130936	0.183632398
N	-0.772926455	-1.407531946	1.847638044
C	-1.105066744	-0.428297759	2.952060020
H	-0.461130339	-0.620032137	3.820743596
H	-2.135284118	-0.606922570	3.271859554

C	-0.925941237	1.024463733	2.478814143
H	-1.012603851	1.704742924	3.340481723
H	0.059294925	1.167275230	2.026206933
C	0.693357757	-1.711760266	1.903343900
H	0.952285030	-2.162273335	2.872299930
H	1.254157949	-0.787357948	1.755956632
H	0.973370264	-2.395144127	1.107516415
C	-2.500581718	2.709577553	-0.667818002
H	-3.543961813	2.908827208	-0.395625109
H	-2.161424598	3.630603657	-1.161771536
C	-2.438068329	1.612603816	-1.757619479
H	-3.037064592	1.948085651	-2.619676201
H	-1.401217638	1.480428536	-2.079825586
C	-1.622175122	2.561871649	0.596908759
H	-1.734171086	3.476747441	1.202315676
H	-0.569519432	2.463283535	0.319664733
N	-1.967840968	1.357288838	1.441896136
N	-2.942669857	0.240014879	-1.336809504
C	-4.367899162	0.294842232	-0.884010814
H	-5.029883844	0.569699443	-1.717833432
H	-4.667370831	-0.686912836	-0.508548922
H	-4.496500052	1.018927812	-0.088828273
C	-3.283612434	1.543655390	2.127178817
H	-4.002754962	2.016276033	1.461848516
H	-3.699295642	0.588971430	2.455470903
H	-3.166992116	2.197352210	3.004135484
H	6.292179100	0.895760288	2.199040305
C	5.852556356	0.654816501	1.236120595
C	6.052036563	-0.618880552	0.677370662
C	5.105544774	1.615914104	0.562026289
C	5.494324427	-0.920420475	-0.578027493
H	6.641738076	-1.360510164	1.205725162
C	4.521467025	1.333044142	-0.711735232
H	4.972650528	2.597156151	1.004094228
C	4.745892785	0.030829662	-1.260867774
H	5.659598526	-1.897361361	-1.021773535
H	4.327639048	-0.201773954	-2.236571671
C	3.743019052	2.284494352	-1.430990274
H	1.971149387	1.384021426	-0.373536092
H	3.397554576	1.995012795	-2.422218147
C	3.511021575	3.706184074	-1.010972236
H	2.669774431	4.145587789	-1.556043907
H	3.301485072	3.801889133	0.061917741
H	4.390992204	4.337236009	-1.217064388
Fe	-1.321921383	-0.321111769	0.054472475

⁴TS_{arom}:

O	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	2.815908216
C	2.545245479	0.000000000	2.764453200
H	3.400051668	0.676867806	2.619344546
H	2.687074250	-0.477623079	3.737962873
C	1.259208975	0.819923719	2.771144802
H	1.294925414	1.516649291	3.625571877
H	1.181249782	1.414070956	1.856578215
C	-0.192611302	-0.823500807	4.053528671
H	-0.334872337	-0.165076002	4.927325417
H	0.726963684	-1.394624515	4.226654709
C	-1.389140853	-1.803544916	3.981627992

H	-2.325499867	-1.252005353	3.849765715
H	-1.469728850	-2.260998900	4.977243893
C	-1.324794967	-2.983258349	2.984382534
H	-0.408145672	-3.560663814	3.161692614
H	-2.174583420	-3.653518744	3.192901217
C	-1.131263384	0.955898289	2.592338926
H	-1.075900606	1.787554954	3.311008466
H	-2.090651923	0.461940180	2.725166339
H	-1.062846888	1.320303216	1.567421088
O	-0.579610221	-0.276768834	-1.345452461
N	-1.326890800	-2.618506327	1.520282848
C	-1.109097678	-3.817148326	0.624415862
H	-2.078604552	-4.235780688	0.323223755
H	-0.592214288	-4.589569963	1.200222003
C	-0.290756698	-3.435707154	-0.620901866
H	-0.299053214	-4.270697138	-1.338892509
H	-0.719818477	-2.558299682	-1.115133209
C	-2.581930700	-1.923496711	1.091526280
H	-3.444572635	-2.598810895	1.186471990
H	-2.473909237	-1.597712633	0.055348277
H	-2.755369743	-1.037723434	1.694665270
C	3.175061219	-1.659479712	-0.737672946
H	3.906118239	-2.433610007	-0.474491704
H	3.618115636	-1.138579420	-1.597578659
C	3.094836515	-0.598487591	0.385159920
H	4.105806680	-0.187814084	0.543003963
H	2.429534927	0.209265785	0.069454263
C	1.866451095	-2.295975556	-1.260557405
H	2.115664535	-2.944823565	-2.117038113
H	1.179836663	-1.518750755	-1.605956718
N	1.120893276	-3.099265959	-0.222111354
N	2.577506966	-1.096894149	1.725728866
C	3.435244693	-2.196344714	2.266640399
H	4.449815954	-1.828980426	2.478869322
H	2.999612720	-2.575143433	3.194620624
H	3.505972393	-3.016413747	1.561834493
C	1.847563367	-4.363538196	0.107558887
H	2.921935739	-4.193215044	0.129843636
H	1.544162020	-4.755534219	1.080498476
H	1.651381352	-5.128810527	-0.657956838
H	1.378448878	0.487229791	-3.427926892
C	0.995597235	1.201500306	-2.705793817
C	-0.415503106	1.141600271	-2.352076205
C	1.840087553	2.100037527	-2.086972809
C	-0.925266641	2.261316983	-1.574756077
H	-1.084954020	0.733101777	-3.108655794
C	1.345188339	3.073077907	-1.177932932
H	2.902447611	2.095337440	-2.320660399
C	-0.060891366	3.149207976	-0.973148062
H	-1.996505445	2.338438890	-1.422599501
H	-0.454186494	3.946218940	-0.346763305
C	2.282518668	4.058149957	-0.513703112
H	3.266269386	3.590637272	-0.371844683
H	1.903850121	4.311569934	0.485887557
C	2.464908536	5.365819778	-1.322444622
H	3.148028190	6.047605705	-0.803694685
H	2.877867653	5.157520079	-2.315409803
H	1.506944780	5.879674648	-1.457568025
Fe	0.466220400	-1.444042339	1.185149448

4Intarom:

O	-0.310999086	-0.331505447	-0.987109904
N	1.376214135	2.146406517	-0.829856775
C	2.976551148	0.824937505	-2.310845558
H	3.096115603	0.489755924	-3.351632600
H	3.886351863	1.376000858	-2.057252255
C	1.768325826	1.755296239	-2.229274966
H	1.976056737	2.653078097	-2.834877779
H	0.882737998	1.268574648	-2.649712325
C	2.421828963	2.900222544	-0.063234195
H	2.585031083	3.888933421	-0.524374160
H	3.363988622	2.347477799	-0.148119928
C	2.091894432	3.103206166	1.434079546
H	1.161976173	3.669569079	1.547211186
H	2.873914023	3.764164379	1.832419437
C	2.077779791	1.867045162	2.361461148
H	3.038130273	1.341354524	2.284113611
H	1.986127196	2.223069825	3.400414676
C	0.091242692	2.904569313	-0.943108043
H	0.185128396	3.717708493	-1.678343166
H	-0.188415923	3.345616451	0.010683346
H	-0.690049026	2.208171568	-1.251156094
O	-1.431277816	-0.718185586	-0.017535039
N	1.001337345	0.843472050	2.092956228
C	1.126799238	-0.365168075	2.992575356
H	0.489255056	-0.238521778	3.877356012
H	2.158394084	-0.426525213	3.349299435
C	0.739673520	-1.643109504	2.235393783
H	0.703266215	-2.494565663	2.934459403
H	-0.247250714	-1.533546241	1.775363716
C	-0.378357559	1.410196175	2.253153944
H	-0.545266709	1.718661694	3.295079094
H	-1.110638014	0.656257877	1.960450636
H	-0.518389095	2.268362096	1.603048845
C	2.143437600	-2.844244819	-1.198447092
H	3.142307304	-3.228206968	-0.959382912
H	1.705538462	-3.603892415	-1.860870375
C	2.260152269	-1.566244322	-2.061962659
H	2.853308045	-1.813581803	-2.958434442
H	1.260364766	-1.258867638	-2.380624967
C	1.252984632	-2.822836589	0.066268756
H	1.197745188	-3.848958648	0.466997097
H	0.243313948	-2.504170437	-0.198744392
N	1.739828984	-1.886625680	1.143945744
N	2.899933429	-0.366116174	-1.385954399
C	4.290784440	-0.676629900	-0.935213140
H	4.941901969	-0.897009038	-1.794303659
H	4.700756506	0.183281482	-0.399175036
H	4.300215445	-1.529724352	-0.267631024
C	3.009688414	-2.385520216	1.755111650
H	3.653958976	-2.830471256	1.000118267
H	3.562100285	-1.577859053	2.239143801
H	2.795291005	-3.162740017	2.504069577
H	-2.647648469	0.598069227	-2.262743557
C	-3.245683136	0.104472987	-1.504768082
C	-2.658063244	-1.104580451	-0.863414794
C	-4.470332842	0.597174519	-1.135550083
C	-3.568590544	-1.779676603	0.104378225

H	-2.232977889	-1.797723268	-1.601206183
C	-5.279585052	-0.046474787	-0.150482070
H	-4.852982436	1.497382585	-1.610410396
C	-4.786792899	-1.245552794	0.442956689
H	-3.221506722	-2.704231960	0.554254184
H	-5.411843252	-1.758497710	1.169616288
C	-6.647436105	0.489206167	0.198202347
H	-6.642908936	1.585088658	0.131331485
H	-6.890560461	0.236294269	1.238219781
C	-7.761558106	-0.063791274	-0.726919903
H	-8.735275209	0.351452840	-0.444740363
H	-7.568812629	0.197578777	-1.773360740
H	-7.822610605	-1.155562586	-0.658547083
Fe	1.250645335	0.120357527	0.055060378

⁶Re:

O	-0.184460906	0.088889744	-0.152286547
N	-0.020456582	0.144731249	2.808519399
C	2.503620579	-0.011550330	2.632333762
H	3.392233276	0.596636755	2.410423971
H	2.678786446	-0.479367095	3.604737135
C	1.278503626	0.894043845	2.702727435
H	1.397452122	1.584629551	3.553405217
H	1.195363472	1.500966818	1.796298954
C	-0.183001169	-0.646879411	4.076158300
H	-0.233455536	0.039973065	4.937357720
H	0.716386052	-1.260072479	4.206699180
C	-1.426063386	-1.566856877	4.108569125
H	-2.341952656	-0.975229416	4.015275095
H	-1.464481925	-1.988123750	5.122478292
C	-1.473993566	-2.777983722	3.149977516
H	-0.566756214	-3.383559953	3.277147233
H	-2.327917628	-3.410877211	3.440217123
C	-1.114686257	1.154587954	2.628609757
H	-0.989392349	1.981076538	3.343386952
H	-2.092774571	0.711164568	2.790997072
H	-1.079518895	1.534925603	1.607669752
O	-1.204423947	-0.203016492	-1.049334688
N	-1.579251765	-2.450633073	1.680057445
C	-1.495322499	-3.682076061	0.805310738
H	-2.505165691	-4.049200667	0.581531930
H	-0.984238623	-4.471648876	1.362864922
C	-0.749543697	-3.362871846	-0.499935133
H	-0.842208614	-4.203819729	-1.203656301
H	-1.177284473	-2.470453345	-0.969938295
C	-2.848929196	-1.720414737	1.349365216
H	-3.717750488	-2.359370257	1.559956898
H	-2.840177099	-1.437486232	0.296705601
H	-2.938834086	-0.805649462	1.926388917
C	2.786187220	-1.768611539	-0.872918383
H	3.496059752	-2.567703104	-0.629448283
H	3.204500272	-1.286772614	-1.767186191
C	2.814229131	-0.682656811	0.229121329
H	3.845124957	-0.301998020	0.305578486
H	2.165987575	0.150157119	-0.061156949
C	1.427106310	-2.363622071	-1.307404527
H	1.601634712	-3.056982110	-2.145783224
H	0.771494341	-1.568221389	-1.664481971
N	0.700059404	-3.081570047	-0.197025275

N	2.377836149	-1.128584268	1.620651371
C	3.211089784	-2.271865834	2.110241869
H	4.258530518	-1.962591993	2.235005067
H	2.829017003	-2.610901627	3.076283214
H	3.175991735	-3.103229449	1.416671956
C	1.381747863	-4.372517213	0.135949176
H	2.462489418	-4.264968670	0.070944554
H	1.131141403	-4.706301800	1.144438842
H	1.085567662	-5.153857347	-0.578447044
H	-6.126711705	-0.424102563	-0.125570500
C	-5.505259391	0.452126282	0.036488451
C	-5.563568434	1.136272379	1.258334948
C	-4.663652026	0.907060796	-0.985447171
C	-4.776366114	2.280168412	1.444810093
H	-6.229963467	0.795526084	2.045028782
C	-3.867389193	2.054437333	-0.813808157
H	-4.627053254	0.374286021	-1.931907313
C	-3.938318627	2.732405601	0.416876265
H	-4.830900957	2.830732387	2.379713287
H	-3.343182849	3.630538059	0.562437733
C	-2.997683541	2.569486656	-1.945452936
H	-2.592365740	1.719591336	-2.506544669
H	-2.133441792	3.102168280	-1.528225065
C	-3.761667523	3.510916403	-2.903502141
H	-3.105525545	3.862608451	-3.707923730
H	-4.615179261	2.997638913	-3.361284765
H	-4.147452552	4.387640377	-2.370767616
Fe	0.223336896	-1.345628719	1.201759331

⁶TS_{aliph}:

O	-0.006927627	0.026055162	0.013206380
N	-0.011897043	-0.009274700	2.972550095
C	2.529019690	-0.005437018	2.989841153
H	3.384833672	0.668515988	2.835177997
H	2.670674614	-0.470434354	3.969376703
C	1.242634401	0.818761994	2.992008750
H	1.254471310	1.483609493	3.871939968
H	1.194500810	1.450390943	2.099671600
C	-0.201623200	-0.870196591	4.187931996
H	-0.329989279	-0.231446585	5.078473340
H	0.716231785	-1.450498779	4.337335181
C	-1.400216941	-1.845049327	4.102963810
H	-2.333491939	-1.293569461	3.950783314
H	-1.497586747	-2.296970538	5.099794504
C	-1.313809041	-3.029380595	3.112567454
H	-0.403874018	-3.607729288	3.318782248
H	-2.170170832	-3.696312055	3.306720463
C	-1.146682443	0.946823388	2.775689960
H	-1.115930286	1.741206052	3.537219865
H	-2.105651355	0.440813363	2.852655514
H	-1.065902252	1.373107151	1.775654347
O	-0.594305218	-0.476735217	-1.260595831
N	-1.284272308	-2.673803232	1.647922181
C	-1.071663799	-3.888589632	0.772831768
H	-2.040379256	-4.294558910	0.451391545
H	-0.578392453	-4.663466695	1.366203186
C	-0.222588544	-3.521804873	-0.454280060
H	-0.192586987	-4.372486885	-1.154084947
H	-0.657185517	-2.663961828	-0.978007931

C	-2.536052555	-1.983968032	1.197421852
H	-3.409549241	-2.634810723	1.350861996
H	-2.441812383	-1.732654201	0.139853513
H	-2.685216216	-1.054570103	1.738935439
C	3.223592239	-1.699489646	-0.480949960
H	3.956050074	-2.459164046	-0.182657490
H	3.686941677	-1.182648029	-1.332698426
C	3.091676047	-0.626979124	0.627254304
H	4.090271837	-0.190778371	0.798528608
H	2.425086646	0.168830100	0.279391886
C	1.942180229	-2.365885228	-1.037549796
H	2.232653001	-3.033594534	-1.866018516
H	1.273363075	-1.603205405	-1.445539645
N	1.161311560	-3.147236257	-0.009082919
N	2.548857090	-1.112319407	1.963707877
C	3.385260956	-2.217792795	2.524985916
H	4.403656121	-1.864628359	2.746733998
H	2.932669151	-2.581093463	3.451374995
H	3.452502905	-3.046104953	1.831029822
C	1.891727533	-4.391033930	0.390332209
H	2.966781066	-4.222438508	0.393892984
H	1.593572413	-4.727462728	1.385699213
H	1.691115013	-5.199104489	-0.328661613
H	-6.416526041	-0.330085218	-0.646721375
C	-5.588223958	0.353715158	-0.489330115
C	-5.607705944	1.234194662	0.604337719
C	-4.519001754	0.363637593	-1.386499003
C	-4.544616108	2.132264365	0.790988358
H	-6.447070949	1.231299859	1.292236883
C	-3.433504447	1.261429140	-1.214211227
H	-4.525728774	-0.317139388	-2.230900061
C	-3.472930065	2.143025910	-0.101172037
H	-4.565124971	2.831400434	1.621407483
H	-2.660044495	2.851106248	0.034765393
C	-2.281626387	1.288694433	-2.114348399
H	-1.386406050	0.356978133	-1.577760988
H	-1.646690067	2.171508295	-1.991050400
C	-2.379466263	0.793211316	-3.545978519
H	-1.392560116	0.791922479	-4.017900489
H	-2.779584659	-0.224682745	-3.611288793
H	-3.036886445	1.444763720	-4.139738261
Fe	0.424682332	-1.371663553	1.277999671

⁶Int_{aliph}:

O	0.275701665	0.519674071	-0.724082223
N	-0.904056363	-2.041368060	-1.205912585
C	-2.759958023	-0.810834332	-2.460592026
H	-2.967099605	-0.347919848	-3.436736185
H	-3.533158673	-1.568326786	-2.304594308
C	-1.389133711	-1.479324083	-2.515761150
H	-1.421232464	-2.272221694	-3.281330111
H	-0.625089474	-0.757378810	-2.818252304
C	-1.725528248	-3.157271688	-0.630131343
H	-1.668366770	-4.044818531	-1.282516910
H	-2.772733394	-2.832813569	-0.617567926
C	-1.305602209	-3.575143629	0.800990224
H	-0.272692156	-3.937514339	0.802428416
H	-1.912855875	-4.455241763	1.053341769
C	-1.516964157	-2.576352374	1.962774244

H	-2.573796829	-2.282204028	2.002694870
H	-1.291447611	-3.100077150	2.905798891
C	0.524133299	-2.439888732	-1.425115743
H	0.612069943	-3.070118430	-2.322407643
H	0.906090096	-3.006572986	-0.579709127
H	1.114037691	-1.529319159	-1.533153563
O	1.133665274	1.361096615	0.227162965
N	-0.715967916	-1.299076671	1.898631783
C	-1.106581347	-0.320964063	2.984450324
H	-0.460427765	-0.465347042	3.860610629
H	-2.128546498	-0.547569041	3.300610076
C	-0.999677699	1.130470616	2.489257634
H	-1.144212563	1.819688681	3.336093655
H	-0.015786249	1.319790153	2.052477792
C	0.762670572	-1.531977379	1.969996522
H	1.037825149	-1.936488756	2.954610108
H	1.279806717	-0.587710480	1.791002665
H	1.077970884	-2.230414326	1.200859179
C	-2.608149397	2.699385894	-0.704225846
H	-3.662370953	2.850938732	-0.443239731
H	-2.306856265	3.635078960	-1.195184719
C	-2.483170614	1.605011614	-1.791332909
H	-3.093406628	1.906823334	-2.658384447
H	-1.438364814	1.526538885	-2.103561019
C	-1.738365227	2.596565881	0.571600277
H	-1.900710280	3.507267795	1.171596829
H	-0.679606589	2.546375925	0.306839692
N	-2.035471557	1.382995065	1.424540059
N	-2.920160975	0.214450874	-1.361934364
C	-4.360073646	0.196367089	-0.955459639
H	-5.009823481	0.400429699	-1.818960065
H	-4.612464371	-0.787574540	-0.552049487
H	-4.559785244	0.940183829	-0.193411753
C	-3.375734079	1.499348160	2.077194641
H	-4.106580692	1.916791172	1.388857981
H	-3.739531804	0.525337372	2.410180013
H	-3.319350876	2.170641453	2.946688157
H	6.117929145	0.373127557	2.084954391
C	5.653536268	0.271680847	1.108935384
C	5.698778586	-0.963233991	0.439986685
C	5.030150975	1.371381979	0.527349221
C	5.112292448	-1.083777495	-0.832883374
H	6.194541561	-1.813514916	0.896388952
C	4.418223445	1.273952047	-0.761130189
H	5.016997915	2.319278697	1.054128423
C	4.485452334	0.006962712	-1.423972482
H	5.162104697	-2.030165521	-1.362800017
H	4.046187869	-0.086427864	-2.413570378
C	3.760579461	2.371427324	-1.386686011
H	1.935575214	1.513228495	-0.329893632
H	3.380958444	2.212282047	-2.394632312
C	3.694091639	3.767478899	-0.841337013
H	2.899606138	4.342243665	-1.327585298
H	3.511462933	3.791988558	0.240258146
H	4.635754696	4.314049208	-1.013953191
Fe	-1.300433718	-0.275433456	0.073892963

⁶TS_{arom}:

O	0.001074071	-0.000970542	0.012865440
---	-------------	--------------	-------------

N	0.009402963	0.011046522	3.001990605
C	2.557505641	0.016675332	2.943103876
H	3.404941566	0.695188144	2.766237998
H	2.724942052	-0.443864043	3.920836606
C	1.266675255	0.835130157	2.970284616
H	1.305401159	1.513344609	3.839332758
H	1.188483979	1.451157988	2.069343310
C	-0.162715538	-0.841576993	4.224835806
H	-0.283768889	-0.199548111	5.113905424
H	0.758810857	-1.418136667	4.365985957
C	-1.362482632	-1.819285524	4.158481756
H	-2.299245125	-1.267346966	4.032232180
H	-1.435253882	-2.282841628	5.151760570
C	-1.300744862	-2.991243128	3.150735803
H	-0.385120485	-3.572067291	3.322620591
H	-2.151127373	-3.661833469	3.356951670
C	-1.125178890	0.972229801	2.813182990
H	-1.040161468	1.810166517	3.521542455
H	-2.082358187	0.484515651	2.984746759
H	-1.094083781	1.336320295	1.784727531
O	-0.808378350	-0.436872263	-1.155144836
N	-1.311372261	-2.611803970	1.691866083
C	-1.135067098	-3.798309560	0.775726107
H	-2.115788487	-4.188727212	0.473904198
H	-0.628528828	-4.593805663	1.330200804
C	-0.313850054	-3.410099071	-0.468610864
H	-0.323743224	-4.240407858	-1.192785288
H	-0.747401884	-2.530202283	-0.955401070
C	-2.573597680	-1.898347791	1.302443182
H	-3.446265815	-2.548574083	1.461823961
H	-2.505672055	-1.603421009	0.253484959
H	-2.696135649	-0.990477215	1.886271983
C	3.168948304	-1.660935830	-0.556074715
H	3.890321417	-2.444029525	-0.292818935
H	3.624066035	-1.137179304	-1.408019325
C	3.094430599	-0.607546779	0.575855263
H	4.112386483	-0.214436374	0.736278575
H	2.449657715	0.216305166	0.255297488
C	1.856111959	-2.280540192	-1.094586656
H	2.107045730	-2.924124812	-1.954642920
H	1.188107014	-1.491679899	-1.449040495
N	1.094564915	-3.076568776	-0.063755949
N	2.561436283	-1.092487449	1.918913226
C	3.389602330	-2.209630253	2.466839369
H	4.412646846	-1.866758437	2.681523333
H	2.941048152	-2.573754864	3.394900685
H	3.442654628	-3.034383366	1.766187756
C	1.805559945	-4.352822580	0.261839410
H	2.884536304	-4.210869321	0.243244386
H	1.525882614	-4.724174814	1.250342394
H	1.564631505	-5.125130265	-0.484290207
H	0.541235787	1.076751256	-3.308678836
C	-0.080312191	1.607764895	-2.594906280
C	-1.329361577	1.015698043	-2.192839357
C	0.354694789	2.786389611	-2.019722747
C	-2.187369079	1.795796156	-1.340226500
H	-1.798870517	0.307048552	-2.871488124
C	-0.450733332	3.492546692	-1.090180675
H	1.320406488	3.200222873	-2.299013285

C	-1.733435131	2.974518316	-0.776696345
H	-3.171249707	1.408061918	-1.096976074
H	-2.377918078	3.536321743	-0.105014134
C	0.011924211	4.811981040	-0.514386303
H	1.105583971	4.815046611	-0.419912830
H	-0.401826304	4.945959379	0.493617048
C	-0.411973503	6.016548848	-1.393749394
H	-0.065539006	6.956902445	-0.950816136
H	0.014530561	5.934748179	-2.399737481
H	-1.502092598	6.064904820	-1.493070792
Fe	0.425907459	-1.361561731	1.312659914

⁶Int_{arom}:

O	-0.313676193	-0.113595759	-0.978725653
N	1.483760944	2.177529092	-0.826316331
C	2.998190366	0.741304839	-2.311436693
H	3.095998604	0.411395163	-3.356274651
H	3.936746864	1.240573616	-2.055060689
C	1.844373408	1.739063107	-2.222776479
H	2.096997142	2.615169544	-2.842461536
H	0.927520056	1.299146316	-2.627659900
C	2.566504568	2.881881473	-0.064883010
H	2.788245644	3.854408072	-0.535573484
H	3.476463496	2.275207779	-0.135205573
C	2.231789802	3.122690463	1.427318582
H	1.333744390	3.741749094	1.520622582
H	3.044358875	3.744688121	1.827112406
C	2.137053114	1.904618888	2.375451276
H	3.076505090	1.338583746	2.336459473
H	2.030043539	2.284406557	3.404311188
C	0.241521231	3.003402315	-0.954701648
H	0.375888811	3.787098792	-1.714873720
H	-0.005768591	3.489647803	-0.013984289
H	-0.576167274	2.338506119	-1.235948366
O	-1.409858023	-0.688282216	-0.078262047
N	1.028699803	0.918418102	2.094417768
C	1.092792953	-0.287201691	3.003708483
H	0.459289493	-0.122460312	3.885301880
H	2.119531659	-0.394843371	3.363640044
C	0.645501154	-1.549822470	2.255207060
H	0.580011715	-2.396332308	2.957690768
H	-0.337518913	-1.401135941	1.799988762
C	-0.335820484	1.530546989	2.209635002
H	-0.529262015	1.838546441	3.246950069
H	-1.082910778	0.803267447	1.886358798
H	-0.422108241	2.397495185	1.561866780
C	1.951410970	-2.868083237	-1.181308038
H	2.921664461	-3.320714995	-0.944580893
H	1.452164087	-3.605082213	-1.825627550
C	2.150458590	-1.615284866	-2.067255995
H	2.722960064	-1.913201751	-2.961591748
H	1.172819440	-1.241618271	-2.382623851
C	1.076092704	-2.763703157	0.090492971
H	0.959408083	-3.776664132	0.510771758
H	0.084209811	-2.384751484	-0.164671303
N	1.625783577	-1.843476800	1.155508462
N	2.868676307	-0.457215309	-1.400401198
C	4.250018296	-0.844680219	-0.979710262
H	4.878457199	-1.061747619	-1.856098680

H	4.705026347	-0.024497067	-0.418337618
H	4.231405336	-1.722955781	-0.345594135
C	2.875713528	-2.397848373	1.759877045
H	3.497612145	-2.867464749	1.001948094
H	3.463020876	-1.614701125	2.243246844
H	2.630191738	-3.166028533	2.508211866
H	-2.706888750	0.907910183	-2.077940959
C	-3.276926800	0.266789918	-1.414869022
C	-2.619052530	-0.994243833	-0.965308197
C	-4.532579378	0.620705893	-0.993628581
C	-3.493535849	-1.861390363	-0.120677725
H	-2.173561038	-1.542892814	-1.807090624
C	-5.307561597	-0.215069337	-0.133591797
H	-4.966280171	1.560039334	-1.328289213
C	-4.743933063	-1.460540582	0.275152844
H	-3.093086647	-2.821404530	0.189130344
H	-5.340026311	-2.115871614	0.905506915
C	-6.708540138	0.174006503	0.273747716
H	-6.781636841	1.266812662	0.349137431
H	-6.929004033	-0.227371331	1.271551623
C	-7.785673111	-0.333111343	-0.718836825
H	-8.785197700	-0.028604532	-0.389296627
H	-7.617546119	0.073977536	-1.722077694
H	-7.768441988	-1.426223247	-0.792150368
Fe	1.304609596	0.167086977	0.071850651

²Re:

O	-0.100579396	0.100472790	-0.049536401
N	0.075771641	0.132948774	2.698306437
C	2.585513566	-0.014054885	2.523250706
H	3.484675301	0.569723971	2.278558140
H	2.753682081	-0.4511004057	3.511401892
C	1.373060115	0.892153236	2.548843716
H	1.476854205	1.625499965	3.362715110
H	1.275529405	1.442862692	1.609460971
C	-0.068470882	-0.575880781	4.022465805
H	-0.034506888	0.165692904	4.835954976
H	0.798285345	-1.234946702	4.144626337
C	-1.363551487	-1.405345639	4.163194546
H	-2.241702157	-0.754254660	4.114681380
H	-1.363954289	-1.805909699	5.185984186
C	-1.548549166	-2.615867708	3.225488400
H	-0.721512305	-3.322947455	3.368543433
H	-2.476258071	-3.137355175	3.509685955
C	-0.998526455	1.175846550	2.519994254
H	-0.766554214	2.049766065	3.143105796
H	-1.971554487	0.802129429	2.816612674
H	-1.030539294	1.457144327	1.468770924
O	-0.936258954	-0.140439138	-1.127032448
N	-1.591756841	-2.283670987	1.755275980
C	-1.629852485	-3.521865797	0.887009021
H	-2.668711087	-3.815682094	0.691792436
H	-1.158787916	-4.346877682	1.427957585
C	-0.895987728	-3.225544368	-0.418755493
H	-0.947127996	-4.084609445	-1.103346401
H	-1.307899982	-2.343804103	-0.918174434
C	-2.797827367	-1.460486575	1.398829494
H	-3.709533613	-2.053073452	1.550317995
H	-2.735695580	-1.145487049	0.357389604

H	-2.866098527	-0.567744091	2.006364953
C	2.711032852	-1.843586681	-0.928351580
H	3.387592076	-2.677460784	-0.705514809
H	3.103331161	-1.408895833	-1.857734700
C	2.852366729	-0.745992594	0.145861831
H	3.907954578	-0.433100182	0.187467541
H	2.245910456	0.119434755	-0.131590469
C	1.297121760	-2.360281165	-1.265230527
H	1.383748834	-3.150652636	-2.026693892
H	0.683693783	-1.558716043	-1.676568217
N	0.539181573	-2.910736125	-0.076109107
N	2.427724174	-1.157285791	1.548177191
C	3.302152093	-2.263711816	2.064046203
H	4.323202127	-1.892318168	2.230311789
H	2.903610838	-2.631095053	3.012677557
H	3.352548383	-3.089054577	1.364455062
C	1.190966433	-4.172261294	0.430425373
H	2.252531160	-4.171430257	0.199814478
H	1.070543656	-4.276203246	1.510380829
H	0.749779155	-5.047387089	-0.061305828
H	-6.098510715	-0.721653880	-0.712244754
C	-5.509019992	0.119770773	-0.359651924
C	-5.665690750	0.584662881	0.953253521
C	-4.605136102	0.747471931	-1.226225777
C	-4.913840777	1.685446578	1.387180498
H	-6.379286066	0.110987334	1.620611351
C	-3.843514845	1.853054421	-0.805581149
H	-4.491422266	0.383562815	-2.243862571
C	-4.013935050	2.311014311	0.514347855
H	-5.045553057	2.069696011	2.395091636
H	-3.447898200	3.175983325	0.852152531
C	-2.904114406	2.561323593	-1.764573738
H	-2.519126830	1.841738981	-2.495941646
H	-2.028753216	2.931169334	-1.215553925
C	-3.581053303	3.739071356	-2.499218651
H	-2.877800059	4.223754622	-3.185817292
H	-4.442763739	3.395031696	-3.081949435
H	-3.939280458	4.493801113	-1.789953503
Fe	0.272474239	-1.362979946	1.275138778

²TS_{aliph}:

O	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	2.724348304
C	2.529473876	0.000000000	2.675511929
H	3.395671853	0.649392791	2.478616227
H	2.690831604	-0.449182761	3.661109094
C	1.259156695	0.837391628	2.686786717
H	1.287474326	1.527026377	3.546275944
H	1.184283876	1.434851895	1.773560378
C	-0.183570249	-0.780783143	4.002389294
H	-0.245026477	-0.088391843	4.859062704
H	0.708197331	-1.403183148	4.151900117
C	-1.442230034	-1.686008052	4.008924808
H	-2.351748731	-1.078922118	3.946213016
H	-1.480063957	-2.159627862	5.000219039
C	-1.504627243	-2.839220395	2.978986958
H	-0.648081755	-3.510906671	3.134479814
H	-2.415960372	-3.428151931	3.176682812
C	-1.115287493	1.000618589	2.538669852

H	-0.928824442	1.885506612	3.164642984
H	-2.077870929	0.590207407	2.833381761
H	-1.143586516	1.280849939	1.485126443
O	-0.520100672	-0.228087607	-1.330092184
N	-1.478707922	-2.421779996	1.525020748
C	-1.428092195	-3.628263091	0.605041222
H	-2.442132856	-3.916879968	0.298930548
H	-1.001431811	-4.477762508	1.147681183
C	-0.578479389	-3.273565734	-0.619253662
H	-0.551293082	-4.113683626	-1.331327898
H	-0.976609215	-2.390778113	-1.127618197
C	-2.699505259	-1.631692126	1.139899499
H	-3.606803868	-2.233059743	1.302902745
H	-2.631713294	-1.355777750	0.086315321
H	-2.777751013	-0.714602182	1.711461451
C	3.006661262	-1.750659321	-0.790886106
H	3.706636473	-2.554023316	-0.525422427
H	3.445281781	-1.277145673	-1.680648587
C	2.996754019	-0.661974616	0.306410834
H	4.029097385	-0.295616949	0.440708383
H	2.362267742	0.169464408	-0.013040582
C	1.647662848	-2.329142758	-1.249210085
H	1.837951884	-3.102722282	-2.012371755
H	1.045638450	-1.540949918	-1.705213111
N	0.811912333	-2.933772217	-0.136539770
N	2.472360273	-1.120870273	1.659652563
C	3.334474348	-2.219988574	2.220217501
H	4.333998683	-1.831150518	2.468352464
H	2.880719650	-2.618469263	3.133719443
H	3.458733199	-3.034120378	1.514257713
C	1.459163489	-4.204645886	0.362635142
H	2.539870244	-4.156026048	0.240655351
H	1.238306331	-4.381643165	1.419301756
H	1.104583055	-5.066489024	-0.219179080
H	-6.133043230	-1.163411063	-2.665400515
C	-5.604592315	-0.430862082	-2.059728116
C	-6.197870552	0.061151059	-0.878973544
C	-4.342784199	0.031599880	-2.467868305
C	-5.514126171	1.026337470	-0.111585384
H	-7.181238816	-0.287242082	-0.573440723
C	-3.637487710	1.002419634	-1.706728835
H	-3.908306624	-0.350053338	-3.387989817
C	-4.250740596	1.485604387	-0.518849304
H	-5.975476292	1.431299155	0.786398864
H	-3.740150950	2.249730207	0.066080212
C	-2.285253645	1.483026836	-2.093379925
H	-1.386440940	0.601504524	-1.613115334
H	-1.989851153	2.384701217	-1.540503703
C	-1.916518268	1.569546962	-3.576485774
H	-0.878117795	1.900816681	-3.692221304
H	-2.012995089	0.603088853	-4.087114306
H	-2.562054954	2.287716422	-4.103693740
Fe	0.366815389	-1.438859594	1.254974313

²Int_{aliph}:

O	0.242207956	0.548682967	-0.709429049
N	-0.893825173	-1.888295026	-1.129031640
C	-2.802199795	-0.843867612	-2.406365871
H	-3.068383562	-0.403470708	-3.378683701

H	-3.530070537	-1.636477228	-2.211243970
C	-1.404379845	-1.424270011	-2.471794874
H	-1.387178560	-2.257436226	-3.191332571
H	-0.685010023	-0.673030594	-2.808106471
C	-1.666408573	-3.048034736	-0.550716528
H	-1.604914988	-3.905211583	-1.239932645
H	-2.719638504	-2.750961983	-0.493058824
C	-1.189708476	-3.504589583	0.846214376
H	-0.155888810	-3.860666911	0.799220783
H	-1.783061671	-4.394063486	1.098369779
C	-1.360237632	-2.525912525	2.026590313
H	-2.423097724	-2.283042248	2.149826974
H	-1.033953151	-3.035015611	2.948047140
C	0.549190905	-2.251490109	-1.369340900
H	0.633190294	-2.843580054	-2.290280201
H	0.947138514	-2.846966544	-0.554246212
H	1.112193595	-1.321853028	-1.446602481
O	1.060566614	1.550219623	0.119778286
N	-0.629894500	-1.217507536	1.884580994
C	-0.975784174	-0.244145434	2.986281527
H	-0.289698763	-0.369694350	3.834382368
H	-1.981322296	-0.470866314	3.350831966
C	-0.897718225	1.179293470	2.435586924
H	-1.108977482	1.913026825	3.227874137
H	0.085031641	1.390168277	2.009297471
C	0.862350440	-1.388174135	1.884271712
H	1.201404150	-1.719371486	2.876281653
H	1.331143777	-0.439020487	1.621397132
H	1.167841096	-2.123569238	1.149624311
C	-2.633532191	2.675582733	-0.717677695
H	-3.684404508	2.824907251	-0.441214639
H	-2.345897275	3.606844705	-1.224677050
C	-2.513973276	1.562201256	-1.777722651
H	-3.124289177	1.840590947	-2.652368033
H	-1.468903144	1.471314377	-2.083718616
C	-1.738466143	2.583489605	0.535248822
H	-1.967384504	3.437173778	1.193149933
H	-0.684026629	2.629858111	0.257170253
N	-1.910364484	1.302753044	1.324643485
N	-2.956604194	0.183119069	-1.311584809
C	-4.413885151	0.181730652	-0.952849264
H	-5.026922650	0.321946493	-1.854735056
H	-4.675952713	-0.775791744	-0.496104293
H	-4.652968171	0.975630002	-0.256219801
C	-3.284980919	1.236036474	1.938105842
H	-3.994536871	1.806208429	1.345524325
H	-3.640317057	0.206233318	2.008532584
H	-3.271364771	1.675524066	2.942860682
H	5.794406085	0.124445283	2.197917460
C	5.406573132	0.080644367	1.184808345
C	5.460098879	-1.127628284	0.469025368
C	4.875436215	1.227636647	0.602537645
C	4.975768783	-1.173130686	-0.850867809
H	5.886773526	-2.014435228	0.925821678
C	4.369605680	1.206918205	-0.734569607
H	4.856350409	2.154050574	1.166090176
C	4.441514877	-0.034623943	-1.443064531
H	5.034376741	-2.098362936	-1.416102054
H	4.083215077	-0.070147581	-2.468403246

C	3.811502369	2.355256791	-1.365399371
H	1.876939444	1.618596249	-0.431935948
H	3.509180450	2.251160633	-2.406069812
C	3.756527238	3.730773373	-0.769185021
H	3.035660231	4.360526805	-1.299530747
H	3.476541779	3.722339655	0.291787581
H	4.733044165	4.238130616	-0.833036731
Fe	-1.324324900	-0.260776813	0.090714740

²TS_{arom}:

O	0.004074787	-0.003786837	0.003265295
N	0.003768594	-0.004365511	2.725705379
C	2.536896711	-0.002840384	2.680274316
H	3.400191411	0.643196496	2.459353317
H	2.699389466	-0.409637792	3.683625203
C	1.263263802	0.831276530	2.654230594
H	1.289526556	1.553818401	3.486143692
H	1.185142357	1.389871126	1.717066132
C	-0.150779149	-0.760373303	4.024441628
H	-0.215710682	-0.047675135	4.863526617
H	0.754538972	-1.360819508	4.178047459
C	-1.387676913	-1.692664561	4.075528659
H	-2.311629010	-1.107845928	4.013289665
H	-1.397515140	-2.139966391	5.079673166
C	-1.442339995	-2.873098623	3.076746824
H	-0.563621000	-3.517264219	3.222643907
H	-2.332212944	-3.481403973	3.310952316
C	-1.117979076	0.990304409	2.538926110
H	-0.918931382	1.891797295	3.136781354
H	-2.070758407	0.583900057	2.872135338
H	-1.175616630	1.245525989	1.479576308
O	-0.275712503	-0.162080351	-1.393652267
N	-1.467785317	-2.478114827	1.618269995
C	-1.431035494	-3.684874297	0.698524734
H	-2.448327892	-3.965197603	0.396626160
H	-1.010014469	-4.539039735	1.237420937
C	-0.583592300	-3.338714467	-0.532093603
H	-0.557856481	-4.186508640	-1.235577005
H	-0.980844080	-2.461588049	-1.052067632
C	-2.706124056	-1.703569829	1.267358140
H	-3.602250725	-2.308459625	1.478537526
H	-2.683261016	-1.444987969	0.208164416
H	-2.767056512	-0.775561392	1.823467489
C	3.020405970	-1.871167390	-0.721926568
H	3.710852816	-2.671447508	-0.425232486
H	3.472418769	-1.428392707	-1.620766690
C	3.011183843	-0.750469603	0.343781650
H	4.044371702	-0.381845211	0.465388380
H	2.382148665	0.075226052	-0.000576893
C	1.660725080	-2.449003141	-1.176143238
H	1.849103253	-3.254418129	-1.906088672
H	1.072529907	-1.670823084	-1.666191284
N	0.803652566	-2.993978718	-0.052174277
N	2.488947985	-1.164421398	1.712768701
C	3.357251583	-2.237663874	2.309629557
H	4.358887113	-1.839395954	2.534214709
H	2.911394087	-2.600481943	3.241507500
H	3.475426070	-3.078970823	1.634287854
C	1.432568338	-4.243941704	0.518051019

H	2.512566774	-4.222200547	0.382939034
H	1.220443874	-4.350204230	1.585732389
H	1.057005404	-5.133507890	-0.005983972
H	-1.101352716	2.827366718	-1.501619041
C	-1.873101944	2.062118369	-1.509575250
C	-1.661339487	0.869835007	-2.284419881
C	-3.034065773	2.226866194	-0.756742663
C	-2.759676378	-0.049295214	-2.384102574
H	-0.946013938	0.909253892	-3.100309819
C	-4.084175785	1.265481300	-0.788625947
H	-3.164775931	3.130691193	-0.162578546
C	-3.921639937	0.132369577	-1.620500884
H	-2.683383609	-0.891141736	-3.069041232
H	-4.736207264	-0.586491757	-1.702714191
C	-5.378618788	1.506835438	-0.031053373
H	-5.164954848	1.958149155	0.949042445
H	-5.887474703	0.551490250	0.158966605
C	-6.350542370	2.442770400	-0.800960460
H	-7.270394647	2.604074804	-0.224769400
H	-5.888910459	3.419894760	-0.988570843
H	-6.623953198	2.009695590	-1.770682017
Fe	0.348623826	-1.458246569	1.277480087

²Int_{arom}:

O	-0.302285114	0.150327298	-0.759453859
N	1.638620988	2.073592315	-0.795964211
C	3.051370451	0.636699806	-2.315380833
H	3.141141254	0.286513787	-3.354197978
H	4.014711416	1.081311941	-2.050268145
C	1.952905085	1.675172938	-2.217797460
H	2.234538351	2.562309751	-2.805865158
H	1.012266232	1.287687288	-2.617938091
C	2.773662104	2.768661422	-0.087210172
H	3.032910090	3.691355155	-0.630258857
H	3.647196982	2.108639100	-0.130249621
C	2.481588167	3.130322183	1.386520118
H	1.653985553	3.843866954	1.447960742
H	3.358614492	3.684877362	1.747209118
C	2.262668473	1.977016087	2.387820307
H	3.159789651	1.346256675	2.420534175
H	2.133577727	2.411084988	3.392489675
C	0.426972428	2.962220778	-0.908536167
H	0.561531155	3.669922336	-1.736970761
H	0.273412734	3.539176537	-0.002455552
H	-0.430466457	2.312320339	-1.082320564
O	-1.440876963	-0.585495858	-0.043371074
N	1.104201390	1.065236830	2.078567782
C	1.052345194	-0.128071493	3.004668460
H	0.433453057	0.098449496	3.882521898
H	2.062668206	-0.333105627	3.368556660
C	0.489557572	-1.326633498	2.242803604
H	0.412606184	-2.203812684	2.902660187
H	-0.496147236	-1.110749114	1.825408481
C	-0.223004523	1.762411686	2.171814450
H	-0.438885702	2.017275975	3.218999121
H	-0.999929639	1.107966628	1.773104901
H	-0.222255807	2.674237462	1.586986047
C	1.656816134	-2.824118746	-1.160488427
H	2.586361610	-3.366090582	-0.947610703

H	1.074114792	-3.511811639	-1.788736348
C	1.946551709	-1.590529976	-2.038578110
H	2.438229542	-1.925514811	-2.966437251
H	1.002803183	-1.100113760	-2.288613527
C	0.828752300	-2.620826482	0.124469765
H	0.729570621	-3.591517253	0.636219278
H	-0.168363223	-2.247177099	-0.113664310
N	1.418344063	-1.618032762	1.091032370
N	2.827821387	-0.534522763	-1.389903844
C	4.189833236	-1.088189622	-1.089150825
H	4.730005195	-1.296440983	-2.023812534
H	4.760518360	-0.358397225	-0.509653792
H	4.128487478	-2.009410941	-0.522833054
C	2.719476281	-2.125146915	1.656501507
H	3.198610400	-2.804791840	0.957705696
H	3.407967740	-1.305378629	1.870017343
H	2.535796449	-2.683982975	2.582112733
H	-2.857252387	1.442240845	-1.466940080
C	-3.376687399	0.571405292	-1.081071726
C	-2.608577567	-0.706052832	-1.023420515
C	-4.673165123	0.661656534	-0.644583031
C	-3.412372586	-1.865934518	-0.534987942
H	-2.102190790	-0.921885489	-1.975026880
C	-5.384540982	-0.469624592	-0.141988214
H	-5.187573746	1.618871080	-0.684283821
C	-4.707602237	-1.724725855	-0.107627848
H	-2.923115013	-2.834715839	-0.511377571
H	-5.248326500	-2.594809325	0.256667830
C	-6.829849498	-0.356344452	0.280081843
H	-7.013288002	0.636880849	0.710572044
H	-7.043219082	-1.087908384	1.070285573
C	-7.816195900	-0.583489849	-0.893616302
H	-8.852169290	-0.491166660	-0.549126416
H	-7.654203196	0.151532181	-1.689902737
H	-7.687198822	-1.581873253	-1.326270903
Fe	1.434568315	0.224502798	0.133978510

²R₃W:

O	-0.119717000	0.274232000	0.047415000
N	0.090967000	0.149460000	2.861131000
C	2.598355000	-0.018798000	2.726158000
H	3.508551000	0.554166000	2.504816000
H	2.756463000	-0.496392000	3.695952000
C	1.401374000	0.903284000	2.783145000
H	1.495725000	1.582067000	3.642838000
H	1.334438000	1.516457000	1.880314000
C	-0.080446000	-0.626233000	4.149944000
H	-0.055486000	0.074801000	4.997080000
H	0.780693000	-1.294894000	4.253319000
C	-1.381332000	-1.452293000	4.222702000
H	-2.257590000	-0.796783000	4.208491000
H	-1.395732000	-1.915886000	5.217902000
C	-1.552930000	-2.602092000	3.213305000
H	-0.725128000	-3.314240000	3.319272000
H	-2.479672000	-3.144414000	3.452043000
C	-0.967972000	1.218147000	2.741959000
H	-0.735188000	2.040936000	3.429239000
H	-1.948783000	0.837542000	3.004487000
H	-0.979280000	1.582021000	1.715801000

O	-0.906730000	0.093092000	-1.078379000
N	-1.585322000	-2.189119000	1.755869000
C	-1.637573000	-3.396755000	0.837737000
H	-2.678138000	-3.647252000	0.601852000
H	-1.212274000	-4.255593000	1.361642000
C	-0.850950000	-3.076950000	-0.427039000
H	-0.891318000	-3.912336000	-1.139225000
H	-1.233840000	-2.179556000	-0.918983000
C	-2.789486000	-1.345453000	1.441926000
H	-3.704741000	-1.930310000	1.599575000
H	-2.736844000	-1.020858000	0.402200000
H	-2.828236000	-0.466219000	2.073539000
C	2.789498000	-1.740032000	-0.778566000
H	3.444391000	-2.591429000	-0.564315000
H	3.216727000	-1.285632000	-1.682475000
C	2.917309000	-0.681626000	0.333603000
H	3.977772000	-0.405625000	0.430366000
H	2.356844000	0.217611000	0.063179000
C	1.377773000	-2.219327000	-1.166661000
H	1.468464000	-2.979403000	-1.956329000
H	0.788091000	-1.392805000	-1.563921000
N	0.579358000	-2.805240000	-0.018794000
N	2.416311000	-1.120831000	1.701943000
C	3.225158000	-2.286298000	2.214271000
H	4.250701000	-1.959682000	2.429089000
H	2.777195000	-2.663808000	3.136138000
H	3.270544000	-3.090998000	1.492145000
C	1.189450000	-4.113718000	0.434604000
H	2.256617000	-4.128219000	0.232640000
H	1.033204000	-4.276998000	1.501803000
H	0.741690000	-4.945536000	-0.120113000
Fe	0.303995000	-1.303057000	1.384337000
H	-1.205299000	1.464928000	-1.668062000
O	-1.390488000	2.400471000	-2.073132000
H	-0.670324000	3.040109000	-1.971044000
H	-3.177966000	3.969042000	-6.372477000
O	-3.404030000	3.170094000	-5.866855000
H	-3.752008000	2.467959000	-6.441742000
H	-2.352413000	2.704740000	-2.741151000
O	-3.283814000	3.034131000	-3.377531000
H	-4.079693000	3.355033000	-2.928513000
H	-3.315735000	3.073942000	-4.410126000

⁴R₃W:

8	-0.394720000	0.365083000	0.179136000
7	0.070907000	0.195773000	3.061085000
6	2.587461000	-0.013525000	2.783957000
1	3.480808000	0.583788000	2.556847000
1	2.792453000	-0.537159000	3.720548000
6	1.391320000	0.914640000	2.957727000
1	1.558709000	1.539083000	3.849028000
1	1.296646000	1.588540000	2.100844000
6	-0.055572000	-0.691693000	4.274155000
1	-0.040255000	-0.072415000	5.184630000
1	0.827437000	-1.339422000	4.310453000
6	-1.326142000	-1.571062000	4.295490000
1	-2.227364000	-0.949789000	4.291046000
1	-1.334640000	-2.066696000	5.275361000
6	-1.449655000	-2.704482000	3.255073000

1	-0.560740000	-3.347083000	3.300727000
1	-2.314472000	-3.329487000	3.523399000
6	-0.989108000	1.258064000	3.054764000
1	-0.801136000	1.987857000	3.854551000
1	-1.974348000	0.828417000	3.217271000
1	-0.979473000	1.759272000	2.087056000
8	-1.033176000	0.151383000	-1.029688000
7	-1.593465000	-2.265304000	1.812646000
6	-1.593377000	-3.439970000	0.852105000
1	-2.625557000	-3.735501000	0.629436000
1	-1.117915000	-4.291428000	1.344643000
6	-0.855500000	-3.077140000	-0.444707000
1	-0.976081000	-3.885350000	-1.180581000
1	-1.259860000	-2.158839000	-0.881676000
6	-2.846283000	-1.470891000	1.586216000
1	-3.726814000	-2.063517000	1.867245000
1	-2.913344000	-1.202370000	0.530815000
1	-2.834378000	-0.553646000	2.167500000
6	2.731915000	-1.593396000	-0.813124000
1	3.416230000	-2.428724000	-0.629399000
1	3.148959000	-1.083301000	-1.691952000
6	2.830206000	-0.572229000	0.344166000
1	3.878000000	-0.245374000	0.420646000
1	2.224517000	0.312782000	0.119097000
6	1.341230000	-2.115188000	-1.241448000
1	1.473170000	-2.778997000	-2.109805000
1	0.703914000	-1.285377000	-1.554662000
7	0.605561000	-2.850396000	-0.146200000
7	2.393054000	-1.072260000	1.717148000
6	3.195321000	-2.269164000	2.142413000
1	4.249006000	-1.992643000	2.280059000
1	2.805893000	-2.647728000	3.090098000
1	3.138656000	-3.060185000	1.405626000
6	1.249007000	-4.180922000	0.127748000
1	2.328795000	-4.115932000	0.016348000
1	1.028328000	-4.530271000	1.137540000
1	0.889899000	-4.928803000	-0.591618000
26	0.236224000	-1.220353000	1.358531000
1	-1.426430000	1.539209000	-1.632318000
8	-1.685366000	2.450510000	-2.024922000
1	-1.187471000	3.201106000	-1.668749000
1	-2.763902000	4.241880000	-6.467073000
8	-2.887666000	3.343050000	-6.118013000
1	-2.901268000	2.679642000	-6.828128000
1	-2.523272000	2.642386000	-2.905725000
8	-3.320902000	2.851900000	-3.716829000
1	-4.253098000	2.910812000	-3.460573000
1	-3.119691000	3.044410000	-4.715645000

⁶R₃W:

O	-0.099996000	0.331949000	0.023814000
N	0.030170000	0.192191000	3.043806000
C	2.555411000	0.002535000	2.825663000
H	3.447507000	0.605276000	2.610129000
H	2.748563000	-0.514460000	3.768382000
C	1.348431000	0.922727000	2.973020000
H	1.487259000	1.545887000	3.869541000
H	1.268423000	1.597023000	2.114988000
C	-0.116783000	-0.699536000	4.252133000

H	-0.136405000	-0.081840000	5.163287000
H	0.775845000	-1.331947000	4.311100000
C	-1.372239000	-1.600097000	4.237694000
H	-2.283475000	-0.993752000	4.228498000
H	-1.388115000	-2.110600000	5.209824000
C	-1.462242000	-2.719899000	3.178013000
H	-0.565528000	-3.351492000	3.227126000
H	-2.322528000	-3.359994000	3.422988000
C	-1.039048000	1.244426000	3.005464000
H	-0.865729000	1.992691000	3.790957000
H	-2.021772000	0.809750000	3.168194000
H	-1.025696000	1.730494000	2.029393000
O	-1.269584000	0.288929000	-0.730477000
N	-1.592436000	-2.257882000	1.740330000
C	-1.584234000	-3.414954000	0.757257000
H	-2.614391000	-3.691665000	0.505587000
H	-1.130306000	-4.282262000	1.242026000
C	-0.813312000	-3.028609000	-0.512824000
H	-0.922530000	-3.814721000	-1.273805000
H	-1.206504000	-2.095001000	-0.928695000
C	-2.849395000	-1.464564000	1.515889000
H	-3.727572000	-2.080602000	1.748654000
H	-2.884898000	-1.141055000	0.475489000
H	-2.864679000	-0.577417000	2.141492000
C	2.804170000	-1.596109000	-0.758160000
H	3.466055000	-2.444429000	-0.553366000
H	3.260682000	-1.093236000	-1.621406000
C	2.882567000	-0.576695000	0.401629000
H	3.934556000	-0.276841000	0.518264000
H	2.305916000	0.319921000	0.151683000
C	1.420316000	-2.092465000	-1.234823000
H	1.568034000	-2.753419000	-2.102508000
H	0.811618000	-1.246603000	-1.559519000
N	0.639395000	-2.822140000	-0.168266000
N	2.383667000	-1.061918000	1.759483000
C	3.145422000	-2.272168000	2.220755000
H	4.198025000	-2.015146000	2.398197000
H	2.712672000	-2.639242000	3.154232000
H	3.102727000	-3.065268000	1.484728000
C	1.259020000	-4.162180000	0.117735000
H	2.341980000	-4.110494000	0.032827000
H	1.010739000	-4.511137000	1.121079000
H	0.908008000	-4.904100000	-0.611664000
Fe	0.237544000	-1.197661000	1.345593000
H	-1.303351000	1.544365000	-1.594710000
O	-1.332167000	2.400618000	-2.175525000
H	-0.533340000	2.946943000	-2.142427000
H	-3.041612000	3.736945000	-6.590641000
O	-3.344726000	3.025561000	-6.001465000
H	-3.798484000	2.320967000	-6.493630000
H	-2.264953000	2.756392000	-2.859871000
O	-3.165986000	3.131872000	-3.513260000
H	-3.905180000	3.589772000	-3.086569000
H	-3.224337000	3.067943000	-4.542989000