Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Electronic structure and bridge geometric distortion in push-pull imine-bridged triads. A theoretical study

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Table of contents

Table S1. Computed ferrocene GDPs for compounds **4**, **5**, **6** and derivatives.

	B3LYP-D4/def2-TZVP			B97-3c		
Comp.	**dFe-Cp$_b$^{c} [a]**	**β_T[b]**	**HOMFc[a]**	**dFe-Cp$_b$^{c} [a]**	**β_T [b]**	**HOMFc [a]**
Ferrocene	1.6791	0.06	0.0000	1.6274	0.02	0.0000
Ferrocene$^{\cdot+}$	1.7029	0.04	0.0000	1.7073	0.45	-0.0100
4a	1.6799	0.67	0.0263	1.6389	1.22	0.0257
4a·H$^+$	1.6961	7.41	0.1452	1.6628	9.54	0.0847
4b	1.6794	0.69	0.0264	1.6371	1.10	0.0277
4b·H$^+$	1.6933	6.09	0.1357	1.6591	8.33	0.0841
4c	1.6824	1.40	0.0058	1.6377	2.25	0.0083
4c·H$^+$	1.6904	3.48	0.0574	1.6583	4.86	0.0440
4d	1.6798	0.46	0.0121	1.6352	0.46	0.0139
4d·H$^+$	1.6909	4.64	0.0682	1.6594	6.15	0.0327
4e	1.6798	0.53	0.0118	1.6342	0.26	0.0140
4e·H$^+$	1.6854	1.87	0.0284	1.6359	0.37	0.0154
5c	1.6809	0.21	0.0198	1.6398	0.94	0.0232
5d	1.6796	0.80	0.0091	1.6326	0.53	0.0135
5d$^{\cdot+}$ Fc$_1$	1.6865	2.72	0.0423	1.6699	4.03	0.0178
5d$^{\cdot+}$ Fc$_2$	1.7473	0.25	0.0152	1.6699	4.00	0.0177
6g	1.68	0.37	0.0112	1.6327	0.59	0.0134
6g·H$^+$	1.6911	5.94	0.1150	1.654	7.60	0.0794
6h	1.6798	0.81	0.0106	1.6335	1.07	0.0127
6h·H$^+$	1.6895	4.41	0.0789	1.6515	5.92	0.0587
6i	1.6805	0.58	0.0198	1.6374	1.62	0.0197
6i·H$^+$	1.691	5.65	0.1180	1.6557	7.63	0.0813
6j Fc$_1$	1.6825	0.96	0.0104	1.6381	0.87	0.0130
6j·H$^+$ Fc$_1$	1.689	4.27	0.0751	1.6515	5.50	0.0572
6j Fc$_2$	1.6795	1.16	0.0114	1.6328	0.49	0.0208

Table S1. Cont.

	B3LYP-D4/def2-TZVP			B97-3c		
Comp.	**dFe-Cp$_b$^{c} [a]**	**β_T[b]**	**HOMFc[a]**	**dFe-Cp$_b$^{c} [a]**	**β_T[b]**	**HOMFc[a]**
6j·H$^+$ Fc$_2$	1.6863	2.18	0.0033	1.6461	3.16	0.0042
6j$^{\cdot+}$ Fc$_1$	1.6894	3.20	0.0487	1.6768	1.26	0.0110
6j$^{\cdot+}$ Fc$_2$	1.7495	0.74	0.0159	1.6513	2.22	0.0187
6n	1.6795	0.69	0.0107	1.6321	0.13	0.0162
6n·H$^+$	1.6902	3.98	0.0210	1.6531	5.48	0.0138
6o	1.6795	1.06	0.0120	1.6329	0.51	0.0203
6o·H$^+$	1.6867	2.30	0.0046	1.6473	3.80	0.0048
6p	1.6805	1.40	0.0228	1.6413	0.09	0.0302
6p·H$^+$	1.6892	3.62	0.0207	1.6583	5.32	0.0107

[a] In Å. [b] In °.

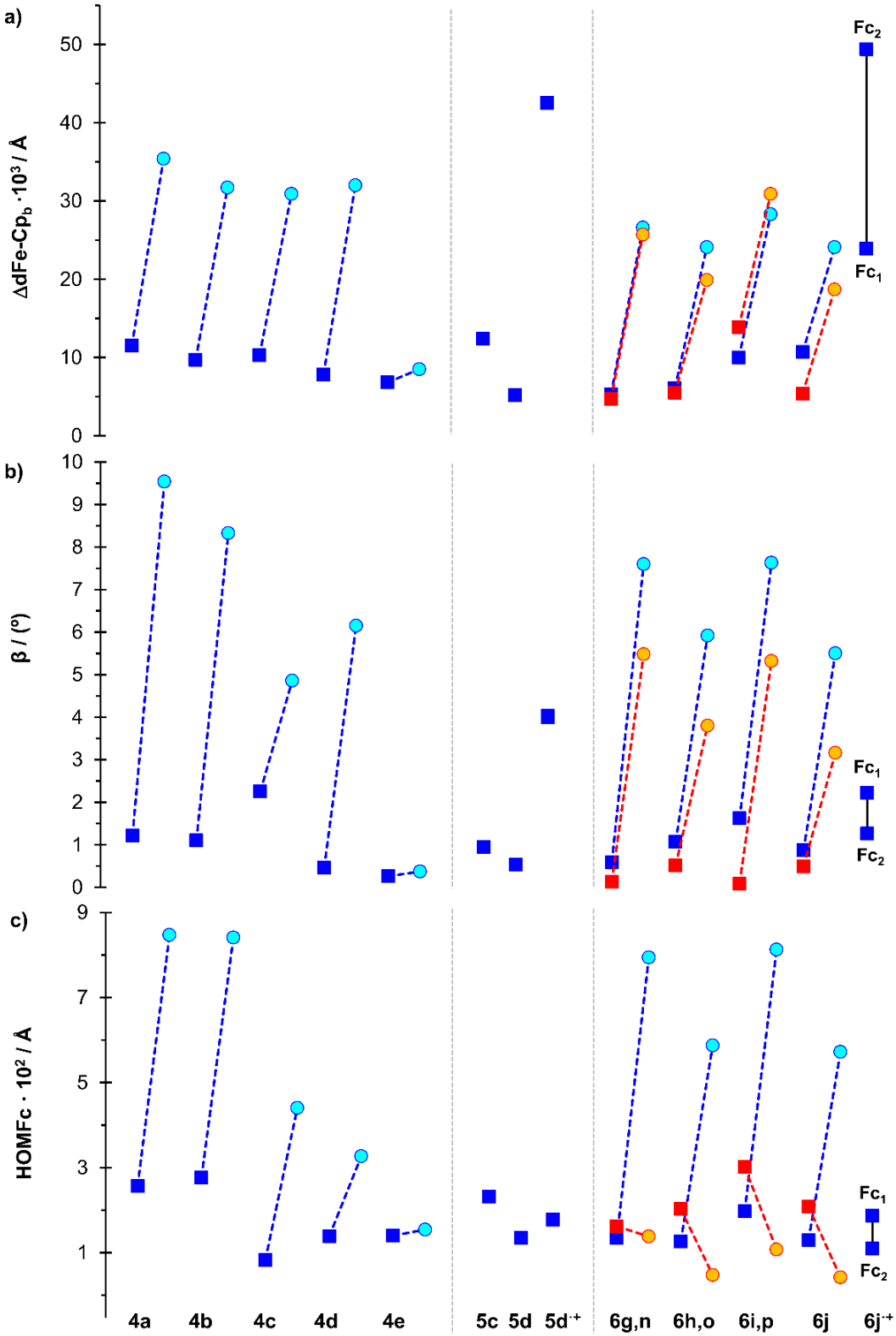

Figure S1. Calculated (B97-3c) ferrocene GDPs for compounds **4**, **5**, **6** and derivatives: a) ΔdFe-Cp$_b$^{c} (Å); b) β_T (º); c) HOMFc (Å). Neutral and protonated species are represented by intense and lighter blue color, respectively. Regiosiomers **6g-p** and their protonated counterparts are represented in red and yellow, respectively.

Transformation of NN into CC virtual bonds

Model compounds **10** and **11** (Figure S2) were employed with the aim of converting NN bonds into virtual CC bonds.

$CH_2{=}N\cdots N{=}CH_2$ **10**

$CH_2{=}CH\cdots N{=}N\cdots CH{=}CH_2$ **11**

Figure S2. Structures used for computing distances for single and double NN links

Single NN ($R_{N\text{-}N}$ = 1.3531 Å) and double N=N ($R_{N=N}$ = 1.2345 Å) bond distances were obtained. From these constants, NN bonds were transformed into the virtual (equivalent) CC distances displaying the same PBO by using constant γ_{NN} which was defined as follows (equation 1):

$$R_{N\text{-}N} - R_{N=N} = \gamma_{NN}\, Ln2 \qquad (1)$$

From γ_{NN} (0.17105 Å), PBOs were obtained for NN bonds as a function of their d_{NN} bond distances (equation 2):

$$PBO_{NN} = e^{(\gamma_{NN} - d_{NN}) / R_{N\text{-}N}} \qquad (2)$$

Next, NN bonds were converted into the corresponding equivalent virtual CC distances as for CN bonds (equations 3 and 4):

$$\frac{\gamma_{CC} - d_{CC}}{R_{C\text{-}C}} = \frac{\gamma_{NN} - d_{NN}}{R_{N\text{-}N}} \qquad (3)$$

$$d_{CC} = \gamma_{CC} - (\gamma_{NN} - d_{NN}) \frac{R_{C\text{-}C}}{R_{N\text{-}N}} \qquad (4)$$

Table S2. Computed GEO, EN and HOMCEc parameters for compounds **5** and **6**.

	B3LYP-D4/def2-TZVP			B97-3c		
Comp.	**GEO[a]**	**EN[a]**	**HOMCEc[a]**	**GEO[a]**	**EN[a]**	**HOMCEc[a]**
5a	-0.2752	0.2307	-0.04449	-0.2776	0.2313	-0.04636
5b	-0.1884	0.3110	0.12258	-0.1932	0.2979	0.10474
5c	-0.1033	0.3613	0.25795	-0.0765	0.3834	0.30687
5d	-0.1419	0.3433	0.20147	-0.1147	0.3633	0.24860
5d$^{\cdot+}$	-0.0632	0.4219	0.35872	-0.0662	0.4016	0.33543
6a	-0.2744	0.2302	-0.04420	-0.2774	0.2312	-0.04630
6a·H^{+}	-0.2451	0.2111	-0.03401	-0.2774	0.2312	-0.04630
6b	-0.1929	0.2876	0.09463	-0.1793	0.2900	0.11073
6b·H^{+}	-0.1297	0.2460	0.11629	-0.1144	0.2491	0.13475
6c	-0.1779	0.2965	0.11862	-0.1597	0.3021	0.14242
6c·H^{+}	-0.1002	0.2713	0.17113	-0.0812	0.2742	0.19298
6d	-0.1189	0.4542	0.33538	-0.1157	0.4629	0.34718
6d·H^{+}	-0.1762	0.2451	0.06889	-0.2038	0.2262	0.02241
6e	-0.3917	0.1479	-0.24379	-0.5874	0.0684	-0.51892
6f	-0.2245	0.3124	0.08787	-0.2202	0.3380	0.11780
6f·H^{+}	-0.2186	0.1592	-0.05945	-0.2124	0.1606	-0.05182
6g	-0.2175	0.2568	0.03926	-0.2050	0.2576	0.05255
6g·H^{+}	-0.0876	0.3039	0.21627	-0.0818	0.2850	0.20319
6h	-0.1720	0.3152	0.14317	-0.1497	0.3229	0.17316
6h·H^{+}	-0.1033	0.2824	0.17915	-0.0802	0.2780	0.19783
6i	-0.1065	0.4094	0.30285	-0.0838	0.4254	0.34162
6i·H^{+}	-0.0530	0.2905	0.23754	-0.0375	0.2782	0.24067
6j	-0.1555	0.3350	0.17950	-0.1250	0.3500	0.22505
6j·H^{+}	-0.0899	0.3083	0.21846	-0.0641	0.3030	0.23891
6j$^{\cdot+}$	-0.0546	0.4449	0.39026	-0.1260	0.3492	0.22315

Table S2. Cont.

	B3LYP-D/def2-TZVP			B97-3c		
Comp.	**GEO[a]**	**EN[a]**	**HOMCEc[a]**	**GEO[a]**	**EN[a]**	**HOMCEc[a]**
6k	-0.2641	0.2176	-0.04652	-0.2755	0.1813	-0.09424
6k·H$^+$	-0.2929	0.1338	-0.15909	-0.3024	0.1020	-0.20046
6l	-0.3409	0.2081	-0.13282	-0.3435	0.1763	-0.16714
6l·H$^+$	-0.3618	0.1339	-0.22787	-0.3738	0.0994	-0.27439
6m	-0.2484	0.2230	-0.02543	-0.2404	0.2219	-0.01847
6m·H$^+$	-0.1450	0.2600	0.11494	-0.1442	0.2660	0.12177
6n	-0.2371	0.2598	0.02265	-0.2250	0.2636	0.03852
6n·H$^+$	-0.1726	0.2132	0.04060	-0.1480	0.2027	0.05468
6o	-0.1624	0.3173	0.15485	-0.1358	0.3285	0.19275
6o·H$^+$	-0.0873	0.2954	0.20812	-0.0644	0.2972	0.23279
6p	-0.1540	0.3389	0.18488	-0.1093	0.3637	0.25438
6p·H$^+$	-0.0796	0.3104	0.23079	-0.0523	0.3237	0.27132

[a] In Å

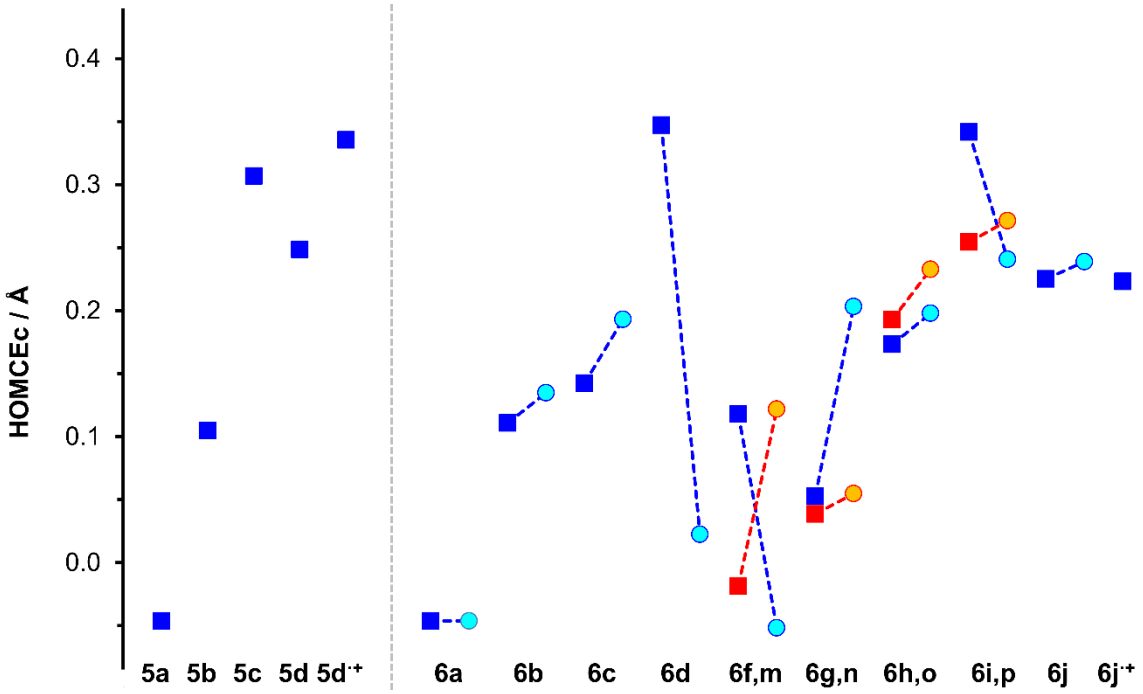

Figure S3. Calculated HOMCEc parameters (B97-3c) for the description of the bridge geometric distortion in compounds **5** and **6**. Type **I** compounds, in dark blue colour (left side of each imine pair) and their N-protonated **I**·$\mathbf{H}^+$ derivatives (right side, light blue colour). Type **II** compounds and their N-protonated derivatives are represented in red (orange for N-protonation derivatives).

Calculated structures

Cartesian coordinates (in Å) and electronic energies (in hartrees) are quoted at the (gas-phase) B3LYP-D4/def2-TZVP level.

Ferrocene: E = -1650.669893747134 au

C	-0.001858	0.008214	0.005487	C	-0.035511	0.021169	-3.351386
C	1.421133	0.006036	0.014141	C	-0.398568	1.397164	-3.365210
C	1.863154	1.358793	0.006852	C	0.797966	2.167693	-3.365739
C	0.713250	2.197119	-0.006764	C	1.900504	1.267863	-3.352276
C	-0.439467	1.362371	-0.007662	C	1.385350	-0.058740	-3.343533
H	2.052827	-0.867292	0.003248	H	-0.717076	-0.813546	-3.327477
H	2.888753	1.690039	-0.009536	H	-1.403288	1.787332	-3.353173
H	0.714942	3.274620	-0.035487	H	0.858408	3.243826	-3.354206
H	-1.463779	1.696625	-0.037874	H	2.942433	1.542954	-3.328611
H	-0.637456	-0.862101	-0.014813	H	1.968687	-0.964609	-3.312166
Fe	0.721170	0.973510	-1.676565				

Ferrocene$^{\cdot+}$: E = -1650.410343158888 au

C	0.000351	0.011395	0.047743	C	0.044578	-0.155995	-3.354437
C	1.425145	0.005212	0.061554	C	-0.404963	1.194199	-3.421439
C	1.871860	1.356898	0.002406	C	0.741700	2.039302	-3.449484
C	0.723023	2.198323	-0.047770	C	1.900243	1.211240	-3.399644
C	-0.433416	1.366709	-0.020010	C	1.469324	-0.145588	-3.340875
H	-0.637067	-0.858010	0.059284	H	-0.583134	-1.030611	-3.296783
H	2.054784	-0.869592	0.085062	H	-1.432525	1.520401	-3.423797
H	2.898687	1.684074	-0.026691	H	0.733958	3.117025	-3.476640
H	0.728280	3.273899	-0.121313	H	2.922741	1.552501	-3.382001
H	-1.456659	1.702741	-0.068519	H	2.108727	-1.010769	-3.270797
Fe	0.733215	0.908102	-1.692215				

4a: E = -2030.909892592258 au

C	0.765934	-0.549795	-1.145498	H	2.054988	-1.127305	2.630068
C	1.616236	0.379627	-1.837347	H	4.536669	-0.634564	1.711296
C	2.908237	-0.193223	-1.933376	H	4.510074	1.763105	0.493606
C	2.884705	-1.465959	-1.298365	H	2.004517	2.744331	0.645264
C	1.573127	-1.691126	-0.813681	C	-0.639750	-0.397955	-0.800487
H	1.317999	1.347250	-2.196144	C	-1.427471	-1.463873	-0.537442
H	3.769809	0.273672	-2.382276	C	-1.247274	0.972912	-0.714143
H	3.724592	-2.130535	-1.178019	C	-2.834823	-1.354646	-0.149293
H	1.246697	-2.555450	-0.259673	H	-1.048843	-2.475173	-0.609476
Fe	2.336310	0.015111	0.055495	C	-2.676453	1.077542	-0.341471
C	1.552879	0.871361	1.768783	C	-3.418771	0.003646	-0.071334
C	2.374848	-0.237525	2.112684	H	-3.065840	2.087386	-0.299863
C	3.687304	0.023724	1.627355	H	-4.463086	0.063917	0.209445
C	3.673325	1.293457	0.984685	O	-0.608426	1.987496	-0.925663
C	2.352452	1.817047	1.069251	O	-3.512759	-2.341398	0.096244
H	0.498795	0.965020	1.973496				

4b: E = -2184.546094662353 au

C	0.737433	-0.534357	-1.149218	H	1.992537	2.763758	0.608186
C	1.602395	0.377491	-1.846091	C	-0.669207	-0.365932	-0.810787
C	2.888710	-0.210444	-1.927223	C	-1.462521	-1.432212	-0.565918
C	2.847380	-1.475553	-1.277946	C	-1.253762	1.012256	-0.716377
C	1.530058	-1.680941	-0.800287	C	-2.868497	-1.346543	-0.172580
H	1.316856	1.344080	-2.217280	H	-1.081203	-2.441241	-0.656455
H	3.758137	0.241950	-2.375886	C	-2.684687	1.137787	-0.325303
H	3.679197	-2.147659	-1.144067	C	-3.465453	0.008864	-0.057791
H	1.190681	-2.534810	-0.237899	O	-0.585541	2.004555	-0.940353
Fe	2.305848	0.026551	0.055226	O	-3.519717	-2.356944	0.047537
C	1.516076	0.909338	1.751259	C	-4.798849	0.154916	0.311858
C	2.325601	-0.202376	2.115234	C	-3.249011	2.407718	-0.220730
C	3.644266	0.041565	1.637715	C	-4.578177	2.548369	0.148224
C	3.646665	1.303767	0.980023	H	-5.013507	3.536270	0.228912
C	2.329719	1.839644	1.047405	C	-5.353792	1.421885	0.414814
H	0.461075	1.014626	1.945264	H	-6.391326	1.535472	0.702369
H	1.993549	-1.083234	2.640175	H	-5.379922	-0.735020	0.512431
H	4.487110	-0.623030	1.736495	H	-2.630713	3.269325	-0.431845
H	4.491502	1.760162	0.490272				

4c: E = -2184.531845970583 au

C	0.817904	-0.542454	-1.229292	H	1.759080	2.677675	0.943988
C	1.672252	0.438250	-1.825810	C	-0.629061	-0.373480	-1.014466
C	2.992521	-0.081524	-1.861424	C	-1.591830	-1.363548	-1.297704
C	2.968166	-1.377228	-1.275018	C	-1.076008	0.842773	-0.484901
C	1.635448	-1.655593	-0.878383	C	-1.269741	-2.598447	-2.068450
H	1.354866	1.398028	-2.200111	C	-2.938226	-1.144446	-0.935861
H	3.862053	0.426491	-2.245337	C	-2.408596	1.071494	-0.190088
H	3.818977	-2.021917	-1.126546	H	-0.341162	1.607447	-0.276796
H	1.296266	-2.554619	-0.392776	C	-2.299360	-3.662848	-2.129632
Fe	2.321253	0.032298	0.093665	C	-3.977277	-2.198512	-1.120764
C	1.471409	0.664105	1.874620	C	-3.341526	0.065394	-0.388232
C	2.395210	-0.387858	2.121705	H	-2.714513	2.025741	0.219785
C	3.674792	0.033878	1.663116	C	-3.550318	-3.481742	-1.704575
C	3.541800	1.347155	1.132957	H	-1.972934	-4.582095	-2.600902
C	2.179330	1.737476	1.263015	H	-4.383712	0.196177	-0.132362
H	0.415172	0.638945	2.088048	H	-4.315286	-4.243844	-1.789918
H	2.161779	-1.346178	2.556170	O	-5.138969	-2.023797	-0.796076
H	4.580660	-0.549678	1.688518	O	-0.237940	-2.752383	-2.696363
H	4.329346	1.933917	0.688854				

4d: E = -2184.544000314708 au

C	0.717601	-0.537988	-1.131521	H	3.701082	-2.065006	-1.244971
C	1.538322	0.416851	-1.816362	H	1.244915	-2.549746	-0.295729
C	2.843145	-0.124919	-1.943581	Fe	2.305917	0.032246	0.055003
C	2.849499	-1.410742	-1.335679	C	1.524816	0.822088	1.799713
C	1.546023	-1.668332	-0.837199	C	2.369484	-0.282134	2.100740
H	1.218379	1.379826	-2.178153	C	3.673024	0.015906	1.612536
H	3.687126	0.363974	-2.402058	C	3.632825	1.304487	1.010307

C	2.304355	1.803002	1.125980
H	0.469441	0.888445	2.009543
H	2.069032	-1.193798	2.590943
H	4.533734	-0.630480	1.668394
H	4.457699	1.805298	0.530155
H	1.945389	2.747176	0.749863
C	-0.687963	-0.367462	-0.765419
C	-1.491033	-1.471399	-0.446530
C	-1.268972	0.902524	-0.722585
C	-2.818343	-1.312519	-0.090510
H	-1.069285	-2.466473	-0.492910
C	-2.598633	1.070186	-0.369803
C	-3.389017	-0.043409	-0.047343
C	-4.810196	0.120805	0.330988
C	-3.174198	2.441489	-0.326093
C	-4.599563	2.564288	0.048606
H	-4.992465	3.573791	0.064957
C	-5.349347	1.500336	0.349942
H	-6.393071	1.588059	0.627033
H	-0.686850	1.785348	-0.945610
H	-3.436169	-2.166521	0.152975
O	-2.515326	3.434010	-0.582419
O	-5.527334	-0.822688	0.619411

4e: E = -2338.179508914748 au

C	0.663571	-0.508370	-1.126354
C	1.479567	0.451534	-1.809373
C	2.784579	-0.087615	-1.946305
C	2.795607	-1.377160	-1.346292
C	1.494750	-1.639414	-0.843085
H	1.155945	1.416268	-2.163131
H	3.625676	0.405187	-2.405931
H	3.648452	-2.030898	-1.263835
H	1.197063	-2.524382	-0.305482
Fe	2.257307	0.056675	0.055764
C	1.482046	0.832394	1.809345
C	2.333596	-0.269540	2.099274
C	3.633074	0.037467	1.605746
C	3.583483	1.329399	1.011335
C	2.253290	1.820914	1.137256
H	0.427382	0.892407	2.024564
H	2.040089	-1.185552	2.585582
H	4.497112	-0.605165	1.653067
H	4.403313	1.836869	0.529509
H	1.887350	2.765195	0.768195
C	-0.740592	-0.341414	-0.752593
C	-1.543617	-1.449139	-0.444281
C	-1.320819	0.926377	-0.691688
C	-2.868432	-1.292122	-0.083051
H	-1.123094	-2.444123	-0.503897
C	-2.650408	1.093793	-0.332567
C	-3.440673	-0.022734	-0.022091
C	-4.862375	0.118257	0.363346
C	-3.207312	2.471535	-0.273444
C	-4.638227	2.614658	0.103100
C	-5.425818	1.495603	0.405435
C	-6.763830	1.667473	0.755209
C	-5.199223	3.889874	0.154729
C	-7.313988	2.938313	0.803003
H	-8.354164	3.066430	1.074579
C	-6.530504	4.051481	0.502287
H	-6.962324	5.043521	0.540158
H	-7.352025	0.789677	0.985216
H	-4.572035	4.738367	-0.082177
H	-3.487238	-2.147522	0.151811
H	-0.739255	1.811701	-0.904845
O	-5.549750	-0.851696	0.635409
O	-2.518389	3.445495	-0.521914

4a·H$^+$: E = -2031.269343238665 au

C	0.073628	-0.000669	0.190309
C	1.521119	-0.008397	0.064288
C	1.952933	1.327561	-0.002486
C	0.818526	2.186267	0.044385
C	-0.336925	1.395324	0.151892
H	2.142078	-0.883122	0.042169
H	2.976981	1.646692	-0.108628
H	0.839697	3.261513	-0.026229
H	-1.345136	1.769554	0.194387
Fe	0.640645	0.855728	-1.588155
C	-0.126914	-0.050573	-3.318742
C	-0.505877	1.318460	-3.270013
C	0.686257	2.094342	-3.251640
C	1.793739	1.202815	-3.274343
C	1.292046	-0.128296	-3.304879
H	-0.803447	-0.890606	-3.323262
H	-1.513242	1.700617	-3.258510
H	0.741819	3.169704	-3.205720
H	2.833250	1.486011	-3.244980
H	1.880181	-1.031080	-3.310069
C	-0.813108	-1.081501	-0.022057
C	-2.197686	-0.933682	0.120046
C	-0.284470	-2.456990	-0.398346
C	-3.054588	-1.991161	-0.096472
H	-2.610579	0.015035	0.437199
C	-1.275142	-3.522469	-0.638748
C	-2.586555	-3.302091	-0.498860
H	-0.872449	-4.486217	-0.920057

H	-3.330287	-4.071636	-0.660019	O	-4.368339	-1.914436	0.054363
O	0.900630	-2.689054	-0.514605	H	-4.659111	-1.035196	0.340047

4b·H$^+$: E = -2184.911571300528 au

C	0.729148	-0.511662	-1.325680	H	1.874312	2.717959	0.824764
C	1.633266	0.480115	-1.882198	C	-0.602531	-0.323797	-0.880404
C	2.921985	-0.082027	-1.914890	C	-1.367601	-1.391467	-0.416174
C	2.871559	-1.391270	-1.359315	C	-1.241706	1.053064	-0.906073
C	1.544869	-1.666402	-0.985170	C	-2.672329	-1.236515	0.019068
H	1.353592	1.458571	-2.221773	H	-0.949411	-2.390128	-0.424239
H	3.810022	0.415448	-2.269238	C	-2.639811	1.167134	-0.426624
H	3.713999	-2.048087	-1.216720	C	-3.343965	0.042291	0.036406
H	1.206145	-2.577309	-0.522444	O	-0.627606	2.027183	-1.285609
Fe	2.166481	0.009354	0.048885	O	-3.396497	-2.266661	0.432478
C	1.402987	0.783639	1.836884	C	-4.658946	0.175596	0.484792
C	2.205551	-0.358835	2.101747	C	-3.261620	2.408541	-0.438279
C	3.516663	-0.085795	1.621496	C	-4.572661	2.536437	0.009360
C	3.516053	1.217788	1.054294	H	-5.051986	3.506286	-0.003410
C	2.204417	1.755093	1.177794	C	-5.267614	1.423642	0.469954
H	0.352475	0.881264	2.060890	H	-6.287194	1.526357	0.816510
H	1.881472	-1.267199	2.582246	H	-5.197438	-0.691441	0.839006
H	4.358528	-0.757569	1.660466	H	-2.710715	3.264880	-0.801758
H	4.356437	1.702758	0.585046	H	-2.904138	-3.099262	0.389497

4c·H$^+$: E = -2184.890836717127 au

C	0.805005	-0.558627	-1.199715	H	1.844283	2.738265	0.887767
C	1.664790	0.416629	-1.824346	C	-0.631112	-0.393724	-0.986799
C	2.977502	-0.111906	-1.865246	C	-1.596813	-1.407966	-1.253213
C	2.974098	-1.385803	-1.237359	C	-1.093589	0.833429	-0.491770
C	1.646911	-1.670723	-0.811391	C	-1.333503	-2.575468	-2.035857
H	1.341821	1.357673	-2.238226	C	-2.953211	-1.199818	-0.862493
H	3.839737	0.385750	-2.277521	C	-2.418376	1.033568	-0.166477
H	3.832812	-2.017005	-1.079529	H	-0.371492	1.618142	-0.319185
H	1.330467	-2.542762	-0.261090	C	-2.345448	-3.566934	-2.317851
Fe	2.294851	0.045478	0.097668	C	-3.992515	-2.247435	-1.078287
C	1.503160	0.763378	1.884508	C	-3.347788	0.000286	-0.318622
C	2.391885	-0.311811	2.147787	H	-2.736590	1.988857	0.230265
C	3.674363	0.048234	1.650330	C	-3.595664	-3.438000	-1.854572
C	3.577184	1.346558	1.080542	H	-2.028852	-4.416199	-2.909424
C	2.233281	1.789755	1.220990	H	-4.384673	0.131130	-0.040619
H	0.453892	0.786740	2.131137	H	-4.360892	-4.182502	-2.032431
H	2.136470	-1.243039	2.626534	O	-5.122926	-2.134289	-0.652507
H	4.561007	-0.563570	1.682292	O	-0.198119	-2.843194	-2.609946
H	4.376737	1.890272	0.604430	H	0.513267	-2.210024	-2.357162

4d·H$^+$: E = -2184.899980914851 au

C	0.685883	-0.481778	-1.220436	C	2.833975	-1.310995	-1.417087
C	1.530005	0.546869	-1.787330	C	1.531355	-1.624479	-0.973519
C	2.830841	0.018617	-1.922354	H	1.222007	1.533200	-2.089326

H	3.685233	0.546594	-2.312842	C	-1.311780	0.940582	-0.881316
H	3.692259	-1.959642	-1.355902	C	-2.723916	-1.255181	0.105610
H	1.230945	-2.558717	-0.530832	H	-0.965229	-2.387047	-0.220333
Fe	2.212743	0.017563	0.079037	C	-2.610813	1.111824	-0.489001
C	1.521237	0.681378	1.932849	C	-3.357560	0.008132	0.013085
C	2.349233	-0.460546	2.101318	C	-4.690729	0.210401	0.384962
C	3.635133	-0.144797	1.579646	C	-3.236597	2.462511	-0.593192
C	3.596258	1.187726	1.086808	C	-4.653240	2.568694	-0.185757
C	2.285797	1.699325	1.298173	H	-5.111571	3.544942	-0.273218
H	0.479333	0.750286	2.202730	C	-5.325999	1.500892	0.274531
H	2.055410	-1.400080	2.539588	H	-6.365099	1.586180	0.575464
H	4.484739	-0.806914	1.545310	H	-0.778483	1.801262	-1.257605
H	4.410728	1.709878	0.611863	H	-3.283964	-2.101183	0.478896
H	1.935909	2.681336	1.025193	O	-2.626109	3.436701	-0.985162
C	-0.671997	-0.322026	-0.792992	O	-5.377249	-0.821639	0.847274
C	-1.422718	-1.410710	-0.284358	H	-6.290038	-0.588717	1.071334

4e·H$^+$: E = -2338.528558509814 au

C	0.681717	-0.175518	-1.127827	C	-1.423041	1.117009	-0.864816
C	1.542080	0.890236	-1.564246	C	-2.639561	-1.000434	0.453318
C	2.804340	0.335669	-1.886558	H	-0.798445	-2.031776	0.175463
C	2.747755	-1.065139	-1.653490	C	-2.743967	1.243406	-0.417297
C	1.452778	-1.386997	-1.181512	C	-3.361041	0.169890	0.260899
H	1.295937	1.938140	-1.616148	C	-4.747845	0.268725	0.765788
H	3.667088	0.886840	-2.222375	C	-3.502854	2.442279	-0.638938
H	3.558099	-1.761978	-1.789906	C	-4.842946	2.610497	-0.166957
H	1.110744	-2.375642	-0.925356	C	-5.466995	1.550938	0.526834
Fe	2.317967	-0.034636	0.106877	C	-6.762885	1.704329	0.985081
C	1.696637	0.290218	2.058513	C	-5.540135	3.810508	-0.388379
C	2.461227	-0.906646	1.985135	C	-7.444409	2.899056	0.763203
C	3.756491	-0.569131	1.503407	H	-8.457924	3.011348	1.125916
C	3.791812	0.834291	1.280290	C	-6.834344	3.948598	0.078745
C	2.518097	1.367041	1.622989	H	-7.371921	4.871904	-0.088796
H	0.667423	0.364390	2.371940	H	-7.227966	0.882941	1.512720
H	2.118358	-1.896905	2.236975	H	-5.063144	4.620668	-0.920393
H	4.563203	-1.259587	1.319409	H	-3.118940	-1.821757	0.968532
H	4.630525	1.392784	0.898119	H	-0.926701	1.922023	-1.393592
H	2.226847	2.402546	1.555828	O	-5.279935	-0.650729	1.353320
C	-0.687894	-0.052355	-0.662052	O	-3.001591	3.458383	-1.293287
C	-1.337417	-1.111361	0.001098	H	-2.100673	3.291458	-1.609244

5a: E = -78.568781709483 au

C	0.079077	0.585006	0.000000	C	0.054052	-0.739746	-0.000000
H	-0.831576	1.172472	0.000000	H	0.964708	-1.327208	0.000000
H	1.011262	1.137666	-0.000000	H	-0.878130	-1.292411	-0.000000

5b: E = -338.446231814569 au

C	0.204715	0.384147	-0.440370	C	-0.039211	-0.497375	0.547627
H	0.454451	-0.007808	-1.418342	H	-0.297844	-0.260665	1.566424

N	0.168050	1.726788	-0.329359	N	0.037339	-1.897971	0.281602
H	-0.055867	2.179721	0.539293	O	-0.195440	-2.646665	1.228376
H	0.363356	2.309966	-1.120900	O	0.324355	-2.287807	-0.850037

5c: E = -2108.297777430373 au

Fe	-0.034577	0.125155	-0.089234	H	-2.669785	-0.625506	0.607191
C	2.007086	0.045675	0.197884	H	-1.075204	-2.451183	-0.555708
C	1.573087	1.394672	0.251857	C	1.402587	-2.097486	1.528691
C	0.623520	1.516096	1.305982	H	0.667147	-2.475542	2.223908
C	0.468560	0.241166	1.904864	C	2.307772	-2.946848	1.002092
C	1.333520	-0.686239	1.231995	H	3.056541	-2.543720	0.326568
H	2.705259	-0.360509	-0.515101	C	2.439367	-4.366242	1.234815
H	1.885872	2.185284	-0.410651	C	1.458782	-5.141449	2.072607
H	0.096873	2.414781	1.582590	C	3.470686	-5.049651	0.675057
H	-0.188753	-0.005811	2.723056	C	1.719494	-6.583201	2.291299
C	-0.464736	-0.777808	-1.901776	C	3.701767	-6.479079	0.862587
C	-0.861662	0.589317	-1.930438	H	4.196248	-4.541454	0.050565
C	-1.822282	0.789749	-0.900153	C	2.751173	-7.212904	1.729318
C	-2.018733	-0.452705	-0.234160	H	0.998649	-7.084980	2.925087
C	-1.181037	-1.420909	-0.854771	H	2.943899	-8.269411	1.869631
H	0.266389	-1.239648	-2.545018	O	0.461420	-4.640005	2.559684
H	-0.484029	1.345019	-2.599802	O	4.641896	-7.058268	0.336242
H	-2.298758	1.724130	-0.651763				

5d: E = -3377.547655977676 au

C	-0.074069	-0.090293	0.001464	H	2.302457	-2.752921	5.808265
C	0.018771	0.077266	1.327216	H	-0.232885	-2.309002	5.026834
H	0.827554	-0.293428	-0.568164	C	-1.298712	-0.030190	-0.775885
H	-0.881825	0.282049	1.897935	C	-2.594556	0.412330	-0.358004
C	1.244312	0.017844	2.102754	C	-3.483345	0.311914	-1.462202
C	1.362956	0.400130	3.477606	C	-2.749203	-0.180265	-2.577391
C	2.704389	0.190025	3.894534	C	-1.407746	-0.386138	-2.158647
C	3.428584	-0.332509	2.786673	H	-2.850226	0.782509	0.621183
C	2.533810	-0.446288	1.688535	H	-4.525260	0.588330	-1.461865
H	0.557913	0.775172	4.089529	H	-3.136989	-0.346463	-3.569192
H	3.098322	0.372654	4.881021	H	-0.596659	-0.740432	-2.774945
H	4.467423	-0.620242	2.787609	Fe	-1.923759	1.596350	-1.908753
H	2.781123	-0.840533	0.716616	C	-0.503152	3.084801	-1.693527
Fe	1.857731	-1.591368	3.266151	C	-0.663220	2.758230	-3.069671
C	0.445958	-3.087216	3.045685	C	-2.018752	3.005616	-3.426320
C	1.719405	-3.549480	2.612411	C	-2.696903	3.483831	-2.270190
C	2.617023	-3.466183	3.714636	C	-1.759468	3.532575	-1.199417
C	1.897197	-2.952150	4.829526	H	0.399326	2.973177	-1.114557
C	0.555673	-2.717332	4.415802	H	0.102121	2.369572	-3.721671
H	-0.434769	-2.994350	2.430986	H	-2.459854	2.837134	-4.395290
H	1.966669	-3.880396	1.616872	H	-3.741601	3.742408	-2.210152
H	3.663066	-3.725941	3.701145	H	-1.969748	3.831909	-0.185553

5d^{-+}: E = -3377.329109457205 au

C	-0.194559	-0.096453	0.037678	H	2.467274	-2.766529	5.794036
C	-0.086287	0.171466	1.361990	H	-0.130432	-2.550073	5.129948
H	0.695667	-0.393680	-0.508456	C	-1.391495	-0.035120	-0.741646
H	-0.965980	0.470056	1.919844	C	-2.678766	0.484308	-0.361165
C	1.139060	0.113501	2.098782	C	-3.532338	0.406190	-1.486827
C	1.273815	0.407491	3.494511	C	-2.794372	-0.136575	-2.576997
C	2.625189	0.209116	3.884914	C	-1.477547	-0.395905	-2.134388
C	3.338988	-0.263981	2.748692	H	-2.949823	0.870722	0.607280
C	2.422940	-0.363973	1.667345	H	-4.558811	0.732381	-1.522463
H	0.473825	0.747249	4.133234	H	-3.168424	-0.293850	-3.575159
H	3.032842	0.380842	4.867891	H	-0.673024	-0.803201	-2.725544
H	4.385966	-0.518627	2.714830	Fe	-1.878976	1.609386	-1.893072
H	2.665238	-0.717793	0.678829	C	-0.437631	3.097343	-1.711573
Fe	1.853996	-1.609021	3.263342	C	-0.579505	2.718253	-3.074973
C	0.517966	-3.297737	3.134434	C	-1.926300	2.967737	-3.458981
C	1.798529	-3.640519	2.635468	C	-2.615054	3.495684	-2.333022
C	2.743717	-3.461837	3.686874	C	-1.694975	3.574012	-1.250127
C	2.038023	-2.998857	4.833013	H	0.459774	3.010345	-1.120254
C	0.661903	-2.892735	4.484046	H	0.192360	2.305944	-3.703965
H	-0.398893	-3.287577	2.566245	H	-2.355821	2.769007	-4.427190
H	2.020154	-3.969851	1.633163	H	-3.657154	3.768382	-2.299809
H	3.803737	-3.646800	3.623879	H	-1.915713	3.923986	-0.255064

5d^{2+}: E = -3377.011739129374 au

C	-0.064228	-0.058448	0.009946	H	2.466799	-2.778582	5.939653
C	-0.001033	0.062890	1.345728	H	-0.127480	-2.615590	5.256221
H	0.836210	-0.280155	-0.552526	C	-1.281000	0.043733	-0.774525
H	-0.901453	0.284550	1.908248	C	-2.562436	0.531598	-0.369960
C	1.215815	-0.039473	2.130109	C	-3.457774	0.411449	-1.466240
C	1.327232	0.331477	3.503485	C	-2.729400	-0.118872	-2.570907
C	2.664402	0.121953	3.926518	C	-1.392361	-0.327920	-2.147676
C	3.392513	-0.407954	2.821401	H	-2.815786	0.926637	0.600699
C	2.497086	-0.527231	1.725260	H	-4.502579	0.678113	-1.461689
H	0.522633	0.710028	4.115042	H	-3.122840	-0.326260	-3.553202
H	3.058110	0.329068	4.908756	H	-0.587562	-0.706387	-2.759038
H	4.437232	-0.674950	2.816580	Fe	-1.941083	1.738305	-2.002886
H	2.750177	-0.922164	0.754481	C	-0.581203	3.414597	-1.973997
Fe	1.875207	-1.734045	3.359365	C	-0.770810	2.982453	-3.309347
C	0.538511	-3.430918	3.292187	C	-2.155131	3.078171	-3.613192
C	1.825205	-3.784722	2.813369	C	-2.824706	3.571373	-2.454824
C	2.763051	-3.554062	3.860675	C	-1.844822	3.776256	-1.440402
C	2.044519	-3.052296	4.985849	H	0.358027	3.431532	-1.443585
C	0.671160	-2.976791	4.627385	H	-0.001836	2.618769	-3.972863
H	-0.378754	-3.465634	2.725409	H	-2.616910	2.819809	-4.552926
H	2.055120	-4.157367	1.827811	H	-3.881753	3.765073	-2.366020
H	3.824917	-3.735862	3.814030	H	-2.031903	4.140555	-0.442810

6a: E = -94.615320831283 au

C	0.057983	0.585986	-0.000000	N	0.049830	-0.677392	-0.000000
H	-0.836099	1.218574	0.000000	H	-0.904271	-1.043364	0.000000
H	1.016057	1.107192	0.000000				

6b: E = -556.650366235714 au

C	-1.840600	0.171045	-0.084272	C	1.825671	-0.224390	0.070446
C	-2.707846	1.199241	-0.460518	C	2.365990	0.982386	0.529865
C	-4.083607	1.026816	-0.384586	C	3.735922	1.201117	0.475336
C	-4.604929	-0.178345	0.069351	C	4.584100	0.227433	-0.039392
C	-3.746354	-1.210007	0.447264	C	4.052689	-0.980231	-0.483163
C	-2.374885	-1.039288	0.372739	C	2.687930	-1.212828	-0.413872
H	-2.297344	2.137913	-0.814622	H	1.713178	1.730854	0.960586
H	-4.747076	1.829990	-0.678879	H	4.143289	2.134081	0.844931
H	-5.677109	-0.316507	0.130098	H	5.651727	0.400944	-0.079488
H	-4.154328	-2.148414	0.801292	H	4.707716	-1.748561	-0.874616
H	-1.695431	-1.829462	0.662221	H	2.263569	-2.152868	-0.741460
C	-0.396644	0.385214	-0.175804	N	0.456142	-0.510963	0.120054
H	-0.086281	1.375300	-0.533862				

6c: E = -785.686070014948 au

C	1.828466	-0.197452	-0.130397	H	-4.141938	-2.252353	-0.681953
C	2.716419	-1.201989	0.251448	H	-4.767369	1.791842	0.597376
C	4.086054	-0.977087	0.305666	H	-2.343199	2.137650	0.676960
C	4.597109	0.267357	-0.059810	C	-0.406029	0.394621	0.108873
C	3.722479	1.271274	-0.481192	H	-0.114166	1.407739	0.414974
C	2.360416	1.043264	-0.514046	O	-5.930459	-0.565961	-0.127917
H	2.312726	-2.169000	0.521824	O	5.920553	0.590902	-0.057912
H	4.739858	-1.776734	0.621368	C	-6.876911	0.438730	0.198393
H	4.136783	2.221517	-0.792264	H	-6.787247	1.301607	-0.468089
H	1.701316	1.822877	-0.873741	H	-7.855167	-0.017786	0.068105
C	-1.841480	0.151303	0.046166	H	-6.765555	0.768949	1.235369
C	-2.367029	-1.092213	-0.339960	C	6.852844	-0.400272	0.334327
C	-3.726892	-1.297682	-0.386403	H	7.833918	0.063777	0.261728
C	-4.610403	-0.262784	-0.049527	H	6.681991	-0.725379	1.365380
C	-4.107289	0.978981	0.333861	H	6.814195	-1.270615	-0.328197
C	-2.731454	1.170849	0.377365	N	0.462394	-0.500765	-0.151947
H	-1.679660	-1.886065	-0.599111				

6d: E = -487.075677471275 au

C	-1.484796	0.265914	-0.017941	F	1.460886	-0.478470	1.098645
H	-1.367508	1.350008	-0.011963	N	-2.759429	-0.160941	-0.029948
C	0.797637	-0.055939	0.001835	H	-3.523089	0.488522	-0.034457
F	1.492387	-0.491751	-1.069459	H	-2.953259	-1.148749	-0.035944
F	0.912878	1.307741	-0.004676	N	-0.502258	-0.549860	-0.014393

6e: E = -354.484691586804 au

C	1.185877	0.255878	0.000009	N	-1.063366	-0.015784	-0.000010
H	0.999126	1.326828	0.000026	O	-1.188416	1.203347	0.000018
N	2.460946	-0.140741	0.000004	O	-1.973665	-0.812645	0.000000
H	3.208881	0.527774	0.000041	N	0.229715	-0.612045	-0.000010
H	2.681948	-1.123589	-0.000000				

6f: E = -474.844005993028 au

N	1.823456	-1.129427	-0.369802	C	-0.700195	1.686768	-0.013254
C	2.834402	-0.917268	0.359158	C	-1.836402	0.992337	0.063014
H	2.820644	-0.295908	1.256332	H	-0.668818	2.769217	-0.003842
C	0.614079	-0.494597	-0.167962	H	-2.807561	1.465443	0.139595
C	-0.548771	-1.172239	-0.093190	O	-2.886700	-1.109003	0.142719
C	0.611308	1.014290	-0.091683	O	1.647598	1.647628	-0.075588
C	-1.836935	-0.492686	0.049061	H	3.774264	-1.396263	0.094935
H	-0.568628	-2.253374	-0.137947				

6g: E = -1744.108376261847 au

N	-3.195376	-1.526585	-0.118930	Fe	0.421608	0.183973	-0.028108
C	-2.465906	-0.793300	0.620428	C	1.313241	-1.387279	-1.039425
H	-2.460898	-1.018573	1.690137	C	2.219078	-0.293583	-0.938351
C	-1.617669	0.332061	0.233114	C	2.428286	-0.022422	0.442750
C	-0.935242	1.192004	1.153130	C	1.651101	-0.947324	1.195111
C	-0.173024	2.126785	0.407456	C	0.962610	-1.790778	0.278468
C	-0.371145	1.852869	-0.975604	H	0.938843	-1.818611	-1.953382
C	-1.255706	0.748965	-1.087750	H	2.652619	0.248482	-1.762943
H	-0.989357	1.124111	2.227921	H	3.047096	0.761817	0.847489
H	0.464024	2.894500	0.815382	H	1.578850	-0.987568	2.269729
H	0.093383	2.375024	-1.796191	H	0.267315	-2.573757	0.534826
H	-1.577083	0.291829	-2.009532	H	-3.144127	-1.232216	-1.096848

6h: E = -2089.638766435100 au

C	-1.288196	-1.291238	0.537814	H	-2.542685	2.363495	1.667483
C	-2.246579	-1.147595	1.592889	C	2.263830	-0.721293	-0.216675
C	-3.519520	-1.512411	1.084492	C	2.646727	0.459469	0.420543
C	-3.359079	-1.879237	-0.283101	C	3.981442	0.848453	0.478651
C	-1.990084	-1.739752	-0.624596	C	4.961558	0.048474	-0.103646
H	-2.032074	-0.807946	2.593675	C	4.587722	-1.127180	-0.760489
H	-4.448822	-1.493594	1.630174	C	3.259466	-1.494522	-0.828247
H	-4.149405	-2.181871	-0.950814	H	1.892203	1.105227	0.851597
H	-1.538404	-1.917350	-1.585609	H	4.238270	1.777717	0.965867
Fe	-2.735183	0.080348	0.008185	H	5.359080	-1.731070	-1.220233
C	-1.797757	1.884240	-0.384150	H	2.964307	-2.397144	-1.347188
C	-2.483157	1.426707	-1.542873	O	6.293864	0.334327	-0.103085
C	-3.864179	1.308164	-1.217524	C	6.725892	1.516318	0.545161
C	-4.030727	1.691631	0.142645	H	6.294048	2.408570	0.080713
C	-2.752780	2.046706	0.658855	H	7.807722	1.542191	0.435233
H	-0.734724	2.043890	-0.304350	H	6.470428	1.505648	1.609484
H	-2.030110	1.184355	-2.490138	C	0.118795	-0.954778	0.631713
H	-4.643193	0.964492	-1.878420	H	0.441966	-0.524352	1.588247
H	-4.957936	1.689888	0.692265	N	0.934797	-1.148805	-0.326989

6i: E = -2124.345338915554 au

Fe	-2.385841	-0.065005	0.042381	C	-2.833243	-2.062649	0.426699
C	-1.464353	-1.802242	0.676668	C	-3.109746	-1.752343	-0.936986

C	-1.910789	-1.297026	-1.537815	H	-0.571545	2.086830	0.027970
C	-0.876819	-1.332150	-0.542489	C	0.470839	-0.854919	-0.728913
H	-0.941285	-1.916256	1.610817	H	0.688564	-0.412706	-1.704109
H	-3.552603	-2.408390	1.151149	C	2.608370	-0.399928	0.065179
H	-4.070549	-1.826785	-1.419500	C	2.712386	1.043437	-0.370969
H	-1.789409	-0.970803	-2.558294	C	3.734151	-1.069535	0.404724
C	-2.096613	1.378067	1.497497	C	4.053831	1.657184	-0.402524
C	-3.486249	1.106825	1.344196	C	5.057003	-0.460221	0.345137
C	-3.845616	1.402933	-0.000185	H	3.684005	-2.100515	0.729720
C	-2.677985	1.856414	-0.676370	C	5.144304	0.963261	-0.074367
C	-1.597869	1.842863	0.249507	H	4.084698	2.695868	-0.707911
H	-1.516462	1.229475	2.393523	H	6.139005	1.391389	-0.093452
H	-4.144967	0.720923	2.105158	O	1.726705	1.683982	-0.687226
H	-4.824050	1.280552	-0.435618	O	6.074669	-1.076455	0.628044
H	-2.616336	2.138739	-1.714755	N	1.366214	-0.967900	0.178206

6j: E = -3393.590801861973 au

N	0.392870	-0.120449	0.233135	H	-2.991655	-2.255063	-1.344622
C	-0.437233	0.186209	-0.684689	C	1.517970	-0.879520	-0.077489
H	-0.309798	-0.149446	-1.720603	C	2.179329	-1.075518	-1.336223
C	-1.616278	0.989344	-0.427063	C	3.306098	-1.913070	-1.112684
C	-2.583198	1.377713	-1.410221	C	3.356057	-2.233377	0.273946
C	-3.616052	2.095295	-0.754549	C	2.264087	-1.589638	0.913854
C	-3.299786	2.152067	0.633296	H	1.900799	-0.636065	-2.279631
C	-2.073874	1.469985	0.839435	H	4.017862	-2.226490	-1.859373
H	-2.535349	1.146847	-2.462641	H	4.107765	-2.836363	0.756656
H	-4.498549	2.502860	-1.220248	H	2.021168	-1.610031	1.963330
H	-3.906246	2.607402	1.399488	Fe	3.464542	-0.182379	0.007898
H	-1.569201	1.309832	1.776959	C	3.367939	1.810556	0.547583
Fe	-3.459841	0.172202	0.019000	C	4.172589	1.092289	1.475813
C	-3.271956	-1.730426	0.807608	C	5.263699	0.519615	0.763088
C	-4.320787	-1.033297	1.467957	C	5.133418	0.883626	-0.606654
C	-5.294538	-0.674870	0.493866	C	3.961682	1.682093	-0.738901
C	-4.848545	-1.154082	-0.769505	H	2.444214	2.318767	0.771649
C	-3.599474	-1.806639	-0.575540	H	3.973638	0.977809	2.528873
H	-2.366771	-2.096661	1.264097	H	6.039097	-0.100541	1.182727
H	-4.354703	-0.787798	2.516999	H	5.793478	0.589062	-1.406265
H	-6.198401	-0.116799	0.676866	H	3.576793	2.095014	-1.657210
H	-5.354882	-1.021503	-1.711842				

6j$^{\cdot+}$: E = -3393.372744461351 au

N	0.343146	-0.108452	0.143766	H	-1.570991	1.499091	1.619283
C	-0.542081	0.131926	-0.768368	Fe	-3.470085	0.167261	0.014488
H	-0.472391	-0.332926	-1.758095	C	-3.321813	-1.674768	0.952585
C	-1.668143	0.978133	-0.557407	C	-4.307826	-0.886239	1.600008
C	-2.683079	1.257689	-1.543889	C	-5.310970	-0.563817	0.644856
C	-3.688106	2.028158	-0.920919	C	-4.950281	-1.165236	-0.592164
C	-3.331016	2.212159	0.446505	C	-3.721105	-1.849570	-0.405629
C	-2.099492	1.563131	0.683588	H	-2.419175	-2.054391	1.403253
H	-2.665114	0.941382	-2.574512	H	-4.283026	-0.557531	2.626189
H	-4.589976	2.386368	-1.389529	H	-6.182696	0.044386	0.822634
H	-3.922817	2.729473	1.183945	H	-5.498959	-1.088056	-1.516674

H	-3.180764	-2.396065	-1.161565	C	3.740576	1.523548	1.223266
C	1.428423	-0.874604	-0.158128	C	4.854410	0.667939	1.449806
C	2.158817	-0.983304	-1.391034	C	5.554428	0.519582	0.226599
C	3.267147	-1.850039	-1.183472	C	4.869696	1.264990	-0.765002
C	3.274891	-2.234338	0.186891	C	3.749092	1.894139	-0.151150
C	2.176839	-1.598313	0.825413	H	3.011197	1.823946	1.957922
H	1.907628	-0.489690	-2.315957	H	5.111608	0.197192	2.385263
H	3.983521	-2.149224	-1.931846	H	6.426443	-0.094666	0.067222
H	3.994698	-2.881845	0.661041	H	5.143291	1.332039	-1.805854
H	1.908910	-1.659823	1.867745	H	3.032921	2.533731	-0.641159
Fe	3.510803	-0.179000	0.019338				

6j^{2+}: E = -3393.049460164889 au

N	0.384217	-0.084162	0.060947	H	-4.527219	-2.050689	-1.652235
C	-0.501315	-0.010576	-0.853955	C	1.523112	-0.847503	-0.146196
H	-0.414954	-0.553074	-1.800935	C	2.289854	-1.019605	-1.338923
C	-1.687587	0.819784	-0.693103	C	3.383176	-1.877852	-1.038498
C	-2.639234	1.117918	-1.722940	C	3.315179	-2.213211	0.344026
C	-3.590503	2.019336	-1.194598	C	2.190552	-1.548819	0.902026
C	-3.256465	2.276810	0.159878	H	2.088233	-0.561794	-2.294574
C	-2.091585	1.537695	0.481888	H	4.135037	-2.208385	-1.737555
H	-2.630326	0.725229	-2.728191	H	4.001888	-2.850708	0.877660
H	-4.448053	2.411559	-1.719207	H	1.867794	-1.575631	1.930502
H	-3.815529	2.903519	0.837328	Fe	3.585147	-0.151394	0.120458
H	-1.581519	1.520241	1.430898	C	3.846409	1.540809	1.320914
Fe	-3.579276	0.161350	-0.070969	C	4.936817	0.654860	1.549011
C	-3.548304	-1.879990	0.352865	C	5.636415	0.493569	0.325268
C	-3.933481	-1.152127	1.517727	C	4.980924	1.267947	-0.663462
C	-5.153561	-0.481772	1.226538	C	3.873543	1.919291	-0.052781
C	-5.521685	-0.793538	-0.106163	H	3.130657	1.867341	2.058030
C	-4.533963	-1.651649	-0.650042	H	5.182217	0.175832	2.483843
H	-2.673949	-2.502881	0.252965	H	6.492714	-0.143121	0.165203
H	-3.401225	-1.118775	2.454837	H	5.261628	1.331775	-1.703141
H	-5.693541	0.171556	1.894130	H	3.182163	2.585351	-0.543633
H	-6.382965	-0.408322	-0.630040				

6k: E = -487.023659265218 au

C	0.844270	-0.008921	-0.001078	H	-3.455327	0.592512	-0.270920
F	1.519995	-0.526061	-1.057323	H	-2.984904	-1.047995	-0.222140
F	0.956772	1.318947	-0.055910	C	-0.571709	-0.491921	0.001820
F	1.498222	-0.434535	1.107717	H	-0.697079	-1.576387	0.025640
N	-2.792389	-0.090571	0.055577	N	-1.524850	0.344969	-0.010024

6l: E = -354.455129227325 au

N	2.479682	-0.081618	-0.026576	N	-1.096630	0.021765	-0.002261
H	3.162205	0.618938	0.205163	O	-1.297500	1.219990	-0.000075
H	2.707815	-1.047037	0.180875	O	-1.961602	-0.850571	-0.004885
C	0.269172	-0.490312	0.001764	N	1.225800	0.338587	0.012287
H	0.312497	-1.574609	-0.009739				

6m: E = -474.851905455299 au

C	-0.748504	-0.124962	0.000018	H	3.091123	0.843107	-0.000020
C	0.186397	-1.088667	0.000020	O	2.465267	-1.669846	0.000044
C	-0.338602	1.309625	0.000051	O	-1.162933	2.206893	-0.000040
C	1.629940	-0.782843	-0.000008	C	-2.197278	-0.418523	0.000010
H	-0.094473	-2.134755	0.000026	H	-2.843998	0.460029	0.000043
C	1.109075	1.613362	-0.000007	N	-2.618022	-1.616051	-0.000028
C	2.026608	0.643851	-0.000006	H	-3.636515	-1.649107	-0.000024
H	1.366082	2.665445	-0.000027				

6n: E = -1744.095104378719 au

C	-1.620753	0.230459	-0.211578	C	2.436597	0.014405	-0.493664
C	-1.238330	0.768395	1.062130	C	2.255396	-0.190580	0.902895
C	-0.399595	1.890229	0.824746	C	1.383823	-1.303592	1.073570
C	-0.256759	2.052492	-0.583096	H	0.343648	-2.592423	-0.426155
C	-0.998384	1.025672	-1.223079	H	1.585771	-1.066121	-2.254880
H	-1.502114	0.371660	2.028432	H	3.025908	0.794241	-0.948015
H	0.073040	2.496205	1.580874	H	2.684368	0.405535	1.691844
H	0.335640	2.806507	-1.075130	H	1.035689	-1.696688	2.014926
H	-1.089169	0.850176	-2.282110	C	-3.247204	-1.314153	0.334300
Fe	0.429662	0.183421	-0.004126	H	-3.844940	-2.187235	0.084488
C	1.026040	-1.784854	-0.216582	H	-3.414136	-0.856231	1.314682
C	1.676804	-0.970844	-1.185251	N	-2.413120	-0.880767	-0.515020

6o: E = -2089.638690930540 au

C	1.222645	-1.134659	-0.557374	H	2.780148	2.437248	-1.502872
C	2.159310	-0.985895	-1.627487	C	-0.973588	-1.138959	0.162889
C	3.412198	-1.496258	-1.197626	H	-0.727296	-1.880367	0.932857
C	3.267588	-1.947783	0.145119	C	-2.363024	-0.699415	0.140848
C	1.923257	-1.723859	0.548348	C	-2.825477	0.243874	-0.779782
H	1.927841	-0.551271	-2.585747	C	-4.148781	0.652194	-0.785347
H	4.321639	-1.514638	-1.775797	C	-5.044445	0.116239	0.145451
H	4.050518	-2.360887	0.760569	C	-4.596773	-0.827833	1.072169
H	1.519390	-1.927941	1.526031	C	-3.274521	-1.225995	1.064414
Fe	2.806809	0.064602	0.022740	H	-2.125555	0.652688	-1.496153
C	2.018197	1.907572	0.527996	H	-4.475158	1.382736	-1.510818
C	2.677092	1.334942	1.651383	H	-5.303933	-1.232021	1.784198
C	4.042429	1.127844	1.303855	H	-2.935035	-1.959829	1.786497
C	4.226692	1.574124	-0.034949	O	-6.357375	0.450613	0.224862
C	2.975644	2.055133	-0.514228	C	-6.873412	1.400804	-0.693273
H	0.968288	2.141971	0.460303	H	-6.374904	2.368767	-0.587670
H	2.217159	1.078398	2.591904	H	-7.927596	1.509711	-0.449811
H	4.798164	0.690178	1.935673	H	-6.773642	1.052626	-1.725457
H	5.146487	1.532766	-0.595477	N	-0.096060	-0.703129	-0.653293

6p: E = -2124.330156128223 au

C	1.273376	-1.270941	-0.472854	C	2.192329	-1.167538	-1.568628

C	3.463909	-1.599666	-1.117232	H	5.099230	1.532383	-0.662412
C	3.352291	-1.952982	0.258661	H	2.743771	2.248082	-1.753475
C	2.007686	-1.754629	0.665494	C	-0.899987	-1.180696	0.306624
H	1.933281	-0.812065	-2.551899	H	-0.675608	-1.894663	1.107685
H	4.367878	-1.627674	-1.703360	C	-2.274358	-0.698174	0.264836
H	4.159559	-2.286512	0.890544	C	-2.606797	0.615247	-0.386087
H	1.623651	-1.899062	1.661573	C	-4.041278	0.917028	-0.602912
Fe	2.790348	0.029714	-0.011733	C	-5.005582	0.181597	-0.045827
C	1.907803	1.879071	0.281449	C	-4.680069	-1.010589	0.767991
C	2.534124	1.439822	1.480981	C	-3.264766	-1.396752	0.857020
C	3.922038	1.258843	1.215776	H	-4.244544	1.813751	-1.175318
C	4.152813	1.586768	-0.149307	H	-3.061752	-2.314102	1.398447
C	2.908127	1.969024	-0.725574	N	-0.036032	-0.832477	-0.563674
H	0.851996	2.046215	0.137147	H	-6.057234	0.422376	-0.141416
H	2.039916	1.252145	2.420425	O	-1.763986	1.446690	-0.652800
H	4.662782	0.914029	1.918819	O	-5.555647	-1.659387	1.317943

6a·H$^+$: E = -94.958452641655 au

N	0.599016	0.000003	-0.000002	H	-1.210948	-0.941922	0.000005
C	-0.672621	-0.000000	0.000002	H	1.136271	0.865415	-0.000005
H	-1.210952	0.941918	0.000003	H	1.136275	-0.865406	-0.000003

6b·H$^+$: E = -557.029426224857 au

C	-1.877097	0.192944	-0.022089	C	1.880751	-0.167370	0.034454
C	-2.755265	1.263236	-0.274021	C	2.413742	1.086651	0.322250
C	-4.123565	1.061680	-0.260250	C	3.788608	1.254445	0.281194
C	-4.629818	-0.205083	0.010550	C	4.621651	0.183084	-0.030518
C	-3.769387	-1.275301	0.271739	C	4.078725	-1.068651	-0.296452
C	-2.404603	-1.083104	0.257999	C	2.704718	-1.249981	-0.262637
H	-2.353077	2.246448	-0.484319	H	1.780615	1.916201	0.606249
H	-4.794961	1.886075	-0.457390	H	4.212854	2.222600	0.510102
H	-5.700085	-0.364881	0.024915	H	5.693904	0.323126	-0.053493
H	-4.175509	-2.253472	0.490241	H	4.723132	-1.904689	-0.531411
H	-1.757981	-1.923242	0.480921	H	2.276161	-2.221341	-0.480135
C	-0.479223	0.473453	-0.073646	N	0.478859	-0.400672	0.039415
H	-0.170043	1.499142	-0.232392	H	0.216503	-1.376619	0.125721

6c·H$^+$: E = -786.080780768789 au

C	1.880865	-0.123777	-0.058076	C	-2.390942	-1.122733	-0.222568
C	2.736984	-1.196382	0.166954	C	-3.738971	-1.345088	-0.235895
C	4.109439	-1.011605	0.184663	C	-4.639903	-0.277634	-0.024458
C	4.637692	0.265610	-0.027029	C	-4.147804	1.018012	0.194984
C	3.767047	1.341096	-0.268472	C	-2.787094	1.229566	0.205523
C	2.404714	1.151326	-0.289666	H	-1.732163	-1.963679	-0.402734
H	2.333363	-2.186922	0.343216	H	-4.147283	-2.330619	-0.412244
H	4.753740	-1.858372	0.364360	H	-4.820003	1.847086	0.354011
H	4.193823	2.317050	-0.454151	H	-2.409966	2.230413	0.376385
H	1.761517	1.991853	-0.511558	C	-0.492816	0.481979	0.049839
C	-1.874456	0.175687	0.005021	H	-0.204652	1.516329	0.185689

O	-5.926195	-0.602045	-0.057361	C	6.898676	-0.477228	0.190613
O	5.943247	0.561564	-0.031735	H	7.871021	0.003280	0.138806
C	-6.927455	0.406322	0.140625	H	6.763390	-0.926094	1.177176
H	-6.861431	1.170268	-0.635680	H	6.826805	-1.244313	-0.583660
H	-7.878002	-0.112370	0.067276	N	0.489650	-0.377642	-0.047961
H	-6.827130	0.857950	1.128875	H	0.245254	-1.358223	-0.117292

6d·H$^+$: E = -487.419183035902 au

C	1.541933	0.283805	-0.000003	N	2.777437	-0.135304	0.000003
H	1.367472	1.353101	-0.000017	H	3.534247	0.534562	-0.000005
C	-0.894773	-0.010073	0.000005	H	3.034193	-1.114402	0.000017
F	-1.508752	-0.462988	1.079298	N	0.486070	-0.499752	0.000007
F	-0.886513	1.315394	-0.000017	H	0.574145	-1.511062	0.000025
F	-1.508762	-0.463024	-1.079268				

6e·H$^+$: E = -354.819087784063 au

C	1.547446	0.253278	0.000000	N	0.513290	-0.553882	0.000020
H	1.313582	1.314281	-0.000019	H	0.519840	-1.569491	0.000036
N	2.795630	-0.120745	0.000004	N	-0.892193	0.014015	0.000009
H	3.527344	0.577582	-0.000011	O	-1.715552	-0.840980	0.000009
H	3.087133	-1.090295	0.000022	O	-0.948144	1.203204	-0.000019

6f·H$^+$: E = -475.184662485103 au

N	1.793125	-1.169690	0.000000	C	-0.768931	1.689839	0.000002
C	2.999325	-0.725728	0.000004	C	-1.909825	0.992447	0.000002
H	3.171268	0.342086	0.000005	H	-0.745136	2.772382	0.000009
C	0.559051	-0.458010	-0.000004	H	-2.882877	1.467268	0.000010
C	-0.577140	-1.165039	-0.000003	O	-2.914128	-1.150432	-0.000001
C	0.551426	1.041186	-0.000011	O	1.588918	1.673252	-0.000002
C	-1.905028	-0.483234	-0.000011	H	3.804684	-1.450029	0.000006
H	-0.607410	-2.250124	0.000001	H	1.672323	-2.182002	-0.000001

6g·H$^+$: E = -1744.499521626297 au

N	3.079584	-1.401560	0.183106	C	-1.271353	-1.450119	1.021620
C	2.369599	-0.636082	-0.614225	C	-2.164711	-0.344261	0.965877
H	2.404582	-0.892417	-1.667199	C	-2.414228	-0.046691	-0.401484
C	1.615912	0.476318	-0.225176	C	-1.675010	-0.964915	-1.196205
C	0.852902	1.286819	-1.158347	C	-0.976605	-1.834811	-0.314379
C	0.054442	2.161475	-0.402835	H	-0.891543	-1.914140	1.917035
C	0.263691	1.894029	0.982116	H	-2.568018	0.187757	1.812012
C	1.205157	0.854906	1.110925	H	-3.036107	0.752461	-0.770719
H	0.924492	1.243550	-2.233009	H	-1.649804	-0.995525	-2.273107
H	-0.630310	2.890920	-0.803003	H	-0.321169	-2.638908	-0.609594
H	-0.240119	2.386400	1.797635	H	3.150399	-1.218550	1.173222
H	1.554652	0.437933	2.041459	H	3.592375	-2.192563	-0.174336
Fe	-0.392291	0.143658	0.012680				

6h·H⁺: E = -2090.034741270726 au

C	1.321487	-1.320716	-0.597425	C	-2.300459	-0.702831	0.146654
C	2.317208	-1.122385	-1.628736	C	-2.695191	0.402939	-0.596582
C	3.566897	-1.485537	-1.090895	C	-4.023393	0.799310	-0.601336
C	3.382738	-1.876016	0.266426	C	-4.967576	0.095164	0.154799
C	2.013411	-1.766431	0.590108	C	-4.555210	-1.005249	0.919760
H	2.121843	-0.787021	-2.634282	C	-3.236421	-1.399348	0.915099
H	4.510622	-1.442633	-1.609032	H	-1.975100	0.982451	-1.158883
H	4.164636	-2.174413	0.945166	H	-4.310457	1.664813	-1.178564
H	1.580053	-1.983271	1.553206	H	-5.293512	-1.535701	1.504947
Fe	2.691824	0.085503	-0.005744	H	-2.931667	-2.261061	1.497375
C	1.814847	1.929308	0.416787	O	-6.270883	0.399989	0.222668
C	2.472231	1.424226	1.570797	C	-6.772809	1.505225	-0.529339
C	3.848584	1.260194	1.249726	H	-6.305978	2.439571	-0.209023
C	4.036988	1.660197	-0.101118	H	-7.838076	1.541264	-0.321755
C	2.778441	2.069390	-0.620612	H	-6.613108	1.354092	-1.599385
H	0.762593	2.151803	0.337696	C	-0.025167	-0.927998	-0.728637
H	2.011875	1.202843	2.519710	H	-0.332423	-0.410941	-1.628689
H	4.611930	0.880694	1.909075	N	-0.958941	-1.157417	0.159982
H	4.967491	1.633129	-0.644249	H	-0.705101	-1.723224	0.961196
H	2.589896	2.421259	-1.621593				

6i·H⁺: E = -2124.722878159823 au

Fe	-2.291138	-0.031391	0.085849	H	-2.580953	2.361595	-1.422190
C	-1.556335	-1.913455	0.509987	H	-0.448902	2.127842	0.184842
C	-2.943257	-2.026736	0.295400	C	0.297538	-0.815750	-0.863010
C	-3.249690	-1.555666	-1.014695	H	0.495673	-0.189881	-1.718956
C	-2.061604	-1.130739	-1.632870	C	2.579428	-0.422443	-0.062680
C	-0.972900	-1.376123	-0.703507	C	2.695887	0.967219	-0.618033
H	-1.040468	-2.181638	1.417792	C	3.643312	-1.038202	0.471257
H	-3.661167	-2.381270	1.016678	C	4.036302	1.570934	-0.636549
H	-4.236123	-1.500342	-1.444790	C	4.976415	-0.397644	0.488215
H	-1.958654	-0.723271	-2.625273	H	3.589513	-2.029838	0.905991
C	-1.889653	1.264445	1.661152	C	5.098262	0.946729	-0.119869
C	-3.288782	1.026503	1.560800	H	4.092681	2.557705	-1.078298
C	-3.718039	1.459599	0.276623	H	6.088017	1.385531	-0.112864
C	-2.586277	1.967493	-0.419251	O	1.711715	1.569846	-1.005892
C	-1.460263	1.853702	0.439442	O	5.928786	-0.967867	0.977872
H	-1.269431	1.043026	2.514265	N	1.309264	-1.025673	-0.030353
H	-3.911398	0.576566	2.316829	H	1.171386	-1.707607	0.704991
H	-4.721940	1.392084	-0.109754				

6j·H⁺: E = -3393.986601912731 au

N	0.386126	-0.014241	0.236630	C	-2.184571	1.512498	0.921996
C	-0.528305	0.317027	-0.637336	H	-2.551668	1.304366	-2.421492
H	-0.381046	-0.051848	-1.644382	H	-4.597366	2.502571	-1.169375
C	-1.660402	1.111764	-0.362542	H	-4.076984	2.537707	1.459389
C	-2.641963	1.475344	-1.361039	H	-1.720696	1.375706	1.885753
C	-3.706581	2.118399	-0.700534	Fe	-3.439938	0.158865	0.003961
C	-3.429566	2.137984	0.696370	C	-3.660645	-1.511327	1.220718

C	-4.897494	-0.817984	1.104603	H	3.887331	-2.358376	-1.753387
C	-5.260975	-0.792555	-0.269137	H	4.018699	-2.826506	0.887788
C	-4.250333	-1.468623	-1.006130	H	2.020067	-1.479982	2.082071
C	-3.266167	-1.917153	-0.083440	Fe	3.465678	-0.178257	0.015696
H	-3.121857	-1.697542	2.135378	C	3.566106	1.865827	0.367991
H	-5.452591	-0.372351	1.913846	C	4.284644	1.160962	1.374094
H	-6.138015	-0.321642	-0.682220	C	5.316887	0.419963	0.736754
H	-4.232233	-1.611069	-2.074199	C	5.235304	0.664058	-0.661262
H	-2.366251	-2.457120	-0.332076	C	4.153237	1.558241	-0.889859
C	1.523125	-0.809211	0.000923	H	2.723409	2.519422	0.529327
C	2.126007	-1.090655	-1.261043	H	4.080755	1.178863	2.432389
C	3.213238	-1.969969	-1.008271	H	6.024174	-0.229733	1.225760
C	3.284237	-2.216085	0.389433	H	5.871008	0.232807	-1.417139
C	2.241674	-1.495570	1.026924	H	3.830683	1.929109	-1.849114
H	1.832444	-0.704951	-2.223128	H	0.280608	0.323643	1.185503

6k·H$^+$: E = -487.344947432406 au

C	0.890977	-0.005594	-0.000632	H	-3.074665	-0.997584	-0.126140
F	1.545028	-0.453921	-1.064025	C	-0.523896	-0.561710	-0.012836
F	0.850984	1.336252	-0.035533	H	-0.675366	-1.634236	0.009679
F	1.507317	-0.398764	1.105870	N	-1.512211	0.249372	-0.035374
N	-2.826144	-0.034111	0.061617	H	-1.298119	1.250745	-0.036488
H	-3.426889	0.666897	-0.353538				

6l·H$^+$: E = -354.764035152934 au

N	2.514488	-0.021788	-0.034069	N	-1.097598	0.047213	-0.002428
H	3.108184	0.745857	0.249885	O	-1.088378	1.267569	0.003565
H	2.830248	-0.967750	0.136197	O	-2.037908	-0.705072	-0.015593
C	0.226919	-0.605902	0.012033	N	1.208490	0.211796	0.029115
H	0.278260	-1.685387	0.000532	H	0.898685	1.202735	0.022585

6m·H$^+$: E = -475.201553264335 au

C	-0.701285	-0.093718	-0.000022	H	3.160759	0.775207	0.000055
C	0.202431	-1.092484	-0.000020	O	2.444009	-1.744523	0.000016
C	-0.247647	1.346287	-0.000042	O	-1.075085	2.232122	-0.000004
C	1.670271	-0.812645	-0.000027	C	-2.131346	-0.267721	-0.000021
H	-0.049052	-2.148763	-0.000021	H	-2.722359	0.644872	-0.000052
C	1.200239	1.598316	0.000015	N	-2.769549	-1.389079	0.000015
C	2.092184	0.599152	0.000020	H	-3.783123	-1.407941	0.000010
H	1.494337	2.640444	0.000046	H	-2.303994	-2.290183	0.000049

6n·H$^+$: E = -1744.464921286670 au

C	-1.586190	0.338026	-0.199796	C	-0.910826	1.169069	-1.157536
C	-1.217094	0.741873	1.122203	H	-1.538090	0.305877	2.053344
C	-0.340681	1.844670	0.971797	H	0.133288	2.376703	1.779849
C	-0.159038	2.107314	-0.414453	H	0.471203	2.874184	-0.833059

H	-0.999613	1.113830	-2.230827	H	3.039405	0.852554	-0.804817
Fe	0.428520	0.148322	0.023418	H	2.629506	0.304880	1.792485
C	1.083975	-1.804869	-0.284603	H	1.036165	-1.855798	1.948198
C	1.738872	-0.920839	-1.186629	C	-3.288697	-1.335835	0.184016
C	2.453589	0.035903	-0.415533	H	-3.874961	-2.132545	-0.249578
C	2.235460	-0.252913	0.958743	H	-3.392129	-1.068932	1.225614
C	1.387396	-1.392098	1.040891	N	-2.451479	-0.699038	-0.557777
H	0.460902	-2.641806	-0.558660	H	-2.402977	-0.964665	-1.538867
H	1.700905	-0.965928	-2.262804				

6o·H$^+$: E = -2090.031635390844 au

C	1.246444	-1.117241	-0.537079	C	-1.069792	-1.097974	0.177586
C	2.172029	-0.998414	-1.619550	H	-0.797537	-1.831465	0.926413
C	3.404640	-1.534580	-1.168069	C	-2.412742	-0.647237	0.135930
C	3.243752	-1.966666	0.176199	C	-2.886194	0.335557	-0.756109
C	1.908186	-1.704918	0.582516	C	-4.205921	0.718840	-0.757932
H	1.962743	-0.597928	-2.598507	C	-5.107527	0.124464	0.147816
H	4.314568	-1.581629	-1.742663	C	-4.649447	-0.852855	1.048923
H	4.012138	-2.394233	0.798432	C	-3.331722	-1.226785	1.040805
H	1.490409	-1.904091	1.555166	H	-2.217853	0.819048	-1.458734
Fe	2.814745	0.063111	0.028217	H	-4.541153	1.475272	-1.450873
C	2.151403	1.956009	0.567683	H	-5.358296	-1.293098	1.736385
C	2.809905	1.338602	1.666228	H	-2.986977	-1.982431	1.735782
C	4.146490	1.054267	1.271494	O	-6.398361	0.425671	0.224592
C	4.313074	1.495610	-0.069414	C	-6.966659	1.404909	-0.655427
C	3.079853	2.051417	-0.506806	H	-6.501888	2.379729	-0.498517
H	1.126387	2.291403	0.553228	H	-8.018569	1.453236	-0.392286
H	2.372845	1.116312	2.626017	H	-6.860535	1.094981	-1.696358
H	4.896439	0.571889	1.876690	N	-0.099035	-0.718087	-0.611574
H	5.210912	1.405137	-0.658574	H	-0.309819	-0.062591	-1.354085
H	2.884730	2.466480	-1.482243				

6p·H$^+$: E = -2124.717282598755 au

C	1.279984	-1.184215	-0.527562	H	5.162748	1.495128	-0.555182
C	2.163242	-0.942040	-1.634295	H	2.837886	2.524488	-1.431235
C	3.437204	-1.419803	-1.250078	C	-0.989408	-1.201350	0.298112
C	3.356286	-1.915089	0.081127	H	-0.714259	-1.867733	1.106529
C	2.026620	-1.763491	0.547718	C	-2.352562	-0.755568	0.192123
H	1.887034	-0.517734	-2.585976	C	-2.768689	0.168973	-0.912273
H	4.326944	-1.385127	-1.856430	C	-4.176114	0.579969	-0.979246
H	4.175790	-2.315556	0.654429	C	-5.075101	0.153484	-0.085791
H	1.660474	-2.040601	1.522016	C	-4.689760	-0.754441	1.016352
Fe	2.780100	0.091215	0.035025	C	-3.272774	-1.178153	1.087860
C	2.059744	1.966584	0.587139	H	-4.430633	1.244783	-1.795039
C	2.694626	1.339610	1.694127	H	-3.022500	-1.848314	1.902540
C	4.048682	1.089535	1.335026	H	-6.116733	0.446934	-0.121546
C	4.246125	1.558731	0.008114	O	-1.952871	0.567685	-1.734426
C	3.015360	2.098008	-0.457547	O	-5.489130	-1.147135	1.840977
H	1.027186	2.274988	0.539988	N	-0.063950	-0.840186	-0.540154
H	2.234956	1.096092	2.638023	H	-0.404164	-0.221447	-1.293388
H	4.790288	0.611371	1.953795				

7: E = -155.946736278184 au

C	0.526433	1.599899	-0.365156	H	0.256094	-1.775035	-1.094370
C	0.527180	0.518990	0.405646	H	1.318552	0.396588	1.142997
C	-0.527180	-0.518990	0.405646	H	-1.318552	-0.396588	1.142997
C	-0.526433	-1.599899	-0.365156	H	1.314585	2.339670	-0.299691
H	-0.256094	1.775036	-1.094370	H	-1.314585	-2.339670	-0.299691

8: E = -171.991891251622 au

C	-1.581569	-0.294566	0.180630	H	-1.434878	-0.790916	1.146245
N	-0.669542	0.336791	-0.418234	H	0.758213	1.411222	0.661440
C	0.608101	0.467515	0.143497	H	1.493944	-1.292315	-0.608690
C	1.616997	-0.377706	-0.042793	H	2.595187	-0.159093	0.360998
H	-2.565665	-0.367320	-0.278660				

9: E = -249.371496625609 au

C	2.799037	0.335338	-0.016169	H	3.800561	0.050136	-0.311782
C	1.796627	-0.531042	-0.049406	H	1.973755	-1.561784	-0.347168
C	0.411970	-0.213724	0.375570	H	0.155189	-0.440686	1.420387
N	-0.451450	0.239991	-0.426931	H	-1.914728	1.572644	0.242915
C	-1.754069	0.524481	0.003813	H	-2.634329	-1.367495	-0.301982
C	-2.768945	-0.334257	-0.008008	H	-3.763049	-0.011090	0.266238
H	2.651397	1.363510	0.292919				

10: E = -188.020759949538 au

C	0.472279	1.438282	-0.371162	H	-0.346078	1.607302	-1.072996
N	0.512710	0.441401	0.410694	H	0.346078	-1.607304	-1.072996
N	-0.512708	-0.441401	0.410694	H	1.281548	2.157096	-0.320107
C	-0.472278	-1.438282	-0.371162	H	-1.281549	-2.157094	-0.320107

11: E = -265.381632374242 au

C	2.709246	0.347104	-0.029288	H	2.556021	1.374632	0.275030
C	1.710225	-0.520071	-0.063157	H	3.709321	0.045893	-0.307044
N	0.393908	-0.228927	0.401338	H	1.846933	-1.567126	-0.314876
N	-0.369439	0.240195	-0.447939	H	-1.822659	1.578249	0.268395
C	-1.685793	0.531257	0.016534	H	-2.531483	-1.363533	-0.321878
C	-2.684703	-0.336043	-0.017447	H	-3.684802	-0.034919	0.260339