Computational Mapping of Redox-Switchable Metal Complexes Based on Ferrocene Derivatives

Electronic Supporting Information

Amy Lai, Jamie Clifton, Paula L. Diaconescu,* Natalie Fey*

Contents

Computational details

DFT calculations were performed in Jaguar 8.5[1] and used the standard B3PW91 density functional.[2] The triple-zeta form of the standard Los Alamos ECP basis set (LACV3P) as implemented in Jaguar was used on the transition metal atoms, employing the 6-31G* basis with five spherical harmonic components of the polarization functions for all other atoms. All optimisations were run as unrestricted, as these showed better convergence behaviour for the oxidised metal complexes; trial calculations with spin-restricted open shell DFT (ROB3PW91) repeatedly failed to converge. "Loose" convergence (five times larger than default criteria) was used for optimizations. Test calculations using default criteria did not lead to significant changes in geometries, but were more time-consuming. Calculations were performed on isolated molecules and NBO atomic charges were calculated.[3] Vibrational frequencies were not computed; complex effects on zero-point and free energy corrections are likely to be small and have been neglected. Stationary points have not been routinely verified as minima but accidental optimisation to transition states seems unlikely for complexes of low symmetry. Trial calculations on two compounds, L1_Y_3a and L4_Al_1d in both oxidation states showed a small negative frequency for the Fe(III) version of L4_Al_1d, likely an artefact of the computational methodology and loose convergence used, while the other compounds were confirmed as true minima. The impact on the energy differences between oxidation states was small in both cases, for L1_Y_3a ΔE = 118.7 kcal mol^{-1}, ΔG = 119.2 kcal mol^{-1} and for L4_Al_1d, ΔE = 150.9 kcal mol^{-1}, ΔG = 148.6 kcal mol^{-1}. Principal component analyses were performed in SIMCA,[4] while all other data analysis used MS Excel.

As these compounds are similar across different metals and oxidation states; here, we supply xyz coordinates for a subset of optimised geometries for representative compounds, along with all processed descriptor data and PC scores.

Table S1: List of metal complexes considered and labels. General format L#_M_R_R'/R''.
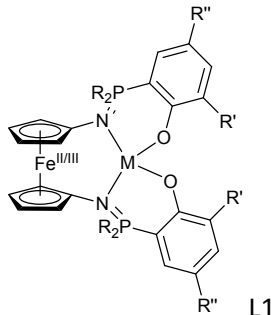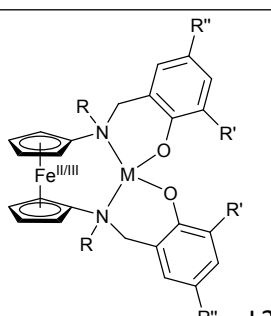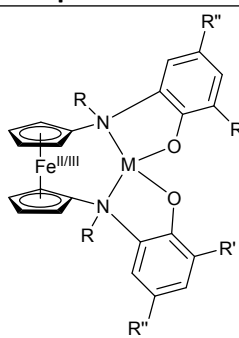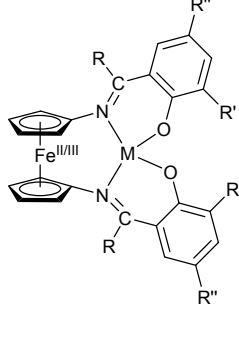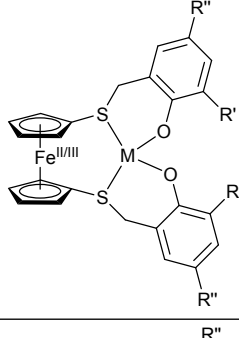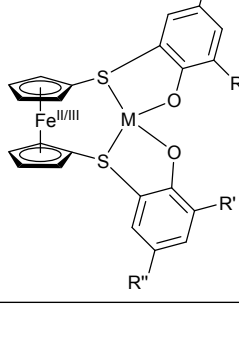
a R' = R'' = H
b R' = R'' = Me
c R' = R'' = tBu
d R' = tBu, R'' = H
e R' = CF$_3$, R'' = H

M = Al(OMe), Sc(OMe), Ti(OMe)$_2$, Y(OMe), Zr(OMe)$_2$, In(OMe), Hf(OMe)$_2$

Complex	Variations	Included	Short label
L1	_1 PH$_2$ _2 PMe$_2$ _3 PPh$_2$ _4 PtBu$_2$ _5 PiPr$_2$ _6 P(CF$_3$)$_2$ _7 P(OMe)$_2$ _8 P(OPh)$_2$ a R' = R'' = H b R' = R'' = Me c R' = R'' = tBu	L1_Al_1a	1
		L1_Al_1c	2
		L1_Al_3c	3
		L1_Sc_1c	4
		L1_Sc_3c	5
		L1_Ti_1a	6
		L1_Ti_3c	7
		L1_Y_1a	8
		L1_Y_1b	9
		L1_Y_1c	10
		L1_Y_2a	11
		L1_Y_3a	12
		L1_Y_3c	13
		L1_Y_4a	14
		L1_Y_5a	15
		L1_Y_6a	16
		L1_Y_7a	17
		L1_Y_8a	18
		L1_Zr_1a	19
		L1_Zr_2a	20
		L1_Zr_3a	21
		L1_Zr_3c	22
		L1_In_1a	23
		L1_In_1c	24
		L1_In_3c	25
		L1_Hf_3c	26
L2	_1 R = H a R' = R'' = H	L2_Y_1a	27

Complex	Variations	Included	Short label
L3	_1 R = H d R' = *t*Bu, R'' = H	L3_Al_1d L3_Sc_1d L3_Ti_1d L3_Y_1d L3_Zr_1d L3_Hf_1d	28 29 30 31 32 33
L4	_1 R = H c R' = R'' = *t*Bu d R' = *t*Bu, R'' = H e R' = CF$_3$, R'' = H	L4_Al_1c L4_Al_1d L4_Al_1e L4_Sc_1d L4_Ti_1c L4_Ti_1d L4_Ti_1e L4_Y_1c L4_Y_1d L4_Y_1e L4_Zr_1c L4_Zr_1d L4_Zr_1e L4_In_1c L4_In_1d L4_Hf_1c L4_Hf_1d	34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50
L5	a R' = R'' = H c R' = R'' = *t*Bu	L5_Ti_a L5_Ti_c L5_Y_c L5_Zr_a L5_Zr_c L5_Hf_c	51 52 53 54 55 56
L6	a R' = R'' = H c R' = R'' = *t*Bu	L6_Al_c L6_Sc_c L6_Ti_a L6_Ti_c L6_Y_a L6_Zr_a L6_Zr_c L6_Hf_c	57 58 59 60 61 62 63 64

Database design

Starting geometries were derived from available crystal structures, changing substituents and metals to access the variations considered here. This approach does not include an exploration of accessible conformers, which may affect some of the substituents and methoxy group placement. However, the metallocene poses problems to standard molecular mechanics approaches - there are multiple ways of dealing with π-coordination of ligands (for an early review, see: N. Fey, "Organometallic molecular modelling – the computational chemistry of metallocenes: a review", *J. Chem. Technol. Biotechnol.*, 1999, 852-862). Arguably, with all ligands coordinated to a second metal centre, treating the ferrocene backbone appropriately is less important here, but it can affect the resilience and speed of conformational searches if the routine to generate new conformers (most commonly, random coordinate changes and rotation around suitable bonds) produces challenging starting geometries. Furthermore, a large-scale search was not feasible without detailed parameterisation, especially for some of the less commonly used metal cations, which lay outside the scope of the present work. Such considerations notwithstanding, there is no reason to expect the molecular mechanics (MM) and DFT potential energy surfaces to be similar, so the lowest energy conformer found with MM is not necessarily optimal for DFT, necessitating extensive sampling of conformers. This is indeed the case for an example investigated here, L1_Y_3c, see Table S2.

The lowest MM structure is highest in terms of DFT potential energy (incidentally, the geometry used for the database is very close to the lowest energy found). This can be addressed by more extensive sampling, but the computational effort escalates quickly. The key here is that we are comparing similar systems and not measuring "softer" changes in dihedral angles. The descriptors used are unlikely to be affected substantially by such conformational changes and it is our assessment that the impact on the descriptors is relatively small in the present case. Most of the data extracted are distances, and here conformational noise gives a standard deviation of less than 0.01 Å for the case of L1_Y_3c, much smaller than the range and STD for the database (as shown in Table S3 below). Clearly, there will be an effect on the energy difference (ΔE) between oxidation states as well, but the differences for different metals are again more substantial than the noise likely to be introduced by working with data for a high energy conformer in one or both oxidation states.

The limiting assumption of this work is that the coordination chemistry and conformational preferences will be similar even as metals and substituents are altered. Recent work on Zr complexes[5] indicates that isomerisation could occur during catalysis; this has not been considered in the present case and would indeed be difficult to capture reliably in a descriptor database.

Table S2: Conformational search results for L1_Y_3c

No.	rel. E, MM	rel. E, DFT	M-D1 (Fe2)	M-D2 (Fe2)	M-OMe (Fe2)	Fe-C	D1-R (Fe2)	D2-R (Fe2)	RDR (Fe2)	Q(M) (Fe2)	Q(OMe) (Fe2)	ΔE (same conf)
original	N/A	-7.54	2.414	2.201	2.061	2.048	1.522	1.314	117.9	2.2155	-0.7536	118.4
1	0.00	0.00	2.413	2.199	2.055	2.052	1.515	1.305	119.4	2.1684	-0.7389	119.2
2	0.28	-3.28	2.415	2.211	2.050	2.044	1.522	1.308	116.3	2.1972	-0.7418	
3	0.94	-7.72	2.427	2.200	2.047	2.048	1.520	1.312	119.1	2.1987	-0.7487	118.5
4	1.08	-6.92	2.445	2.196	2.060	2.052	1.517	1.316	119.2	2.2160	-0.7584	
5	1.11	-2.15	2.433	2.215	2.044	2.045	1.520	1.311	117.8	2.2143	-0.7428	
6	1.53	-6.66	2.422	2.204	2.046	2.046	1.523	1.311	116.4	2.2108	-0.7494	
7	1.78	-5.16	2.422	2.195	2.049	2.048	1.521	1.310	118.9	2.2006	-0.7518	
8	4.46	-4.95	2.428	2.202	2.047	2.048	1.521	1.312	119.0	2.2038	-0.7522	
9	4.59	-3.79	2.426	2.219	2.044	2.045	1.520	1.312	118.1	2.2171	-0.7445	
Mean			2.425	2.204	2.050	2.048	1.520	1.311	118.2	2.2042	-0.7482	
STD			0.010	0.008	0.006	0.003	0.002	0.003	1.1	0.0147	0.0061	

Calculations focussed on compounds of the following metals: Al^{3+}, Sc^{3+}, Ti^{4+}, Y^{3+}, Zr^{4+}, In^{3+}, Hf^{4+}, and the supporting ligand structures as shown in Table S1. In these metal complexes, methoxy was used as a model ligand for the alkoxide; the number of methoxy groups coordinated to the active metal centre was adjusted to achieve a neutral complex for the Fe(II) case, and both neutral and cationic complexes, assumed to correspond to Fe(II) and Fe(III) backbone oxidation states, were fully optimised. For DFT calculations in Jaguar, initial formal charges can be set, but there is ultimately no control over which metal centre is oxidised; Fe-C distances and NBO charges on Fe suggest that for all compounds reported here, the iron centre has been oxidised, but, as noted below, Ce complexes were ultimately left out as these proved more difficult to control. In all schemes and tables, M = Al(OMe), Sc(OMe), Ti(OMe)$_2$, Y(OMe), Zr(OMe)$_2$, In(OMe), Hf(OMe)$_2$.

We also attempted an evaluation of Zr^{3+} and Ce^{3+} or Ce^{4+} complexes, but these calculations proved persistently difficult to converge and unreliable with respect to determining whether the oxidation occurred on the ferrocene or the reacting metal. This also occurred for some of the other complexes, most notably with L2, limiting the variation captured in the database in this case. This ties in with mechanistic study of the cerium catalysis,[6] where the oxidation process was found to change the oxidation state of the reacting metal (confirmed by XANES and Mössbauer spectroscopy), rather than the metallocene backbone and will be investigated further in a future study.

DFT calculations can be unreliable in cases where multiple electronic configurations can be accessed energetically, and we are exploring whether wavefunction stability checks, available e.g. in Gaussian, would help to improve data robustness and convergence. However, the computational approach was chosen to capture spin state energy differences well. While dispersion and solvation effects are likely to affect geometries and energies, this matters less for a systematic evaluation of metal complexes as all will be affected by similar errors, with trends being captured more reliably.

Our selection of metal complexes to consider was driven by curiosity and pragmatism, with the most extensive structural variations explored for Y complexes as these generally converged well in both oxidation states. We have not sought to achieve a full exploration of all structural variations for all metal centres, but instead focussed on different subsets to map out the importance of variable effects, as discussed in the text. For some of the metal centres considered, we only managed to optimise one of the oxidation states, despite repeated attempts; these have not been included in the present analysis, making the sampling of the different ligands and metal centres uneven.

Descriptors:

Initially, a large number of structural parameters and NBO charges, as well as the energy differences between the Fe(II) and Fe(III) oxidation states, were extracted from each successful geometry optimisation. Some structural parameters did not respond strongly to the variations explored here, and were not included in our final analysis, e.g., the O-C distances in the methoxy groups. For the Fe-C distances and charges, we found the net change on oxidation more useful than the raw data, whereas for most of the descriptors further removed from the Fe centres, the variation with the Fe oxidation state was small and showed no clear trend, leading us to focus on the descriptors as measured directly. We have used averages of distances and angles to avoid complications around extracting data consistently across varied chemistries and coordination geometries. This may mask outlier responses, but is computationally more convenient. It is worth noting that we perform PCA on the correlation matrix, so all descriptors are standardised and means-centered in this process.

We initially considered treating each oxidation state as a separate entry in the database, but found that the distribution of metal complexes in the Fe(II) and Fe(III) version tended to shadow rather closely (Figure S1), making the data analysis difficult. In addition, the present version captures

differences between catalysts, rather than those due to changing the oxidation state. To achieve detailed insight in differences in catalytic behaviour when changing the oxidation state, additional mechanistic study is necessary and we envisage introducing reaction-specific descriptors to improve resolution in due course.
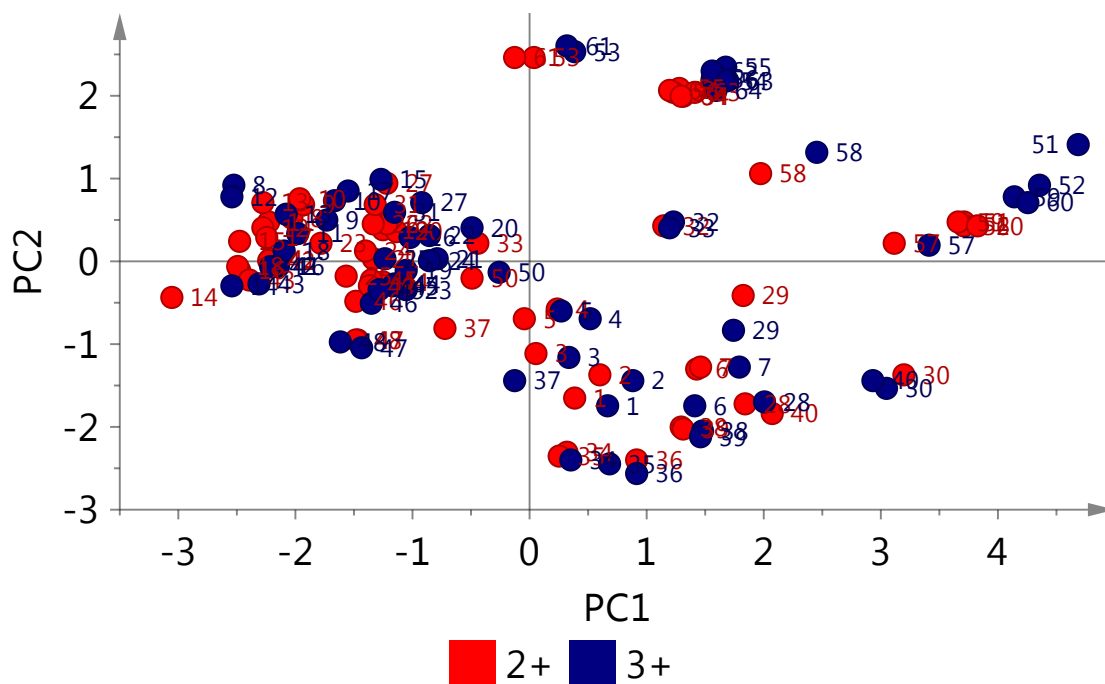
Figure S1: PC1 and PC2 score plot treating each oxidation state as a separate entry.

Table S3: Descriptor labels, details, and standard descriptive statistics.

Descriptor	Details (unit)	Mean	STD	Min.	Max.
M-D1(Fe2), M-D1(Fe3)	r(M-D1), both oxidation states (Å)	2.546 2.713	0.388 0.517	2.016 2.070	3.854 4.177
M-D2(Fe2), M-D2(Fe3)	r(M-D2), both oxidation states (Å)	2.050 2.024	0.130 0.127	1.753 1.748	2.224 2.192
M-OMe(Fe2), M-OMe(Fe3)	r(M-OMe), both oxidation states (Å)	1.928 1.916	0.109 0.119	1.704 1.677	2.082 2.204
D1-R(Fe2), D1-R(Fe3)	av. r(D1-R), both oxidation states (Å)	1.512 1.504	0.169 0.169	1.273 1.259	1.806 1.800
D2-R(Fe2), D2-R(Fe3)	r(D2-R), both oxidation states (Å)	1.318 1.323	0.015 0.015	1.292 1.289	1.357 1.353
$\angle$R-D1-R(Fe2), $\angle$R-D1-R(Fe3)	av. $\angle$R-D1-R, both oxidation states (°)	113.8 114.4	5.6 6.3	104.9 101.7	129.8 128.7
Q(M)(Fe2), Q(M)(Fe3)	NBO charge on M, both oxidation states	2.018 2.047	0.255 0.229	1.393 1.528	2.412 2.402
Q(OMe)(Fe2), Q(OMe)(Fe3)	NBO charge on OMe group, both oxidation states	-0.604 -0.589	0.127 0.131	-0.757 -0.748	-0.357 -0.334
ΔFe-C	change in av. Fe-C distances due to oxidation state, av. r(Fe-C,Fe3) – av. r(Fe-C,Fe2) (Å)	0.053	0.006	0.039	0.068
ΔQ(Fe)	change in NBO charge on Fe centre, Q(Fe3) – Q(Fe2)	0.493	0.017	0.454	0.525
ΔE	E_{opt}(Fe3 complex) – E_{opt}(Fe2 complex) (kcal mol^{-1})	132.35	9.24	115.03	150.98

Most of the structural descriptors are highly correlated between the two oxidation states, giving rise to correlation coefficients >0.8. These include M-D1, M-D2, M-OMe, D1-R, D2-R, <R-D1-R, Q(OMe).

Table S4 lists additional correlations >0.6.

Table S4: Correlations >0.6 (not including the same descriptor in different oxidation states, as noted above).

Descriptor 1	Descriptor 2	Correlation
M-D1(Fe2)	D2-R(Fe2)	0.732
M-D2(Fe2)	M-OMe(Fe2)	0.940
	M-OMe(Fe3)	0.941
M-OMe(Fe2)	Q(M) (Fe2)	0.607
	Q(M) (Fe3)	0.612
	M-OMe(Fe3)	0.947
D1-R(Fe2)	<RDR(Fe2)	-0.655
	<RDR(Fe3)	-0.691
D2-R(Fe2)	M-D1(Fe3)	0.724
<RDR(Fe2)	D1-R(Fe3)	-0.628
Q(M)(Fe2)	Q(OMe)(Fe2)	-0.606
	M-OMe(Fe2)	0.617
M-D1(Fe3)	D2-R(Fe2)	0.623
M-D2(Fe3)	M-OMe(Fe3)	0.946
M-OMe(Fe3)	Q(M) (Fe3)	0.617
D1-R(Fe3)	<RDR(Fe3)	-0.674

Correlations between structural descriptors and the three descriptors capturing the change experienced after oxidation change (ΔE, $\Delta Q(Fe)$ and ΔFe-C) are not as high, but $\Delta Q(Fe)$ has a correlation coefficient of -0.531 with <RDR(Fe3) (-0.460 with <RDR(Fe)), while ΔFe-C has a number of correlation coefficients >0.5 (M-D1(Fe2) = 0.519, M-D2(Fe2) = -0.514, D2-R(Fe2) = 0.555, <RDR(Fe2) = -0.583, M-D1(Fe2) = 0.500, <RDR(Fe3) = 0.500. No variable correlates particularly highly with the vertical ionisation energy, ΔE, and it does not load highly on the first two PCs (see below), suggesting perhaps that its relationship with the remainder of this database is not described well by a linear regression equation.

PCA results

Table S5: Autofit diagnostics:

Component	R^2X	R^2X(cum)	Eigenvalue	Q^2	Limit	Q^2(cum)
0	Cent.					
1	0.399	0.399	7.58	0.288	0.065	0.288
2	0.165	0.563	3.13	0.079	0.068	0.344
3	0.144	0.707	2.74	0.160	0.071	0.449
4	0.101	0.808	1.92	0.099	0.074	0.504
5	0.072	0.880	1.37	0.255	0.078	0.630
6	0.036	0.916	0.682	0.165	0.083	0.691
7	0.024	0.941	0.461	-0.005	0.087	0.690
8	0.021	0.961	0.396	0.100	0.093	0.721
9	0.014	0.975	0.257	-0.050	0.100	0.707

Descriptor loadings
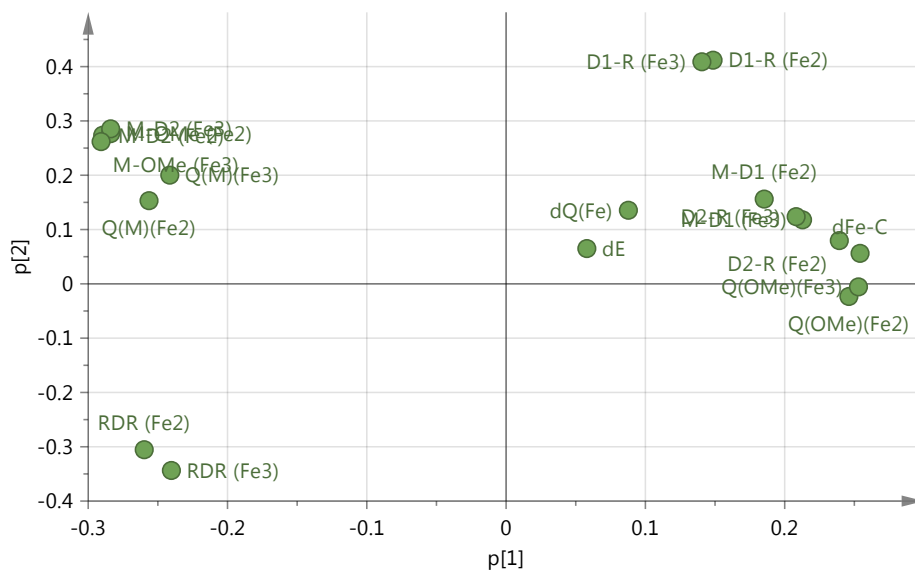
Figure S2: Descriptor loadings plot, PC1 and PC2.

Table S6: Descriptor loadings, PC1-4.

Var ID (Primary)	M1.p[1]	M1.p[2]	M1.p[3]	M1.p[4]
Cumulative % of variation	39.9	56.3	70.7	80.8
M-D1 (Fe2)	0.185	0.157	-0.399	0.008
M-D2 (Fe2)	-0.289	0.274	0.010	-0.162
M-OMe (Fe2)	-0.283	0.276	-0.095	-0.104
D1-R (Fe2)	0.148	0.413	0.165	-0.162
D2-R (Fe2)	0.239	0.079	-0.387	0.090
RDR (Fe2)	-0.259	-0.305	-0.134	-0.132
Q(M)(Fe2)	-0.257	0.153	-0.184	0.278
Q(OMe)(Fe2)	0.246	-0.022	0.064	-0.352
M-D1 (Fe3)	0.212	0.119	-0.396	0.003
M-D2 (Fe3)	-0.284	0.287	0.003	-0.143
M-OMe (Fe3)	-0.291	0.261	-0.106	-0.114
D1-R (Fe3)	0.140	0.409	0.173	-0.173
D2-R (Fe3)	0.208	0.124	-0.350	-0.009
RDR (Fe3)	-0.240	-0.344	-0.164	-0.119
Q(M)(Fe3)	-0.241	0.200	-0.183	0.271
Q(OMe)(Fe3)	0.253	-0.005	0.043	-0.343
ΔE	0.058	0.064	0.138	0.543
ΔQ(Fe)	0.088	0.135	0.438	0.269
ΔFe-C	0.254	0.056	-0.070	0.272
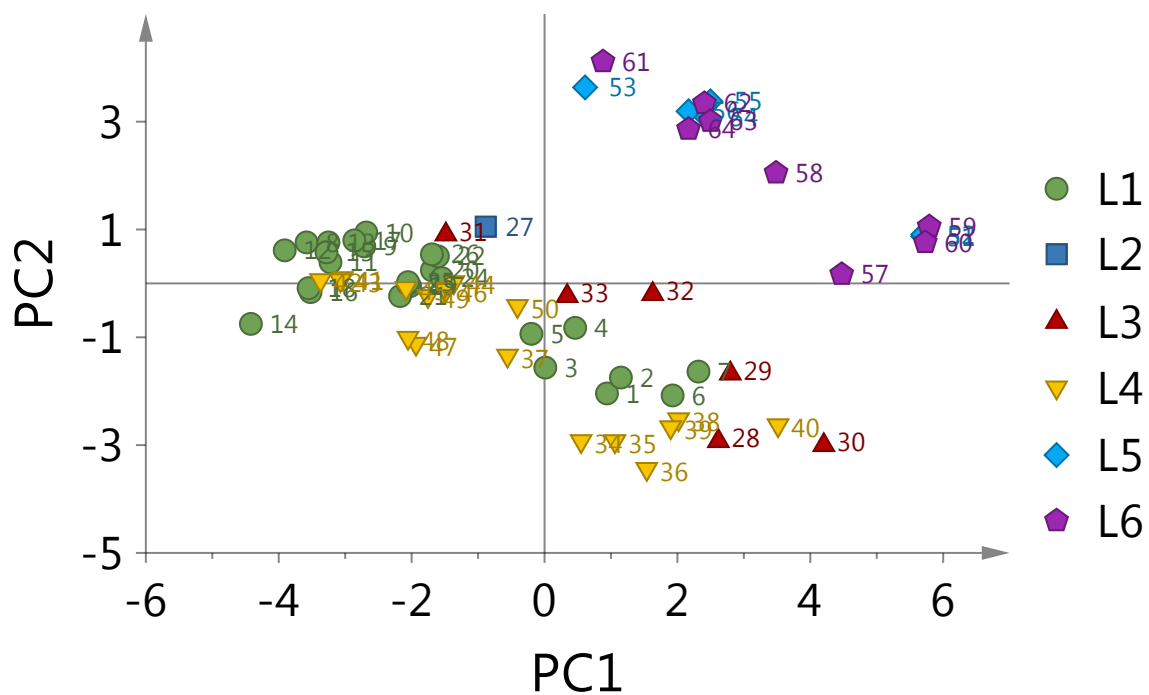
Figure S3: PC1 and PC2 score plot, short labels, coloured by L (Table S1).
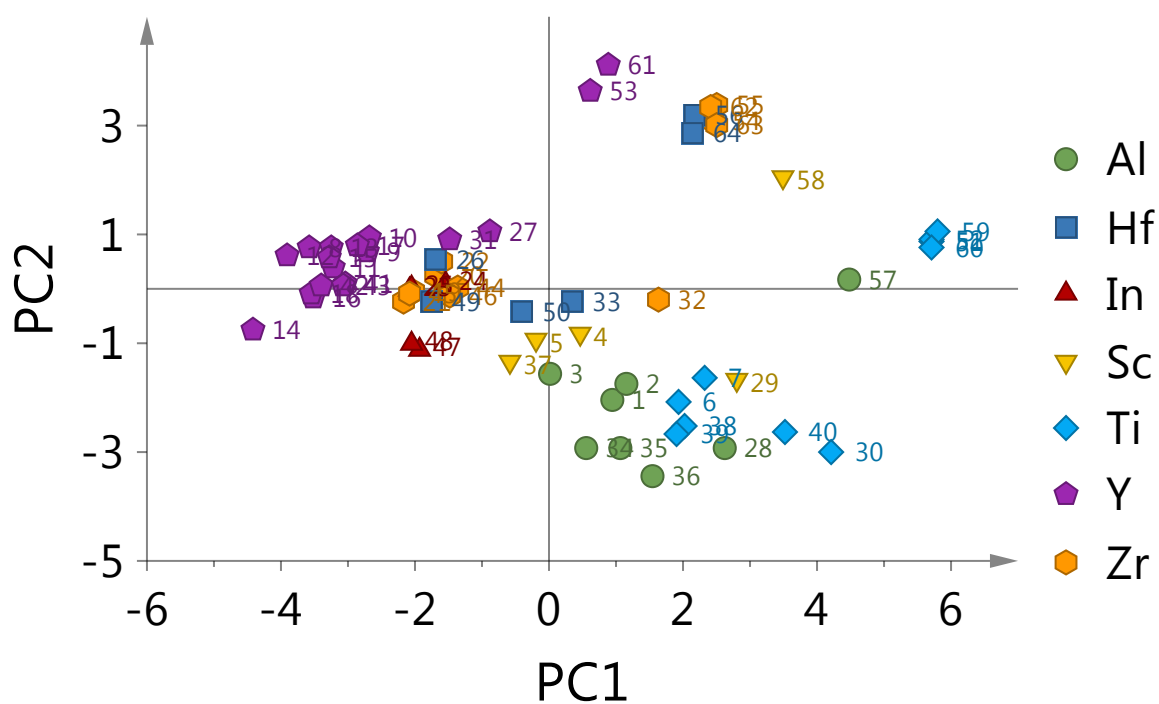
Figure S4: PC1 and PC2 score plot, short labels, coloured by M (Table S1).

Figure S5: PC1 and PC2 score plot, overview, full labels, coloured by L (Table S1).

Figure S6: PC1 and PC2 score plot. Symbols marked in bright red correspond to metal complexes found active in ring-opening polymerisation catalysis.
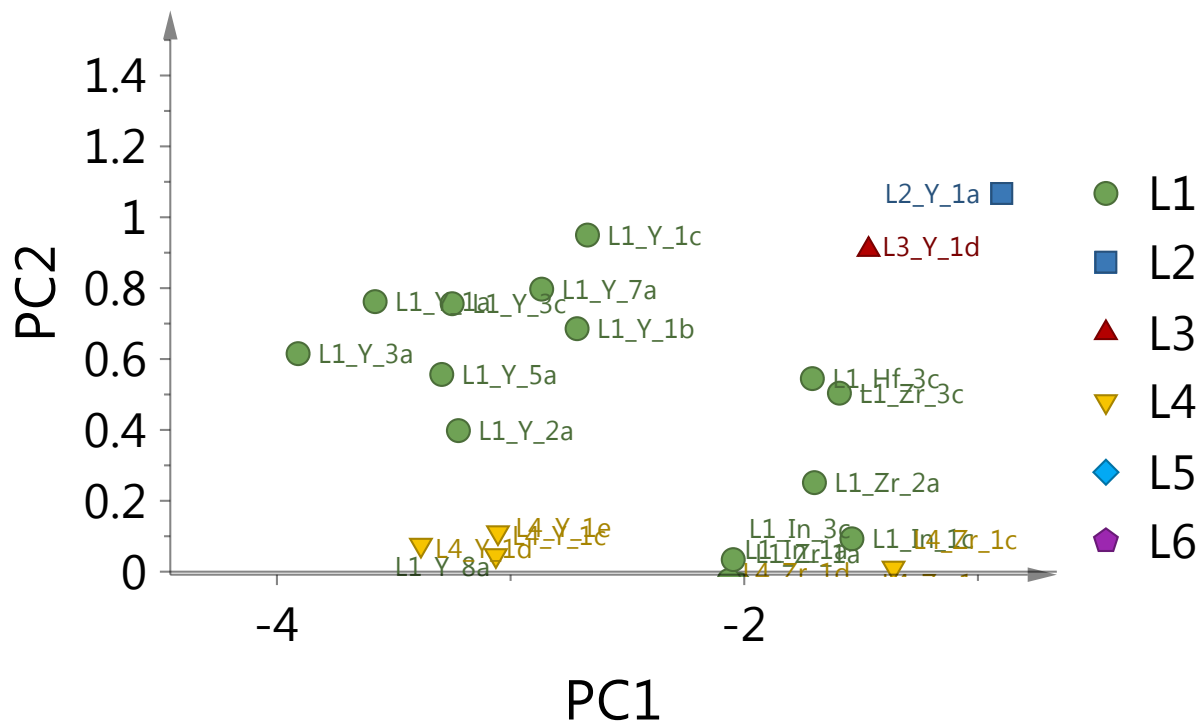
Figure S7: PC1 and PC2 score plot, upper left quadrant, full labels, coloured by L (Table S1).
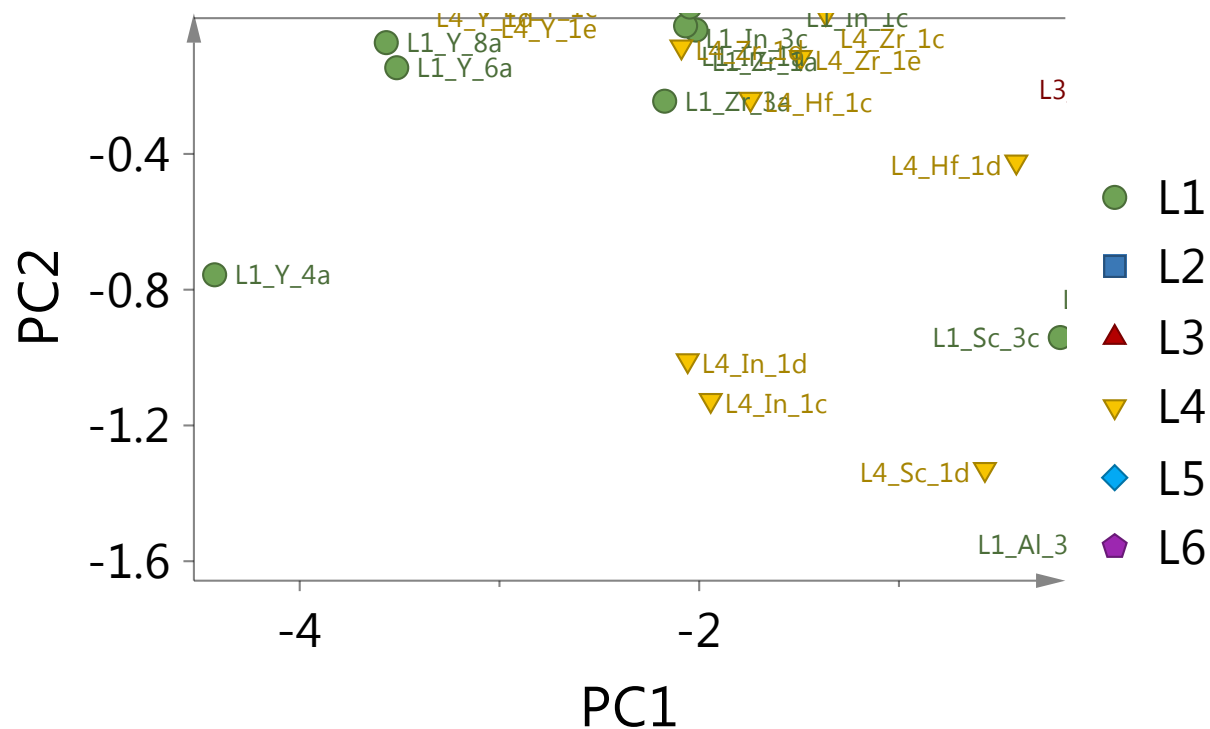
Figure S8: PC1 and PC2 score plot, lower left quadrant, full labels, coloured by L (Table S1).
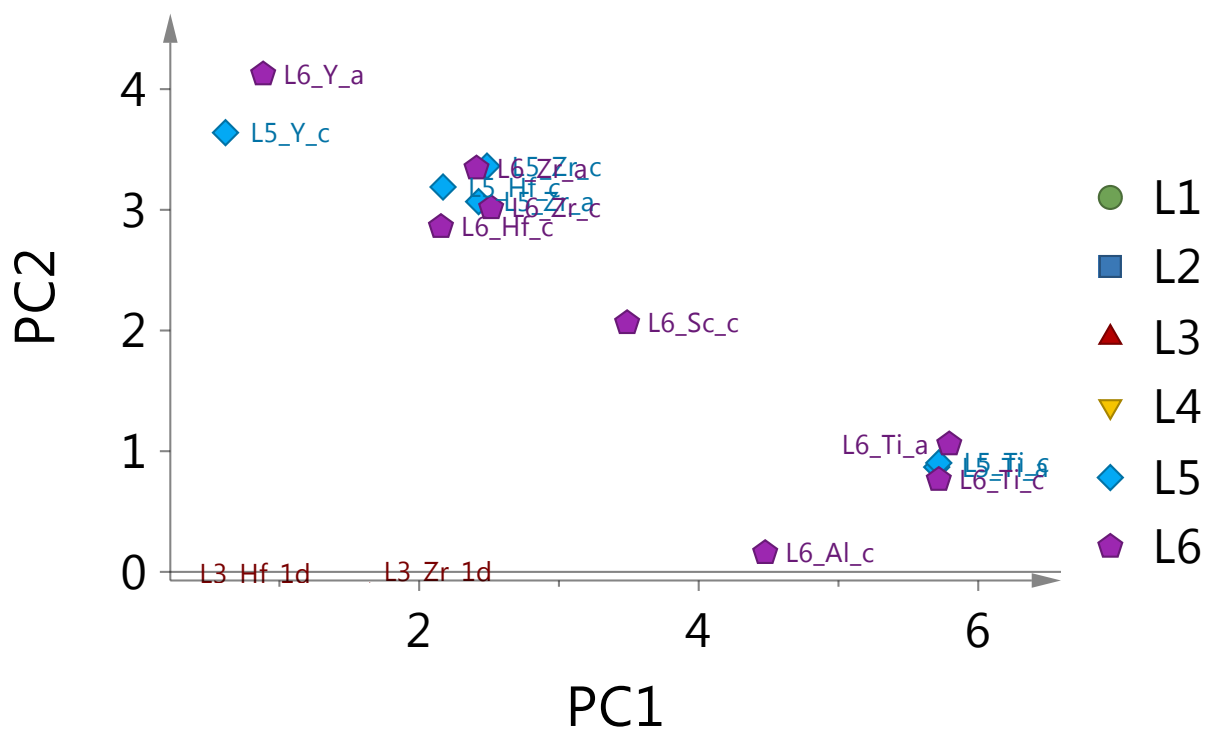
Figure S9: PC1 and PC2 score plot, upper right quadrant, full labels, coloured by L (Table S1).
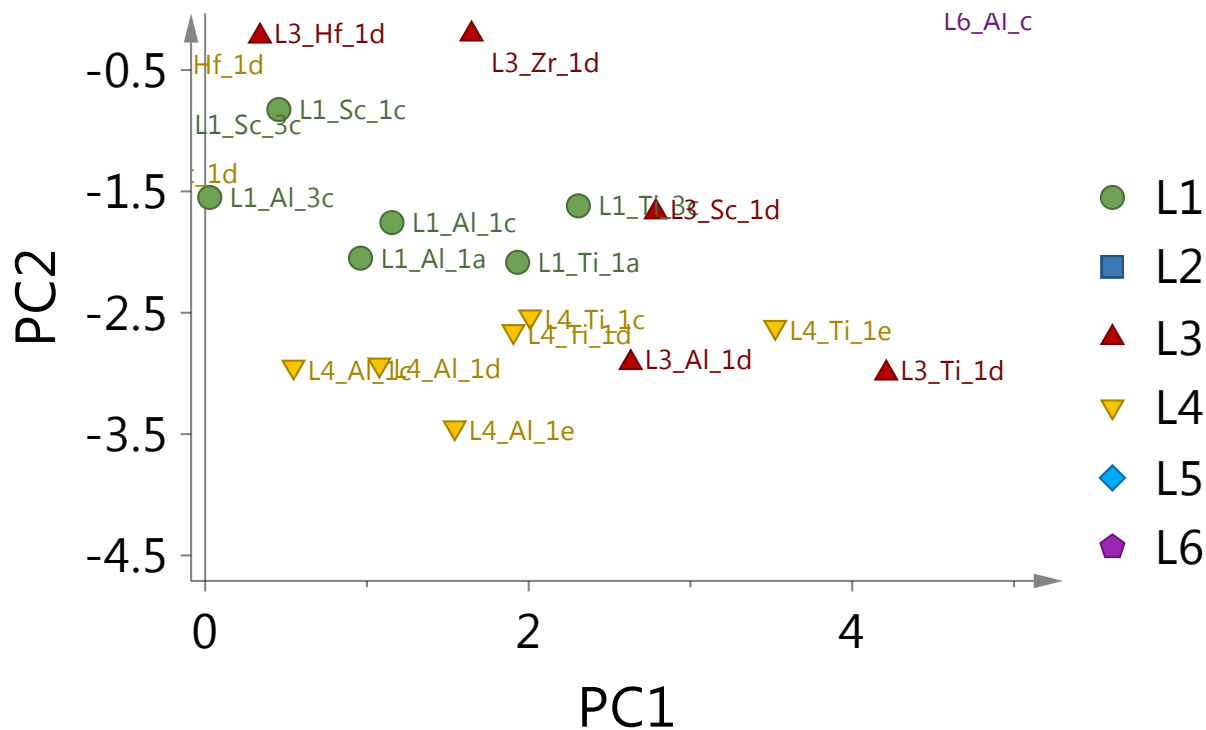
Figure S10: PC1 and PC2 score plot, lower right quadrant, full labels, coloured by L (Table S1).
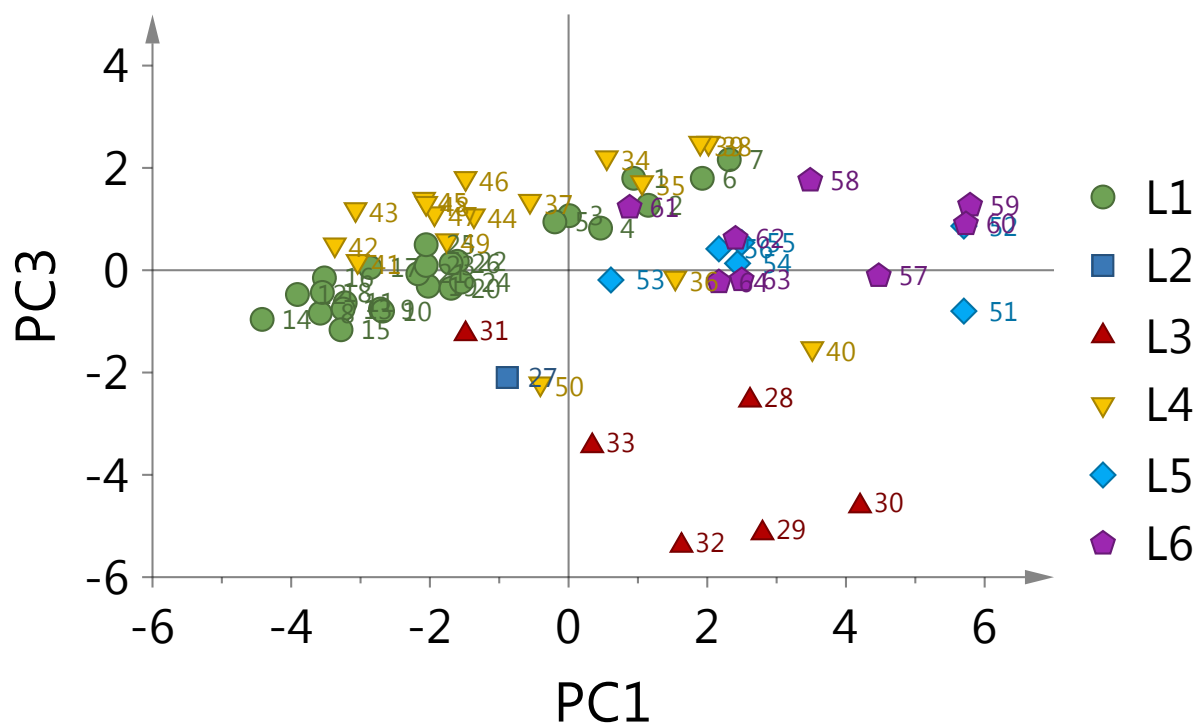
Figure S11: PC1 and PC3 score plot, short labels, coloured by L (Table S1).

References

1. Jaguar, version 8.5, L. Schrödinger, Schrödinger, LLC, 2014, New York, NY.

2. a) J. C. Slater, *Quantum Theory of Molecules and Solids, Vol. 4: The Self-Consistent Field for Molecules and Solids*, McGraw-Hill, New York, 1974; b) J. P. Perdew, P. Ziesche and H. Eschrig, eds., in *Electronic Structure Theory of Solids*, Akademie Verlag, Berlin, 1991; c) J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh and C. Fiolhais, *Phys. Rev. B*, 1992, **46**, 6671; d) A. D. Becke, *Phys. Rev. A*, 1998, **38**, 3098.

3. NBO 5.0 E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales and F. Weinhold, 2001, Madison.

4. SIMCA, version 15, 2018, Sartorius Stedim Data Analytics AB.

5. R. Dai, A. Lai, A. N. Alexandrova and P. L. Diaconescu, *Organometallics*, 2018, **37**, 4040-4047.

6. E. M. Broderick, N. Guo, T. Wu, C. S. Vogel, C. Xu, J. Sutter, J. T. Miller, K. Meyer, T. Cantat and P. L. Diaconescu, *Chem. Commun.*, 2011, **47**, 9897-9899.

XYZ coordinates for representative compounds (related compounds in each set were built by altering metal atoms, substituents and oxidation states; all data extracted have been provided as a separate Excel file)

L1_Y_3c
Fe(II)

Y1	1.9882602479	3.4918309115	3.5408533153
Fe2	-0.2156613170	4.7087339686	6.6626906496
P3	-1.2740520670	3.3531795296	2.4148691890
P4	3.2369008348	1.6936097167	6.3713245211
N5	-0.3912427928	3.7596513792	3.7212175211
N6	2.0393300917	2.6552536270	5.8192172263
O7	1.3904380822	3.6960094679	1.4127982786
O8	3.3824664560	1.8234212011	3.3674216122
O9	2.9433464191	5.2764152767	3.9266571504
C10	-0.9011070543	4.6086101777	4.7205015194
C11	-0.4228323898	5.9275213027	5.0206423129
H12	0.3975770693	6.4172835475	4.5120324458
C13	-1.1698165909	6.4352893864	6.1223499228
H14	-1.0229843089	7.3947441682	6.6022433685
C15	-2.1147742645	5.4400300158	6.5121915273
H16	-2.8077014882	5.5110204442	7.3412068094
C17	-1.9420543006	4.3098790019	5.6616530609
H18	-2.4814887818	3.3735558437	5.7174248224
C19	1.3954226520	3.4210132756	6.8284254834
C20	1.7458997841	4.7450725569	7.2621079053
H21	2.5038497357	5.3659099394	6.8052381268
C22	0.8865794384	5.1108512362	8.3365356141
H23	0.8818746304	6.0643553413	8.8497688980
C24	-0.0105259822	4.0270252969	8.5730607578
H25	-0.8124093379	4.0122213542	9.3005739023
C26	0.2945008414	2.9927060575	7.6423886602
H27	-0.2200584201	2.0465555739	7.5421998474
C28	-0.8555705027	4.1910666144	0.8818204934
C29	-1.8294031526	4.7261544048	0.0295708384
H30	-2.8778669696	4.6262678162	0.2975054317
C31	-1.4706779796	5.3737045217	-1.1482780560
C32	-0.0966051831	5.4588043801	-1.4222168632
H33	0.2037069539	5.9680282454	-2.3296893960
C34	0.5363855546	4.2572129371	0.5859246351
C35	3.6919556679	0.3807908943	5.2293387020
C36	4.1377640292	-0.8387216613	5.7614921221
H37	4.0777419049	-1.0001362586	6.8341756116
C38	4.6554948036	-1.8411689833	4.9498951873
C39	4.7322236661	-1.5546033852	3.5788127936
H40	5.1385439797	-2.3174573196	2.9263361474
C41	3.7806246279	0.6630296424	3.8361077300
C42	3.5209916023	6.5293554642	3.8022193954
H43	2.8011301314	7.2828492728	3.4399545049
H44	3.9063156869	6.8943047283	4.7711513079
H45	4.3677829695	6.5250911832	3.0964294376

C46	4.3296494747	-0.3543620684	2.9935626775
C47	0.9164600628	4.9380826899	-0.6144845975
C48	2.3938185618	5.0991053395	-1.0087474670
C49	-2.5481443050	5.9572920981	-2.0746238704
C50	4.4924418673	-0.1210603516	1.4822989953
C51	5.1118302326	-3.1769079647	5.5566271029
C52	6.2097404463	-2.9231614604	6.6090611586
H53	5.8528846137	-2.2838665273	7.4248988044
H54	6.5449773519	-3.8695055245	7.0537979738
H55	7.0797279119	-2.4326746984	6.1564727156
C56	3.9127080625	-3.8705098169	6.2319576270
H57	3.4864793665	-3.2512227687	7.0290259349
H58	3.1179351964	-4.0730535590	5.5038405536
H59	4.2170210428	-4.8265533509	6.6782041855
C60	5.6826871590	-4.1334669446	4.4988507875
H61	5.9807537400	-5.0753909605	4.9752774886
H62	4.9451540423	-4.3744096640	3.7238324499
H63	6.5702681306	-3.7168513883	4.0081068298
C64	5.1226690640	-1.3272142778	0.7674793285
H65	4.5044859941	-2.2300657927	0.8496901939
H66	5.2247401929	-1.0981642734	-0.3001120151
H67	6.1244184527	-1.5587529485	1.1501384159
C68	3.1145796976	0.1264571532	0.8374752362
H69	2.4570838230	-0.7394168080	0.9834857594
H70	2.6227118218	1.0044644804	1.2595384448
H71	3.2261253161	0.2870688745	-0.2427212628
C72	5.4175829880	1.0891337480	1.2418364971
H73	5.5210296155	1.2777449146	0.1654416223
H74	5.0205896324	1.9890752241	1.7149270162
H75	6.4182297029	0.8979138936	1.6497432844
C76	3.0499987773	3.7124284591	-1.1537493542
H77	2.9762384376	3.1418408610	-0.2262621112
H78	2.5649005925	3.1365694099	-1.9520883333
H79	4.1114149292	3.8221362752	-1.4129831153
C80	3.1288577959	5.9191801251	0.0689059236
H81	3.0501134985	5.4487575296	1.0504917658
H82	4.1932537098	6.0129698895	-0.1848838700
H83	2.7083999008	6.9302491762	0.1396977937
C84	2.5692255794	5.8368602290	-2.3465493432
H85	3.6392637468	5.9221269385	-2.5719306166
H86	2.1007671674	5.3011132850	-3.1815231694
H87	2.1599392191	6.8544990273	-2.3165666221
C88	-3.3742179278	7.0085845119	-1.3063000648
H89	-3.8722661379	6.5745396725	-0.4317588373
H90	-2.7341576587	7.8265044641	-0.9543613639
H91	-4.1514661152	7.4383892582	-1.9520713069
C92	-3.4833300951	4.8290903353	-2.5562421431
H93	-3.9809148402	4.3275116443	-1.7182277425
H94	-4.2655199661	5.2280424202	-3.2157240033
H95	-2.9234758485	4.0694230747	-3.1150781780
C96	-1.9480962682	6.6378496473	-3.3142311461

H97	-2.7530380603	7.0397372713	-3.9415139427
H98	-1.2911665101	7.4733711443	-3.0445643896
H99	-1.3722655735	5.9343645386	-3.9276931652
X100	-1.2116000000#	4.9630670000#	5.7891090000#
X101	0.3323850000#	3.5837900000#	7.4084670000#
C102	1.7591977730	-0.2152388451	10.3241069510
C103	1.3792634381	-0.7482624045	9.0912860438
C104	1.8614144988	-0.1916967423	7.9097965658
C105	2.7460005103	0.8979939291	7.9432030707
C106	3.1083376243	1.4360683157	9.1829844812
C107	2.6196814379	0.8793456318	10.3649791964
H108	1.3817115656	-0.6489824317	11.2469080703
H109	0.7034922844	-1.5993036136	9.0495155749
H110	1.5578293688	-0.6111603596	6.9538655144
H111	3.7696101826	2.2965734764	9.2301360715
H112	2.9110812081	1.3093671059	11.3202291293
C113	7.2131238984	3.9359825313	7.1726610242
C114	7.0251168347	2.6506407472	7.6846850547
C115	5.8255873411	1.9799867406	7.4659910465
C116	4.7912943982	2.5927083170	6.7420769861
C117	4.9892705419	3.8737956684	6.2166166083
C118	6.1972066363	4.5385040591	6.4347789420
H119	8.1508798365	4.4594555930	7.3435821532
H120	7.8164230321	2.1676335221	8.2533616791
H121	5.6972490280	0.9743816155	7.8601536212
H122	4.2128473078	4.3485779634	5.6184776147
H123	6.3402673556	5.5335785589	6.0203368253
C124	-5.7706225297	4.1055736092	3.1538329899
C125	-4.8764711925	5.1732150854	3.0749230475
C126	-3.5259397925	4.9367408267	2.8394475692
C127	-3.0556579961	3.6241689003	2.6769795165
C128	-3.9580600403	2.5577579351	2.7613696522
C129	-5.3107621495	2.8004668615	2.9974048706
H130	-6.8260142463	4.2924484452	3.3383131913
H131	-5.2301792481	6.1932868905	3.2021595741
H132	-2.8350078264	5.7737656185	2.7842292969
H133	-3.6079045940	1.5367338640	2.6392374681
H134	-6.0049628016	1.9656703336	3.0583558361
C135	-0.9456561224	-1.2016137593	1.8416956807
C136	-1.2462460264	-0.3868702890	0.7494699397
C137	-1.3063506733	0.9950641416	0.9046037990
C138	-1.0715455965	1.5672251925	2.1606636030
C139	-0.7644311886	0.7486854549	3.2539133546
C140	-0.6984886407	-0.6339437852	3.0900472512
H141	-0.8953050026	-2.2807797907	1.7163210459
H142	-1.4270841242	-0.8291776330	-0.2271642906
H143	-1.5265966438	1.6333994329	0.0522144865
H144	-0.5761619414	1.2025742092	4.2246022382
H145	-0.4486350668	-1.2671829261	3.9377194728

Fe(III)

Y1	2.0480496858	3.6090874947	3.5711198243
Fe2	-0.3297859462	4.7299435081	6.7629696963
P3	-1.2395601228	3.4099220084	2.4374539710
P4	3.2155433458	1.6610280099	6.3417467220
N5	-0.3706666383	4.0330165342	3.6975334024
N6	1.9813714279	2.6644336500	5.8936526119
O7	1.4528628139	3.8250883592	1.4955666464
O8	3.4337177896	1.9615186356	3.4581404945
O9	2.8491845865	5.4213080742	4.1382408407
C10	-0.9015884259	4.8495862811	4.6578211250
C11	-0.2623263250	6.0413794099	5.1520435760
H12	0.6669706479	6.4340066903	4.7580641823
C13	-1.0364585387	6.5704291720	6.2266200558
H14	-0.8245163382	7.4802980242	6.7732276399
C15	-2.1293192307	5.6833109923	6.4568369269
H16	-2.8916832133	5.7911870519	7.2178680211
C17	-2.0239127262	4.6092152804	5.5286419823
H18	-2.6765004417	3.7480794506	5.4797875199
C19	1.3164412123	3.2954549382	6.9416989064
C20	1.6300966484	4.5636315386	7.5363923353
H21	2.4428941580	5.2043235275	7.2231970437
C22	0.6846830563	4.8467687104	8.5611656655
H23	0.6786141746	5.7258585723	9.1929052066
C24	-0.2681309666	3.7857868947	8.5820850233
H25	-1.1182271021	3.7020426711	9.2469390757
C26	0.1032237155	2.8508449669	7.5687367088
H27	-0.4207279654	1.9387290546	7.3167383150
C28	-0.8003589226	4.1408316893	0.8685423030
C29	-1.7777717133	4.5255543584	-0.0628696321
H30	-2.8267376890	4.3612779248	0.1664684240
C31	-1.4131837006	5.1031273838	-1.2731300687
C32	-0.0388018642	5.3045088179	-1.4861736302
H33	0.2594407835	5.7783342228	-2.4127350329
C34	0.5908864267	4.2921117703	0.6155600619
C35	3.5468062220	0.3456369559	5.1742534726
C36	3.8622341720	-0.9408128255	5.6358991200
H37	3.7451904469	-1.1736447087	6.6902940435
C38	4.3431821519	-1.9110785120	4.7634722551
C39	4.5083818856	-1.5247618237	3.4245859179
H40	4.8960165491	-2.2631656593	2.7341649912
C41	3.7214297433	0.7232630767	3.8168622090
C42	3.5602730404	6.6138450323	4.0195383445
H43	2.9476744340	7.4088756757	3.5649150848
H44	3.8925944950	6.9808645184	5.0054280512
H45	4.4577567984	6.4959778246	3.3935920230
C46	4.2287243886	-0.2556562057	2.9146779600
C47	0.9745962009	4.9364576023	-0.5995113016
C48	2.4506338421	5.2257951273	-0.9227901556
C49	-2.4871841047	5.4970317528	-2.2995446454
C50	4.4805419990	0.0727794314	1.4341603770
C51	4.7023850052	-3.3123852776	5.2818488045

C52	5.8074054790	-3.1909177660	6.3511097735
H53	5.4819272779	-2.5891662674	7.2079460720
H54	6.0881878803	-4.1811880034	6.7313915021
H55	6.7062215179	-2.7219724625	5.9334056680
C56	3.4560523842	-3.9693338081	5.9065483485
H57	3.0616408593	-3.3825853389	6.7445141882
H58	2.6557680708	-4.0772036284	5.1644186914
H59	3.6991475816	-4.9685456269	6.2889414068
C60	5.2189970704	-4.2308323277	4.1656364711
H61	5.4544481252	-5.2176521016	4.5807087556
H62	4.4727953690	-4.3746100285	3.3751764313
H63	6.1357315520	-3.8428097153	3.7061914499
C64	5.0887588654	-1.1132183889	0.6674172815
H65	4.4220634774	-1.9843113723	0.6463840341
H66	5.2645205263	-0.8140628179	-0.3724005304
H67	6.0541208392	-1.4266666463	1.0834015889
C68	3.1460850452	0.4259778909	0.7493623634
H69	2.4510638423	-0.4211907686	0.7988795230
H70	2.6643745975	1.2906757956	1.2103394157
H71	3.3165973216	0.6597554700	-0.3087996292
C72	5.4723560318	1.2490154706	1.3214688404
H73	5.6417327552	1.4991393885	0.2667360780
H74	5.0991982620	2.1390311793	1.8317734510
H75	6.4404361089	0.9809896440	1.7623339299
C76	3.2508066872	3.9111871562	-0.9951988195
H77	3.2019220377	3.3588867732	-0.0555767905
H78	2.8625516781	3.2659942303	-1.7927671163
H79	4.3042356933	4.1241434461	-1.2184599015
C80	3.0410509894	6.1471098626	0.1634830169
H81	2.9612333587	5.7033829550	1.1583502757
H82	4.1020309339	6.3387781733	-0.0420593101
H83	2.5222304701	7.1138925487	0.1784582583
C84	2.6213018777	5.9434569606	-2.2702202858
H85	3.6855628342	6.1460048739	-2.4376616198
H86	2.2708514185	5.3333080964	-3.1111421062
H87	2.0980547065	6.9069907286	-2.2973211239
C88	-3.4585574394	6.5135363585	-1.6667664508
H89	-3.9653934029	6.1009121598	-0.7864091860
H90	-2.9287745270	7.4215424016	-1.3552274453
H91	-4.2334394182	6.8041376020	-2.3872804807
C92	-3.2708770207	4.2379906824	-2.7222601953
H93	-3.7664519272	3.7587688047	-1.8696603906
H94	-4.0475019486	4.4949897686	-3.4534849161
H95	-2.6055348049	3.4978954633	-3.1824467374
C96	-1.8857360082	6.1310461352	-3.5629276783
H97	-2.6882161343	6.3828225620	-4.2661306524
H98	-1.3436317306	7.0576353184	-3.3399640370
H99	-1.2012209003	5.4473440363	-4.0788436504
X100	-1.2903698000#	5.0372404000#	5.7063048000#
X101	0.4272162000#	3.5033964000#	7.5095546000#
C102	2.0454615691	-0.1662991444	10.4256842257

C103	1.4448247181	-0.6170271038	9.2488371887
C104	1.8225677269	-0.0811476901	8.0210917565
C105	2.8184361723	0.9073273150	7.9527880842
C106	3.4111298693	1.3593497854	9.1386512521
C107	3.0250046401	0.8225735685	10.3667673992
H108	1.7531429996	-0.5885188087	11.3834629666
H109	0.6846585823	-1.3932700399	9.2878915737
H110	1.3563399467	-0.4441592008	7.1079999226
H111	4.1798739743	2.1261984860	9.1063151672
H112	3.4974499731	1.1779044534	11.2788845884
C113	7.2664392884	3.8215529562	6.8326259703
C114	7.1397983760	2.4739477827	7.1727863855
C115	5.9135548955	1.8327377718	7.0360707861
C116	4.7956643149	2.5422210413	6.5689092223
C117	4.9321410322	3.8867222996	6.2100215486
C118	6.1665972084	4.5219897439	6.3462925984
H119	8.2275098576	4.3191750436	6.9353710306
H120	8.0012689692	1.9194096768	7.5359454793
H121	5.8300788442	0.7766370740	7.2823069350
H122	4.0924169698	4.4302678702	5.7827689265
H123	6.2683741135	5.5654118690	6.0591999198
C124	-5.7480363832	4.0700325570	3.1200379924
C125	-4.9066931115	5.1552724534	2.8693683908
C126	-3.5490535189	4.9485734710	2.6456133813
C127	-3.0217637754	3.6469721776	2.6753974072
C128	-3.8714023881	2.5621281540	2.9231756709
C129	-5.2307829046	2.7766915840	3.1447107979
H130	-6.8091901597	4.2336461751	3.2899745952
H131	-5.3097648327	6.1642663257	2.8430100846
H132	-2.9015906874	5.7970426023	2.4380879699
H133	-3.4752614189	1.5503634918	2.9380505995
H134	-5.8861724126	1.9296760325	3.3304019866
C135	-0.6419428755	-1.1445005869	2.3914411596
C136	-0.9737464959	-0.4724706355	1.2146883033
C137	-1.1158612705	0.9122868636	1.2164770275
C138	-0.9371163100	1.6279869545	2.4071994846
C139	-0.5994973366	0.9522193830	3.5872261207
C140	-0.4475857828	-0.4328212907	3.5738665090
H141	-0.5242622153	-2.2251172435	2.3837637085
H142	-1.1140696273	-1.0276681452	0.2910770493
H143	-1.3583617635	1.4388185339	0.2966676756
H144	-0.4513154176	1.5108407352	4.5089963035
H145	-0.1719668753	-0.9567181568	4.4851776557

L1_Zr_3c

Fe(II)
Zr1	5.1874319633	11.0156666119	3.9171238447
Fe2	3.2201102284	7.5010641892	4.1813954770
N3	2.9079794808	10.5809885286	3.6454666186
N4	5.2409152079	9.3916198604	5.5692166165

O5	4.6421165613	12.6114369134	2.6527787143
O6	4.7997930662	12.2001052348	5.6996072845
O7	5.7429785959	9.7627984972	2.4691772023
O8	7.0766959554	11.5720583177	4.1528058198
C9	6.8018761637	9.4562959235	1.6250641216
C10	8.1459813646	12.3768684147	4.5245612158
C11	3.7153971564	13.5258978640	2.5085265291
C12	3.9804147307	14.7530668750	1.8147693100
C13	2.9912509010	15.7300493616	1.8221603070
H14	3.2053345259	16.6693440463	1.3224532331
C15	1.7276218551	15.5922068504	2.4312285849
C16	1.4464511439	14.3584560703	2.9920239716
H17	0.4682031183	14.1660154421	3.4217097483
C18	2.4025149826	13.3272435531	3.0091397781
P19	1.7570923316	11.6852921068	3.3036440641
C20	5.5142032738	12.3885139557	6.7805925626
C21	5.5586255506	13.6680407394	7.4451319231
C22	6.3997401935	13.8190965442	8.5397639150
H23	6.4363273636	14.7926489285	9.0176339797
C24	7.2190077384	12.8051342467	9.0738417779
C25	7.1342793291	11.5687236070	8.4642398403
H26	7.7240809238	10.7420027086	8.8455568314
C27	6.2893995553	11.3429938566	7.3604405704
P28	6.1743172872	9.6192652094	6.8891340637
C29	2.4554865320	9.2462992812	3.4504736802
C30	2.8514963632	8.3906921721	2.3708957684
H31	3.6212529821	8.6387316575	1.6541106874
C32	2.1320596011	7.1690392685	2.4769054494
H33	2.2438576356	6.3081511869	1.8297725573
C34	1.2773407380	7.2535925796	3.6161602140
H35	0.6274905627	6.4700133075	3.9855330591
C36	1.4753409743	8.5295288055	4.2225331654
H37	1.0049661704	8.8868830686	5.1282711462
C38	4.8001337607	8.0612710993	5.3448075962
C39	5.2405147210	7.1814985833	4.3017666082
H40	5.9293092111	7.4567571695	3.5173090340
C41	4.5362105724	5.9507841680	4.4232189894
H42	4.6212578092	5.1032262646	3.7547861851
C43	3.6592366730	6.0494043981	5.5439143209
H44	2.9644789678	5.2891335668	5.8779195140
C45	3.8089464752	7.3495221084	6.1076903666
H46	3.2524640006	7.7550331610	6.9408403248
H47	6.5836824645	9.7663226130	0.5910174997
H48	7.7265846853	9.9659645212	1.9427281365
H49	6.9979496797	8.3704055686	1.6075655099
H50	8.9313672513	11.7754110480	5.0075802002
H51	8.5901161524	12.8656234181	3.6441537200
H52	7.8380266363	13.1598244543	5.2320915273
C53	4.4492365682	7.3984083342	10.5740254897
C54	5.2394952149	6.7085819461	9.6549131601
C55	5.7811092991	7.3739210929	8.5575155525

C56	5.5428757952	8.7433647633	8.3697462456
C57	4.7475928089	9.4299608103	9.2962022360
C58	4.2038733504	8.7592182385	10.3904128752
H59	4.0279244652	6.8776420622	11.4305922233
H60	5.4328265809	5.6467640615	9.7878021924
H61	6.3861759702	6.8225638793	7.8431088924
H62	4.5638232243	10.4931086510	9.1639830367
H63	3.5909625215	9.3045405921	11.1042432188
C64	10.4474415106	7.9701285270	6.2043266953
C65	9.6577085844	8.3877214974	5.1349960239
C66	8.3693090801	8.8682678186	5.3581125129
C67	7.8581872668	8.9323872108	6.6605415062
C68	8.6562765547	8.5064417369	7.7319271254
C69	9.9449331057	8.0303942228	7.5033472533
H70	11.4525209070	7.5945783984	6.0262698184
H71	10.0442194848	8.3420294088	4.1195702440
H72	7.7617360297	9.2100666351	4.5253611696
H73	8.2695260454	8.5273482886	8.7475830141
H74	10.5541773033	7.7006072227	8.3416567905
C75	-1.2234100834	11.9706424333	6.8299823832
C76	-1.6931961910	12.1864177941	5.5352847144
C77	-0.8237337518	12.0951719109	4.4490357030
C78	0.5270698806	11.7858848989	4.6525026595
C79	0.9953962881	11.5693381699	5.9555218769
C80	0.1218067264	11.6628358545	7.0366127753
H81	-1.9042030125	12.0396303422	7.6750260073
H82	-2.7413201987	12.4225254570	5.3664977279
H83	-1.2024069965	12.2534590586	3.4422528539
H84	2.0435401311	11.3233017645	6.1106118979
H85	0.4942143769	11.4927752912	8.0439465986
C86	-0.5082477916	10.5485069723	-0.5710056025
C87	0.4666680746	11.5436862240	-0.5873346767
C88	1.1206434587	11.9022561631	0.5887899846
C89	0.8064680876	11.2658187591	1.7966170042
C90	-0.1736767326	10.2627928710	1.8043696916
C91	-0.8264852531	9.9095610431	0.6260634721
H92	-1.0197536627	10.2706833906	-1.4898978401
H93	0.7193654088	12.0470908101	-1.5174998789
H94	1.8749971669	12.6832246720	0.5697372739
H95	-0.4218678931	9.7480458474	2.7275456073
H96	-1.5833510793	9.1289594091	0.6446505252
C99	5.2989467617	14.9541790312	1.0463976235
C100	6.5039133832	14.9429064283	2.0068865643
H101	6.5623563129	14.0042641607	2.5599421416
H102	7.4347778151	15.0697971179	1.4376396759
H103	6.4354011629	15.7667365570	2.7269542195
C104	5.3275815713	16.2885233222	0.2832844235
H105	5.2597734133	17.1529630502	0.9555173254
H106	6.2773548707	16.3717986605	-0.2585882746
H107	4.5211714192	16.3620371826	-0.4570359727
C108	5.4525941900	13.8231446600	0.0071119040

H109	6.3912601090	13.9482153829	-0.5483636644
H110	5.4652705134	12.8415895893	0.4868846248
H111	4.6289364184	13.8469841305	-0.7180818557
C112	0.7314196698	16.7586755115	2.4102118192
C113	-0.5840334013	16.4072650006	3.1189093654
H114	-1.1028932300	15.5754608153	2.6270443252
H115	-0.4206372656	16.1364503764	4.1686223299
H116	-1.2589229343	17.2714562451	3.1001975802
C117	1.3475995544	17.9769142525	3.1251593197
H118	1.5782358649	17.7403027278	4.1703664393
H119	2.2760786345	18.3046104999	2.6447010355
H120	0.6496927557	18.8242312305	3.1136674356
C121	0.4012995571	17.1346591121	0.9515197564
H122	-0.3114082461	17.9691878886	0.9208974575
H123	1.2940768348	17.4411906660	0.3951734890
H124	-0.0469459588	16.2857352068	0.4213815082
C125	4.7183985993	14.8536322931	6.9384301926
C126	4.8607960582	16.0996151802	7.8268433505
H127	4.5358189847	15.9144133547	8.8583752632
H128	5.8891449408	16.4808990708	7.8518671577
H129	4.2291351753	16.8997081896	7.4223120012
C130	3.2258371202	14.4738861013	6.9252381829
H131	2.8797472794	14.2230792119	7.9365180120
H132	2.6246285256	15.3176557905	6.5630422717
H133	3.0448126175	13.6200161188	6.2718676411
C134	5.1761006530	15.2414003236	5.5195573379
H135	4.5674868834	16.0700768508	5.1352159682
H136	6.2239680259	15.5672833601	5.5288009130
H137	5.0820223675	14.4026441121	4.8293350717
C138	8.1270340128	13.0941238638	10.2755541217
C139	7.2705636018	13.5300720285	11.4814791206
H140	6.6828668374	14.4284275187	11.2626277204
H141	6.5709483164	12.7365000887	11.7707720391
H142	7.9080223751	13.7529380038	12.3470395293
C143	9.1157902781	14.2211540127	9.9151243513
H144	8.5949531157	15.1454172448	9.6419157021
H145	9.7734608863	14.4475530319	10.7648041351
H146	9.7448467821	13.9302233522	9.0657310067
C147	8.9391143147	11.8600826186	10.6923909638
H148	9.5883528240	12.1106568136	11.5401639648
H149	8.2901058789	11.0338129809	11.0079338287
H150	9.5810148052	11.5010265383	9.8787617232

Fe(III)

Zr1	5.3368248983	11.0113925296	3.7367808666
Fe2	3.1359774543	7.4813512305	4.0791057808
N3	2.9261019739	10.5979344085	3.5141696356
N4	5.3357155833	9.3188198863	5.4405741515
O5	4.7069262385	12.5440647999	2.5124241502
O6	5.0121881860	12.1702064866	5.4954851485
O7	5.6811162662	9.5941624192	2.3609071304

O8	7.2304115507	11.4388881899	3.8731996945
C9	6.7150926989	9.1995365989	1.5090668454
C10	8.4407895834	12.0909618658	4.1005035452
C11	3.7842532549	13.4729917064	2.3581296582
C12	4.0436375263	14.6375448832	1.5642503798
C13	3.0730965151	15.6327140370	1.5310131387
H14	3.2837446140	16.5222058323	0.9478850143
C15	1.8284895637	15.5700392184	2.1908365907
C16	1.5595192571	14.3994944521	2.8743202650
H17	0.5958099464	14.2741468897	3.3557916455
C18	2.5008710072	13.3523309682	2.9471929776
P19	1.8112694049	11.8131435118	3.5379204654
C20	5.4473488684	12.3494947476	6.7245390129
C21	5.4100294961	13.6321564195	7.3725833298
C22	5.8438718937	13.7135581325	8.6898319536
H23	5.8013953927	14.6836817655	9.1716493538
C24	6.3331255153	12.6376056322	9.4538853159
C25	6.3964329401	11.4152435509	8.8150201474
H26	6.7610911160	10.5474443246	9.3548984160
C27	5.9699576088	11.2633017845	7.4773949583
P28	6.2289249334	9.6374257694	6.7927283650
C29	2.3946380281	9.3433564858	3.2788773163
C30	2.8484954518	8.4303078368	2.2673886920
H31	3.6707940458	8.6436018424	1.5985722143
C32	2.0732353956	7.2348484193	2.3465803557
H33	2.1636123708	6.3751314416	1.6948735528
C34	1.1651670409	7.3715449659	3.4372770510
H35	0.4554627995	6.6277248683	3.7769610479
C36	1.3825125889	8.6471352157	4.0260318517
H37	0.8965065678	9.0271798873	4.9152417678
C38	4.8539223375	8.0277267067	5.2837889552
C39	5.1636539773	7.1184375415	4.2149921840
H40	5.8299213718	7.3456656673	3.3958224956
C41	4.4141525964	5.9159613985	4.3967549501
H42	4.4609012978	5.0377563378	3.7654945275
C43	3.5882632929	6.0873950303	5.5458519580
H44	2.8826861860	5.3680230379	5.9414879830
C45	3.8313943641	7.3883271318	6.0649325964
H46	3.3192064538	7.8399673086	6.9024022860
H47	6.5166793311	9.5243770441	0.4772551847
H48	7.6765210821	9.6306205833	1.8251465123
H49	6.8210529248	8.1011754926	1.4909520437
H50	9.2025727415	11.3733065080	4.4313137757
H51	8.7936688592	12.5704553571	3.1779959116
H52	8.3293085321	12.8642495112	4.8721775533
C53	5.1889197430	6.5784996774	10.0961800559
C54	6.2415381764	6.3237634887	9.2200720820
C55	6.5770089434	7.2544960455	8.2382313351
C56	5.8534936496	8.4472550075	8.1228174341
C57	4.7930809120	8.6971039589	9.0076585861
C58	4.4660905184	7.7675526351	9.9901739136

H59	4.9364076910	5.8559463827	10.8682492405
H60	6.8123699083	5.4027925718	9.3057486010
H61	7.4096955950	7.0535523998	7.5696872674
H62	4.2399259625	9.6304640948	8.9387417280
H63	3.6519581798	7.9744128352	10.6804899326
C64	10.6889580897	8.7675072651	5.9850764403
C65	9.7090182272	8.2717236326	5.1270321277
C66	8.3677218469	8.5755416836	5.3495320422
C67	7.9972298676	9.3728900866	6.4380737413
C68	8.9875697122	9.8821973709	7.2888154219
C69	10.3267413684	9.5773382902	7.0610704914
H70	11.7354737335	8.5309590852	5.8103721567
H71	9.9887793731	7.6529339095	4.2781021889
H72	7.6085477386	8.2102534119	4.6662013472
H73	8.7183349051	10.5257911219	8.1211081683
H74	11.0895903954	9.9785644319	7.7232556291
C75	-0.0505369113	12.2292710951	7.7451003437
C76	-0.7176692835	12.7806048780	6.6516903684
C77	-0.1796602673	12.6627937283	5.3733583757
C78	1.0392608292	11.9946084487	5.1793122540
C79	1.7075309234	11.4477523876	6.2820034230
C80	1.1600030640	11.5642864624	7.5579751020
H81	-0.4752783961	12.3192635927	8.7419167319
H82	-1.6632424163	13.2980538876	6.7917600857
H83	-0.7261492543	13.0754553500	4.5297848436
H84	2.6614139671	10.9475033474	6.1353000858
H85	1.6856376730	11.1430075782	8.4113364193
C86	-1.4994176254	10.7511672465	0.4930832225
C87	-0.3155825762	11.3649586887	0.0844197714
C88	0.6552201337	11.7053821644	1.0211539774
C89	0.4528734939	11.4268937391	2.3814323050
C90	-0.7369912341	10.8046633907	2.7839318097
C91	-1.7087872723	10.4728888798	1.8419246045
H92	-2.2610341824	10.4954490684	-0.2394257949
H93	-0.1517828734	11.5892800520	-0.9664571575
H94	1.5673938383	12.2013499152	0.6993487357
H95	-0.9180313652	10.5878264823	3.8326577588
H96	-2.6329402974	10.0003566342	2.1655503423
C99	5.3357061587	14.7583867571	0.7338478891
C100	6.5819659927	14.7549382003	1.6419467758
H101	6.6522792143	13.8376234065	2.2284521159
H102	7.4879088912	14.8416395795	1.0282819790
H103	6.5637582483	15.6059649406	2.3325075019
C104	5.3715709039	16.0570593873	-0.0874674960
H105	5.3722723090	16.9508335799	0.5480619243
H106	6.2931085627	16.0806975680	-0.6801494138
H107	4.5311470839	16.1299716251	-0.7883404375
C108	5.4068898547	13.5833616763	-0.2646812003
H109	6.3218559063	13.6578962620	-0.8654543611
H110	5.4121832829	12.6194550221	0.2489814800
H111	4.5533156192	13.6066314675	-0.9537693828

C112	0.8336513198	16.7341124475	2.0873726915
C113	-0.4600929479	16.4577900368	2.8667581623
H114	-0.9953346463	15.5839285284	2.4744051556
H115	-0.2679332632	16.2978192382	3.9347455013
H116	-1.1349622140	17.3168376804	2.7800916140
C117	1.4783623910	18.0125327646	2.6594558623
H118	1.7370618186	17.8822335743	3.7167875581
H119	2.3935958776	18.2855418404	2.1228039567
H120	0.7846446313	18.8587407500	2.5823948134
C121	0.4605476508	16.9622338745	0.6085962538
H122	-0.2502920653	17.7926901839	0.5179603618
H123	1.3351574183	17.2087371419	-0.0030128488
H124	-0.0071567037	16.0681710633	0.1795174633
C125	4.9231594839	14.8958412016	6.6434611803
C126	5.0443311361	16.1583677944	7.5118464068
H127	4.4207779497	16.1080702496	8.4128982719
H128	6.0787392188	16.3598937986	7.8151682654
H129	4.7017767299	17.0220538281	6.9304763437
C130	3.4390927381	14.7411285057	6.2683164882
H131	2.8216058639	14.6114473633	7.1655118926
H132	3.0869900752	15.6362304494	5.7411315809
H133	3.2841292723	13.8835233163	5.6143539439
C134	5.7711351918	15.1331452208	5.3797159449
H135	5.4179696658	16.0306290520	4.8572486460
H136	6.8245708104	15.2916003573	5.6424740574
H137	5.7091996795	14.2927100001	4.6882509784
C138	6.7513746604	12.8503562286	10.9143516257
C139	5.5330189784	13.3353250548	11.7251686771
H140	5.1291304689	14.2752342130	11.3333231048
H141	4.7275584508	12.5915159255	11.7052852930
H142	5.8110899321	13.5047530854	12.7726517601
C143	7.8688368755	13.9098128812	10.9846645169
H144	7.5471491427	14.8744145433	10.5775748910
H145	8.1735139896	14.0756840095	12.0252674684
H146	8.7519256693	13.5872676073	10.4206651440
C147	7.2736188918	11.5596254908	11.5610823146
H148	7.5524332786	11.7530989644	12.6031377191
H149	6.5156867401	10.7667476225	11.5666441872
H150	8.1668943612	11.1774820100	11.0516640734

L2_Y_1a

Fe(II)
Y1	4.6583824861	10.9994676586	3.8866129852
Fe2	2.1526366665	8.7177817758	6.3282922949
N3	2.2423400723	11.3456179243	4.6705419058
N4	5.1206827610	9.0627396094	5.5719763425
O5	4.0493245330	12.6667888196	2.6925152880
O6	6.1027166573	11.8565841931	5.2017982650
O7	5.0491765881	9.4305602050	2.5988841784
C9	5.3892982357	8.8111350455	1.4009128076

C11	3.3139390087	13.7225648565	3.0151634800
C12	3.8001758369	15.0343222066	2.8654995929
C13	3.0169891089	16.1249419904	3.2237725869
H14	3.4172353717	17.1296664710	3.1038906872
C15	1.7293611001	15.9472843623	3.7356143951
C16	1.2350009564	14.6544436719	3.8818626719
H17	0.2297483969	14.4992056188	4.2731265543
C18	2.0041353831	13.5434784498	3.5270915469
C19	1.4698882257	12.1507904227	3.6569626865
H20	1.5460349865	11.6042337683	2.7090692181
H21	0.4123061653	12.1700955083	3.9509889107
H22	2.3146791990	11.9254043051	5.5095205961
C23	6.5035623328	11.6814430707	6.4561185664
C24	6.7102005624	12.7845936455	7.3040075776
C25	7.1098350675	12.6029385525	8.6238050684
H26	7.2585851709	13.4729481956	9.2603968927
C27	7.3180383267	11.3216723416	9.1366029914
C28	7.1187674436	10.2224659123	8.3045883601
H29	7.2737730009	9.2159096897	8.6913832635
C30	6.7192517176	10.3804189479	6.9763398113
C31	6.5235575609	9.1959301190	6.0772341168
H32	6.8229901716	8.2745130842	6.5962984877
H33	7.1460051108	9.2912733928	5.1774393208
H34	5.1292977388	8.3815845526	4.8111630154
C35	1.5521388318	10.1381115045	5.0180808476
C36	1.7063183585	8.8899582283	4.3391074843
H37	2.3924644604	8.6903311968	3.5228904788
C38	0.8269392583	7.9522361020	4.9538560944
H39	0.7408139178	6.9048644299	4.6958667640
C40	0.1237276117	8.6169422727	5.9993980185
H41	-0.5850693632	8.1601085045	6.6780343206
C42	0.5593486938	9.9719132058	6.0367924048
H43	0.2359788548	10.7318659736	6.7376839041
C44	4.1787856359	8.6460258059	6.5552732816
C45	3.6196388591	7.3379748358	6.7128843587
H46	3.8306461690	6.4802770521	6.0858253550
C47	2.6918941236	7.3850675071	7.7934704573
H48	2.0692661880	6.5666843044	8.1316637843
C49	2.6865413285	8.7114374991	8.3129312996
H50	2.0641992326	9.0754411781	9.1204507234
C51	3.6014860394	9.4935219795	7.5501873605
H52	3.8271928056	10.5423018349	7.6919149244
H53	5.0649287011	7.7572710985	1.3893802862
H54	4.9216998837	9.3083789110	0.5358274304
H55	6.4790424869	8.8175226862	1.2356867107
H59	4.8027801089	15.1672163889	2.4677212551
H60	1.1216138655	16.8035159962	4.0156487938
H61	6.5492622305	13.7798459091	6.8973218264
H62	7.6274414867	11.1806665038	10.1689212273

Fe(III)

Y1	4.6646059560	11.1347768054	3.5005815410
Fe2	2.4638880154	8.6572584544	6.4623865015
N3	2.5441445264	11.5745766896	4.8460109844
N4	5.7152048655	8.6388792879	5.6565244094
O5	3.8277371034	12.5729104362	2.2241656541
O6	5.6758792184	11.6013879614	5.2523656100
O7	5.2087808234	9.2114324943	2.9179894264
C9	5.4781386855	8.3159467187	1.8639749862
C11	3.2416168564	13.7098733486	2.6379113117
C12	3.7122925401	14.9619444239	2.2182553388
C13	3.1055210389	16.1285217026	2.6699956287
H14	3.4831951475	17.0907241086	2.3332122033
C15	2.0185309965	16.0770818545	3.5450797047
C16	1.5397761856	14.8398131591	3.9602550106
H17	0.6825848403	14.7884289521	4.6300690566
C18	2.1327359301	13.6521951200	3.5153331101
C19	1.5812570822	12.3247285657	3.9336666141
H20	1.3944314151	11.6769105664	3.0697842756
H21	0.6349851675	12.4606833512	4.4693558184
H22	2.9641051790	12.2705270188	5.4682163192
C23	5.8165435984	11.6253743756	6.5808958477
C24	5.4597464846	12.7648205567	7.3189552756
C25	5.5939501265	12.7807642074	8.7052534004
H26	5.3219834897	13.6757178288	9.2596662135
C27	6.0897829242	11.6652934770	9.3794368056
C28	6.4511370439	10.5348011482	8.6487088966
H29	6.8614880848	9.6688234994	9.1675262507
C30	6.3163234601	10.4925487169	7.2590668776
C31	6.7518698420	9.2758238635	6.4777807793
H32	7.1559545378	8.5234296931	7.1660604496
H33	7.5552566171	9.5370980561	5.7809333366
H34	5.7803867939	8.6968886905	4.6290499731
C35	1.8721173755	10.6252242060	5.6609623530
C36	1.0148434063	9.5910231252	5.1892758661
H37	0.8382048943	9.3317465149	4.1528888028
C38	0.4039338563	8.9715744977	6.3169012245
H39	-0.3235490852	8.1712198635	6.2766097159
C40	0.9374305030	9.5716781485	7.4919452057
H41	0.6717097469	9.3323549176	8.5132652795
C42	1.8704709971	10.5806512368	7.0854781800
H43	2.4462390038	11.2264615852	7.7378737581
C44	4.6462149174	8.0121020163	6.1376173459
C45	3.6318073710	7.3528953078	5.3438768572
H46	3.6511179320	7.2770157675	4.2645385319
C47	2.7464462062	6.6643056071	6.2264899331
H48	1.9512701887	5.9941752894	5.9258669557
C49	3.0691518192	7.0562790926	7.5579190508
H50	2.5638043857	6.7351686654	8.4600683267
C51	4.1653233632	7.9692253536	7.4966601882
H52	4.6256179340	8.4701545441	8.3370312519
H53	5.1016443140	7.3100809955	2.0994584824

H54	5.0032080838	8.6392127989	0.9272714906
H55	6.5590142566	8.2361657477	1.6874139781
H59	4.5514896566	14.9955118726	1.5288590640
H60	1.5457844162	16.9912050901	3.8920841785
H61	5.1128378717	13.6452630091	6.7817392315
H62	6.2093684350	11.6809217191	10.4589547387

L3_Y_1d

Fe(II)
Y1	2.0795504253	3.3461004529	3.5250856253
Fe2	-0.2024907460	4.1271821607	6.7127511596
O3	1.4955154319	4.1111724816	1.5925901680
O4	2.7731799971	1.3269154776	3.1718345692
O5	3.4249495306	4.5415563193	4.4903770816
C6	-0.6334280066	4.9044066409	4.8672189240
C7	0.1686706117	5.8181192775	5.6165724563
H8	1.1536284604	6.1674789493	5.3334748773
C9	-0.5459053617	6.1450629116	6.8047188509
H10	-0.1895230736	6.7898003355	7.5973284556
C11	-1.7781279006	5.4275930409	6.7993815509
H12	-2.5231230409	5.4348393366	7.5843810076
C13	-1.8382808936	4.6638725318	5.5976871685
H14	-2.6421198153	4.0030493979	5.2962330732
C15	0.7827910037	2.3482494615	6.4969490421
C16	1.6042451414	3.2889958247	7.1907546967
H17	2.5615278125	3.6583330352	6.8448730875
C18	0.9108567968	3.6795691038	8.3718989351
H19	1.2558171587	4.4086929444	9.0932135839
C20	-0.3391240141	2.9932565683	8.4065553531
H21	-1.1087473012	3.1066299442	9.1593486486
C22	-0.4176870632	2.1618682436	7.2511499088
H23	-1.2472390919	1.5211724193	6.9761162073
C24	-0.3645685531	5.2751519239	2.4592577358
C25	-1.3402981145	6.2628436073	2.3937156233
H26	-2.0465184879	6.3878373387	3.2109902741
C27	-1.3847563828	7.0818828917	1.2726444612
C28	-0.4665911120	6.8839660043	0.2398858445
H29	-0.5310441781	7.5340614582	-0.6268427714
C30	0.5884219088	5.0720888130	1.4348302619
C31	2.1487079710	0.6627118879	5.3487235864
C32	2.2729395049	-0.1420919079	6.4746562811
H33	1.6278607365	0.0219833889	7.3348172907
C34	3.2363795906	-1.1419987773	6.4801507142
C35	4.0410424820	-1.3229259732	5.3533997995
H36	4.7804201379	-2.1171112114	5.3813504208
C37	2.9630827030	0.5048821238	4.2033194861
C38	4.5223377946	5.3074344197	4.8667312555
H39	4.2335791634	6.0889397697	5.5886866674
H40	5.3013916903	4.6900680986	5.3411173098
H41	4.9798317580	5.8134907324	4.0021927113

C42	3.9376892308	-0.5342572230	4.2037424518
C43	0.5250441365	5.8993477756	0.2772673720
N44	1.1355310746	1.7214108109	5.2595479980
N45	-0.2710934655	4.3523176470	3.5982661566
C46	1.5199248742	5.7083272755	-0.8765446346
C47	1.2578716917	6.6843396950	-2.0329944425
H48	0.2576549392	6.5543093330	-2.4639747544
H49	1.3667387171	7.7305550556	-1.7221668482
H50	1.9864195248	6.5021460270	-2.8320083922
C51	2.9569909354	5.9542618139	-0.3740778497
H52	3.0668117209	6.9796310543	0.0004150602
H53	3.2164418292	5.2625265062	0.4304580209
H54	3.6734755408	5.8154463801	-1.1942748499
C55	1.3983121048	4.2755439300	-1.4353742308
H56	2.1160691960	4.1269675326	-2.2528163784
H57	1.5972864197	3.5318090690	-0.6602030893
H58	0.3916367166	4.1002223726	-1.8349659906
C59	4.8352607636	-0.7689544526	2.9798357442
C60	3.9610288767	-1.0889204102	1.7500475453
H61	3.2696816843	-0.2705589860	1.5356071398
H62	4.5943213321	-1.2502399328	0.8677641247
H63	3.3775078788	-2.0028531018	1.9176379169
C64	5.6875968630	0.4863153050	2.7035218962
H65	5.0557727868	1.3546068301	2.5044571431
H66	6.3328943662	0.7149185819	3.5608358232
H67	6.3320705123	0.3215134127	1.8301428126
C68	5.7989932757	-1.9469960312	3.1872843561
H69	6.4028787977	-2.0835113532	2.2822211229
H70	6.4913780232	-1.7730992023	4.0201031461
H71	5.2662962341	-2.8878435385	3.3721641656
X72	-1.6700556444#	4.7970981656#	5.4075773579#
X73	0.6145324225#	4.1123818282#	7.7180422565#
H74	-2.1329098578	7.8661865662	1.1947656216
H75	3.3638462725	-1.7788777135	7.3510873448
H76	0.2895625208	1.3162250447	4.8527044154
H77	-0.8858017872	3.5564656616	3.4119990414

Fe(III)

Y1	1.8553588185	3.1204138793	3.3801369558
Fe2	-0.2452713916	4.1322856146	6.7336480596
O3	1.2619014479	3.9604653328	1.5228396469
O4	2.5399998611	1.1070474690	3.1670537957
O5	3.0426115532	4.3764781210	4.4555329835
C6	-0.7733825585	4.9729388674	4.7816553264
C7	0.1009960333	5.8324345002	5.5094359436
H8	1.0800865173	6.1478991257	5.1711665834
C9	-0.5365549439	6.1774738120	6.7361313365
H10	-0.1318794053	6.8368190210	7.4932230479
C11	-1.7807472643	5.4825652400	6.8013586657
H12	-2.5019760448	5.5277980651	7.6072110704

C13	-1.9096463476	4.7090962037	5.6060370969
H14	-2.7478441767	4.0741901424	5.3445877409
C15	0.7678380269	2.1964748051	6.5881069672
C16	1.5875795877	3.1833285901	7.2136633039
H17	2.5479868333	3.5129443847	6.8378052677
C18	0.9077503130	3.6554175937	8.3732808843
H19	1.2864668692	4.3921449511	9.0700389911
C20	-0.3627954064	3.0089408771	8.4369582807
H21	-1.1206751034	3.1498636238	9.1972535539
C22	-0.4616571550	2.1312135231	7.3130617644
H23	-1.3063880206	1.4961254726	7.0731629869
C24	-0.3432669010	5.4154056917	2.4472158924
C25	-1.1188850057	6.5732891690	2.4419124154
H26	-1.8333709913	6.7702339555	3.2379626432
C27	-0.9633286346	7.4599139374	1.3887790133
C28	-0.0618750992	7.1621253274	0.3634151784
H29	0.0301775589	7.8758344738	-0.4478354852
C30	0.5750506426	5.0982393347	1.4237391341
C31	2.3187421168	0.6949837634	5.4800405818
C32	2.7194285198	0.1068356894	6.6785223344
H33	2.1552839595	0.2705651785	7.5941977527
C34	3.8483502442	-0.6950247620	6.6740075376
C35	4.5249212849	-0.9231665717	5.4715605825
H36	5.3923749439	-1.5732882218	5.4988306727
C37	3.0004267183	0.4927464938	4.2593069687
C38	4.1521004064	5.1399136319	4.8367731317
H39	3.8811903340	5.8583941321	5.6267268396
H40	4.9598986776	4.5034754680	5.2245899016
H41	4.5497504795	5.7158214433	3.9899529386
C42	4.1321183934	-0.3719906609	4.2495615325
C43	0.7146248694	6.0016730739	0.3329163713
N44	1.0968884221	1.5096003322	5.4145448195
N45	-0.4880782771	4.4204245082	3.5230669405
C46	1.6791335493	5.7027648465	-0.8241781628
C47	1.6465462275	6.7995538047	-1.8998183143
H48	0.6537540126	6.9059892699	-2.3529092653
H49	1.9564338319	7.7755331588	-1.5071612286
H50	2.3443047138	6.5363295427	-2.7025591350
C51	3.1239370834	5.6158821161	-0.2931213321
H52	3.4259844738	6.5603291170	0.1755863318
H53	3.2341594367	4.8124825394	0.4393405042
H54	3.8147444309	5.4165368260	-1.1212665733
C55	1.2832596757	4.3715606857	-1.4956824761
H56	1.9675534078	4.1536233629	-2.3247226106
H57	1.3235427351	3.5384612727	-0.7898803568
H58	0.2679993179	4.4299606415	-1.9061338920
C59	4.8782772134	-0.6862226458	2.9434223836
C60	3.9042707309	-1.3370976859	1.9397879338
H61	3.0606549949	-0.6801021215	1.7148452143
H62	4.4286656952	-1.5574432665	1.0021078171
H63	3.5133407681	-2.2825245091	2.3348140988

C64	5.4643104548	0.6064999776	2.3422119094
H65	4.6765618896	1.3141941131	2.0733814594
H66	6.1488845438	1.0928904174	3.0478012689
H67	6.0308162035	0.3726117496	1.4327975962
C68	6.0435147587	-1.6634149268	3.1660072031
H69	6.5337190418	-1.8616857815	2.2064309680
H70	6.8051713471	-1.2561236911	3.8418629158
H71	5.7045685881	-2.6273605849	3.5634902863
X72	-1.6700556444#	4.7970981656#	5.4075773579#
X73	0.6145324225#	4.1123818282#	7.7180422565#
H74	-1.5494486528	8.3734156578	1.3491868482
H75	4.1961867799	-1.1596173500	7.5917689515
H76	0.3130300854	0.9331456389	5.1038730641
H77	-1.2113503220	3.7460002348	3.2645315616

L3_Zr_1d

Fe(II)

Zr1	6.0470504222	12.2290474739	4.1169150427
Fe2	1.9393349912	8.8081488881	6.0835687987
N3	2.2667530898	11.6884464766	5.0187694124
N4	4.8403921750	9.9628622510	6.5117813083
O5	4.2909319042	13.1018773887	3.8970618512
O6	6.5866233827	11.9527220991	5.9974138232
O7	5.9940511318	10.4740303145	3.2748022447
O8	7.4448758350	13.3093724063	3.3373513326
C9	3.0316546037	13.4140064265	3.4839578158
C10	2.7680511970	14.4268007421	2.5342347850
C11	1.4304556409	14.6192780638	2.1596025741
H12	1.1820594080	15.3841632678	1.4331983599
C13	0.3988691612	13.8506014831	2.6876689109
C14	0.6672163732	12.8695268266	3.6296672361
H15	-0.1316981576	12.2723901038	4.0591749646
C16	1.9830869226	12.6474026293	4.0454035152
C17	3.8820955787	15.2763695430	1.8964676078
C18	4.8021890192	14.3815279513	1.0419808971
H19	4.2251988772	13.8664977913	0.2649009295
H20	5.3141085048	13.6235723602	1.6394867146
H21	5.5717983183	14.9874533672	0.5460000476
C22	4.6906160673	16.0117414890	2.9830785016
H23	5.4909121773	16.6069973426	2.5240889466
H24	5.1449094655	15.3212290398	3.6960374646
H25	4.0423191770	16.6948746910	3.5444438832
C26	3.3195177010	16.3545520123	0.9527265153
H27	4.1483229521	16.9482620851	0.5489465265
H28	2.6424433301	17.0423142209	1.4719791432
H29	2.7835030121	15.9198480891	0.1010705116
C30	6.6493969213	11.4124876452	7.2337512452
C31	7.5861614795	11.8669171728	8.1904202113
C32	7.5743953282	11.2418505701	9.4440782885

H33	8.2700155247	11.5645529567	10.2103309257
C34	6.6987900268	10.2030608915	9.7387931724
C35	5.8002189968	9.7492165718	8.7821870597
H36	5.1379079667	8.9194361146	9.0027609813
C37	5.7584051850	10.3560474259	7.5258584944
C38	8.5822556015	12.9963971122	7.8789303400
C39	7.8239507615	14.2970955114	7.5475918840
H40	8.5339030989	15.1028558014	7.3198544891
H41	7.2125926264	14.6164511551	8.3999046538
H42	7.1629341189	14.1714369799	6.6874936056
C43	9.4929313948	12.5896979239	6.7025013985
H44	8.9224341736	12.4099677084	5.7891047588
H45	10.0507423498	11.6766199780	6.9438924175
H46	10.2218168247	13.3847310708	6.4982242136
C47	9.4997147481	13.2965203300	9.0756442749
H48	10.1074708287	12.4280596875	9.3562323920
H49	8.9355787289	13.6230471732	9.9571345333
H50	10.1879849748	14.1069070634	8.8075884097
C51	1.5025746073	10.5038319355	5.0573891689
C52	1.5956576813	9.3940914751	4.1523968472
H53	2.3030500121	9.3120948613	3.3369464495
C54	0.6344206716	8.4220050489	4.5441385504
H55	0.4832891921	7.4523779641	4.0866222806
C56	-0.0675702375	8.9268799176	5.6801739892
H57	-0.8382064170	8.4032246431	6.2317655475
C58	0.4595270591	10.2110124537	5.9940214467
H59	0.1703974528	10.8496046655	6.8185500004
C60	3.8720127817	8.9830073988	6.8124555984
C61	3.6926053666	7.7250492798	6.1577157826
H62	4.2552445741	7.3746506120	5.3011020317
C63	2.6310259754	7.0303725659	6.8098012815
H64	2.2413845171	6.0604919195	6.5283480166
C65	2.1526040643	7.8538435467	7.8701916815
H66	1.3320975469	7.6220304683	8.5367725678
C67	2.8969167592	9.0712915274	7.8564028853
H68	2.7584334925	9.9202870521	8.5124439388
C69	6.2276033712	9.4058488011	2.4038273862
H70	5.3989003274	8.6874458769	2.4553214148
H71	6.3127872604	9.7593319775	1.3680135111
H72	7.1565986679	8.8855726973	2.6726719636
C73	8.4487742181	14.0987555416	2.7759179614
H74	9.2083046722	13.4651805632	2.2993172293
H75	8.0264541672	14.7699531813	2.0176008440
H76	8.9355047334	14.7047218281	3.5504881738
X77	1.1652069999#	9.6570340001#	5.7153150001#
X78	2.6512790000#	8.4138540000#	7.5004090000#
H79	3.2433412543	11.5805150387	5.2633367075
H80	5.3012696818	9.7795315281	5.6242124484
H81	-0.6251361762	14.0264942215	2.3667091593
H82	6.7269073200	9.7307447430	10.7177493446

Fe(III)

Zr1	6.1624743821	11.9572144510	3.9074276742
Fe2	2.0421782849	8.7589212053	6.0340740038
N3	2.5426023527	11.7893977885	5.3384301436
N4	5.2286642808	9.1966245502	6.7078178095
O5	4.4606827272	12.9552811425	3.8414571042
O6	6.4487051919	11.4202492539	5.8136906412
O7	5.9215388950	10.2811080118	2.9491471705
O8	7.6299398891	12.9459287606	3.1655689174
C9	3.2312097999	13.5334860503	3.7783242405
C10	2.9580079586	14.6735490734	2.9880131863
C11	1.6421559810	15.1545947028	3.0126810575
H12	1.3855979533	16.0254026501	2.4213399158
C13	0.6390844877	14.5617237232	3.7733170223
C14	0.9224913985	13.4495790339	4.5526586784
H15	0.1539225824	12.9896931989	5.1674886001
C16	2.2139773325	12.9303836264	4.5506076567
C17	4.0299006921	15.3617077873	2.1253985052
C18	4.5790434471	14.3750149553	1.0751999124
H19	3.7771243274	14.0274443551	0.4133861177
H20	5.0400913435	13.4942539974	1.5312639786
H21	5.3376116812	14.8668679475	0.4540255244
C22	5.1641826905	15.8975659386	3.0209387358
H23	5.9238639923	16.3984427231	2.4080858366
H24	5.6581943400	15.1043640505	3.5865508622
H25	4.7749950820	16.6298015352	3.7376838849
C26	3.4621222067	16.5639224976	1.3507313903
H27	4.2600912259	17.0119686516	0.7478138558
H28	3.0818205282	17.3439450937	2.0198810722
H29	2.6589030027	16.2725632191	0.6642618669
C30	6.4670832909	11.2364977281	7.1469275602
C31	7.1166262322	12.1184970299	8.0481151090
C32	7.0281102005	11.8108873411	9.4113973101
H33	7.5020349198	12.4684465854	10.1303379370
C34	6.3725368500	10.6801810369	9.8963481286
C35	5.7764716103	9.7997068902	9.0090418167
H36	5.3195665220	8.8783678986	9.3591545138
C37	5.8099659312	10.0892543607	7.6438138680
C38	7.8894163340	13.3596192101	7.5699841987
C39	6.9339999748	14.3493781063	6.8744658642
H40	7.4917378383	15.2168687169	6.5018042118
H41	6.1738305342	14.7133350265	7.5755308364
H42	6.4033092826	13.9066068290	6.0266940255
C43	9.0330321230	12.9334301442	6.6268611362
H44	8.6723426450	12.4190849132	5.7336426839
H45	9.7285527181	12.2625352730	7.1444193426
H46	9.5987853942	13.8151701288	6.3021723250
C47	8.5375467699	14.1210495526	8.7386258021
H48	9.2551260732	13.5004264923	9.2874072775
H49	7.7953375667	14.5063962882	9.4470049605

H50	9.0867907596	14.9833050394	8.3440995236
C51	1.7356246313	10.6540000858	5.1565428928
C52	1.8813251612	9.6269850786	4.1653579576
H53	2.6502517052	9.5923619190	3.4040461505
C54	0.8202787919	8.6870990854	4.3448829287
H55	0.6540520144	7.7926798866	3.7574490792
C56	0.0168097874	9.1294214755	5.4307040542
H57	-0.8453821648	8.6130516576	5.8338373397
C58	0.5946574412	10.3169205678	5.9499642704
H59	0.2579010270	10.8734210188	6.8155667241
C60	4.1076276600	8.4817436596	6.9034028976
C61	3.6196586461	7.4107904090	6.0720794644
H62	4.1351321552	7.0000502392	5.2129242088
C63	2.4401062379	6.8733046379	6.6760933196
H64	1.8960560564	6.0040778427	6.3295093700
C65	2.0992671768	7.7023920385	7.7809901872
H66	1.2399685812	7.5872388667	8.4290795683
C67	3.0672792184	8.7468583273	7.8633730519
H68	3.0754766721	9.5546515413	8.5820843228
C69	6.0429089746	9.3413237004	1.9136993118
H70	5.2988350118	8.5444042041	2.0413128538
H71	5.8784476387	9.8145325312	0.9381737668
H72	7.0420790914	8.8892445783	1.9211913488
C73	8.6699722967	13.6385628744	2.5263292561
H74	9.4202524882	12.9297339564	2.1577782174
H75	8.2729181884	14.2110863046	1.6807924705
H76	9.1467707661	14.3280677771	3.2314189563
X77	1.1371166003#	9.6829265992#	5.5807159998#
X78	2.7341582000#	8.3574472000#	7.6135586000#
H79	3.5287294691	11.5801565702	5.2332537132
H80	5.7500650670	9.0370063318	5.8535894538
H81	-0.3644618979	14.9780130207	3.7642881657
H82	6.3592849505	10.4742960013	10.9624961178

L4_Y_1c

Fe(II)

Y1	2.3121337467	4.1130712605	4.2399902613
Fe2	-0.2704362329	4.5059219301	7.3360438953
O3	1.8264099699	4.6603115761	2.1649175092
O4	3.0964907301	2.1539994705	3.7278596803
O5	3.5087010018	5.5723488320	5.0280708728
C6	-0.8315896185	4.7676444458	5.3848909279
C7	-0.7626526506	6.0257146409	6.0655040964
H8	-0.1194528706	6.8502196511	5.7869497479
C9	-1.6748327706	5.9817704361	7.1585134665
H10	-1.8317915825	6.7696977151	7.8837397365
C11	-2.2992297442	4.6997678739	7.1675648753
H12	-3.0085462586	4.3424541667	7.9035429709
C13	-1.7829314890	3.9469287124	6.0723680888

H14	-2.0220873323	2.9199733758	5.8261502086
C15	1.4273679496	3.3608306132	7.3919234949
C16	1.7053260007	4.6959999039	7.8289106695
H17	2.4120674013	5.3651695133	7.3547423664
C18	0.8846972330	4.9623811425	8.9625033701
H19	0.8419628827	5.8972403526	9.5061067955
C20	0.0924489617	3.8059394361	9.2243999779
H21	-0.6652536575	3.7140202129	9.9920691877
C22	0.4203880528	2.8150108185	8.2553845910
H23	-0.0478504739	1.8450442628	8.1468422163
C24	-0.3942769428	3.8720812128	1.8345420806
C25	-1.3770826801	3.3721266701	0.9503952255
H26	-2.3188482559	3.0328554865	1.3807112312
C27	-1.1711557577	3.3106982098	-0.4126688242
C28	0.0375623875	3.8675486007	-0.8842848601
H29	0.1918734166	3.8895994438	-1.9563501366
C30	0.8787425947	4.3166196918	1.3398266922
C31	2.9163312841	0.5690625530	5.4894268472
C32	3.0923790488	-0.7530350790	5.9520925215
H33	2.7854372196	-0.9762436828	6.9735659506
C34	3.6227418246	-1.7471003215	5.1530100106
C35	3.9906449435	-1.3634671663	3.8480608704
H36	4.4092786678	-2.1253417545	3.2021450136
C37	3.2889408304	0.9340421552	4.1563023325
C38	4.4397814528	6.5536139321	5.3371665673
H39	4.1854687072	7.0637078258	6.2818609388
H40	5.4507961383	6.1316600907	5.4550553465
H41	4.4901166245	7.3255601158	4.5525871309
C42	3.8487121781	-0.0831234614	3.3202357407
C43	1.0392839975	4.4011280322	-0.0812975585
C44	-0.8100231842	4.0620125145	3.1915660444
C45	2.3356705579	1.4806306903	6.4309660182
N46	2.0335826833	2.7397528904	6.2823494338
N47	-0.1008657815	4.4586440433	4.2155524439
C48	2.2721636832	5.0854755852	-0.6935771637
C49	2.1993880203	5.1489891136	-2.2274257755
H50	2.1982140434	4.1521775029	-2.6857273540
H51	1.3128477232	5.6915752856	-2.5780581491
H52	3.0808188005	5.6793707262	-2.6068927939
C53	2.3466386224	6.5367157602	-0.1737971831
H54	1.4521287431	7.0998396222	-0.4678497792
H55	2.4295655493	6.5639781741	0.9153281819
H56	3.2208780593	7.0451883100	-0.6005170986
C57	3.5641880275	4.3326212137	-0.3242389814
H58	4.4339203202	4.8482650436	-0.7525020447
H59	3.6963049897	4.2742250309	0.7573014867
H60	3.5467724294	3.3123073351	-0.7242369182
C61	4.2572547082	0.2183861079	1.8694156617
C62	3.0146942822	0.6515417028	1.0658798546
H63	2.5652727168	1.5570920073	1.4774829626
H64	3.2895000950	0.8479558289	0.0216611370

H65	2.2582112531	-0.1434151222	1.0692579882
C66	5.3298844411	1.3255841701	1.8409158170
H67	4.9648311563	2.2448159740	2.3024161076
H68	6.2314544529	1.0034520879	2.3768799993
H69	5.6150669779	1.5491127509	0.8049304890
C70	4.8517428279	-1.0097798543	1.1609311456
H71	5.1401130368	-0.7296811389	0.1406968950
H72	5.7515720268	-1.3851471294	1.6640095511
H73	4.1314593775	-1.8333791406	1.0802303117
H76	-1.8841907262	3.9138054231	3.3596468474
H77	2.1282340970	1.0347669429	7.4116156979
C80	-2.2286793343	2.7027383189	-1.3460661891
C83	-2.4758640256	1.2350072916	-0.9478345780
H84	-2.8313090114	1.1500501819	0.0856979263
H85	-3.2332095493	0.7800212023	-1.6002259990
H86	-1.5545065247	0.6463689994	-1.0332774279
C86	-3.5473449470	3.4911093529	-1.2267555222
H87	-3.9434817761	3.4710842923	-0.2047239204
H88	-3.4031080576	4.5408977610	-1.5092013318
H89	-4.3129994776	3.0627026390	-1.8873027917
C89	-1.7909424569	2.7271613557	-2.8179930693
H90	-2.5684280462	2.2684195457	-3.4415039229
H91	-1.6371532974	3.7497090268	-3.1841819035
H92	-0.8644032383	2.1622359469	-2.9777859187
C92	3.7750629345	-3.1845538740	5.6730684467
C95	2.3845885983	-3.7524539101	6.0178290980
H96	1.8808255426	-3.1535426748	6.7856455412
H97	1.7391711431	-3.7699120993	5.1311303541
H98	2.4693764055	-4.7795509943	6.3975462911
C98	4.6558591214	-3.1903786826	6.9366354560
H99	4.2242023699	-2.5783861579	7.7370400332
H100	4.7681878018	-4.2120175348	7.3234024967
H101	5.6558900981	-2.7971213155	6.7176464708
C101	4.4233555305	-4.1146842011	4.6378101738
H102	4.5174836784	-5.1240503963	5.0573481551
H103	3.8218074955	-4.1937915367	3.7238936701
H104	5.4293357860	-3.7781885924	4.3584816299

Fe(III)

Y1	2.3187858589	4.0946825017	4.2094523611
Fe2	-0.2574628345	4.5462663039	7.3724110805
O3	1.8013587561	4.6469533810	2.1677948263
O4	3.0977718807	2.1248897760	3.7530338102
O5	3.3754644362	5.5881569573	5.1058906862
C6	-0.8712153581	4.8381494694	5.3154362088
C7	-0.7234776383	6.0751627778	6.0186735545
H8	-0.0455757487	6.8692215209	5.7316256090
C9	-1.6203082655	6.0758474740	7.1268651443
H10	-1.7532779691	6.8856768882	7.8330133089
C11	-2.2920367943	4.8176452690	7.1495987232

H12	-3.0265662354	4.4970161755	7.8777784579
C13	-1.8149377143	4.0460648656	6.0472841665
H14	-2.0963409150	3.0276323195	5.8092807706
C15	1.5045591180	3.3092515761	7.4266136531
C16	1.7600968453	4.6660080752	7.8161937401
H17	2.4538312242	5.3216866002	7.3018145761
C18	0.9673973202	4.9557266195	8.9686459367
H19	0.9588937197	5.8914741492	9.5126691271
C20	0.1817927808	3.8038419956	9.2664940346
H21	-0.5480756428	3.7150116373	10.0616773211
C22	0.4895758143	2.8015414480	8.3048737274
H23	0.0091611206	1.8346186477	8.2204409285
C24	-0.3964086356	3.8078849319	1.8371758724
C25	-1.3719444216	3.2874012970	0.9414790960
H26	-2.3044426861	2.9173603030	1.3645764738
C27	-1.1610189421	3.2514318379	-0.4161011684
C28	0.0393643963	3.8490105932	-0.8806436140
H29	0.1895634122	3.8868862146	-1.9522110711
C30	0.8689560793	4.2913863701	1.3373110343
C31	2.8387846567	0.5138085510	5.4750392954
C32	2.9899797072	-0.8256445693	5.9255234765
H33	2.6667612841	-1.0608978210	6.9384235748
C34	3.5169734374	-1.8067801882	5.1208914000
C35	3.9179753834	-1.4016718122	3.8235803675
H36	4.3393822270	-2.1615152611	3.1781187418
C37	3.2507018496	0.8945307741	4.1485303127
C38	4.3203678172	6.5709130310	5.4108856882
H39	4.0883023809	7.0580226108	6.3716780595
H40	5.3300994420	6.1436766697	5.4916094051
H41	4.3421192961	7.3544346587	4.6402707405
C42	3.8168538274	-0.1152464044	3.3079832903
C43	1.0296577269	4.4009436508	-0.0805189793
C44	-0.8174696221	4.0057627279	3.1724785761
C45	2.2958077732	1.4146607842	6.4167208510
N46	2.0369845117	2.7071660613	6.2986059008
N47	-0.1226215774	4.4786379863	4.2004494323
C48	2.2461767047	5.1179778493	-0.6883766038
C49	2.1649154741	5.1894681298	-2.2213584052
H50	2.1877834222	4.1969270241	-2.6877376051
H51	1.2660692213	5.7150448019	-2.5655770156
H52	3.0314853053	5.7430247383	-2.5998453978
C53	2.2891543115	6.5669975592	-0.1588213484
H54	1.3802446537	7.1117342376	-0.4416847119
H55	2.3854279945	6.5964980909	0.9293674522
H56	3.1458980749	7.0967749991	-0.5926302574
C57	3.5549104339	4.3887928893	-0.3304051439
H58	4.4082222345	4.9238159506	-0.7652360757
H59	3.7044205164	4.3299125260	0.7493542743
H60	3.5565960337	3.3704524380	-0.7349662890
C61	4.2759038106	0.1991753676	1.8754760129
C62	3.0671743770	0.6697986346	1.0421876615

H63	2.6279976534	1.5852669373	1.4439714929
H64	3.3790555064	0.8658818169	0.0092779636
H65	2.2909154432	-0.1049621553	1.0146439071
C66	5.3748664126	1.2806459010	1.8959552870
H67	5.0202402059	2.2099786058	2.3459838780
H68	6.2489687940	0.9350343081	2.4609883447
H69	5.7030404517	1.4999123647	0.8727518418
C70	4.8631118071	-1.0342219796	1.1704384165
H71	5.1844078345	-0.7499964563	0.1620881284
H72	5.7421897205	-1.4326817002	1.6911997722
H73	4.1286601789	-1.8413025086	1.0593396888
H76	-1.8851889332	3.8226627308	3.3412732267
H77	2.0986670839	0.9651448907	7.3969041953
C80	-2.2020533653	2.6360142636	-1.3661797726
C83	-2.4365272121	1.1628923917	-0.9747840604
H84	-2.8052688396	1.0673648070	0.0535385379
H85	-3.1818054897	0.7058696620	-1.6379829262
H86	-1.5102934501	0.5806774947	-1.0545873792
C86	-3.5277546241	3.4155255491	-1.2532057729
H87	-3.9370638161	3.3817735019	-0.2364096732
H88	-3.3909993369	4.4689026746	-1.5258105486
H89	-4.2809219346	2.9868523066	-1.9262386285
C89	-1.7485702735	2.6727103610	-2.8331365718
H90	-2.5167298621	2.2127838190	-3.4659968831
H91	-1.6008823416	3.6979205714	-3.1942175344
H92	-0.8182877662	2.1128928005	-2.9899094541
C92	3.6468772509	-3.2562407154	5.6176901180
C95	2.2458766608	-3.7937666175	5.9734413884
H96	1.7698999058	-3.1977415309	6.7615403671
H97	1.5848124992	-3.7827343053	5.0981059523
H98	2.3128548212	-4.8280513541	6.3337963752
C98	4.5461500354	-3.2925555151	6.8699915363
H99	4.1349041446	-2.6896305419	7.6883014239
H100	4.6459649289	-4.3213699396	7.2377738422
H101	5.5507302312	-2.9141248164	6.6461675392
C101	4.2618807542	-4.1844962040	4.5598108904
H102	4.3429910550	-5.1997331374	4.9656164541
H103	3.6449482618	-4.2453084404	3.6547150964
H104	5.2710643908	-3.8665594468	4.2704895565

L4_Zr_1c

Fe(II)

Zr1	5.0232051572	11.1555262632	4.3493071581
Fe2	2.2179973471	8.4043087228	5.6177194183
N3	2.6685587303	11.4081349003	4.7926391800
N4	5.0238531099	9.4952925972	6.0289258441
O5	4.5290162340	12.9492890632	3.4139181930
O6	5.3591809240	12.2495815665	6.1836875094
O7	4.6080211211	9.8802763184	2.8844446710

O8	6.9471406664	11.1642354842	4.0325885055
C9	3.7391760141	13.9753579220	3.6170303943
C10	3.9619080419	15.2274994773	2.9620431029
C11	3.1374300635	16.2895197857	3.3116865515
H12	3.3265799681	17.2498098612	2.8425842154
C13	2.0572370687	16.2147057663	4.2197650059
C14	1.7882740623	14.9703140574	4.7494929889
H15	0.9341037432	14.8179310193	5.4042800164
C16	2.5993511039	13.8491809201	4.4610523757
C17	5.0414115906	15.3745408775	1.8769073157
C18	4.7347200725	14.3859802219	0.7314311126
H19	3.7539142962	14.5982089904	0.2879411445
H20	4.7367486206	13.3525737986	1.0861409593
H21	5.4901447781	14.4808521798	-0.0594058559
C22	6.4463339492	15.0956704058	2.4449209647
H23	7.1946090119	15.1951261029	1.6474633528
H24	6.5190216419	14.0892445301	2.8607213291
H25	6.6982648877	15.8149517619	3.2329899159
C26	5.0627992451	16.7875609694	1.2731539612
H27	5.8298460919	16.8322895661	0.4909217772
H28	5.3127303817	17.5528504542	2.0185227524
H29	4.1056940921	17.0556444332	0.8089111373
C30	2.1017160526	12.5752612067	4.8950539960
C31	6.1639070539	12.0487055375	7.1881388663
C32	6.7045655227	13.1308618608	7.9641966652
C33	7.5974192006	12.8173363697	8.9781895915
H34	8.0286649350	13.6395184540	9.5404690878
C35	7.9841069317	11.5068435158	9.3513304131
C36	7.3912569532	10.4766932134	8.6584628869
H37	7.5954586066	9.4408176577	8.9157766191
C38	6.4959608276	10.7178026715	7.5893526071
C39	6.3077582941	14.5864930988	7.6733959068
C40	4.7810669469	14.7418446551	7.8282129225
H41	4.4846661912	15.7766268770	7.6135171684
H42	4.4702917652	14.5068363121	8.8542224863
H43	4.2446980707	14.0835455798	7.1421506170
C44	6.7331491166	14.9752722122	6.2449685938
H45	6.2569555325	14.3364441920	5.5000211672
H46	7.8211860791	14.8939275723	6.1278603014
H47	6.4485922447	16.0151803836	6.0381283641
C48	6.9731384868	15.5789713444	8.6400483478
H49	8.0673451161	15.5672176728	8.5599955494
H50	6.7002404615	15.3877385345	9.6852191868
H51	6.6402654990	16.5946143251	8.3951893423
C52	5.8003334193	9.5818617558	7.0793211296
C53	1.7972881436	10.3166776917	5.0478766337
C54	1.3613864644	9.3868989734	4.0515476639
H55	1.7322692680	9.3553386749	3.0364214434
C56	0.4156948362	8.5104893701	4.6576880980
H57	-0.0723678254	7.6743316847	4.1735356191
C58	0.2710579567	8.8860825312	6.0263290811

H59	-0.3457845392	8.3861934965	6.7625874897
C60	1.1205570198	10.0055283039	6.2706809448
H61	1.2703332022	10.5114193142	7.2160650272
C62	4.2058803754	8.3430303838	6.0021540336
C63	3.8961677308	7.5343572403	4.8633570892
H64	4.2571668420	7.7130794391	3.8624904584
C65	2.9762927580	6.5306175514	5.2805379066
H66	2.5220423933	5.7859625843	4.6391071361
C67	2.7088068693	6.7125051426	6.6697971727
H68	2.0161190990	6.1331057530	7.2664820398
C69	3.4685130014	7.8281265630	7.1221912191
H70	3.4475750819	8.2624639083	8.1137735321
C71	5.0586018531	9.2266867928	1.7432137817
H72	4.8453412666	8.1458490885	1.7906942521
H73	4.5571033847	9.6213124988	0.8468060657
H74	6.1443371997	9.3504660767	1.6121759010
C75	8.3177206637	11.3695674887	3.9522117572
H76	8.8504414564	10.4084777127	3.9101646797
H77	8.5713307724	11.9400809680	3.0471427606
H78	8.6835931442	11.9277757259	4.8254545880
H81	1.0783643473	12.5998096188	5.2886341659
H82	5.8891189656	8.6784658644	7.6928830716
C85	1.2330054147	17.4703704308	4.5346899165
C88	0.1231373831	17.1892385951	5.5573127905
H89	-0.5930738672	16.4446692593	5.1883472822
H90	0.5301838345	16.8320755683	6.5109925680
H91	-0.4365406589	18.1102334117	5.7606748479
C91	2.1583407696	18.5577900144	5.1180058389
H92	2.6263325481	18.2159410852	6.0490386160
H93	2.9605042648	18.8275040012	4.4214860422
H94	1.5887170110	19.4702222616	5.3381858758
C94	0.5719923655	17.9987340988	3.2453375045
H95	-0.0180712338	18.8998508661	3.4578093598
H96	1.3135915381	18.2615745518	2.4825698588
H97	-0.0994859876	17.2471704726	2.8129412375
C97	8.9883668613	11.2962816142	10.4918123578
C100	8.4377251177	11.9172916845	11.7912604427
H101	8.2555480002	12.9927770033	11.6853370139
H102	7.4905873723	11.4453514356	12.0796347683
H103	9.1507222520	11.7809818705	12.6148755020
C103	10.3269453473	11.9696742055	10.1271976474
H104	10.2091367791	13.0459811047	9.9575559054
H105	11.0576453767	11.8381238772	10.9359748665
H106	10.7480434209	11.5322281393	9.2139112279
C106	9.2591014541	9.8073932341	10.7523195046
H107	9.9884527597	9.6977469661	11.5638720381
H108	8.3487311588	9.2752432327	11.0541080773
H109	9.6718382901	9.3091141366	9.8668852481

Fe(III)

Zr1	5.0748720022	11.1971183156	4.4113168520
Fe2	2.2365896695	8.3751175376	5.5356837598
N3	2.6801424219	11.4201444288	4.8513314968
N4	5.0173894298	9.5057290280	6.1271420903
O5	4.5318269929	12.9664428207	3.5044446595
O6	5.4133071656	12.2446426409	6.2519895874
O7	4.4995836147	9.8520511444	3.0386995271
O8	6.9569190979	11.1316052728	3.9880952340
C9	3.7392400079	13.9919934090	3.7084763216
C10	3.9321597686	15.2291375555	3.0226807410
C11	3.1047905096	16.2861280650	3.3798942641
H12	3.2716359327	17.2390847636	2.8892386906
C13	2.0444070408	16.2216742199	4.3168795077
C14	1.7990339745	14.9894996195	4.8769928268
H15	0.9617587476	14.8425329437	5.5535572801
C16	2.6173888315	13.8670992345	4.5847752115
C17	4.9751032413	15.3713698413	1.9011362896
C18	4.6418511924	14.3627829972	0.7806690148
H19	3.6445629602	14.5560706274	0.3670079379
H20	4.6713119519	13.3322651259	1.1431771696
H21	5.3677095736	14.4591907026	-0.0360280675
C22	6.4002314671	15.1202087893	2.4292283627
H23	7.1204819498	15.2252144162	1.6082858697
H24	6.5071717934	14.1188930475	2.8505305948
H25	6.6655756312	15.8513792931	3.2012972296
C26	4.9579822596	16.7753667532	1.2760532508
H27	5.7062947763	16.8204995900	0.4768621404
H28	5.2121066815	17.5569751713	2.0024043824
H29	3.9879916946	17.0194281700	0.8262992477
C30	2.1244874737	12.6024221363	5.0067411749
C31	6.1186146045	12.0648279447	7.3295582747
C32	6.6530380259	13.1558345138	8.0920847269
C33	7.4333702222	12.8399274037	9.1927043571
H34	7.8637547742	13.6646338787	9.7508757812
C35	7.7164803888	11.5289352190	9.6642902320
C36	7.1391079729	10.4963619632	8.9713732481
H37	7.2786063677	9.4655073983	9.2850797138
C38	6.3478063886	10.7338759737	7.8126616313
C39	6.3809973407	14.6156663060	7.6996042372
C40	4.8616632165	14.8799473972	7.7238261749
H41	4.6595700517	15.9206219400	7.4423657984
H42	4.4552155816	14.7200592830	8.7303647724
H43	4.3285190543	14.2307524035	7.0262455469
C44	6.9489114945	14.8984701508	6.2955195259
H45	6.4858549461	14.2657971952	5.5367760502
H46	8.0328374994	14.7317518406	6.2727616472
H47	6.7661111493	15.9455789166	6.0244889593
C48	7.0369617961	15.6078833682	8.6716988496
H49	8.1305733377	15.5246517256	8.6775933492
H50	6.6722590006	15.4865939888	9.6989855042
H51	6.7923962626	16.6291059092	8.3583737051

C52	5.7058225319	9.6111594211	7.2563174497
C53	1.7902451099	10.3503442908	5.0000275051
C54	1.3976565060	9.4736947955	3.9368585057
H55	1.8286122647	9.4940124879	2.9446776999
C56	0.4157106739	8.5787855248	4.4324165928
H57	-0.0517108569	7.7788694010	3.8713422021
C58	0.2148686206	8.8536228157	5.8116692393
H59	-0.4472657713	8.3139400426	6.4776770618
C60	1.0677967850	9.9417860559	6.1756235301
H61	1.1537067728	10.3931707497	7.1561308459
C62	4.2740690517	8.3324667411	6.0265726557
C63	4.0724986273	7.5443721814	4.8529695428
H64	4.4853270831	7.7840396137	3.8847280233
C65	3.1674283237	6.4989972107	5.1630065714
H66	2.7962408063	5.7611940387	4.4623735554
C67	2.7786718824	6.6238172728	6.5255016508
H68	2.0799180910	5.9850341158	7.0507123423
C69	3.4465219543	7.7630592250	7.0664136718
H70	3.3498898371	8.1456841092	8.0749431538
C71	4.9528095870	9.3401482928	1.8152105688
H72	4.8476098798	8.2427464292	1.7806084505
H73	4.3648920515	9.7533745896	0.9837288593
H74	6.0107373790	9.5809997448	1.6422905775
C75	8.3312501868	11.2196521158	3.7561761434
H76	8.7433273930	10.2280235677	3.5295586970
H77	8.5306930118	11.8837337705	2.9060356326
H78	8.8420968039	11.6187697070	4.6411856451
H81	1.1081397265	12.6283647919	5.4178662479
H82	5.7860610927	8.6995147392	7.8577579046
C85	8.6161576375	11.3339428968	10.8905287007
C88	10.0087624802	11.9279321180	10.5935018008
H89	9.9575968482	12.9987094545	10.3643777212
H90	10.6676980346	11.8073336403	11.4621037891
H91	10.4777141850	11.4244607564	9.7396004772
C91	7.9965720429	12.0504622612	12.1076658467
H92	7.8855187888	13.1279216709	11.9411950123
H93	7.0055973610	11.6435657995	12.3427878498
H94	8.6343980533	11.9189902923	12.9901673547
C94	8.7897453161	9.8492996208	11.2435662106
H95	9.4387773139	9.7506414031	12.1209863093
H96	7.8323861267	9.3730751702	11.4900196792
H97	9.2573743269	9.2866085587	10.4261714736
C97	1.2134331927	17.4763083588	4.6162774162
C100	0.1235463555	17.2096567461	5.6641989342
H101	-0.5929634093	16.4505132022	5.3261105695
H102	0.5489307329	16.8844638402	6.6214705032
H103	-0.4420614445	18.1293784372	5.8524921418
C103	2.1424261217	18.5831162492	5.1557001217
H104	2.6266746694	18.2720718570	6.0890992162
H105	2.9305546384	18.8425124602	4.4393792759
H106	1.5683742714	19.4953829809	5.3592167058

C106	0.5291055311	17.9643799005	3.3227028883
H107	-0.0698852447	18.8607544617	3.5251737399
H108	1.2556010166	18.2238930036	2.5444374794
H109	-0.1388485370	17.1958287513	2.9153492970

L5_Y_c

Fe(II)

Y1	0.3033849334	16.7508161629	4.9574767243
Fe2	2.2219200848	12.9732761975	7.1558315858
S3	-0.8762554150	14.6321180423	6.4743831293
S4	3.1712374780	16.0139479055	5.6346731940
O5	0.4398572477	17.5281023258	6.9486314010
O6	1.1393327211	15.7048267086	3.2911726568
O7	-1.2451029694	17.7982723597	4.1805382715
C8	0.2023157281	13.2745336972	6.8321951409
C9	0.4180755927	12.6370193385	8.0916392654
H10	0.1498364907	13.0362170679	9.0592539466
C11	1.0960475291	11.4092416685	7.8433227546
H12	1.4403534297	10.7167640904	8.6008793713
C13	1.3048544910	11.2902566419	6.4395004263
H14	1.8314077745	10.4888356985	5.9378207584
C15	0.7652850623	12.4472904569	5.8086899221
H16	0.7893639573	12.6709680757	4.7494402894
C17	3.4380537434	14.5615392872	6.6108875500
C18	4.0126065955	13.3168802097	6.2094408063
H19	4.2216783089	13.0136406496	5.1938470082
C20	4.2038260471	12.5310713174	7.3834284062
H21	4.5905485976	11.5198173605	7.4066949248
C22	3.7339934395	13.2782901931	8.5007617233
H23	3.7006872020	12.9383135544	9.5279120469
C24	3.2502028257	14.5312660024	8.0283940239
H25	2.8114906535	15.3193227175	8.6264499730
C26	-1.1757498396	15.5447301425	8.0626829335
H27	-1.8810013678	16.3086681839	7.7097446382
H28	-1.7322925769	14.8528353518	8.7022798562
C29	-0.0404294139	16.1711039333	8.8102722582
C30	0.1983966080	15.7780258148	10.1234954024
H31	-0.4014533808	14.9678826428	10.5377848408
C32	1.1535497270	16.4161623438	10.9214896059
C33	1.8274694967	17.4879995109	10.3331723406
H34	2.5546462884	18.0230653753	10.9352109450
C35	1.6298554304	17.9402063545	9.0172705291
C36	0.6901027011	17.2398567161	8.2158815251
C37	3.8598400747	15.6417770460	3.9672101627
H38	3.7841094552	16.6307516046	3.4942409714
H39	4.9252573263	15.4300657860	4.1033116643
C40	3.2120918554	14.5931346895	3.1121762204
C41	4.0019735520	13.5712480779	2.5943689532
H42	5.0546895971	13.5404817378	2.8760011714

C43	3.4855774253	12.6119088342	1.7182174863
C44	2.1371702591	12.7448498459	1.3857088135
H45	1.7137473257	12.0297633950	0.6893750879
C46	1.2834919389	13.7479147201	1.8747294040
C47	1.8375698220	14.7047923480	2.7675714324
C48	-2.2672739384	18.5734930797	3.6495966029
H49	-3.0747823295	17.9425977772	3.2472964551
H50	-2.7059182714	19.2365082551	4.4120031313
H51	-1.9004286466	19.2065970743	2.8264992521
C54	2.4311625657	19.1920812404	8.5919312414
C55	2.0361055522	20.3632594340	9.5187203952
H56	2.2345203606	20.1443414156	10.5734152730
H57	2.6033996348	21.2649941197	9.2537420287
H58	0.9685233951	20.5936156753	9.4206458798
C59	2.1998781692	19.6738608723	7.1496964966
H60	1.1480114493	19.8892284725	6.9485039389
H61	2.7776913747	20.5949196063	6.9949477324
H62	2.5495208977	18.9386626692	6.4184270239
C63	3.9422934241	18.9154066791	8.7377255449
H64	4.5189473370	19.8047053845	8.4517646733
H65	4.2240037234	18.6571123280	9.7643909479
H66	4.2507435568	18.0892849428	8.0863584811
C67	1.3858307838	15.9622509357	12.3697820209
C68	2.4930123546	16.7670225366	13.0647143488
H69	3.4533248366	16.6738904609	12.5434263406
H70	2.2420161705	17.8321120334	13.1337179540
H71	2.6341013766	16.3962733953	14.0872846545
C72	0.0858338007	16.1398240154	13.1789140721
H73	-0.2268134523	17.1904645500	13.1889285634
H74	-0.7376981841	15.5511587567	12.7589866040
H75	0.2296856327	15.8168211571	14.2183185059
C76	1.7949810122	14.4761136580	12.3913324438
H77	1.9520319599	14.1336569564	13.4224925554
H78	1.0272329096	13.8350171469	11.9431271901
H79	2.7281357816	14.3199870065	11.8367760786
C80	-0.1609561436	13.7592442805	1.3206845560
C81	-1.1477634355	14.6857858720	2.0499817218
H82	-1.2623196981	14.4102633555	3.1050886531
H83	-0.8547750866	15.7350112108	2.0004857160
H84	-2.1350476906	14.5824847627	1.5800724483
C85	-0.1008642996	14.2125797624	-0.1535607980
H86	0.3058870504	15.2277020132	-0.2314021320
H87	0.5337518703	13.5506965082	-0.7540230984
H88	-1.1052028568	14.2135739713	-0.5977674319
C89	-0.7705191883	12.3418802875	1.3858522964
H90	-1.8008592076	12.3640430338	1.0095838199
H91	-0.2242018005	11.6088611623	0.7836951114
H92	-0.7988765522	11.9729299374	2.4182910603
C93	4.3863395840	11.4936139480	1.1732536534
C94	3.6348433313	10.5471409482	0.2272952816
H95	2.8014781964	10.0448428713	0.7325796889

H96	3.2379804812	11.0748269477	-0.6481590885
H97	4.3166874157	9.7695703693	-0.1380819392
C98	5.5663873108	12.1091530879	0.3959700158
H99	5.2075360689	12.7028892992	-0.4529073543
H100	6.1729103750	12.7660364944	1.0294866725
H101	6.2254061165	11.3219661546	0.0068094101
C102	4.9342128121	10.6563192577	2.3467580911
H103	5.5818981955	9.8500292654	1.9781687884
H104	5.5262055114	11.2653973391	3.0396849854
H105	4.1154933458	10.1999395512	2.9163119061

Fe(III)

Y1	0.2607033315	16.8758059999	4.8990520416
Fe2	2.2578378921	12.9942463908	7.1382999815
S3	-0.9010739813	14.6558108207	6.4312298643
S4	3.3137573191	16.0495709555	5.6151965188
O5	0.4241410263	17.4611402554	6.9333418956
O6	1.2001269989	15.6993133784	3.3992986055
O7	-1.3359594611	17.8318436113	4.1595142850
C8	0.1149059947	13.2800287528	6.8026019575
C9	0.3464438197	12.6729749606	8.0696783060
H10	0.0689630767	13.0871017811	9.0289591426
C11	1.0360963159	11.4484050959	7.8567982248
H12	1.3552715519	10.7662301380	8.6348421987
C13	1.2772735501	11.3112635638	6.4611333751
H14	1.7933140375	10.4924361382	5.9765394947
C15	0.7427440084	12.4623586184	5.8057565345
H16	0.7757096421	12.6667654823	4.7416277015
C17	3.6092170881	14.6260051906	6.5698558251
C18	4.1209666316	13.3549510072	6.1729500224
H19	4.3314189163	13.0509454393	5.1561709407
C20	4.2741221029	12.5536156821	7.3406928026
H21	4.6529295894	11.5389932871	7.3591953846
C22	3.8033208196	13.3014209120	8.4575741829
H23	3.7706580666	12.9678630249	9.4870628164
C24	3.3471223096	14.5666090354	7.9802983390
H25	2.9184208776	15.3646902546	8.5765529957
C26	-1.2233463196	15.5323951097	8.0417852664
H27	-1.9019038830	16.3184520875	7.6860273002
H28	-1.8092595749	14.8413755891	8.6551692431
C29	-0.0670676948	16.1075025801	8.7909026568
C30	0.1611286377	15.6992639758	10.1040925068
H31	-0.4754208143	14.9221707857	10.5271840798
C32	1.1275630134	16.3192825780	10.9028349991
C33	1.8344359041	17.3678645731	10.3089073843
H34	2.5685202846	17.8874935300	10.9148299502
C35	1.6488115178	17.8339784596	8.9949056535
C36	0.6856639218	17.1616010084	8.1992718580
C37	3.9395864010	15.6753961783	3.9179186575
H38	3.8083596328	16.6595472878	3.4480843603

H39	5.0161829142	15.4992389138	4.0060667850
C40	3.2664714909	14.5990426894	3.1262514521
C41	4.0471596001	13.5766176024	2.5919360137
H42	5.1154625746	13.5708996117	2.8094046919
C43	3.5000128390	12.5981150919	1.7575020234
C44	2.1356966794	12.7148610241	1.4877043687
H45	1.6896992129	11.9862465868	0.8202209700
C46	1.2925967066	13.7221880214	1.9900186379
C47	1.8768508746	14.6939802765	2.8459486262
C48	-2.3979630268	18.5716120490	3.6330356599
H49	-3.1894009424	17.9049881143	3.2644985987
H50	-2.8313098030	19.2333944714	4.3957151432
H51	-2.0593424679	19.1928260633	2.7924430431
C54	2.4572640571	19.0889497077	8.5909852431
C55	2.0323984625	20.2519407190	9.5149452148
H56	2.2162713605	20.0320916582	10.5715926617
H57	2.5949093550	21.1589708359	9.2627834136
H58	0.9651828819	20.4724208966	9.3996086427
C59	2.2552243122	19.5766662756	7.1462394661
H60	1.2086735280	19.8010250500	6.9277904205
H61	2.8378267034	20.4951564139	7.0050393698
H62	2.6206416352	18.8459535908	6.4166851862
C63	3.9663583476	18.8225436896	8.7743402253
H64	4.5405172230	19.7229510810	8.5241633705
H65	4.2251813281	18.5476230649	9.8023198173
H66	4.3081256183	18.0164590605	8.1132165069
C67	1.3137123390	15.9042349878	12.3696035123
C68	2.4684211854	16.6556659637	13.0468741818
H69	3.4245642287	16.4875857506	12.5364882740
H70	2.2862909267	17.7355402810	13.0887739485
H71	2.5802230830	16.3064712514	14.0794646763
C72	0.0182906208	16.2100262172	13.1477834679
H73	-0.2182191308	17.2790954764	13.1076317273
H74	-0.8406473403	15.6623176522	12.7436984702
H75	0.1276567066	15.9261274658	14.2015438946
C76	1.6105177153	14.3948732272	12.4549305952
H77	1.7196690142	14.0834314253	13.5004638001
H78	0.8057712979	13.7915770200	12.0182443275
H79	2.5442533626	14.1489158916	11.9336100848
C80	-0.1622076018	13.7236908115	1.4639923771
C81	-1.1146858448	14.7166471868	2.1486494032
H82	-1.2121668589	14.5186160379	3.2236186956
H83	-0.8075141182	15.7543024757	2.0115259096
H84	-2.1142386965	14.6016524905	1.7120961891
C85	-0.1183453605	14.0877126446	-0.0358975239
H86	0.3133351035	15.0842883595	-0.1826260081
H87	0.4829445296	13.3748196908	-0.6102618719
H88	-1.1306804144	14.0910096476	-0.4586907459
C89	-0.7950258956	12.3249747323	1.6242772975
H90	-1.8207649267	12.3354993236	1.2371330493
H91	-0.2562518357	11.5420226120	1.0820310380

H92	-0.8433392765	12.0287367397	2.6799613471
C93	4.3884447412	11.4921309037	1.1710252457
C94	3.6000989797	10.5225125789	0.2800100267
H95	2.7989547738	10.0176170677	0.8329410270
H96	3.1563430594	11.0291129632	-0.5847055822
H97	4.2715182214	9.7473219200	-0.1059792877
C98	5.5084260850	12.1259520670	0.3228311454
H99	5.0908105881	12.7062138684	-0.5075592363
H100	6.1421815351	12.7965717279	0.9141295610
H101	6.1550432773	11.3470080940	-0.0991482117
C102	5.0191586154	10.6797459138	2.3195606205
H103	5.6599820881	9.8837707131	1.9218753029
H104	5.6418336230	11.3054207805	2.9702414977
H105	4.2441296282	10.2090308585	2.9373651053

L5_Zr_c

Fe(II)

Zr1	10.1352798640	0.4776890772	4.8470245942
Fe2	11.1957799058	4.4451147954	7.0947152785
S3	12.4126010086	1.2025189714	6.5075404018
S4	8.6090135296	2.8823423465	5.3076746128
O5	8.4548241556	-0.0519184014	4.0522108326
O6	11.3514166030	-0.9436453917	4.3611438126
O7	10.7413602689	1.9522535993	3.5056109603
O8	9.7280934084	0.0898249076	6.8342636168
C9	10.4185259084	0.0313113093	7.9675626226
C10	9.8845976435	-0.5584504434	9.1440988902
C11	10.6960954541	-0.5840980644	10.2824829326
H12	10.2859792714	-1.0336293032	11.1781546566
C13	12.0072547422	-0.0901762679	10.3373292602
C14	12.5183619320	0.4651556287	9.1650998968
H15	13.5437218348	0.8249270304	9.1198429122
C16	11.7314017892	0.5536675228	8.0181927155
C17	8.4723069137	-1.1682659890	9.1488583919
C18	8.0945502559	-1.7491153275	10.5201928300
H19	7.0768375542	-2.1543945672	10.4704558630
H20	8.1059501370	-0.9869315919	11.3090359270
H21	8.7581333618	-2.5687597635	10.8211057776
C22	8.3979867553	-2.3147470926	8.1188799658
H23	8.6166861273	-1.9572234807	7.1100556599
H24	7.3922039384	-2.7548318589	8.1182290463
H25	9.1133994110	-3.1081346521	8.3680366341
C26	7.4295119862	-0.0857609133	8.8027448548
H27	7.6233572033	0.3536447591	7.8216873819
H28	7.4386747568	0.7154441822	9.5526874662
H29	6.4220343904	-0.5215644166	8.7919532877
C30	12.8778069768	-0.1658467226	11.6002113629
C31	12.1188071550	-0.7600133528	12.7952132034
H32	11.2319455309	-0.1671049157	13.0499252639

H33	12.7713018101	-0.7741771073	13.6766271486
H34	11.7997595761	-1.7914346750	12.6058142283
C35	14.1085728455	-1.0504761721	11.3224928009
H36	13.8045835582	-2.0693054535	11.0549857208
H37	14.7496424292	-1.1082650293	12.2119238777
H38	14.7143862692	-0.6562632656	10.4988364412
C39	13.3442536588	1.2509477430	11.9912704951
H40	13.9429577648	1.7162085730	11.2001379789
H41	13.9637493286	1.2176432268	12.8966288918
H42	12.4856624190	1.9030917797	12.1918647707
C43	9.2834707116	4.0280727049	6.4860124626
C44	9.4448793344	3.7095220495	7.8697391817
H45	9.3284141981	2.7286417300	8.3103716804
C46	9.8227671134	4.9051314042	8.5462351409
H47	10.0580791763	4.9852833684	9.5997251412
C48	9.9013498740	5.9540731931	7.5860528527
H49	10.2087437603	6.9738678546	7.7799439857
C50	9.5696936913	5.4154510416	6.3082252472
H51	9.5657218898	5.9416964138	5.3634774000
C52	12.5559778090	2.9535861229	6.7704210951
C53	12.8713892911	3.6563435082	7.9733852642
H54	12.8936508891	3.2295647347	8.9665805820
C55	13.0865441613	5.0228070420	7.6302088114
H56	13.2985087076	5.8227587795	8.3282937888
C57	12.9101528284	5.1632863689	6.2236014830
H58	12.9660173159	6.0874882984	5.6629585300
C59	12.5785798995	3.8868300111	5.6876847153
H60	12.3462904708	3.6543841508	4.6578657880
C61	9.0275906427	3.5872007382	3.7316550147
C62	10.0722359375	2.9858088874	2.9955686295
C63	10.3674107549	3.5119171884	1.7040274117
C64	9.6006640479	4.5875836971	1.2563823146
H65	9.8235587183	4.9902186791	0.2735007997
C66	8.5469366889	5.1799166371	1.9746355162
C67	8.2674198926	4.6463179398	3.2268980471
H68	7.4551174757	5.0306217522	3.8357623128
C69	11.4720779152	2.8980169643	0.8258929466
C70	12.8327249722	2.9767700549	1.5464665822
H71	13.6193593665	2.5426438362	0.9158242643
H72	12.8121947055	2.4284656304	2.4906527559
H73	13.1051963144	4.0198557916	1.7504585405
C74	11.1320095776	1.4254602223	0.5161080679
H75	10.1794003216	1.3506839913	-0.0226862614
H76	11.0583075532	0.8352662519	1.4318214805
H77	11.9128100494	0.9838435741	-0.1168115609
C78	11.6170207986	3.6306506041	-0.5167917765
H79	12.4138360629	3.1555311650	-1.1012524157
H80	11.8899975313	4.6848163506	-0.3855151948
H81	10.6994096856	3.5820801907	-1.1158464729
C82	7.7580074882	6.3448490682	1.3590019981
C83	6.6207450793	6.8193062744	2.2733571742

H84	6.0874492409	7.6522879310	1.7998731381
H85	6.9940834514	7.1749931663	3.2412451317
H86	5.8907064022	6.0223866015	2.4584560431
C87	7.1381613659	5.8991766552	0.0193207638
H88	6.5725658757	6.7229756187	-0.4347267887
H89	6.4524870652	5.0565231229	0.1668421532
H90	7.9017443704	5.5856520411	-0.7009140153
C91	8.7058442437	7.5344290960	1.1101043284
H92	9.5246201721	7.2679978604	0.4323014387
H93	9.1506612634	7.8836525615	2.0496246523
H94	8.1599214385	8.3732737747	0.6594270708
C96	12.2210390874	-1.9442246345	3.9422307141
H97	11.7617347304	-2.9322233916	4.0789829141
H98	12.4703259843	-1.8176084040	2.8805614491
H99	13.1510562535	-1.9093576658	4.5249975853
C99	7.4065775876	-0.5232209392	3.2686952512
H100	6.4801637530	-0.5613926779	3.8562761324
H101	7.2459306719	0.1365660726	2.4060539410
H102	7.6264187661	-1.5336326985	2.8974706579

Fe(III)

Zr1	10.1350972635	0.2745882097	4.7130996153
Fe2	11.1495552290	4.3093831211	7.0379608396
S3	12.4890017656	1.0818887352	6.3901833284
S4	8.4710005157	2.6748016423	5.2994388597
O5	8.4254576520	-0.2057236502	3.9861759445
O6	11.3875691404	-1.0878544274	4.1983665681
O7	10.6665991696	1.9040527971	3.5414995696
O8	9.8105298085	0.0223132167	6.7308496927
C9	10.4773023114	0.0190947938	7.8844040672
C10	9.8935146112	-0.4214107201	9.1034826842
C11	10.6824431142	-0.3583366766	10.2581581594
H12	10.2308463873	-0.6814967735	11.1868451358
C13	12.0179894625	0.0699727419	10.2972148319
C14	12.5829765827	0.4658815478	9.0856509703
H15	13.6284955907	0.7593686735	9.0292994477
C16	11.8126035653	0.4825366035	7.9222079442
C17	8.4517756394	-0.9574177343	9.1521285826
C18	8.0313990184	-1.3588271118	10.5744664416
H19	7.0011050456	-1.7306955104	10.5522102360
H20	8.0560462241	-0.5114292780	11.2703824028
H21	8.6578279253	-2.1609163960	10.9814636787
C22	8.3411667268	-2.2102574649	8.2597222741
H23	8.5823978657	-1.9855703448	7.2183231867
H24	7.3194881958	-2.6070450595	8.2964015112
H25	9.0196786508	-2.9966605781	8.6099762041
C26	7.4644086253	0.1232520277	8.6682504792
H27	7.6795182994	0.4355888998	7.6435644753
H28	7.4969849140	1.0025341949	9.3249473269
H29	6.4394535283	-0.2654874342	8.6948605334

C30	12.8481846075	0.1079693525	11.5896650803
C31	12.0312228433	-0.3181678543	12.8176164558
H32	11.1653361581	0.3340953096	12.9825151687
H33	12.6591266382	-0.2617096338	13.7137158857
H34	11.6745788384	-1.3509798193	12.7345283403
C35	14.0547308264	-0.8416140743	11.4558087321
H36	13.7255621933	-1.8737364403	11.2926869680
H37	14.6602477447	-0.8192365623	12.3697595632
H38	14.7066437502	-0.5619983737	10.6205043017
C39	13.3542561904	1.5445668455	11.8307433123
H40	14.0074050128	1.8907380393	11.0203198606
H41	13.9363587563	1.5953225588	12.7583180396
H42	12.5166499913	2.2470917769	11.9222859641
C43	9.1111700819	3.8397779691	6.4519637202
C44	9.3659170072	3.5651550870	7.8330423110
H45	9.2703239038	2.5993682466	8.3121457248
C46	9.7393858468	4.7913208137	8.4646241893
H47	9.9811185318	4.9159465077	9.5125147731
C48	9.7625937954	5.8078251394	7.4679295173
H49	10.0436991145	6.8433405199	7.6143907412
C50	9.4048804571	5.2167724955	6.2254804170
H51	9.3647528414	5.7104606552	5.2636077691
C52	12.6283044429	2.8182604592	6.6787496913
C53	12.9143517368	3.4952329242	7.9027345159
H54	12.9399930427	3.0386718905	8.8827152757
C55	13.1102263673	4.8705640208	7.6150787123
H56	13.3114635338	5.6435608650	8.3467065058
C57	12.9162113000	5.0657034791	6.2207098140
H58	12.9676408967	6.0116057578	5.6963985762
C59	12.6035715808	3.8019542201	5.6374555146
H60	12.3873940232	3.6041088273	4.5962861449
C61	8.8745492198	3.4531869399	3.7563203016
C62	9.9897412457	2.9491913520	3.0534302082
C63	10.3571186789	3.6057333225	1.8424608774
C64	9.5817234172	4.6959963851	1.4453385049
H65	9.8623894356	5.2009224005	0.5280742386
C66	8.4527395859	5.1860929995	2.1288469739
C67	8.0992434645	4.5242906671	3.2977215719
H68	7.2285859771	4.8218805396	3.8739370401
C69	11.5455407946	3.1245793908	0.9908290930
C70	12.8465048013	3.1458806726	1.8170922433
H71	13.6937337094	2.8414570042	1.1913356222
H72	12.7930218972	2.4581099626	2.6644101234
H73	13.0583770669	4.1582758479	2.1853710270
C74	11.2703628571	1.6925027004	0.4909835982
H75	10.3655902746	1.6637489709	-0.1267995226
H76	11.1441238793	0.9944699899	1.3219030198
H77	12.1084993572	1.3424033399	-0.1236094682
C78	11.7738412210	4.0154013465	-0.2407936022
H79	12.6323177275	3.6346359745	-0.8049678603
H80	11.9989889864	5.0531274273	0.0337721195

H81	10.9141383880	4.0142876376	-0.9203697816
C82	7.6808591284	6.3926796083	1.5791362173
C83	6.4956442311	6.7738385240	2.4763122606
H84	5.9727906560	7.6371041358	2.0504815388
H85	6.8183183682	7.0560057307	3.4863507876
H86	5.7667412797	5.9594536626	2.5608183623
C87	7.1384373667	6.0642635297	0.1739240531
H88	6.5893761118	6.9230070758	-0.2301959266
H89	6.4543523163	5.2088167490	0.2051956277
H90	7.9422195628	5.8256148612	-0.5307566452
C91	8.6278760792	7.6062420997	1.4912490445
H92	9.4840827893	7.4137428681	0.8357808347
H93	9.0169401180	7.8760929219	2.4807007659
H94	8.0949455270	8.4766859418	1.0911915760
C96	12.1285081476	-2.1928286140	3.7610135272
H97	11.4594199768	-3.0230994149	3.5080315717
H98	12.7132714527	-1.9232239857	2.8741113282
H99	12.8142265583	-2.5170526887	4.5524337973
C99	7.2957226801	-0.6729493813	3.3027421085
H100	6.4149514569	-0.6068969999	3.9514191408
H101	7.1243738367	-0.0683335865	2.4048094249
H102	7.4405661207	-1.7179431246	3.0062207936

L6_Y_a

Fe(II)

Y1	0.2485893030	16.5701235410	5.4357942609
Fe2	2.3920932040	13.3220338373	6.8533681257
S3	3.0345910105	16.8178749824	6.4148340883
S4	-0.8201222972	13.8841332711	5.3670169888
O5	-0.9836611881	17.9949663311	4.7168210624
O7	0.2883592511	16.7962694073	7.5924757995
O8	1.0885608856	15.5196210705	3.7220967395
C9	-1.7496812090	19.0227024749	4.1767997774
C10	1.2150423003	17.1530899022	8.4560881223
C11	0.8892206266	17.5015945916	9.7834038943
C12	1.8709637665	17.9046950622	10.6779463952
H13	1.5849945405	18.1741084769	11.6924770951
C14	3.2140962399	17.9830008097	10.2942191955
C15	3.5643668806	17.6426975989	8.9927305453
H16	4.5979383560	17.7092706494	8.6612884686
C17	2.5852802176	17.2173414985	8.0900715813
C18	3.4347012811	15.0794141445	6.4840641212
C19	4.0028948236	14.3685400180	7.5837552563
H20	4.0905200671	14.7411130377	8.5953846892
C21	4.4025349051	13.0869226855	7.1051819719
H22	4.8334653086	12.2961979791	7.7062042708
C23	4.0726461423	13.0044030181	5.7207263515
H24	4.2099129258	12.1415706891	5.0816847608
C25	3.4654540807	14.2310571010	5.3341174304

H26	3.0798385549	14.4903279215	4.3583006519
C27	0.3608231379	13.1354315160	6.4777733767
C28	0.5808628202	13.5954309367	7.8148110685
H29	0.2195523010	14.5281770974	8.2277111590
C30	1.3657081314	12.6145777178	8.4814458307
H31	1.7329221857	12.6869529701	9.4970494527
C32	1.6389604220	11.5607190114	7.5611831622
H33	2.2536844344	10.6904675032	7.7531332373
C34	1.0216343300	11.8806471467	6.3177052451
H35	1.0608341137	11.3021099965	5.4044821793
C36	0.6746318276	14.4320061072	3.1106716432
C37	-0.2150789063	13.5145084270	3.7323035962
C38	-0.6723844823	12.3707726761	3.0709978279
H39	-1.3744761624	11.7110720374	3.5754168701
C40	-0.2348753122	12.0875283103	1.7825219572
C41	0.6542041125	12.9702361914	1.1598770119
H42	0.9979943899	12.7628388461	0.1487043033
C43	1.0998367847	14.1166321062	1.8021760177
H45	-1.7953939888	18.9515557060	3.0793831056
H46	-2.7803644351	18.9898059732	4.5608740527
H47	-1.3291417004	20.0068327717	4.4333058517
H48	-0.1563119379	17.4572554515	10.0767459203
H49	3.9727428238	18.3162029161	10.9966982381
H50	-0.5888844997	11.1997692537	1.2663734683
H51	1.7798680045	14.8075883806	1.3110446925

Fe(III)

Y1	0.2396446168	16.6354781202	5.4018209238
Fe2	2.4367527652	13.2943578743	6.8434874208
S3	3.0623473040	16.8432572189	6.3641832828
S4	-0.8964360979	13.9258128949	5.4736194069
O5	-0.8864142740	18.0862650442	4.6143230392
O7	0.3908739278	16.5522789138	7.5585613481
O8	1.1507023559	15.3486457333	3.9120961875
C9	-1.6283960676	19.1434426398	4.0728680591
C10	1.2678295652	17.0493770469	8.4135781577
C11	0.9141315745	17.3968712801	9.7307475813
C12	1.8558988332	17.9339521242	10.5994551263
H13	1.5509075811	18.2037707883	11.6072794216
C14	3.1797798464	18.1495063230	10.2000265450
C15	3.5613392888	17.8145321657	8.9068464866
H16	4.5788644447	17.9868832388	8.5655175587
C17	2.6204126115	17.2571959382	8.0342093931
C18	3.5268095206	15.1395257637	6.4978966405
C19	4.0175266823	14.4919034818	7.6677775809
H20	4.0096266137	14.9144449465	8.6644737963
C21	4.4967063090	13.2087779687	7.2929976098
H22	4.9125444036	12.4708188545	7.9681434306
C23	4.2721022309	13.0393921821	5.8974910451
H24	4.5034576873	12.1548389939	5.3170464083

C25	3.6443728154	14.2208595737	5.4031708907
H26	3.3190075542	14.4161751460	4.3899323921
C27	0.2820756959	13.0755529225	6.4846590336
C28	0.5902448819	13.3943930477	7.8459864240
H29	0.2439127069	14.2740657015	8.3734861880
C30	1.4081671126	12.3431654471	8.3596901869
H31	1.8016888970	12.2812357880	9.3666417530
C32	1.6460739404	11.4144954457	7.3052411389
H33	2.2656288765	10.5277953732	7.3596767474
C34	0.9728763004	11.8802707277	6.1430156722
H35	0.9806565623	11.4220476050	5.1621977215
C36	0.6265431703	14.3356568322	3.2442309899
C37	-0.3699196314	13.5092811741	3.8291205951
C38	-0.9538941059	12.4402107609	3.1412553026
H39	-1.7348342207	11.8530436826	3.6174962347
C40	-0.5332524158	12.1494475820	1.8499457332
C41	0.4593814608	12.9409025827	1.2601064185
H42	0.7851664390	12.7217677114	0.2465217702
C43	1.0310728211	14.0120202269	1.9350671395
H45	-1.2436179697	19.4183636859	3.0819552280
H46	-2.6822237866	18.8554509747	3.9644912469
H47	-1.5792792371	20.0271433727	4.7228509295
H48	-0.1177373952	17.2558658578	10.0403917512
H49	3.8997821118	18.5863030709	10.8853318858
H50	-0.9802982647	11.3249107312	1.3032172226
H51	1.7852534783	14.6345861339	1.4615266136

L6_Zr_a

Fe(II)

Zr1	-2.2662225799	9.3693528319	9.2997669493
Fe2	-0.7810512580	10.1646683184	4.6740397404
S3	0.2810548007	9.5829035614	7.9734521777
S4	-3.5782532814	9.7853284479	6.7661989946
O5	-1.9787323134	11.4050024819	9.2217906994
O6	-2.2679234569	7.4797530159	8.4882966566
O7	-4.1030138245	9.3597956495	9.9378446996
O8	-1.1715437352	9.0062146158	10.8645042794
C9	0.4755267805	9.6579498545	6.2195160896
C10	1.0474477640	10.7024725283	5.4295369138
H11	1.2857068534	11.6991129890	5.7713127469
C12	1.1830752098	10.2125637791	4.0980611870
H13	1.5501954648	10.7815123412	3.2533169236
C14	0.6913194749	8.8769448708	4.0630281894
H15	0.6213930291	8.2453510886	3.1869946349
C16	0.2466779042	8.5302861950	5.3704624962
H17	-0.2027829420	7.5925000368	5.6705158994
C18	-2.7380305581	10.2849520874	5.2943577582
C19	-2.6501961802	9.6087968008	4.0386599346
H20	-2.9391731861	8.5859668755	3.8458451713

C21	-2.0521533138	10.5054086731	3.1058609165
H22	-1.8146851830	10.2738656293	2.0753485375
C23	-1.7647563092	11.7248902766	3.7820190522
H24	-1.2725009571	12.5899125476	3.3569218819
C25	-2.1800143714	11.5923566316	5.1373151216
H26	-2.0769279192	12.3347099952	5.9184224833
C27	0.7740950112	11.2372208788	8.5950680755
H28	0.7721491475	11.0532191962	9.6772280873
H29	1.8140851997	11.3969588037	8.2921683440
C30	-0.0709285506	12.4285323209	8.2590704393
C31	0.5287168541	13.5226930191	7.6284611634
H32	1.5718527232	13.4328765307	7.3345980525
C33	-0.1624564868	14.7109177892	7.4114128616
C34	-1.4753884145	14.7688904966	7.9022665312
H35	-2.0173097675	15.7008067740	7.7803185710
C36	-2.1272340219	13.7159720247	8.5501138004
C37	-1.4181041695	12.4865617448	8.6794063211
C38	-3.5276583700	13.9126313976	9.1609101686
C39	-4.5538993222	12.9525286991	8.5325257354
H40	-5.5538770438	13.1592466988	8.9367522703
H41	-4.3151067038	11.9099455117	8.7451506185
H42	-4.6014596333	13.0837449792	7.4445254779
C43	-4.0559310425	15.3410769897	8.9499899040
H44	-3.4003490116	16.0980765306	9.3970546322
H45	-5.0375232628	15.4335717553	9.4300855244
H46	-4.1893781835	15.5810780637	7.8877387614
C47	-3.4530597018	13.6675993851	10.6828147638
H48	-2.7696459731	14.3815162588	11.1591472348
H49	-3.1059752772	12.6555518573	10.9049105917
H50	-4.4456491500	13.7984401545	11.1336697820
C51	0.4495239939	15.9272868957	6.7016616433
C52	-0.3842055062	16.2636181055	5.4485868036
H53	0.0290884036	17.1400918696	4.9327121607
H54	-1.4263136958	16.4872892804	5.7020593492
H55	-0.3855888572	15.4239180769	4.7430803800
C56	1.8967814821	15.6717064120	6.2583336079
H57	2.5538165349	15.4581557547	7.1101882192
H58	2.2919637427	16.5610533288	5.7529284335
H59	1.9658354477	14.8341489004	5.5533075165
C60	0.4492791469	17.1408389411	7.6531066721
H61	1.0399630989	16.9328981896	8.5531656150
H62	-0.5637138342	17.4071853484	7.9742451457
H63	0.8821503377	18.0195200027	7.1572001076
C64	-4.1518255691	8.0680172496	6.4634281578
H65	-4.7962313545	7.9152134801	7.3381467481
H66	-4.8009754025	8.0974891417	5.5823009261
C67	-3.1453010603	6.9627051340	6.3500875788
C68	-3.1559878361	6.1605487637	5.2056440402
H69	-3.8499041313	6.4192343505	4.4088761619
C70	-2.3300615530	5.0475987537	5.0832834346
C71	-1.5246574639	4.7426756882	6.1915603574

H72	-0.8998440803	3.8580665235	6.1303530434
C73	-1.4838357140	5.4893179635	7.3728577482
C74	-2.2830966904	6.6682639822	7.4293317174
C75	-0.6622723166	5.0036179555	8.5831615525
C76	0.4145264904	6.0284365769	8.9829937960
H77	1.0817205335	6.2495033725	8.1409209852
H78	1.0299032884	5.6229533797	9.7973043442
H79	-0.0250136702	6.9647099261	9.3284948965
C80	-1.6138879508	4.7651391198	9.7741175537
H81	-2.1500443310	5.6787670129	10.0422861436
H82	-1.0427193362	4.4300299387	10.6499546086
H83	-2.3499766823	3.9879039387	9.5342390243
C84	0.0617023254	3.6765935068	8.2996708380
H85	-0.6335133092	2.8683194962	8.0430007223
H86	0.6050294507	3.3669681787	9.2005529572
H87	0.7986045586	3.7707394802	7.4922520966
C88	-2.2877578165	4.1584651812	3.8323917562
C89	-0.8601948346	4.1666166151	3.2495958385
H90	-0.5628577853	5.1811555047	2.9582545122
H91	-0.8011754269	3.5268709167	2.3595027372
H92	-0.1242667959	3.7994220048	3.9733526694
C93	-2.6755498696	2.7132055086	4.2033871415
H94	-1.9964977118	2.2868979118	4.9500134643
H95	-2.6412325016	2.0669151900	3.3167596294
H96	-3.6909716251	2.6733243103	4.6148998469
C97	-3.2536090528	4.6442426764	2.7418927042
H98	-4.2959336920	4.6269467896	3.0825394878
H99	-3.1827464845	3.9894121179	1.8651755900
H100	-3.0172766713	5.6632136292	2.4113696532
C114	-0.6270855621	8.8040672506	12.1266892760
H115	0.1538302786	9.5499656966	12.3343599092
H116	-1.3998334307	8.8917263587	12.9034927411
H117	-0.1776840427	7.8040823115	12.1969101312
C105	-5.3649031282	9.0345599677	10.4210228746
H106	-6.1319780071	9.6579083426	9.9409829891
H107	-5.6015171691	7.9778609822	10.2267314550
H108	-5.4169068085	9.2030991814	11.5055827546

Fe(III)

Zr1	-2.3644345761	9.3409378505	9.4814716135
Fe2	-0.9777466924	10.1589329147	4.6379016358
S3	0.1893503052	9.4415121490	7.8978837706
S4	-3.7360907385	9.7591169312	6.8307721737
O5	-1.9431395606	11.3224937796	9.2119557668
O6	-2.3814162225	7.5111065828	8.5613483645
O7	-4.1931278295	9.4145766308	10.0782527466
O8	-1.2020127653	8.9783861179	10.9751688350
C9	0.4160874933	9.5559607266	6.1735509234
C10	0.9450852498	10.6327746134	5.4021274511
H11	1.1993392983	11.6137479141	5.7769177637

C12	1.0217934359	10.2140695314	4.0451764253
H13	1.3782714802	10.8198190258	3.2214044369
C14	0.5026401098	8.8915628518	3.9598918723
H15	0.4108570156	8.2951319881	3.0616079880
C16	0.0990140956	8.4900605402	5.2687808740
H17	-0.3429782126	7.5388069487	5.5416816369
C18	-3.0197887143	10.3069757571	5.3385214262
C19	-2.9648173121	9.6560048982	4.0713699219
H20	-3.2819269041	8.6442585401	3.8647107647
C21	-2.3726411859	10.5479333739	3.1348958019
H22	-2.1946844437	10.3314420960	2.0890239698
C23	-2.0196132390	11.7425670025	3.8236612940
H24	-1.5397432167	12.6129622960	3.3954291140
C25	-2.3870177559	11.5864131118	5.1940774440
H26	-2.2375410444	12.3101087367	5.9873494181
C27	0.7757871590	11.0570398774	8.5575349912
H28	0.7424838638	10.8541649815	9.6350023309
H29	1.8275193066	11.1645458483	8.2739395009
C30	-0.0225510275	12.2718990848	8.2055210972
C31	0.6085003797	13.3270586462	7.5369464832
H32	1.6548551103	13.2105955095	7.2627576287
C33	-0.0535437878	14.5217137138	7.2738284834
C34	-1.3634180460	14.6291873110	7.7690610838
H35	-1.8789094075	15.5711936631	7.6187330300
C36	-2.0396360016	13.6242189692	8.4696664357
C37	-1.3629606977	12.3803579279	8.6352606439
C38	-3.4143321106	13.9022970024	9.1088446905
C39	-4.4964869634	12.9591378499	8.5541111899
H40	-5.4733796329	13.2248106456	8.9767600514
H41	-4.2970486625	11.9167429010	8.8068270747
H42	-4.5770668101	13.0488140839	7.4630593858
C43	-3.8911445040	15.3415169529	8.8518258867
H44	-3.2006741071	16.0884943031	9.2602078078
H45	-4.8586611245	15.4903972928	9.3441415859
H46	-4.0361915553	15.5482069458	7.7840968419
C47	-3.2956317749	13.7198258526	10.6366777239
H48	-2.5686061980	14.4247037150	11.0568187285
H49	-2.9824038513	12.7059358230	10.8977927700
H50	-4.2645730795	13.9126395367	11.1133681411
C51	0.5916376032	15.7006321023	6.5311973335
C52	-0.2603942594	16.0587253389	5.2976815978
H53	0.1756327744	16.9130153311	4.7662652392
H54	-1.2863561053	16.3278848521	5.5706121739
H55	-0.3087283334	15.2167807034	4.5949379172
C56	2.0137902108	15.3767007366	6.0515962399
H57	2.6909831716	15.1609891450	6.8862693178
H58	2.4268022477	16.2361714066	5.5119407186
H59	2.0305096365	14.5216272356	5.3630591391
C60	0.6684159350	16.9236085377	7.4677920159
H61	1.2735984750	16.7020871691	8.3542486031
H62	-0.3230152622	17.2393833013	7.8100453785

H63	1.1260252850	17.7743212726	6.9482313746
C64	-4.2227821300	8.0129864762	6.5139615003
H65	-4.8257615962	7.8099961966	7.4067336712
H66	-4.8983996053	8.0076364869	5.6528855758
C67	-3.1180671849	7.0157904670	6.3684610529
C68	-3.0003509485	6.2941289113	5.1761774074
H69	-3.6948585644	6.5138285824	4.3685246665
C70	-2.0572970339	5.2811677103	5.0298160745
C71	-1.2939435591	4.9744929430	6.1676636625
H72	-0.5971204335	4.1478350466	6.0934726803
C73	-1.3867761405	5.6327488797	7.3985334953
C74	-2.2783592006	6.7417065612	7.4721013599
C75	-0.6243892843	5.0989333929	8.6267587795
C76	0.3775936398	6.1292258690	9.1751192184
H77	1.0942667869	6.4346197749	8.4030516715
H78	0.9503450283	5.6847053421	9.9985580354
H79	-0.1215206714	7.0196424707	9.5602433403
C80	-1.6485571961	4.7388182678	9.7235924374
H81	-2.2400174474	5.6084021985	10.0213754951
H82	-1.1274037648	4.3576354657	10.6104270443
H83	-2.3343468769	3.9576072145	9.3754239733
C84	0.1737913620	3.8242230841	8.3041292169
H85	-0.4656111309	3.0107326916	7.9427619556
H86	0.6640849461	3.4700150603	9.2177606302
H87	0.9633705778	4.0027905285	7.5635329218
C88	-1.8704137292	4.4749427312	3.7371266373
C89	-0.4040520555	4.5764948724	3.2701404368
H90	-0.1319079771	5.6163335472	3.0469941713
H91	-0.2512645194	3.9888211018	2.3570759804
H92	0.2968260174	4.2022616834	4.0238908040
C93	-2.2173809713	2.9951665739	3.9979799525
H94	-1.5741335075	2.5560007265	4.7680815293
H95	-2.0892071955	2.4052659608	3.0822429265
H96	-3.2566415607	2.8876893670	4.3286892467
C97	-2.7692113764	4.9851756406	2.6024031637
H98	-3.8337678435	4.8764641432	2.8404991972
H99	-2.5800817768	4.4081681473	1.6903608495
H100	-2.5732208672	6.0400118417	2.3684710601
C114	-0.6098144545	8.7127011194	12.2151595828
H115	0.4799634319	8.6534679522	12.1035837683
H116	-0.8474731482	9.5107267356	12.9289917175
H117	-0.9716964846	7.7579232706	12.6147855617
C105	-5.4373023671	9.2424079568	10.6949466537
H106	-6.1440731270	9.9955853968	10.3269094472
H107	-5.8362863771	8.2428622527	10.4795200564
H108	-5.3395274862	9.3544984594	11.7813444261