Proton or Metal? The H/D Exchange of Arenes in Acidic Solvents

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Content:

Experimental Details

All catalytic reactions were performed in either screw-cap or J. Young NMR tubes. All chemicals were obtained from common commercial suppliers and were used without further purification. Measurement of the NMR spectra were performed on Bruker AC 300-P, Avance III 600, and Varian Inova 500 MHz instruments. The bis-NHC complexes were synthesized according to procedures reported in the literature.[1,2]

Standard procedure for H/D exchange reaction. The metal compound was weighed directly into the NMR tube in a N_2 filled glovebox. The NMR tube was brought out of the glovebox, and the indicated amount of toluene-D_8 was quickly added. Silver triflate was rapidly added in form of 0.8 mL of freshly prepared diluted solution in HOTFA or HOAc (containing 5% acetic anhydride). The diluted solutions were prepared in the glovebox. The NMR tube was sealed and immersed in a hot oil bath for the indicated time. After cooling to room temperature, 30 μL of a 1 : 9 v : v solution of $MeNO_2$: HOTFA (HOAc) as standard and a capillary, which contained DMSO-D_6, were added. The reaction was then analyzed by ^{1}H-NMR spectroscopy.

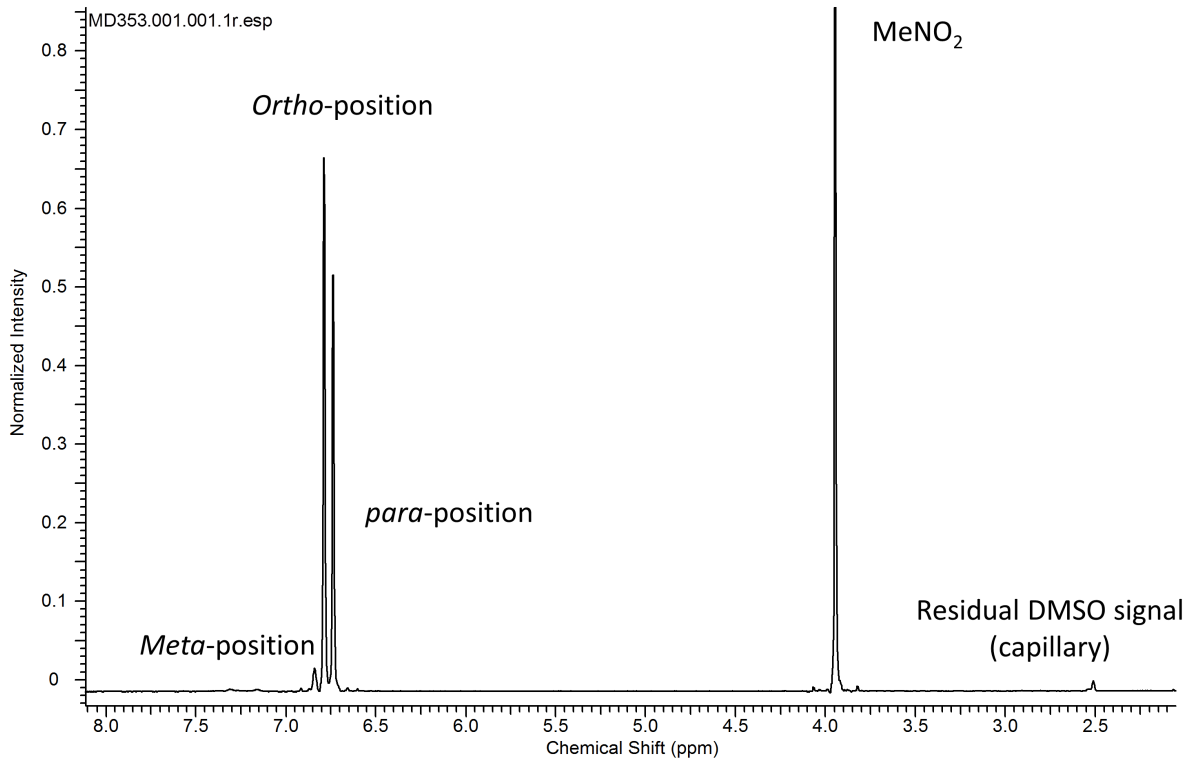

Figure S1. Representative ^{1}H NMR spectrum of H/D exchange of toluene-D_8 in HOTFA with comparably low yield (186 μmol) of H/D exchange.

Kinetic Experiment

Reaction Conditions

80 ºC, 28 µL Toluene-D_8, 0.8 mL HOTFA, 0.021 mmol $AgBF_4$. Determination of product formation by addition of 30 µL of dilute 9:1 v:v $MeNO_2$: HOTFA solution as internal standard to the reaction mixture at the beginning of the reaction.

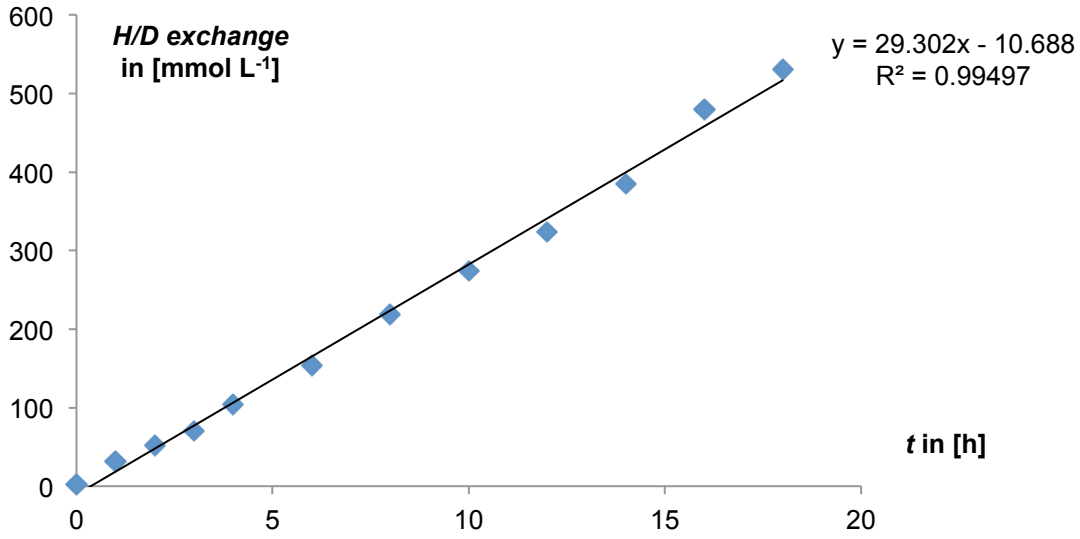

Figure S2. Kinetic experiment for the H/D exchange of toluene-D_8 in HOTFA.

Isotope Effect

The isotope effect was determined for the exchange of the *ortho*/*para* positions only. The reaction rate for the exchange of toluene-D_8 with HOTFA was determined according to Figure S2 (after subtraction of the exchange of the *meta* position). The reaction rate for the exchange of toluene-H_8 with DOTFA (Figure S3) was assessed by measuring the yield for the exchange of the *ortho* and *para* positions after 2, 8, and 17 h (each data point is the mean of two runs).

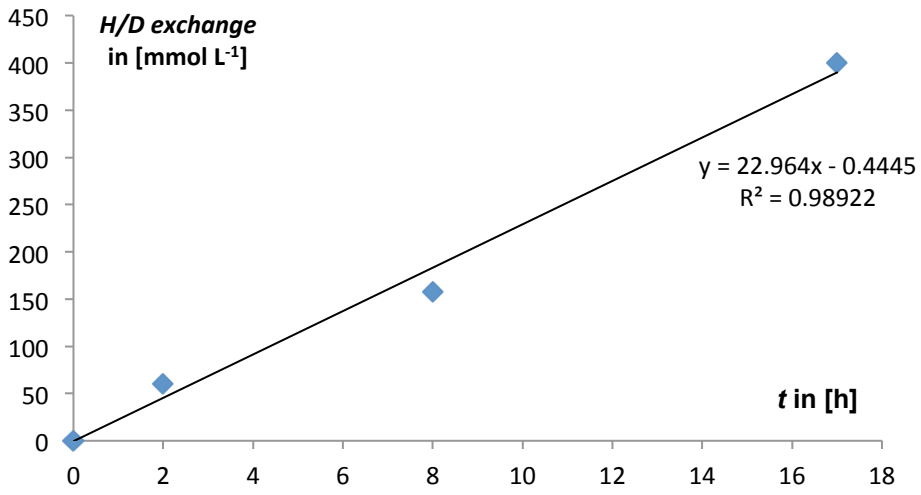

Figure S3. Reaction rate for H/D exchange of toluene-H_8 in DOTFA.

Comparison Tetrafluoroborate and Triflate Anions

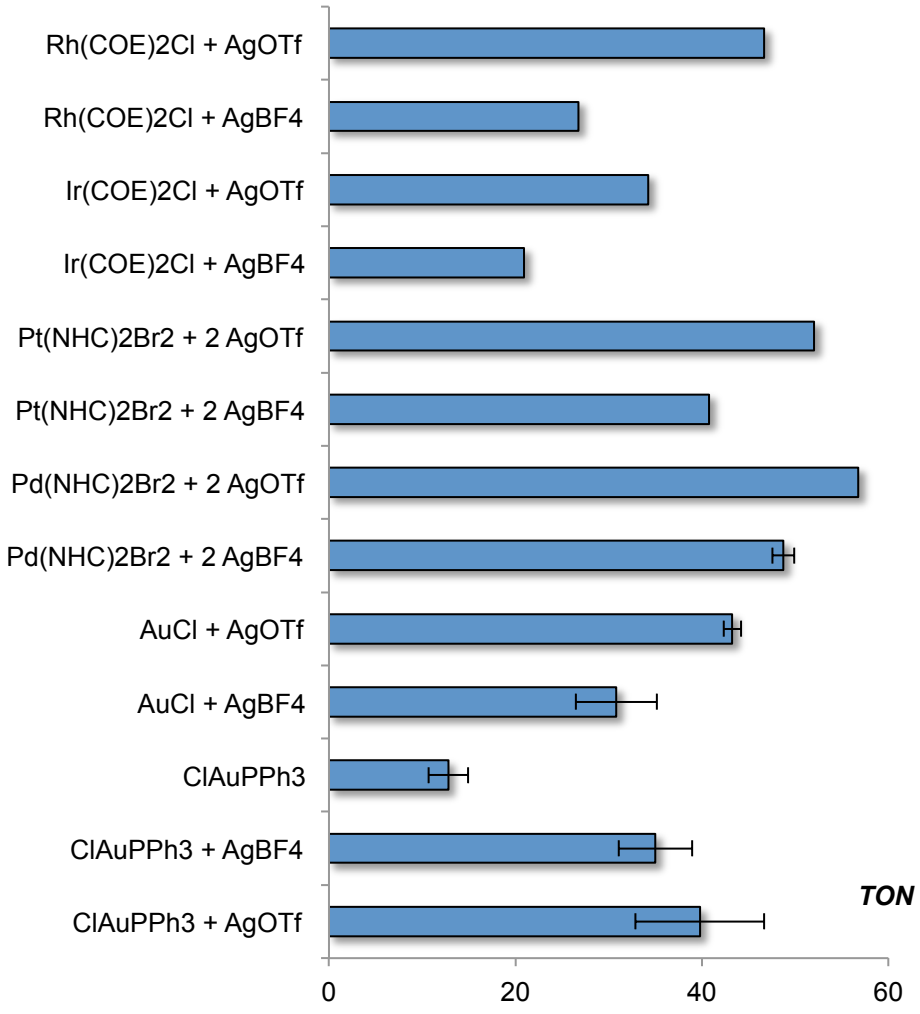

Figure S4. Triflate anion leads to faster catalysis than tetrafluoroborate anion.

Computational Details

All quantum mechanical calculations were carried out using the Jaguar software version 7.6 developed by Schrödinger Inc.[3] Geometry optimizations were carried out on initial guess structures, and vibrational frequencies were gathered to confirm the optimized geometries as intermediates or transition states and to construct a free energy profile. Solvation energies were calculated using the PBF Poisson-Boltzmann implicit continuum solvation model[4] in Jaguar, with a dielectric constant of 8.55 and a probe radius of 2.451 Å for HOTFA.

Geometry optimization and vibrational data were calculated using the B3LYP density functional,[5] whereas single point gas-phase and solvated energies were calculated using the M06 functional.[6] Calculations involving uncatalyzed H/D exchange of toluene in HOTFA used the 6-311G**++ basis set.[7] Geometry optimization and frequency calculations involving metal salts used a modified double-ζ Los Alamos basis set and pseudopotential[6] that includes *f* functions for transition metals[8], and the 6-31G** basis set[9] for the other atoms; whereas single point gas-phase and solvated energies used a modified triple-ζ Los Alamos basis set and pseudopotential (LACV3P**++) that includes *f* functions and diffuse functions for metals, and the 6-311G**++ basis set[10] for the other atoms.

The free energy for each molecular species in solution was calculated using the formula

$$G = E_{gas} + \Delta G_{solv} + ZPE + H_{tot} - TS_{tot}$$

where E_{gas} and ΔG_{solv} are the single point gas-phase and solvation energies, respectively, ZPE the zero-point energy, and H_{tot} and S_{tot} the total sum of vibrational, rotational, translational, and electronic enthalpy and entropy at standard conditions, respectively. The energies of uncatalyzed H/D exchange of toluene in HOTFA were calculated and Δ*G*s were reported relative to an energetically minimized assemblage of one toluene and two HOTFA molecules.

For metal ions M^{n+}, the relevant species in the equation $M(HOTFA)_c^{n+}$ + benzene ⇌ $M(HOTFA)_{c-1}(OTFA)^{(n-1)+}$ + benzeneH^+ were calculated, and the metals ranked by ΔG values. To ensure consistency, the coordination number c was taken to be 6 for most metals, with octahedral species being calculated; whereas for M = Pt, Pd, Au, and other platinum-group metals c was taken to be 4 and square planar species were calculated.

XYZ Coordinates of Calculated Structures

Al-III.6tfah.3+

Al1	0	0	0
O7	-0.86707	1.273666	1.128297
O8	-0.66949	-1.38774	1.128297
O9	-1.53656	-0.11407	-1.1283
O10	0.66949	1.387741	-1.1283
O11	1.536564	0.114075	1.128297
O12	0.867073	-1.27367	-1.1283
C13	-0.89155	2.281807	1.855492
O14	-1.90255	2.644672	2.55691
C15	-2.42188	0.368797	-1.85549
O16	-3.24163	-0.32532	-2.55691
C17	-1.53033	-1.91301	1.855492
O18	-1.33908	-2.97	2.55691
C19	2.421879	-0.3688	1.855492
O20	3.24163	0.325325	2.55691
C21	0.891552	-2.28181	-1.85549
O22	1.902555	-2.64467	-2.55691
C23	1.530327	1.91301	-1.85549
O24	1.339076	2.969997	-2.55691
C25	0.343274	3.215429	2.021865
F21	1.257434	2.522598	2.744532
F22	0.860048	3.458086	0.809002
F23	0.038918	4.330039	2.629096
C28	2.956281	1.310431	-2.02187
F25	2.813351	0.172329	-2.74453
F26	3.769383	2.131316	-2.6291
F27	3.424814	0.98422	-0.809
C31	2.613006	-1.905	2.021865
F29	1.555917	-2.35027	2.744532
F30	2.564766	-2.47387	0.809002
F31	3.730465	-2.19872	2.629096
C34	-0.34327	-3.21543	-2.02187
F33	-1.25743	-2.5226	-2.74453
F34	-0.03892	-4.33004	-2.6291
F35	-0.86005	-3.45809	-0.809
C37	-2.95628	-1.31043	2.021865
F37	-2.81335	-0.17233	2.744532
F38	-3.42481	-0.98422	0.809002
F39	-3.76938	-2.13132	2.629096
C40	-2.61301	1.904999	-2.02187
F41	-1.55592	2.350269	-2.74453
F42	-3.73047	2.198723	-2.6291
F43	-2.56477	2.473866	-0.809
H44	-3.08797	-1.29244	-2.50327
H45	-0.42469	-3.32048	2.503268
H46	2.663273	-2.02804	-2.50327
H47	3.087967	1.292444	2.503268
H48	0.424694	3.32048	-2.50327
H49	-2.66327	2.028035	2.503268

Ag-I.6tfah.1+

Ag1	0.110646	0.108558	-0.00281
O7	-1.14529	1.488121	1.695811
O8	-0.57987	-1.63035	1.718671
O9	-1.64499	-0.20496	-1.81917
O10	0.815285	1.788683	-1.73133
O11	1.900111	0.303491	1.752552
O12	1.121062	-1.53308	-1.6381
C13	-0.92064	2.191532	2.657717
O14	-1.62171	2.213226	3.777146
C15	-2.29859	0.368402	-2.66546
O16	-2.85294	-0.19539	-3.7217
C17	-1.4069	-1.8669	2.573234
O18	-1.19285	-2.54395	3.68648
C19	2.292584	-0.35387	2.692939
O20	2.516064	0.103092	3.912707
C21	0.695598	-2.1911	-2.56297
O22	1.174752	-2.19261	-3.79536
C23	1.536445	1.827245	-2.70522
O24	1.234216	2.378006	-3.86759
C25	0.265974	3.181628	2.727563
F21	1.146665	2.753348	3.676078
F22	0.896766	3.233267	1.55884
F23	-0.14763	4.39778	3.071001
C28	2.952093	1.20453	-2.73885
F25	2.968363	0.181431	-3.64064
F26	3.856571	2.101331	-3.12045
F27	3.273932	0.71897	-1.54468
C31	2.600767	-1.86722	2.605465
F29	1.807574	-2.54523	3.48112
F30	2.36331	-2.32102	1.379539
F31	3.86898	-2.10369	2.934456
C34	-0.49712	-3.16769	-2.43595
F33	-1.45644	-2.85137	-3.34806
F34	-0.09821	-4.41563	-2.67768
F35	-1.02972	-3.09795	-1.2193
C37	-2.8695	-1.36977	2.494565
F37	-3.0546	-0.39533	3.429425
F38	-3.1199	-0.85364	1.294189
F39	-3.72723	-2.35286	2.748702
C40	-2.54548	1.895135	-2.64469
F41	-1.74643	2.475744	-3.58439
F42	-3.80752	2.189135	-2.93649

F43	-2.22842	2.398399	-1.45487
H44	-2.63854	-1.14866	-3.71331
H45	-0.25327	-2.81059	3.712163
H46	1.93064	-1.57502	-3.83604
H47	2.308024	1.057319	3.930681
H48	0.324904	2.731055	-3.81914
H49	-2.33842	1.553192	3.709403

Bi-III.6tfah.3+

Bi1	0.002024	0.004288	0.003985
O7	-1.14742	1.318734	1.647669
O8	-0.57035	-1.6505	1.640485
O9	-1.71625	-0.29651	-1.63629
O10	0.58933	1.641124	-1.65063
O11	1.715502	0.321656	1.652294
O12	1.123114	-1.33604	-1.63645
C13	-1.00959	2.395776	2.249455
O14	-1.83493	2.873844	3.1153
C15	-2.56897	0.367524	-2.24721
O16	-3.39339	-0.10497	-3.11713
C17	-1.56769	-2.0707	2.249066
O18	-1.56065	-3.02346	3.116081
C19	2.577664	-0.3348	2.257746
O20	3.3998	0.142843	3.127244
C21	0.974006	-2.40791	-2.24477
O22	1.799333	-2.89285	-3.10698
C23	1.592741	2.046934	-2.25803
O24	1.600185	2.9962	-3.12927
C25	0.243571	3.288992	2.048174
F21	1.133126	2.98457	2.998498
F22	0.779464	2.964442	0.842681
F23	-0.0526	4.565275	2.073332
C28	2.987655	1.396087	-2.05938
F25	3.152552	0.462231	-3.0024
F26	3.953339	2.28099	-2.10063
F27	2.977442	0.781384	-0.84833
C31	2.729379	-1.86665	2.05848
F29	2.012366	-2.48498	3.003255
F30	2.193798	-2.17144	0.848879
F31	3.983359	-2.24544	2.098094
C34	-0.29346	-3.28453	-2.05932
F33	-1.17277	-2.95574	-3.01198
F34	-0.01561	-4.56462	-2.09862
F35	-0.83185	-2.96635	-0.85426
C37	-2.97116	-1.43618	2.056978
F37	-3.14473	-0.50889	3.004795
F38	-2.97204	-0.81673	0.848876
F39	-3.92547	-2.33347	2.097644
C40	-2.70386	1.901975	-2.05556
F41	-1.98497	2.50777	-3.00657
F42	-3.95444	2.292531	-2.09189
F43	-2.16034	2.208097	-0.84972
H44	-3.29455	-1.06741	-3.26841
H45	-0.67327	-3.4087	3.267779
H46	2.587203	-2.33039	-3.25473
H47	3.291299	1.103466	3.283142
H48	0.718147	3.39217	-3.28475
H49	-2.61383	2.301468	3.272255

Cu-II.6tfah.2+

Cu1	0.00877	-0.0063	0.00124
O7	-1.04792	1.216694	1.273042
O8	-0.72116	-1.61772	1.436374
O9	-1.55661	-0.23131	-1.22547
O10	0.723882	1.621891	-1.42356
O11	1.571586	0.219557	1.22409
O12	1.063328	-1.22369	-1.27556
C13	-0.96529	2.168915	2.045845
O14	-1.89015	2.497351	2.897609
C15	-2.34036	0.334913	-1.9874
O16	-3.12771	-0.29676	-2.80418
C17	-1.5947	-1.99244	2.20247
O18	-1.47757	-2.94276	3.093752
C19	2.346821	-0.35066	1.992488
O20	3.131887	0.278001	2.813157
C21	0.974142	-2.17161	-2.05255
O22	1.888931	-2.49063	-2.91858
C23	1.58416	1.999147	-2.20356
O24	1.449867	2.945563	-3.09655
C25	0.280182	3.089532	2.141255
F21	1.149736	2.505076	3.005507
F22	0.868244	3.174537	0.945925
F23	-0.03194	4.2896	2.583276
C28	2.988329	1.343492	-2.26629
F25	2.905257	0.27129	-3.10216
F26	3.91153	2.167525	-2.7171
F27	3.326873	0.894612	-1.05159
C31	2.474508	-1.89242	2.127975
F29	1.619134	-2.28815	3.093842
F30	2.126495	-2.47872	0.979133
F31	3.704339	-2.23676	2.456441
C34	-0.26761	-3.09845	-2.137
F33	-1.14355	-2.52457	-3.00166
F34	0.049441	-4.29979	-2.57232
F35	-0.85041	-3.17911	-0.93886
C37	-2.99686	-1.32982	2.250086

F37	-2.91717	-0.25622	3.084537
F38	-3.32222	-0.88165	1.031523
F39	-3.92855	-2.14844	2.693365
C40	-2.47906	1.876004	-2.1214
F41	-1.62815	2.278663	-3.08877
F42	-3.71167	2.212431	-2.44776
F43	-2.13326	2.464336	-0.97294
H44	-2.97308	-1.26236	-2.76842
H45	-0.57181	-3.30749	3.091298
H46	2.621258	-1.84079	-2.90583
H47	2.981893	1.244287	2.774402
H48	0.542387	3.305659	-3.08336
H49	-2.6259	1.851484	2.878847

Fe-II.6tfah.2+ (quintet)

Fe1	0	0	0
O7	-0.989	1.36763	1.290166
O8	-0.6899	-1.54031	1.290166
O9	-1.6789	-0.17268	-1.29017
O10	0.689905	1.540311	-1.29017
O11	1.678901	0.17268	1.290166
O12	0.988996	-1.36763	-1.29017
C13	-0.9241	2.293499	2.090214
O14	-1.85407	2.61054	2.944312
C15	-2.44828	0.346457	-2.09021
O16	-3.18783	-0.30041	-2.94431
C17	-1.52418	-1.94704	2.090214
O18	-1.33376	-2.91094	2.944312
C19	2.448277	-0.34646	2.090214
O20	3.187831	0.300405	2.944312
C21	0.924098	-2.2935	-2.09021
O22	1.854074	-2.61054	-2.94431
C23	1.524179	1.947041	-2.09021
O24	1.333757	2.910945	-2.94431
C25	0.332357	3.193403	2.21388
F21	1.195438	2.569263	3.056168
F22	0.920095	3.30292	1.018227
F23	0.04341	4.386129	2.691546
C28	2.931747	1.308872	-2.21388
F25	2.822766	0.249352	-3.05617
F26	3.820204	2.15547	-2.69155
F27	3.32046	0.854635	-1.01823
C31	2.59939	-1.88453	2.21388
F29	1.627328	-2.31991	3.056168
F30	2.400365	-2.44829	1.018227
F31	3.776794	-2.23066	2.691546
C34	-0.33236	-3.1934	-2.21388
F33	-1.19544	-2.56926	-3.05617
F34	-0.04341	-4.38613	-2.69155
F35	-0.92009	-3.30292	-1.01823
C37	-2.93175	-1.30887	2.21388
F37	-2.82277	-0.24935	3.056168
F38	-3.32046	-0.85463	1.018227
F39	-3.8202	-2.15547	2.691546
C40	-2.59939	1.884531	-2.21388
F41	-1.62733	2.319912	-3.05617
F42	-3.77679	2.230658	-2.69155
F43	-2.40037	2.448285	-1.01823
H44	-3.01381	-1.26163	-2.89857
H45	-0.4143	-3.24085	2.898568
H46	2.599508	-1.97922	-2.89857
H47	3.013809	1.26163	2.898568
H48	0.414301	3.24085	-2.89857
H49	-2.59951	1.97922	2.898568

Fe-III.6tfah.3+ (sextet)

Fe1	0	0	0
O7	-0.94382	1.322893	1.216293
O8	-0.67375	-1.47882	1.216293
O9	-1.61757	-0.15592	-1.21629
O10	0.67375	1.478816	-1.21629
O11	1.617568	0.155923	1.216293
O12	0.943817	-1.32289	-1.21629
C13	-0.92821	2.317996	1.961161
O14	-1.90939	2.685625	2.704678
C15	-2.47155	0.355144	-1.96116
O16	-3.28051	-0.31077	-2.70468
C17	-1.54334	-1.96285	1.961161
O18	-1.37113	-2.99639	2.704678
C19	2.471549	-0.35514	1.961161
O20	3.280513	0.310765	2.704678
C21	0.928211	-2.318	-1.96116
O22	1.909387	-2.68563	-2.70468
C23	1.543338	1.962852	-1.96116
O24	1.371126	2.99639	-2.70468
C25	0.331015	3.223039	2.10109
F21	1.219229	2.534564	2.856608
F22	0.861273	3.403646	0.884167
F23	0.050929	4.368692	2.663088
C28	2.956741	1.324852	-2.10109
F25	2.804612	0.211399	-2.85661
F26	3.808863	2.14024	-2.66309
F27	3.37828	0.955939	-0.88417
C31	2.625726	-1.89819	2.10109
F29	1.585383	-2.32317	2.856608
F30	2.517007	-2.44771	0.884167
F31	3.757934	-2.22845	2.663088
C34	-0.33102	-3.22304	-2.10109

F33	-1.21923	-2.53456	-2.85661
F34	-0.05093	-4.36869	-2.66309
F35	-0.86127	-3.40365	-0.88417
C37	-2.95674	-1.32485	2.10109
F37	-2.80461	-0.2114	2.856608
F38	-3.37828	-0.95594	0.884167
F39	-3.80886	-2.14024	2.663088
C40	-2.62573	1.898187	-2.10109
F41	-1.58538	2.323165	-2.85661
F42	-3.75793	2.228452	-2.66309
F43	-2.51701	2.447707	-0.88417
H44	-3.14484	-1.28112	-2.66461
H45	-0.46294	-3.36408	2.664612
H46	2.681907	-2.08295	-2.66461
H47	3.144844	1.281123	2.664612
H48	0.462937	3.364077	-2.66461
H49	-2.68191	2.082954	2.664612

Mg-II.6tfah.2+

Mg1	0	0	0
O7	-0.94933	1.351383	1.281482
O8	-0.69566	-1.49784	1.281482
O9	-1.645	-0.14646	-1.28148
O10	0.695665	1.497839	-1.28148
O11	1.644999	0.146456	1.281482
O12	0.949334	-1.35138	-1.28148
C13	-0.91494	2.274613	2.085372
O14	-1.86662	2.587213	2.915598
C15	-2.42734	0.344946	-2.08537
O16	-3.1739	-0.32294	-2.9156
C17	-1.5124	-1.92967	2.085372
O18	-1.30728	-2.91015	2.915598
C19	2.427343	-0.34495	2.085372
O20	3.173904	0.322936	2.915598
C21	0.914939	-2.27461	-2.08537
O22	1.866622	-2.58721	-2.9156
C23	1.512403	1.929667	-2.08537
O24	1.307281	2.910149	-2.9156
C25	0.335968	3.176854	2.244413
F21	1.190595	2.532839	3.082732
F22	0.938482	3.313072	1.058506
F23	0.041732	4.358003	2.74563
C28	2.91922	1.29747	-2.24441
F25	2.788801	0.235334	-3.08273
F26	3.795007	2.14286	-2.74563
F27	3.338445	0.843786	-1.05851
C31	2.583252	-1.87938	2.244413
F29	1.598206	-2.29751	3.082732
F30	2.399963	-2.46929	1.058506
F31	3.753275	-2.21514	2.74563
C34	-0.33597	-3.17685	-2.24441
F33	-1.1906	-2.53284	-3.08273
F34	-0.04173	-4.358	-2.74563
F35	-0.93848	-3.31307	-1.05851
C37	-2.91922	-1.29747	2.244413
F37	-2.7888	-0.23533	3.082732
F38	-3.33845	-0.84379	1.058506
F39	-3.79501	-2.14286	2.74563
C40	-2.58325	1.879384	-2.24441
F41	-1.59821	2.297505	-3.08273
F42	-3.75328	2.215143	-2.74563
F43	-2.39996	2.469285	-1.05851
H44	-2.99364	-1.2822	-2.85336
H45	-0.3864	-3.23367	2.85336
H46	2.607243	-1.95147	-2.85336
H47	2.993645	1.282203	2.85336
H48	0.386402	3.233674	-2.85336
H49	-2.60724	1.951471	2.85336

Tl-III.6tfah.3+

Tl1	0.000416	0.000615	2.48E-05
O7	-1.03746	1.327227	1.308726
O8	-0.6271	-1.56031	1.305033
O9	-1.6631	-0.23572	-1.3137
O10	0.628681	1.562988	-1.30259
O11	1.66413	0.2369	1.312974
O12	1.035344	-1.32763	-1.30933
C13	-0.96396	2.316623	2.060846
O14	-1.91218	2.706118	2.835411
C15	-2.48556	0.322327	-2.06356
O16	-3.29423	-0.30423	-2.84079
C17	-1.52018	-1.99312	2.056989
O18	-1.38164	-3.00938	2.830458
C19	2.48609	-0.32115	2.06338
O20	3.2922	0.305389	2.843282
C21	0.959225	-2.31654	-2.06183
O22	1.904529	-2.70521	-2.84039
C23	1.521748	1.993624	-2.0559
O24	1.38484	3.010685	-2.82857
C25	0.321648	3.183096	2.182792
F21	1.14822	2.540673	3.037264
F22	0.914056	3.231099	0.97892
F23	0.06106	4.387692	2.619235
C28	2.913194	1.310786	-2.18057
F25	2.765488	0.273507	-3.03368
F26	3.826927	2.136476	-2.61936
F27	3.251941	0.821786	-0.97689
C31	2.601247	-1.86775	2.176075

F29	1.626856	-2.27237	3.020497
F30	2.358326	-2.39795	0.966823
F31	3.773193	-2.24127	2.619141
C34	-0.32641	-3.18369	-2.17926
F33	-1.15523	-2.54313	-3.03285
F34	-0.06626	-4.38889	-2.6143
F35	-0.91603	-3.23009	-0.9739
C37	-2.91356	-1.31377	2.179065
F37	-2.76935	-0.27431	3.030024
F38	-3.25262	-0.82829	0.974
F39	-3.82547	-2.14089	2.618941
C40	-2.59779	1.868919	-2.17902
F41	-1.62199	2.270225	-3.02333
F42	-3.76864	2.244044	-2.62354
F43	-2.35461	2.400743	-0.97045
H44	-3.18477	-1.27816	-2.82025
H45	-0.48469	-3.40415	2.805531
H46	2.695506	-2.12665	-2.81847
H47	3.180907	1.279133	2.824469
H48	0.489063	3.407975	-2.80216
H49	-2.70334	2.127906	2.810753

Zn-II.6tfah.2+

Zn1	0.000235	-0.00034	-0.00019
O7	-1.00422	1.330189	1.315417
O8	-0.65057	-1.5356	1.316375
O9	-1.65472	-0.20524	-1.31805
O10	0.648438	1.535877	-1.31729
O11	1.656021	0.202566	1.31672
O12	1.006614	-1.32912	-1.3164
C13	-0.92407	2.260165	2.110442
O14	-1.84239	2.587303	2.972343
C15	-2.41988	0.328071	-2.11365
O16	-3.16032	-0.30442	-2.97708
C17	-1.49545	-1.93188	2.111555
O18	-1.31951	-2.89229	2.971866
C19	2.420015	-0.33134	2.113062
O20	3.162537	0.300671	2.97502
C21	0.92727	-2.25885	-2.11176
O22	1.845188	-2.58383	-2.97495
C23	1.492825	1.933523	-2.11229
O24	1.315105	2.89304	-2.97327
C25	0.336422	3.156184	2.22059
F21	1.180736	2.563975	3.103336
F22	0.945585	3.212545	1.031586
F23	0.046624	4.369997	2.641731
C28	2.899955	1.292052	-2.22424
F25	2.80913	0.264211	-3.10661
F26	3.804248	2.151057	-2.64745
F27	3.256077	0.793517	-1.03577
C31	2.563956	-1.87102	2.225429
F29	1.626865	-2.30386	3.107228
F30	2.309373	-2.42803	1.036787
F31	3.758849	-2.22786	2.649172
C34	-0.33155	-3.15739	-2.22077
F33	-1.17715	-2.56786	-3.10408
F34	-0.03933	-4.37111	-2.64062
F35	-0.94044	-3.21362	-1.03165
C37	-2.90098	-1.28713	2.224565
F37	-2.80667	-0.25901	3.106275
F38	-3.25715	-0.78839	1.036207
F39	-3.80694	-2.14363	2.649242
C40	-2.56834	1.86753	-2.2231
F41	-1.6333	2.304793	-3.10487
F42	-3.76468	2.221534	-2.64517
F43	-2.31445	2.423091	-1.03365
H44	-2.99158	-1.26708	-2.94141
H45	-0.4021	-3.22911	2.934942
H46	2.594069	-1.95583	-2.93975
H47	2.996441	1.26371	2.937713
H48	0.396989	3.22798	-2.93675
H49	-2.59241	1.96073	2.936531

Zn-II.6tfah.2+

Zn1	0.000235	-0.00034	-0.00019
O7	-1.00422	1.330189	1.315417
O8	-0.65057	-1.5356	1.316375
O9	-1.65472	-0.20524	-1.31805
O10	0.648438	1.535877	-1.31729
O11	1.656021	0.202566	1.31672
O12	1.006614	-1.32912	-1.3164
C13	-0.92407	2.260165	2.110442
O14	-1.84239	2.587303	2.972343
C15	-2.41988	0.328071	-2.11365
O16	-3.16032	-0.30442	-2.97708
C17	-1.49545	-1.93188	2.111555
O18	-1.31951	-2.89229	2.971866
C19	2.420015	-0.33134	2.113062
O20	3.162537	0.300671	2.97502
C21	0.92727	-2.25885	-2.11176
O22	1.845188	-2.58383	-2.97495
C23	1.492825	1.933523	-2.11229
O24	1.315105	2.89304	-2.97327
C25	0.336422	3.156184	2.22059
F21	1.180736	2.563975	3.103336

F22	0.945585	3.212545	1.031586
F23	0.046624	4.369997	2.641731
C28	2.899955	1.292052	-2.22424
F25	2.80913	0.264211	-3.10661
F26	3.804248	2.151057	-2.64745
F27	3.256077	0.793517	-1.03577
C31	2.563956	-1.87102	2.225429
F29	1.626865	-2.30386	3.107228
F30	2.309373	-2.42803	1.036787
F31	3.758849	-2.22786	2.649172
C34	-0.33155	-3.15739	-2.22077
F33	-1.17715	-2.56786	-3.10408
F34	-0.03933	-4.37111	-2.64062
F35	-0.94044	-3.21362	-1.03165

Al-III.tfa.5tfah.2+

Al1	0.281799	-0.04077	0.141625
O7	-0.1074	0.12685	1.990833
O8	-1.49663	-0.39491	-0.36447
O9	0.128396	1.821728	-0.10691
O10	2.128794	0.289784	0.617903
O11	0.669478	-1.93224	0.471075
O12	0.798936	-0.3272	-1.65331
C13	-0.64817	-0.07948	3.089566
O14	-1.85509	0.216038	3.400452
C15	-0.27262	2.94668	0.245675
O16	-1.42365	3.218786	0.73445
C17	-2.62632	0.050398	0.072801
O18	-2.77871	0.924721	0.939937
C19	0.254386	-3.03976	0.838656
O20	1.004651	-4.07413	1.014349
C21	0.342661	-0.68601	-2.75749
O22	-0.86474	-1.0481	-3.00741
C23	3.19228	0.842037	0.295418
O24	4.149136	1.072286	1.131742
C25	0.186106	-0.7767	4.192895
F21	1.341292	-0.12001	4.325267
F22	-0.45251	-0.8397	5.338785
F23	0.446636	-2.02294	3.735967
C28	3.546175	1.265247	-1.1621
F25	2.528456	1.965904	-1.6726
F26	4.649298	1.984481	-1.18918
F27	3.708711	0.135909	-1.86183
C31	-1.25353	-3.33922	1.074498
F29	-1.77224	-2.34122	1.823866
F30	-1.84883	-3.3328	-0.12244
F31	-1.43607	-4.48841	1.680659
C34	1.317746	-0.72488	-3.96553
C37	-2.90098	-1.28713	2.224565
F37	-2.80667	-0.25901	3.106275
F38	-3.25715	-0.78839	1.036207
F39	-3.80694	-2.14363	2.649242
C40	-2.56834	1.86753	-2.2231
F41	-1.6333	2.304793	-3.10487
F42	-3.76468	2.221534	-2.64517
F43	-2.31445	2.423091	-1.03365
H44	-2.99158	-1.26708	-2.94141
H45	-0.4021	-3.22911	2.934942
H46	2.594069	-1.95583	-2.93975
H47	2.996441	1.26371	2.937713
H48	0.396989	3.22798	-2.93675
H49	-2.59241	1.96073	2.936531
F33	1.844105	0.492937	-4.10299
F34	2.280961	-1.60259	-3.66734
F35	0.690475	-1.08631	-5.06865
C37	-3.86831	-0.64302	-0.55288
F37	-3.55156	-1.09192	-1.78764
F38	-4.1886	-1.68859	0.216555
F39	-4.88382	0.195414	-0.6347
C40	0.703689	4.139364	0.075087
F41	1.873371	3.763933	0.632758
F42	0.883651	4.347074	-1.22638
F43	0.250473	5.224738	0.668591
H44	-2.00473	2.402561	0.812307
H46	-1.45076	-1.00186	-2.2129
H47	1.948627	-3.89955	0.826663
H48	3.933159	0.779763	2.039568
H49	-2.35452	0.576874	2.616765

Ag-I.tfa.5tfah.0

Ag1	0.804195	0.020846	-0.08105
O2	0.023286	0.186194	2.400832
O3	-1.47074	0.231889	-1.09555
O4	0.853954	2.531459	0.174318
O5	3.19937	0.806439	0.282802
O6	0.9247	-2.37517	0.906175
O7	1.125949	-1.33337	-2.12921
C8	-0.85988	-0.22276	3.131097
O9	-2.14989	-0.01026	3.036201
C10	0.241864	3.316108	0.88245
O11	-0.99796	3.247598	1.26874
C12	-2.43069	0.417316	-0.31533
O13	-2.45997	1.184698	0.688652
C14	0.196761	-3.32753	1.062583
O15	0.543606	-4.48412	1.611983
C16	0.341901	-1.65051	-3.00866

O17	-0.92184	-1.33621	-3.11516
C18	3.525417	1.896606	-0.13283
O19	4.151529	2.834924	0.567454
C20	-0.52177	-1.16998	4.305929
F21	0.709918	-0.92876	4.764054
F22	-1.38828	-1.07068	5.316773
F23	-0.55476	-2.44758	3.846814
C24	3.331952	2.343282	-1.59869
F25	2.426228	1.563481	-2.20133
F26	2.940189	3.616658	-1.68359
F27	4.505351	2.210249	-2.24509
C28	-1.27883	-3.31595	0.601426
F29	-1.89727	-2.24986	1.14794
F30	-1.31742	-3.1838	-0.7332
F31	-1.93841	-4.41738	0.950302
C32	0.807795	-2.5804	-4.1539
F33	2.12101	-2.4391	-4.36207
F34	0.568912	-3.85987	-3.80116
F35	0.161476	-2.32967	-5.29889
C36	-3.74993	-0.35007	-0.59818
F37	-3.53751	-1.41368	-1.39317
F38	-4.30286	-0.78643	0.545304
F39	-4.62803	0.462885	-1.21082
C40	0.992995	4.553322	1.42917
F41	1.970663	4.126572	2.260072
F42	1.567157	5.218231	0.417555
F43	0.203344	5.390802	2.104508
H44	-1.46502	2.406801	0.935857
H45	-1.22517	-0.7694	-2.33792
H46	1.479481	-4.41749	1.873615
H47	4.238693	2.517777	1.483332
H48	-2.35919	0.485787	2.190559

Bi-III.tfa.5tfah.2+

Bi1	0.853987	-0.0563	0.553383
O2	-0.3432	-0.22516	2.602227
O3	-1.02387	-0.03759	-0.54846
O4	0.557008	2.208249	0.959495
O5	2.873182	1.141371	-0.29518
O6	0.567882	-2.47105	0.9323
O7	1.426926	-1.03289	-1.47499
C8	-1.25454	-0.52646	3.383698
O9	-2.47164	-0.09478	3.340662
C10	0.023913	3.329921	0.944131
O11	-1.2379	3.579368	0.954503
C12	-2.18876	0.423141	-0.1798
O13	-2.41062	1.134236	0.798585
C14	-0.20816	-3.4227	1.039641
O15	0.094035	-4.59718	1.494108
C16	0.984834	-1.42745	-2.56756
O17	-0.23844	-1.3712	-2.97413
C18	3.128405	1.89396	-1.23318
O19	4.251735	2.512274	-1.4314
C20	-0.97456	-1.55877	4.505122
F21	0.178883	-1.26258	5.09436
F22	-1.95238	-1.61717	5.385389
F23	-0.85173	-2.75752	3.881572
C24	2.107221	2.155044	-2.36861
F25	0.861712	1.870819	-1.88455
F26	2.130645	3.399544	-2.79237
F27	2.35275	1.308294	-3.37119
C28	-1.68456	-3.2988	0.585625
F29	-2.23917	-2.26803	1.268141
F30	-1.68253	-2.97407	-0.71972
F31	-2.38116	-4.39082	0.785834
C32	1.95458	-2.04592	-3.61476
F33	2.084359	-1.17818	-4.61904
F34	3.135953	-2.25984	-3.04398
F35	1.445693	-3.18958	-4.05942
C36	-3.36957	-0.03212	-1.09057
F37	-2.89926	-0.5601	-2.23783
F38	-4.06427	-0.96496	-0.43716
F39	-4.14191	1.005471	-1.36757
C40	0.947417	4.57592	0.913405
F41	1.817147	4.395471	-0.10459
F42	0.264577	5.686595	0.72475
F43	1.624347	4.624705	2.058437
H44	-1.77392	2.74251	0.966569
H45	-0.84465	-0.95944	-2.31733
H46	1.029933	-4.65913	1.77073
H47	4.909493	2.313151	-0.73627
H48	-2.6219	0.481387	2.554696

Cu-II.tfa.5tfah.1+

Cu1	0.511022	0.072709	0.038812
O2	0.424056	-0.35038	2.042608
O3	-1.31954	-0.31898	-0.52682
O4	0.25038	2.245059	0.494394
O5	2.460977	0.467108	0.432953
O6	0.527938	-2.63028	0.189929
O7	1.163713	-0.47651	-1.79836
C8	-0.28204	-0.34999	3.051708
O9	-1.45861	0.160367	3.201029
C10	-0.33143	3.314765	0.603616
O11	-1.6125	3.493293	0.779836
C12	-2.41218	0.136361	-0.0464

O13	-2.54362	0.900298	0.926273
C14	-0.09764	-3.51373	0.737886
O15	0.399963	-4.61846	1.258763
C16	0.675851	-1.22251	-2.65333
O17	-0.53503	-1.67615	-2.70078
C18	3.312971	1.209825	-0.04351
O19	4.485219	1.39691	0.503781
C20	0.268229	-1.07622	4.303497
F21	1.493129	-0.61494	4.57718
F22	-0.51652	-0.91912	5.360289
F23	0.356059	-2.38516	4.001387
C24	3.189832	1.990242	-1.38089
F25	1.904341	2.155741	-1.71348
F26	3.771868	3.179071	-1.27568
F27	3.796574	1.269216	-2.32847
C28	-1.63612	-3.43603	0.896358
F29	-1.9312	-2.38968	1.705945
F30	-2.18146	-3.19064	-0.30642
F31	-2.1658	-4.53488	1.406997
C32	1.57534	-1.73688	-3.80473
F33	2.672193	-0.9865	-3.88942
F34	1.92272	-3.00096	-3.52406
F35	0.915698	-1.70354	-4.95999
C36	-3.70395	-0.35303	-0.76075
F37	-3.40662	-1.0204	-1.88819
F38	-4.36914	-1.16872	0.062729
F39	-4.46944	0.69462	-1.06551
C40	0.450551	4.6492	0.531485
F41	1.76314	4.388682	0.460827
F42	0.080025	5.325205	-0.55986
F43	0.208761	5.385291	1.617422
H44	-2.07379	2.618769	0.826143
H45	-1.07083	-1.32964	-1.93873
H46	1.367105	-4.6222	1.138195
H47	4.56442	0.867933	1.320171
H48	-1.82738	0.521124	2.33803

Fe-II.tfa.5tfah.1+ (quintet)

Fe1	0.408055	-0.0495	0.015306
O2	0.014995	0.155365	2.124342
O3	-1.5571	-0.35073	-0.58521
O4	0.22468	2.053292	-0.16603
O5	2.451043	0.380651	0.506161
O6	0.743831	-2.15282	0.517109
O7	1.00351	-0.44667	-1.9653
C8	-0.65234	-0.07697	3.128208
O9	-1.91937	0.147348	3.294145
C10	-0.2067	3.047219	0.411399
O11	-1.37637	3.183091	0.955306
C12	-2.6429	0.055621	-0.05889
O13	-2.75977	0.899861	0.854857
C14	0.247102	-3.16889	0.978216
O15	0.919282	-4.1964	1.432761
C16	0.428044	-0.86713	-2.96786
O17	-0.83662	-1.14862	-3.07889
C18	3.40198	1.08288	0.185252
O19	4.331938	1.476524	1.017682
C20	0.03308	-0.75857	4.334254
F21	1.189209	-0.1418	4.598255
F22	-0.72784	-0.77144	5.417927
F23	0.303207	-2.03243	3.965245
C24	3.662221	1.549023	-1.27261
F25	2.565127	2.141357	-1.75263
F26	4.684276	2.394137	-1.33386
F27	3.932068	0.461124	-2.00363
C28	-1.28718	-3.3736	1.050874
F29	-1.81559	-2.36927	1.782781
F30	-1.78022	-3.29991	-0.19088
F31	-1.6167	-4.52983	1.600079
C32	1.240386	-1.15845	-4.25169
F33	2.38962	-0.48469	-4.21706
F34	1.501403	-2.47409	-4.28969
F35	0.549626	-0.8128	-5.33629
C36	-3.93324	-0.63209	-0.58046
F37	-3.75282	-1.08564	-1.83226
F38	-4.20285	-1.67871	0.219229
F39	-4.96306	0.207974	-0.5641
C40	0.693677	4.30181	0.507871
F41	1.960603	3.89603	0.725752
F42	0.647458	4.965819	-0.64945
F43	0.31911	5.101953	1.500605
H44	-1.91329	2.339653	0.864846
H45	-1.31565	-0.96727	-2.22653
H46	1.877482	-4.02917	1.358541
H47	4.13526	1.146147	1.914427
H48	-2.32668	0.487453	2.448525

Fe-III.tfa.5tfah.2+ (sextet)

Fe1	0.361943	-0.03319	0.200105
O2	-0.08175	0.144315	2.153109
O3	-1.51108	-0.35518	-0.40715
O4	0.184645	1.932533	-0.0844
O5	2.351287	0.375417	0.646995
O6	0.747299	-2.04283	0.605964
O7	0.894943	-0.4231	-1.69751

C8	-0.69885	-0.14034	3.19478
O9	-1.92834	0.133512	3.438245
C10	-0.25745	3.053452	0.230499
O11	-1.41595	3.29652	0.721356
C12	-2.62333	0.092559	0.074696
O13	-2.73622	0.96063	0.952096
C14	0.26268	-3.13459	0.925998
O15	0.951763	-4.19665	1.1838
C16	0.395847	-0.71813	-2.80159
O17	-0.83531	-1.01418	-3.02756
C18	3.380075	0.934759	0.242962
O19	4.393186	1.207944	1.000451
C20	0.049058	-0.91998	4.307619
F21	1.212188	-0.31659	4.543294
F22	-0.66367	-1.01705	5.407857
F23	0.289798	-2.15222	3.803318
C24	3.611851	1.32848	-1.24646
F25	2.532976	1.984568	-1.69275
F26	4.684444	2.082094	-1.37793
F27	3.754002	0.190045	-1.93522
C28	-1.27173	-3.36489	1.006413
F29	-1.80298	-2.37466	1.758646
F30	-1.75784	-3.2648	-0.23662
F31	-1.57163	-4.52955	1.530359
C32	1.334799	-0.73996	-4.04201
F33	1.836997	0.488393	-4.18323
F34	2.319183	-1.60376	-3.78798
F35	0.672649	-1.09722	-5.12637
C36	-3.89099	-0.59678	-0.51109
F37	-3.6273	-1.02198	-1.76166
F38	-4.17501	-1.65476	0.256842
F39	-4.90989	0.242181	-0.52909
C40	0.663416	4.281525	-0.00886
F41	1.873169	3.970929	0.487923
F42	0.75929	4.470051	-1.32294
F43	0.190616	5.357821	0.587368
H44	-1.9646	2.463075	0.824684
H45	-1.39218	-0.9626	-2.21187
H46	1.915806	-4.05278	1.1014
H47	4.251727	0.930721	1.927278
H48	-2.37456	0.549736	2.6522

Mg-II.tfa.5tfah.1+

Mg1	0.447043	-0.02217	0.138664
O2	0.053442	0.081004	2.174475
O3	-1.51691	-0.3262	-0.49232
O4	0.262068	2.016538	-0.02018
O5	2.477992	0.376523	0.563017
O6	0.728926	-2.1084	0.55281
O7	0.97983	-0.43456	-1.80978
C8	-0.63369	-0.1534	3.165081
O9	-1.88913	0.116546	3.322196
C10	-0.24285	3.073443	0.348287
O11	-1.43802	3.240246	0.816536
C12	-2.60744	0.080805	0.006795
O13	-2.73762	0.917762	0.933263
C14	0.249361	-3.16979	0.919995
O15	0.935292	-4.23914	1.231139
C16	0.420638	-0.81075	-2.83983
O17	-0.84157	-1.07692	-2.98061
C18	3.468576	0.990999	0.194847
O19	4.483686	1.284731	0.969023
C20	0.016003	-0.89767	4.353519
F21	1.190969	-0.33135	4.644604
F22	-0.75455	-0.91821	5.429982
F23	0.243116	-2.16811	3.944153
C24	3.680651	1.465729	-1.26816
F25	2.576773	2.086675	-1.69572
F26	4.716856	2.290151	-1.36565
F27	3.897525	0.380832	-2.0223
C28	-1.28199	-3.39036	1.024128
F29	-1.80861	-2.39879	1.771319
F30	-1.79685	-3.31574	-0.20974
F31	-1.58727	-4.55485	1.570608
C32	1.274844	-1.04169	-4.10803
F33	2.118133	-0.01626	-4.25629
F34	1.981992	-2.16849	-3.92613
F35	0.520798	-1.16269	-5.19519
C36	-3.89658	-0.57674	-0.55292
F37	-3.69247	-1.01773	-1.80738
F38	-4.2015	-1.63076	0.224454
F39	-4.91486	0.277619	-0.55324
C40	0.603964	4.363049	0.240275
F41	1.821234	4.105526	0.753692
F42	0.738982	4.678014	-1.05234
F43	0.056974	5.378886	0.89625
H44	-1.93895	2.367571	0.847066
H45	-1.32138	-0.91335	-2.12062
H46	1.890424	-4.06709	1.13106
H47	4.319141	0.952026	1.871242
H48	-2.27652	0.4892	2.474363

Tl-III.tfa.5tfah.2+

Tl1	0.356053	0.016126	0.178079
O2	0.037655	0.044331	2.27746
O3	-1.56077	-0.34126	-0.53556
O4	0.269898	2.130176	0.063961

O5	2.405775	0.31832	0.655499
O6	0.794827	-2.14562	0.599806
O7	0.962097	-0.44657	-1.79738
C8	-0.64602	-0.24841	3.274411
O9	-1.8893	0.013873	3.460615
C10	-0.32541	3.200302	0.291836
O11	-1.52884	3.338411	0.720454
C12	-2.64092	0.084694	0.040039
O13	-2.66477	0.882574	0.986959
C14	0.268137	-3.21342	0.93199
O15	0.911579	-4.29787	1.218456
C16	0.443043	-0.80883	-2.87258
O17	-0.80128	-1.05746	-3.08742
C18	3.457949	0.818202	0.223299
O19	4.527162	0.939797	0.937249
C20	0.037525	-1.05292	4.409495
F21	1.206501	-0.48762	4.699715
F22	-0.72012	-1.14456	5.480951
F23	0.262699	-2.28656	3.89802
C24	3.649696	1.30801	-1.24169
F25	2.52277	1.913073	-1.6407
F26	4.665885	2.141074	-1.3323
F27	3.862655	0.224445	-1.99401
C28	-1.27282	-3.38668	0.990889
F29	-1.77872	-2.3452	1.697195
F30	-1.7355	-3.30619	-0.26238
F31	-1.63345	-4.51634	1.549993
C32	1.387794	-0.99723	-4.0923
F33	2.031379	0.154671	-4.2876
F34	2.263613	-1.95405	-3.77263
F35	0.707473	-1.33681	-5.17128
C36	-3.95279	-0.53973	-0.51719
F37	-3.78869	-0.8432	-1.81356
F38	-4.18272	-1.66498	0.171736
F39	-4.96224	0.299205	-0.3719
C40	0.426858	4.526947	-0.00763
F41	1.711607	4.361556	0.321604
F42	0.325965	4.749757	-1.31956
F43	-0.09537	5.529636	0.675245
H44	-1.99956	2.470168	0.848697
H45	-1.3636	-0.92066	-2.28366
H46	1.880699	-4.18997	1.146072
H47	4.411573	0.602389	1.84798
H48	-2.30909	0.435858	2.665719

Zn-II.tfa.5tfah.1+

Zn1	0.405142	0.143878	0.096046
O2	0.042178	0.140666	2.188228
O3	-1.54612	-0.1977	-0.58385
O4	0.328668	2.233111	0.048827
O5	2.477033	0.387949	0.579938
O6	0.734127	-2.0474	0.501353
O7	1.014003	-0.38001	-1.8412
C8	-0.62593	-0.18479	3.165774
O9	-1.89311	0.015612	3.350078
C10	-0.30263	3.212601	0.448206
O11	-1.50293	3.232303	0.930119
C12	-2.62898	0.117318	8.14E-06
O13	-2.7433	0.905454	0.966745
C14	0.242181	-3.11726	0.822777
O15	0.914347	-4.20222	1.116785
C16	0.467072	-0.91449	-2.80763
O17	-0.79007	-1.21057	-2.9285
C18	3.525901	0.863132	0.167463
O19	4.618159	0.960692	0.885078
C20	0.062029	-0.97234	4.304466
F21	1.24737	-0.42168	4.578225
F22	-0.67339	-1.03155	5.404007
F23	0.270598	-2.22809	3.84173
C24	3.731399	1.368659	-1.28454
F25	2.618913	1.977121	-1.70431
F26	4.753041	2.214097	-1.3586
F27	3.974249	0.302735	-2.05878
C28	-1.29072	-3.33039	0.885833
F29	-1.82311	-2.36756	1.667841
F30	-1.78348	-3.18896	-0.35318
F31	-1.62171	-4.51499	1.368593
C32	1.343198	-1.34603	-4.00701
F33	2.25418	-0.40275	-4.25192
F34	1.971629	-2.48274	-3.65959
F35	0.61422	-1.56076	-5.09651
C36	-3.91754	-0.57855	-0.51266
F37	-3.71175	-1.13363	-1.71766
F38	-4.24912	-1.54847	0.355475
F39	-4.91866	0.293881	-0.59945
C40	0.360616	4.608414	0.350153
F41	1.651925	4.499312	0.689586
F42	0.276252	5.02439	-0.91965
F43	-0.23233	5.48989	1.148819
H44	-1.93496	2.322346	0.935417
H45	-1.29571	-0.93028	-2.11382
H46	1.871868	-4.03089	1.045291
H47	4.457212	0.609649	1.78084
H48	-2.30745	0.413876	2.533002

HD_meta

C	2.33687	2.31462	1.54543
C	2.29766	3.54136	0.86842
C	1.54843	3.74936	-0.30962
C	0.82487	2.67219	-0.79562
C	0.81366	1.39778	-0.13133
C	1.61230	1.24516	1.05264
H	2.93753	2.21474	2.44403
H	0.22596	2.78340	-1.69634
H	1.62492	0.27660	1.54404
H	0.88488	0.49539	-0.82362
O	1.23622	-1.14438	-1.43104
C	1.23890	-1.83221	-0.39999
O	0.39924	-1.83681	0.55985
C	2.47673	-2.72606	-0.13416
F	3.31015	-2.05796	0.70801
F	3.15861	-2.99285	-1.25625
F	2.15430	-3.89048	0.44931
H	-0.30292	1.09776	0.09250
O	-1.91207	0.86727	0.19593
C	-2.46678	-0.23579	0.12107
O	-1.95888	-1.40947	0.14000
C	-4.01370	-0.25883	0.03056
F	-4.52770	-0.54503	1.24271
F	-4.43583	-1.18925	-0.83802
F	-4.49102	0.93106	-0.35835
H	-0.85021	-1.49358	0.29183
H	2.87291	4.37486	1.26785
C	1.55053	5.09643	-0.99134
H	1.12125	5.86862	-0.34194
H	2.56955	5.41166	-1.24369
H	0.96661	5.07395	-1.91551

HD_ortho

C	-1.85547	3.33921	-1.08504
C	-1.06550	4.33845	-0.48549
C	0.01539	4.04032	0.35164
C	0.35591	2.71828	0.61540
C	-0.42527	1.65891	-0.00080
C	-1.54669	2.02085	-0.84045
H	-2.69460	3.61428	-1.71545
H	-2.14958	1.21827	-1.25652
H	-0.74700	0.84119	0.72459
O	-1.61000	-0.56379	1.33138
C	-1.80255	-1.40361	0.43783
O	-0.96699	-1.99802	-0.31291
C	-3.28025	-1.70467	0.07847
F	-3.68636	-0.77830	-0.84016
F	-4.08761	-1.59401	1.14243
F	-3.45845	-2.91528	-0.46327
H	0.28735	0.93971	-0.53712
O	1.73492	0.05439	-0.96358
C	2.10765	-0.97224	-0.38156
O	1.41712	-1.92330	0.11717
C	3.63499	-1.11332	-0.16601
F	4.29773	-0.88819	-1.31185
F	3.99553	-2.31101	0.30416
F	4.03076	-0.17461	0.73141
H	0.27386	-1.86855	-0.06231
H	-1.30660	5.38227	-0.67342
H	0.58906	4.84896	0.79488
C	1.51151	2.35828	1.49568
H	2.24193	1.76143	0.93660
H	2.00824	3.24493	1.89786
H	1.17420	1.73307	2.33188

HD_para

C	-2.75007	1.97633	-0.96837
C	-2.86368	3.15815	-0.20405
C	-2.03165	3.35141	0.92260
C	-1.10442	2.39643	1.27272
C	-0.94298	1.19121	0.49842
C	-1.82625	1.01244	-0.62863
H	-3.40510	1.83374	-1.82303
H	-2.13710	4.26073	1.50757
H	-0.45978	2.54747	2.13435
H	-1.73895	0.09600	-1.20514
C	-3.84772	4.22091	-0.60026
H	-3.35974	4.94610	-1.26667
H	-4.70000	3.80187	-1.14272
H	-4.21421	4.77554	0.26877
H	-0.82745	0.24415	1.10750
O	-0.84934	-1.54330	1.50846
C	-0.78767	-2.05770	0.38394
O	0.01763	-1.80615	-0.57261
C	-1.90654	-3.05291	-0.01815
F	-2.81883	-2.38210	-0.77759
F	-2.55341	-3.55042	1.04426
F	-1.44695	-4.07938	-0.74967
H	0.16804	1.12525	0.14608
O	1.81312	1.21018	-0.10686
C	2.56684	0.23103	-0.11062
O	2.28445	-1.01716	-0.15433
C	4.09397	0.49407	-0.10525
F	4.57604	0.34994	-1.35545
F	4.73652	-0.36823	0.69654

F	4.36697	1.73906	0.30895
H	1.20537	-1.28768	-0.28151

HOTFA_dimer

C	-3.44200	-0.03004	0.00005
C	-1.89719	-0.02062	-0.00011
O	-1.42511	1.20061	0.00013
H	-0.42071	1.18341	-0.00010
O	-1.26099	-1.06330	-0.00036
F	-3.90184	0.60360	1.09046
F	-3.90052	-1.28162	0.00023
F	-3.90202	0.60339	-1.09034
O	1.42507	-1.20061	-0.00006
H	0.42068	-1.18334	-0.00021
C	1.89719	0.02064	-0.00020
O	1.26095	1.06331	-0.00059
C	3.44202	0.03003	0.00009
F	3.90053	1.28162	0.00026
F	3.90172	-0.60357	1.09055
F	3.90218	-0.60344	-1.09023

HOTFA

C	-0.60102	-0.00094	-0.00001
F	-1.18841	1.19611	-0.00036
F	-0.99721	-0.68008	-1.09019
F	-0.99726	-0.67941	1.09056
C	0.93459	0.16012	0.00000
O	1.49808	1.22234	-0.00003
O	1.52169	-1.04611	0.00003
H	2.48638	-0.89447	-0.00000

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C	0.19441	-1.20225	-0.00901
C	0.91390	0.00027	-0.01140
C	0.19410	1.20241	-0.00901
C	-1.20149	1.20527	0.00220
C	-1.90512	-0.00018	0.00851
C	-1.20101	-1.20551	0.00220
H	0.73478	-2.14661	-0.01793
H	0.73416	2.14693	-0.01791
H	-1.73908	2.15014	0.00154
H	-2.99187	-0.00040	0.01399
H	-1.73838	-2.15052	0.00154
C	2.42554	0.00012	0.00940
H	2.80998	-0.01633	1.03834
H	2.83437	-0.87798	-0.50242
H	2.83404	0.89399	-0.47444

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