

# Supporting Information

## A Water Molecule Residing in the $\text{Fe}_{\text{a}3}^{3+}\cdots\text{Cu}_{\text{B}}^{2+}$ Dinuclear Center of the Resting Oxidized as-Isolated Cytochrome *c* Oxidase: A Density Functional Study

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## Calculation Results for the DNC Model Clusters with Low/Intermediate-Spin

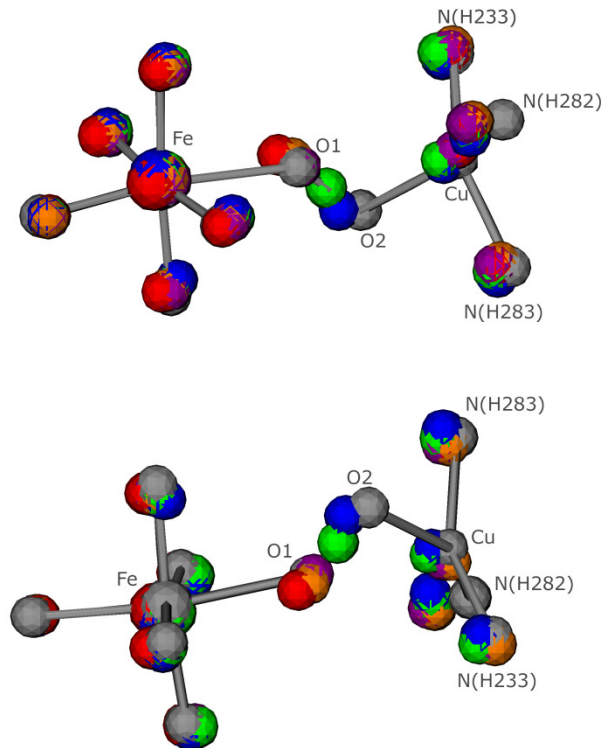
### $\text{Fe}_{\text{a}3}^{3+}$

We have geometry optimized our DNC model clusters (See Fig. 4 in the main text) with the  $\text{Fe}_{\text{a}3}^{3+}$  site in different spin state (low-spin (LS), intermediate-spin (IS), and high-spin (HS)). Our calculations show that the IS- $\text{Fe}_{\text{a}3}^{3+}$  state is generally lower in energy by 2-7 kcal mol<sup>-1</sup> than the corresponding HS- $\text{Fe}_{\text{a}3}^{3+}$  state for each model cluster studied here. However, the resonance Raman and EPR experimental data suggest that the  $\text{Fe}_{\text{a}3}^{3+}$  is HS in both the active  $\mathbf{O}_{\text{H}}$  and the resting  $\mathbf{O}$  states.<sup>1,2</sup> One needs more experimental data and higher-level theoretical calculations to determine whether different spin states of  $\text{Fe}_{\text{a}3}^{3+}$  can coexist in the  $\mathbf{O}_{\text{H}}$  and the resting  $\mathbf{O}$  states. In fact, the existence of IS/LS- $\text{Fe}_{\text{a}3}$  states in the resting  $\mathbf{O}$  DNCs may be temperature-dependent, since Mössbauer spectroscopy experiments on *Thermus thermophilus ba*<sub>3</sub><sup>3</sup> and *c<sub>1</sub>aa*<sub>3</sub><sup>4</sup> have shown the coexistence of different HS and “LS” (might also be IS according to the isomer shift and quadrupole splitting values)  $\text{Fe}_{\text{a}3}^{3+}$  species at very low temperature (4.2 K), and the “LS”  $\text{Fe}_{\text{a}3}^{3+}$  species changes to HS as temperature increases above 190 K.<sup>3</sup> For simplicity, we have presented our calculation results in which the HS- $\text{Fe}_{\text{a}3}^{3+}$  site is antiferromagnetically (AF) coupled with the  $\text{Cu}_{\text{B}}^{2+}$  site, and will put the results of the LS- and IS- $\text{Fe}_{\text{a}3}^{3+}$  states here as the Supporting Information. Note that, all conclusions we find for the HS- $\text{Fe}_{\text{a}3}^{3+}$  states (Table 1) will remain the same if the  $\text{Fe}_{\text{a}3}^{3+}$  is in the IS state.

Similar to Table 1, our calculated properties of the optimized  $\text{Fe}_{\text{a}3}^{3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+}$ ,  $\text{Fe}_{\text{a}3}^{3+}\text{-H}_2\text{O}\cdots\text{OH}^{-}\text{-Cu}_{\text{B}}^{2+}$ ,  $\text{Fe}_{\text{a}3}^{3+}\text{-OH}^{-}\cdots\text{H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$ , and  $\text{Fe}_{\text{a}3}^{3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$  DNC clusters with LS- and IS- $\text{Fe}_{\text{a}3}^{3+}$  spin states are given in Table S1. We did not obtain the optimized  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-H}_2\text{O}\cdots\text{OH}^{-}\text{-Cu}_{\text{B}}^{2+}$  state, since during the  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-H}_2\text{O}\cdots\text{OH}^{-}\text{-Cu}_{\text{B}}^{2+}$  geometry optimization calculation, the proton on the  $\text{H}_2\text{O}$  ligand transferred to the  $\text{OH}^{-}$  ligand, and as the result, the  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-OH}^{-}\cdots\text{H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$  state was obtained. The  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+}$ ,  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O}\cdots\text{OH}^{-}\text{-Cu}_{\text{B}}^{2+}$ ,  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-OH}^{-}\cdots\text{H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$  and  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-OH}^{-}\cdots\text{H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$  structures are all in higher energy (by 8.2–10.7 kcal mol<sup>-1</sup>) than the  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+}$  state. The four structures are also in higher energy (by 1.5–4.0 kcal mol<sup>-1</sup>) than the  $\text{Fe}_{\text{a}3}^{\text{HS},3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+}$  (see Table 1) state. Therefore, the  $\text{Fe}_{\text{a}3}^{3+}$  in the active  $\mathbf{O}_{\text{H}}$  state is very unlikely in the LS state, and the  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O}\cdots\text{OH}^{-}\text{-Cu}_{\text{B}}^{2+}$ ,  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-OH}^{-}\cdots\text{H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$ , and  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-OH}^{-}\cdots\text{H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$  are also unlikely to represent the DNC structure of the resting  $\mathbf{O}$  state.

Very similar to  $\text{Fe}_{\text{a}3}^{\text{HS},3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}\text{(a)-(d)}$  (see Fig. 4V-VIII and the Results and Discussion section in the main text), we also obtained four  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}\text{(a)-(d)}$  optimized DNC geometries, which are similar in energies, and similar to the structures shown in Fig. 4V-VIII. Further, an optimized

LS- $\text{Fe}_{\text{a}3}^{3+}$  structure  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}$  (very similar to Fig. 4V) was also obtained (see Table S1), which is higher in energy than the four  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{a})\text{-(d)}$  structures, but in lower energy than the four  $\text{Fe}_{\text{a}3}^{\text{HS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{a})\text{-(d)}$  structures. The calculated  $\text{p}K_{\text{a}}$ 's for the ligand  $\text{H}_2\text{O}$  in  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}$  and in the four  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{a})\text{-(d)}$  structures are very high (9.1-12.0), indicating that the  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}$  and  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{a})\text{-(d)}$  structures are energetically more stable than the  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-OH}^-\text{-Cu}_{\text{B}}^{2+}$  state. Similar to Fig. 5 in the main text, we also stacked the Cartesian coordinates of the central portions of the X-ray crystal structure 3S8G<sup>5</sup> and the five geometry optimized structures  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}$  and  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{a})\text{-(d)}$  together. The overlapped structures are shown in Fig. S1 with two different orientations. The colors of the atoms in different structures are as the following: 3S8G: silver,  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}$ : red,  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{a})$ : orange,  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{b})$ : purple,  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{c})$ : blue, and  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{d})$ : green.



**Figure S1.** The overlap of the central portions of the following DNC structures (see Table S1): Silver: 3S8G X-ray crystal structure; Red:  $\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}$ ; Orange:  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{a})$ ; Purple:  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{b})$ ; Blue:  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{c})$ ; and Green:  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{d})$ . The two pictures are the views of this overlap from two different angles. For clarity, the H-bonding water molecules and the hydrogen atoms are not shown. For comparison, see Fig. 5 in the main text.

Very similar to the corresponding HS-Fe<sub>a3</sub><sup>3+</sup> results, the H<sub>2</sub>O molecules in Fe<sub>a3</sub><sup>LS,3+</sup>-H<sub>2</sub>O-Cu<sub>B</sub><sup>2+</sup>, Fe<sub>a3</sub><sup>IS,3+</sup>-H<sub>2</sub>O-Cu<sub>B</sub><sup>2+</sup>(a), and Fe<sub>a3</sub><sup>IS,3+</sup>-H<sub>2</sub>O-Cu<sub>B</sub><sup>2+</sup>(b) are close to the O1 position in 3S8G, the H<sub>2</sub>O ligand in Fe<sub>a3</sub><sup>IS,3+</sup>-H<sub>2</sub>O-Cu<sub>B</sub><sup>2+</sup>(c) is near O2, and the H<sub>2</sub>O ligand in Fe<sub>a3</sub><sup>IS,3+</sup>-H<sub>2</sub>O-Cu<sub>B</sub><sup>2+</sup>(d) is in about the middle between O1 and O2. Therefore, the LS/IS-Fe<sub>a3</sub><sup>3+</sup> calculations also support our proposal that the electron density around O1-O2 in the X-ray crystal structures represents the overlap of the electron density of one water molecule that locates at different positions along O1-O2 in different CcO molecules in the crystal. More calculations and experiments are needed to examine whether these Fe<sub>a3</sub><sup>LS,3+</sup>-H<sub>2</sub>O-Cu<sub>B</sub><sup>2+</sup> and Fe<sub>a3</sub><sup>IS,3+</sup>-H<sub>2</sub>O-Cu<sub>B</sub><sup>2+</sup>(a)-(d) structures represent the “low-spin” species found in Mössbauer experiments on the resting **O** state *Thermus thermophilus* ba<sub>3</sub> at low temperature (4.2 – 190 K).<sup>3</sup>

**Table S1.** OLYP-D3-BJ Calculated Geometrical, Energetic, and Net Spin Properties of the Optimized  $\text{Fe}_{\text{a}3}^{3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+}$ ,  $\text{Fe}_{\text{a}3}^{3+}\text{-H}_2\text{O}\cdots\text{OH}^{-}\text{-Cu}_{\text{B}}^{2+}$ ,  $\text{Fe}_{\text{a}3}^{3+}\text{-OH}^{-}\cdots\text{H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$ , and  $\text{Fe}_{\text{a}3}^{3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$  DNC Clusters with LS- and IS- $\text{Fe}_{\text{a}3}^{3+}$  Spin States.<sup>a</sup>

Structure	Geometry (Å)					$E^b$	$Q^c$	$\text{p}K_{\text{a}}(\text{H}_2\text{O})^d$	Net Spin <sup>e</sup>			
	Fe-N(H384)	Fe-O	Cu-O	O $\cdots$ O	Fe $\cdots$ Cu				$\text{Fe}_{\text{a}3}$	O(Fe)/O(Cu)	$\text{Cu}_{\text{B}}$	Y237
$\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+}$	2.11	1.88	2.10		3.73	9.3	0		0.94	0.07	-0.36	-0.41
$\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+}$	2.46	2.01	2.00		3.71	0.0	0		2.55	0.02	-0.41	-0.05
$\text{Fe}_{\text{a}3}^{\text{HS},3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+}$	2.50	1.99	2.04		3.73	6.7	0		4.08	0.12	-0.39	-0.25
$\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O}\cdots\text{OH}^{-}\text{-Cu}_{\text{B}}^{2+}$	2.23	2.20	1.96	2.51	4.76	8.2	0		2.73	0.07/-0.16	-0.49	-0.04
$\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-OH}^{-}\cdots\text{H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$	2.02	1.87	2.14	2.47	4.85	10.7	0		0.98	0.06/-0.03	-0.40	-0.34
$\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-OH}^{-}\cdots\text{H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$	2.35	2.05	2.09	2.40	4.60	10.7	0		2.72	0.15/-0.05	-0.41	-0.30
$\text{Fe}_{\text{a}3}^{\text{LS},3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$	1.94	2.37	3.10		5.04	2.6	1	9.1	0.98	0.00	-0.22	-0.64
$\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}(\text{a})$	2.18	2.40	2.90		4.94	-1.0	1	11.8	2.73	0.04	-0.24	-0.61
$\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}(\text{b})$	2.19	2.46	2.67		4.78	-1.3	1	12.0	2.72	0.03	-0.25	-0.60
$\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}(\text{c})$	2.12	3.44	2.26		4.71	1.0	1	10.3	2.68	0.00	-0.33	-0.49
$\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}(\text{d})$	2.17	3.00	2.24		4.56	-0.3	1	11.2	2.72	-0.01	-0.33	-0.47
3S8G <sup>f</sup>	2.22	2.39	2.25	1.52	4.92							

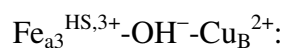
<sup>a</sup> LS: low-spin; IS: intermediate-spin, HS: high-spin. For comparison, we also list the  $\text{Fe}_{\text{a}3}^{\text{HS},3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+}$  (see Table 1) results in this table.

<sup>b</sup> Calculated broken-symmetry state energies (offset by  $-26343.3 \text{ kcal mol}^{-1}$ ). <sup>c</sup> The net charge of the model clusters. <sup>d</sup> The  $\text{p}K_{\text{a}}(\text{H}_2\text{O})$  values were calculated for the process  $\text{Fe}_{\text{a}3}^{\text{IS},3+}\text{-OH}^{-}\text{-Cu}_{\text{B}}^{2+} \rightarrow \text{Fe}_{\text{a}3}^{\text{LS/IS},3+}\text{-H}_2\text{O}\text{-Cu}_{\text{B}}^{2+}$ . <sup>e</sup> The Mulliken net spin populations on  $\text{Fe}_{\text{a}3}^{3+}$ , O of the bridging OH<sup>-</sup>/H<sub>2</sub>O,  $\text{Cu}_{\text{B}}^{2+}$ , and on the heavy atoms of the Tyr237-O<sup>-</sup> side chain (the sum total). <sup>f</sup> The X-ray crystal structure.<sup>5</sup>

## References

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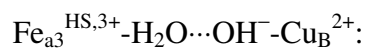
## Cartesian Coordinates of the Geometry Optimized DNC Clusters Listed in Table 1:



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C	1.298871	4.585726	20.031207	H	-9.053409	-3.090292	17.189682
C	2.274393	3.527164	19.661137	C	-10.945615	-3.409142	22.799456
N	1.938741	2.181439	19.559187	C	-10.870916	-2.083530	23.466291
C	3.605777	3.651760	19.363646	N	-9.715774	-1.334829	23.459003
C	3.026693	1.512898	19.193059	C	-11.788028	-1.315341	24.154963
N	4.078634	2.377984	19.070152	C	-9.953426	-0.176154	24.126852
H	0.372039	4.146726	20.398549	N	-11.209692	-0.122358	24.567025
H	1.060714	5.225373	19.174117	H	-10.963760	-3.302852	21.708332
H	1.715167	5.225326	20.815386	H	-11.850109	-3.937757	23.108013
H	4.242351	4.517634	19.313602	H	-8.824081	-1.682330	23.073963
H	3.120635	0.451775	19.043656	H	-12.820877	-1.554170	24.374483
C	8.822503	3.511934	19.825854	H	-9.195261	0.583118	24.264947
C	7.783928	2.600978	19.240280	C	-0.106485	-7.227867	24.323223
C	8.134608	1.456225	18.504863	C	0.506426	-6.151464	23.484629
C	6.424299	2.860155	19.421565	N	1.385466	-6.397227	22.442346
C	7.174764	0.618230	17.967830	C	0.276285	-4.788888	23.419916
C	5.443232	2.040485	18.872305	C	1.652553	-5.224736	21.802171
C	5.776341	0.870226	18.103049	N	0.988647	-4.227332	22.369816
O	4.873330	0.118308	17.570263	H	-0.766309	-7.849589	23.704725
H	8.577798	4.563003	19.636101	H	-0.724264	-6.761531	25.094388
H	9.808882	3.301917	19.405427	H	1.765319	-7.300029	22.196333
H	9.187212	1.227187	18.355147	H	-0.354611	-4.184762	24.053361
H	6.127205	3.721018	20.010523	H	2.325783	-5.140530	20.962490
H	7.467649	-0.260309	17.400540	C	-7.335965	-2.844604	29.407724
C	-3.849775	1.852200	16.263523	N	-6.393167	-1.913514	29.989289
C	-2.559433	1.820499	16.996949	C	-5.648110	-1.064578	29.271351
N	-1.340347	2.051244	16.381408	N	-5.764802	-1.018735	27.943013
C	-2.245480	1.547813	18.304723	N	-4.764326	-0.280399	29.894827
C	-0.347818	1.931795	17.291932	H	-6.849441	-3.518739	28.696350
N	-0.873240	1.621804	18.474631	H	-8.147350	-2.315009	28.902534
H	-4.065460	0.878799	15.808604	H	-6.154303	-2.025643	30.961323
H	-3.824352	2.600389	15.465763	H	-6.532886	-1.487007	27.468203
H	-1.212005	2.290388	15.408267	H	-5.355191	-0.205734	27.470956
H	-2.902147	1.324802	19.126460	H	-4.702906	-0.307074	30.899416
H	0.698418	2.079767	17.079722	H	-4.180640	0.392225	29.377540
C	-4.727813	3.847469	21.544491	Fe	1.158923	-1.817097	21.736082
C	-3.459469	3.072669	21.619921	C	-1.912642	-1.594598	23.239825
N	-3.264961	2.019549	22.497643	C	-0.342231	-2.091689	18.657264
C	-2.288041	3.167731	20.905434	C	4.197448	-2.573035	20.292735
C	-2.030456	1.510225	22.295316	C	2.685547	-1.462273	24.771953
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H	-5.090397	4.105357	22.544135	C	-0.842306	-1.152968	25.494329
H	-3.970624	1.648881	23.165142	C	0.466671	-1.099787	25.919713
H	-2.039410	3.851818	20.110590	C	1.294001	-1.406049	24.765961
H	-1.623580	0.676985	22.836964	C	0.981761	-0.759206	27.271655
C	-8.508134	-3.736798	17.876003	O	-3.146503	-1.781101	17.355697
C	-8.379670	-3.061649	19.219022	C	-2.040181	-0.759083	26.279972
O	-8.755618	-1.906817	19.433439	C	-2.182445	0.776931	26.307533
O	-7.795217	-3.822650	20.141115	C	-3.299666	1.159691	27.260387
H	-7.503486	-3.922560	17.480454	O	-3.005518	1.336735	28.477067

O	-4.492714	1.201858	26.800447	H	-7.280330	0.870101	20.240382
N	1.800077	-2.335583	19.836197	H	-7.869076	-0.450805	20.702296
C	1.027763	-2.314582	18.697397	O	-7.729827	-2.163693	26.005333
C	1.867284	-2.570891	17.535603	H	-7.256169	-1.920872	25.168298
C	3.147765	-2.760525	18.003804	H	-8.589884	-1.732587	25.906317
C	3.096455	-2.580636	19.446709	O	-5.179598	1.034378	24.217771
C	1.366847	-2.629488	16.136685	H	-4.865536	1.040473	25.162333
N	3.099263	-2.004523	22.418698	H	-5.520432	0.127944	24.065505
C	4.210232	-2.291489	21.655383	H	-7.688900	-3.288858	21.027483
C	5.400113	-2.195454	22.469426	H	-2.392395	1.142850	25.302849
C	4.979523	-1.849661	23.753244	H	-1.243141	1.210195	26.652631
C	3.523205	-1.758587	23.700497	H	-1.941061	-1.117877	27.307745
C	6.786951	-2.425839	21.991825	H	-2.948588	-1.206042	25.871026
C	5.761990	-1.626925	24.947546	H	1.628214	-1.554412	27.658555
C	7.092957	-1.442542	25.024204	H	1.581723	0.157733	27.242006
N	-0.802593	-1.940152	21.060800	H	0.164747	-0.607814	27.978218
C	-1.192365	-1.915285	19.748129	H	-2.881072	-1.450276	23.700711
C	-2.624622	-1.674787	19.690283	H	3.159577	-1.262349	25.723808
C	-3.066805	-1.548177	21.006935	H	5.200110	-1.595086	25.877537
C	-1.912088	-1.734277	21.849534	H	7.562556	-1.280783	25.990593
C	-3.478168	-1.582790	18.528232	H	7.733422	-1.421189	24.152619
C	-4.426328	-1.258354	21.515114	H	7.345377	-3.032439	22.710701
C	-5.167926	-2.532821	21.932948	H	6.801362	-2.930486	21.025660
C	-6.393284	-2.207587	22.767877	H	7.327348	-1.477892	21.882400
O	-7.532436	-2.626142	22.368691	H	5.146859	-2.736399	19.804678
O	-6.225476	-1.555300	23.835751	H	4.127360	-3.003002	16.150554
C	4.355658	-3.168187	17.211976	H	3.775833	-5.245641	17.103938
O	5.534934	-2.441395	17.561000	H	4.860102	-4.860465	18.456561
C	4.642822	-4.652923	17.405857	H	2.186872	-2.726899	15.424658
H	5.503654	-4.946333	16.797442	H	0.693398	-3.482858	15.996278
Cu	0.158264	1.432750	20.191170	H	0.799254	-1.726803	15.886731
H	8.891071	3.392425	20.913366	H	-0.818732	-2.061061	17.686909
H	-4.673318	2.104938	16.938342	H	-4.527906	-1.311450	18.758383
H	-5.531462	3.294703	21.032083	H	-5.021397	-0.713576	20.782329
H	-9.006487	-4.710142	17.956797	H	-4.343147	-0.613465	22.386314
H	-10.071117	-4.017669	23.050776	H	-4.507062	-3.141430	22.557371
H	0.595659	-7.919075	24.825694	H	-5.435858	-3.119816	21.054900
H	-7.746920	-3.426171	30.227401	H	5.297813	-1.468073	17.538843
O	1.127878	0.154003	21.452781	H	4.558025	0.138784	22.305861
O	4.177877	0.986850	22.027285	H	2.043814	0.476009	21.531270
O	-7.471395	0.369407	21.047260	H	4.748890	1.264099	21.294424



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C	1.482539	4.917766	19.782216	H	1.715167	5.225326	20.815386
C	2.315894	3.744686	19.409250	H	4.275772	4.515527	18.671290
N	1.913067	2.429855	19.621713	H	2.975867	0.564927	19.428433
C	3.609972	3.719887	18.960245	C	8.754740	3.433648	19.816417
C	2.941068	1.634059	19.328874	C	7.708028	2.480854	19.296855
N	4.007227	2.387377	18.931219	C	8.038732	1.213381	18.789802
H	0.415973	4.688432	19.717931	C	6.352488	2.818407	19.309463
H	1.692620	5.767128	19.127531	C	7.071527	0.338840	18.320556



C	5.364788	1.955469	18.837296	C	-7.202385	-2.921462	29.432703
C	5.676714	0.654209	18.311145	N	-6.218499	-2.062754	30.057785
O	4.773769	-0.157093	17.865370	C	-5.440309	-1.211995	29.377559
H	8.492318	4.468814	19.573248	N	-5.535622	-1.117778	28.055743
H	9.727899	3.215501	19.366257	N	-4.579092	-0.421195	30.037294
H	9.082745	0.906621	18.771388	H	-6.734262	-3.668167	28.782663
H	6.053445	3.776713	19.720555	H	-7.910516	-2.329654	28.847759
H	7.360906	-0.635918	17.940260	H	-6.012784	-2.200179	31.034186
C	-4.162819	1.158630	17.169151	H	-6.248109	-1.614455	27.527335
C	-2.793968	1.371683	17.706759	H	-5.035670	-0.350248	27.590077
N	-1.671702	1.544932	16.914455	H	-4.381129	-0.638397	31.002095
C	-2.328128	1.443484	18.994291	H	-3.851974	0.075106	29.496927
C	-0.587617	1.728021	17.702570	Fe	1.631816	-2.334067	21.807799
N	-0.960301	1.676097	18.980260	C	-1.311020	-1.563284	23.403224
H	-4.763426	0.630398	17.910178	C	-0.013071	-2.314217	18.771771
H	-4.135406	0.550061	16.261750	C	4.572622	-3.040002	20.192426
H	-1.661215	1.540083	15.904184	C	3.333343	-1.949891	24.754563
H	-2.878779	1.340338	19.909335	N	1.094925	-1.855687	23.737910
H	0.412852	1.895909	17.338844	C	-0.171334	-1.596524	24.195010
C	-4.897714	3.930768	21.659766	C	-0.125667	-1.318706	25.619908
C	-3.575050	3.286077	21.834700	C	1.199608	-1.387804	25.994310
N	-3.390092	2.146607	22.596443	C	1.953856	-1.746610	24.802857
C	-2.360173	3.533686	21.240858	C	1.790131	-1.135609	27.335462
C	-2.114916	1.732365	22.454092	O	-2.891296	-2.018291	17.617031
N	-1.463552	2.553726	21.631369	C	-1.302699	-0.975290	26.458250
H	-4.778619	4.893239	21.158271	C	-1.732469	0.496625	26.320459
H	-5.406811	4.086212	22.615019	C	-2.868183	0.776061	27.293789
H	-4.091404	1.698089	23.228808	O	-2.580661	0.805729	28.524332
H	-2.090691	4.307277	20.539456	O	-4.054060	0.902004	26.831734
H	-1.707048	0.845862	22.908677	N	2.159321	-2.711507	19.854704
C	-8.411061	-3.800557	17.838137	C	1.338909	-2.631708	18.753133
C	-8.175562	-3.149553	19.174078	C	2.110614	-2.902285	17.551201
O	-8.600353	-2.026072	19.456166	C	3.405046	-3.137198	17.955933
O	-7.461640	-3.891821	20.014885	C	3.429553	-2.991585	19.402600
H	-7.451682	-4.092056	17.400385	C	1.549563	-2.883125	16.173395
H	-8.928907	-3.107543	17.176522	N	3.611434	-2.573913	22.400964
C	-10.747880	-3.301559	22.572792	C	4.674088	-2.806813	21.562184
C	-10.598948	-1.953668	23.178430	C	5.912055	-2.704696	22.303601
N	-9.376375	-1.326076	23.265556	C	5.565905	-2.392335	23.614212
C	-11.493299	-1.070062	23.746237	C	4.107318	-2.310011	23.650811
C	-9.555634	-0.124839	23.871034	C	7.268101	-2.890079	21.729992
N	-10.836044	0.075876	24.177297	C	6.418283	-2.182669	24.762072
H	-10.503965	-3.286307	21.505395	C	7.730814	-1.887311	24.749860
H	-11.774677	-3.653255	22.691299	N	-0.316295	-1.963001	21.181364
H	-8.494380	-1.754643	22.959404	C	-0.787861	-2.029326	19.894355
H	-12.561736	-1.194996	23.867019	C	-2.216258	-1.772570	19.903600
H	-8.737725	0.553493	24.073246	C	-2.583423	-1.559597	21.233683
C	-0.101381	-7.294945	24.249767	C	-1.385862	-1.704929	22.016559
C	0.574647	-6.274927	23.404520	C	-3.142949	-1.748379	18.795943
N	1.500723	-6.589418	22.422612	C	-3.930018	-1.259225	21.776855
C	0.423817	-4.909974	23.317750	C	-4.826548	-2.496400	21.851930
C	1.873191	-5.456340	21.781857	C	-6.076292	-2.255632	22.683447
N	1.231294	-4.418065	22.304602	O	-7.174370	-2.771856	22.285133
H	-0.705390	-7.969060	23.631403	O	-5.973144	-1.591709	23.753177
H	-0.768863	-6.790634	24.951704	C	4.585034	-3.461352	17.094986
H	1.840144	-7.517016	22.211664	O	5.694306	-2.598955	17.364356
H	-0.204722	-4.258733	23.902617	C	5.028757	-4.910519	17.272720
H	2.593147	-5.416863	20.980153	H	5.883193	-5.120174	16.621810

Cu	0.180417	2.061459	20.607932	H	1.021247	-0.867707	28.061185
H	8.891071	3.392425	20.913364	H	-2.243719	-1.378702	23.919863
H	-4.673318	2.104939	16.938341	H	3.862671	-1.785216	25.684347
H	-5.531462	3.294705	21.032081	H	5.931538	-2.270444	25.731376
H	-9.006491	-4.710140	17.956796	H	8.269076	-1.761505	25.685518
H	-10.071119	-4.017667	23.050778	H	8.284949	-1.734287	23.832271
H	0.595655	-7.919074	24.825695	H	7.926797	-3.388780	22.445976
H	-7.746920	-3.426172	30.227401	H	7.237785	-3.480411	20.812765
O	2.322854	-0.289221	21.614742	H	7.722881	-1.921371	21.487263
O	1.194537	1.839687	22.264236	H	5.494133	-3.190151	19.650089
O	-6.707989	-0.024992	20.129581	H	4.274275	-3.339609	16.048406
H	-6.874176	0.498837	19.333217	H	4.210418	-5.584946	17.004646
H	-7.350064	-0.758502	20.039089	H	5.313481	-5.105112	18.309040
O	-7.377042	-2.089492	26.038442	H	2.332174	-2.984492	15.420708
H	-6.969521	-1.932106	25.150502	H	0.832226	-3.699500	16.028970
H	-7.879856	-2.908352	25.923944	H	1.012323	-1.947085	15.986518
O	-5.107863	0.984715	24.355824	H	-0.533424	-2.293573	17.824217
H	-4.646595	0.905292	25.232245	H	-4.171935	-1.457185	19.078492
H	-5.386497	0.072056	24.125984	H	-4.432429	-0.506919	21.167534
H	-7.334918	-3.388651	20.917832	H	-3.837445	-0.849751	22.778925
H	-2.047541	0.704801	25.299274	H	-4.280567	-3.313163	22.337866
H	-0.882769	1.139983	26.562403	H	-5.096160	-2.838646	20.853703
H	-1.077712	-1.169037	27.508108	H	5.329846	-1.678383	17.554418
H	-2.148651	-1.616725	26.189982	H	0.550494	1.771362	22.983269
H	2.324259	-2.017415	27.706417	H	1.819375	0.550268	21.974685
H	2.515883	-0.315786	27.291787	H	3.178655	-0.294475	22.063392

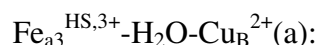


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C	1.468229	4.908902	19.790230	H	7.345006	-0.653406	18.009812
C	2.309645	3.738025	19.439904	C	-4.220246	1.145987	17.226495
N	1.940843	2.426073	19.737523	C	-2.845419	1.317657	17.759701
C	3.588629	3.720228	18.951402	N	-1.721622	1.431457	16.959355
C	2.965070	1.638532	19.424296	C	-2.370819	1.395382	19.044389
N	4.004570	2.393893	18.953501	C	-0.627748	1.580718	17.743018
H	0.403634	4.668677	19.742782	N	-0.994784	1.564147	19.021827
H	1.670510	5.749696	19.122580	H	-4.851345	0.692562	17.991945
H	1.715167	5.225326	20.815386	H	-4.220536	0.488212	16.353698
H	4.233149	4.514978	18.615263	H	-1.717362	1.407914	15.949303
H	3.016668	0.576230	19.584085	H	-2.919821	1.334702	19.965100
C	8.756231	3.434760	19.815822	H	0.376696	1.703962	17.370699
C	7.701576	2.487545	19.311418	C	-4.894631	3.983717	21.597071
C	8.030620	1.204130	18.832658	C	-3.574403	3.350314	21.819009
C	6.350408	2.843526	19.314432	N	-3.420435	2.211511	22.587761
C	7.064893	0.329591	18.374496	C	-2.336294	3.592996	21.271564
C	5.358795	1.978211	18.861121	C	-2.139492	1.798199	22.490552
C	5.670871	0.663765	18.353773	N	-1.449512	2.614469	21.693612
O	4.765561	-0.135411	17.914610	H	-4.776100	4.900288	21.016262
H	8.498029	4.469960	19.570754	H	-5.399909	4.221678	22.538090
H	9.725852	3.204300	19.365316	H	-4.137908	1.760700	23.191737
H	9.073961	0.896305	18.824895	H	-2.042880	4.366410	20.579191
H	6.060590	3.812608	19.705643	H	-1.761013	0.907274	22.960234

C	-8.394875	-3.810640	17.842435	C	1.336080	-2.740702	18.732244
C	-8.175094	-3.142104	19.173646	C	2.115080	-2.983834	17.526063
O	-8.632657	-2.029418	19.447052	C	3.408785	-3.216214	17.932042
O	-7.435057	-3.853573	20.018756	C	3.422194	-3.111150	19.385211
H	-7.432878	-4.121215	17.424814	C	1.558760	-2.933816	16.147001
H	-8.892783	-3.119168	17.163763	N	3.610891	-2.723223	22.406704
C	-10.745066	-3.308705	22.558701	C	4.666568	-2.940158	21.555666
C	-10.606956	-1.948478	23.139802	C	5.912740	-2.801212	22.282047
N	-9.391384	-1.306410	23.220630	C	5.576155	-2.477156	23.591691
C	-11.513614	-1.063465	23.687591	C	4.114755	-2.415460	23.639958
C	-9.586915	-0.095640	23.802757	C	7.265910	-2.945819	21.688263
N	-10.870894	0.097548	24.099614	C	6.431417	-2.219799	24.728848
H	-10.494204	-3.310976	21.492863	C	7.748338	-1.941746	24.715939
H	-11.771822	-3.661337	22.676181	N	-0.294728	-1.949983	21.152634
H	-8.500239	-1.730664	22.932579	C	-0.772037	-2.057227	19.870161
H	-12.580591	-1.200531	23.810690	C	-2.199617	-1.792842	19.879018
H	-8.777442	0.594267	23.999552	C	-2.563462	-1.551905	21.204234
C	-0.131597	-7.275060	24.311061	C	-1.360724	-1.668934	21.985246
C	0.509179	-6.268316	23.423305	C	-3.126109	-1.767186	18.771097
N	1.368620	-6.609020	22.392529	C	-3.913774	-1.253926	21.743352
C	0.400251	-4.896831	23.346107	C	-4.782857	-2.509203	21.886410
C	1.744773	-5.482183	21.738087	C	-6.038967	-2.257754	22.708070
N	1.167604	-4.425773	22.294468	O	-7.149310	-2.726157	22.284904
H	-0.799135	-7.929933	23.738419	O	-5.922569	-1.629611	23.797917
H	-0.729340	-6.759971	25.065968	C	4.598685	-3.491593	17.067359
H	1.667805	-7.546405	22.164838	O	5.694015	-2.617474	17.369470
H	-0.170412	-4.227144	23.969464	C	5.080527	-4.931952	17.198896
H	2.423030	-5.465513	20.900074	H	5.943751	-5.094776	16.546100
C	-7.204522	-2.910844	29.436923	Cu	0.170947	1.977543	20.635320
N	-6.237842	-2.032570	30.065203	H	8.891071	3.392425	20.913364
C	-5.420037	-1.223983	29.372071	H	-4.673318	2.104939	16.938341
N	-5.515041	-1.133138	28.048893	H	-5.531462	3.294705	21.032081
N	-4.500405	-0.500102	30.019060	H	-9.006491	-4.710140	17.956796
H	-6.721183	-3.652069	28.791414	H	-10.071119	-4.017667	23.050778
H	-7.917485	-2.330703	28.847516	H	0.595655	-7.919074	24.825695
H	-5.982166	-2.224609	31.020962	H	-7.746920	-3.426172	30.227401
H	-6.235926	-1.619741	27.519778	O	2.435919	-0.462958	21.456591
H	-5.007896	-0.372343	27.580176	O	1.151555	1.378032	22.430466
H	-4.441123	-0.549853	31.022780	O	-6.770376	-0.008517	20.184949
H	-3.830530	0.082194	29.492828	H	-6.932394	0.512842	19.385344
Fe	1.670595	-2.268275	21.758626	H	-7.401954	-0.750148	20.085854
C	-1.280916	-1.491961	23.367864	O	-7.393912	-2.074127	26.049198
C	-0.009464	-2.390847	18.752917	H	-6.953338	-1.934860	25.172823
C	4.561129	-3.165677	20.182908	H	-7.797495	-2.949781	25.973222
C	3.347950	-2.008997	24.733676	O	-5.156747	0.991945	24.343840
N	1.119620	-1.824980	23.704047	H	-4.663284	0.919385	25.201847
C	-0.141204	-1.534091	24.160647	H	-5.405290	0.068824	24.122077
C	-0.089245	-1.257532	25.586753	H	-7.310248	-3.338758	20.914990
C	1.232128	-1.369182	25.962718	H	-1.988924	0.794954	25.300843
C	1.978051	-1.752197	24.772925	H	-0.846228	1.204782	26.593882
C	1.827483	-1.143654	27.306805	H	-1.028963	-1.118756	27.479397
O	-2.879051	-2.056446	17.595761	H	-2.110194	-1.544680	26.163310
C	-1.260081	-0.909529	26.433737	H	2.328575	-2.045247	27.676140
C	-1.689075	0.564836	26.321794	H	2.582545	-0.350392	27.268988
C	-2.847399	0.814213	27.278068	H	1.066941	-0.850392	28.031411
O	-2.580986	0.865602	28.513096	H	-2.211762	-1.292176	23.882506
O	-4.028403	0.890884	26.795933	H	3.879614	-1.839135	25.661060
N	2.148730	-2.851793	19.831436	H	5.938821	-2.247063	25.698848

H	8.275474	-1.772618	25.651107	H	1.010557	-2.000148	15.982707
H	8.318642	-1.848722	23.800458	H	-0.535289	-2.371682	17.808271
H	7.945314	-3.447716	22.382168	H	-4.149965	-1.455713	19.049936
H	7.237857	-3.514384	20.757568	H	-4.436304	-0.543791	21.101147
H	7.697394	-1.961888	21.464153	H	-3.822614	-0.789869	22.722298
H	5.485624	-3.298344	19.641403	H	-4.216118	-3.282847	22.416640
H	4.291804	-3.339709	16.023940	H	-5.040816	-2.908988	20.906446
H	4.282576	-5.618892	16.903380	H	5.319456	-1.713689	17.569185
H	5.366343	-5.152161	18.229714	H	0.555708	0.946381	23.058021
H	2.345175	-3.005951	15.395020	H	1.745628	0.574093	22.052596
H	0.852200	-3.755124	15.977463	H	3.334543	-0.474597	21.811465



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C	1.444244	4.972027	19.784998	C	-2.270238	3.468424	21.159118
C	2.300630	3.831440	19.391951	C	-2.012450	1.630187	22.302484
N	1.937245	2.499994	19.619210	N	-1.352854	2.482594	21.511611
C	3.595543	3.856906	18.963226	H	-4.680080	4.847467	21.163699
C	2.986443	1.743436	19.313999	H	-5.253264	4.021455	22.624984
N	4.032969	2.537179	18.925996	H	-3.987018	1.568969	23.088818
H	0.381265	4.723574	19.744632	H	-2.004672	4.278957	20.498962
H	1.634212	5.845138	19.157811	H	-1.606818	0.728603	22.728496
H	1.715167	5.225326	20.815386	C	-8.403078	-3.803505	17.832919
H	4.237144	4.675457	18.686089	C	-8.185024	-3.125548	19.159904
H	3.052442	0.671574	19.353431	O	-8.603970	-1.993581	19.415106
C	8.736141	3.618212	19.847249	O	-7.488760	-3.857965	20.023178
C	7.711478	2.696342	19.264282	H	-7.437684	-4.111669	17.420275
C	8.073263	1.430428	18.746378	H	-8.901722	-3.121041	17.145711
C	6.358641	3.036745	19.282238	C	-10.789516	-3.256945	22.727626
C	7.128458	0.543344	18.290788	C	-10.544949	-1.960922	23.413411
C	5.383829	2.157939	18.832007	N	-9.295468	-1.384870	23.458550
C	5.724430	0.850432	18.310697	C	-11.368926	-1.073711	24.076649
O	4.829492	0.043617	17.888348	C	-9.391766	-0.205769	24.126886
H	8.415768	4.661267	19.781142	N	-10.642882	0.023163	24.521778
H	9.701295	3.504896	19.346448	H	-10.683953	-3.154854	21.641633
H	9.124675	1.156365	18.722230	H	-11.799567	-3.610525	22.944901
H	6.060696	3.990218	19.702350	H	-8.448160	-1.826690	23.071728
H	7.422311	-0.425275	17.901777	H	-12.432729	-1.165369	24.255294
C	-4.347554	1.085209	17.170526	H	-8.538794	0.436294	24.300504
C	-2.941160	1.111024	17.629151	C	-0.036228	-7.457798	24.053879
N	-1.860433	1.142176	16.767161	C	0.666544	-6.402033	23.278642
C	-2.397268	1.190620	18.884444	N	1.744192	-6.659187	22.445001
C	-0.719977	1.248124	17.489573	C	0.437959	-5.052814	23.149652
N	-1.018861	1.279229	18.785579	C	2.133771	-5.513530	21.847397
H	-4.991031	0.689820	17.958171	N	1.354571	-4.515969	22.258497
H	-4.467841	0.466467	16.277767	H	-0.383521	-8.257567	23.390375
H	-1.915769	1.099454	15.759248	H	-0.906555	-7.019388	24.546487
H	-2.899351	1.200530	19.833945	H	2.166251	-7.564711	22.294890
H	0.267601	1.306416	17.059404	H	-0.307710	-4.441097	23.629634
C	-4.809999	3.871073	21.635752	H	2.953546	-5.434873	21.151106
C	-3.489776	3.191907	21.736605	C	-7.341350	-2.814733	29.426135
N	-3.292320	2.030074	22.460441	N	-6.390658	-1.898940	30.022863

C	-5.671464	-1.019322	29.317606	H	5.908316	-4.912248	16.553065
N	-5.686980	-1.036696	27.990010	Cu	0.139371	2.026772	20.252458
N	-4.926458	-0.099110	29.965972	H	8.891071	3.392424	20.913364
H	-6.844906	-3.463049	28.700831	H	-4.673318	2.104940	16.938341
H	-8.158244	-2.282018	28.929618	H	-5.531463	3.294706	21.032081
H	-6.426601	-1.761971	31.020688	H	-9.006492	-4.710138	17.956795
H	-6.383979	-1.558193	27.457124	H	-10.071120	-4.017666	23.050777
H	-5.162582	-0.300855	27.502934	H	0.595653	-7.919075	24.825693
H	-4.714804	-0.306502	30.932175	H	-7.746921	-3.426171	30.227400
H	-4.143593	0.315297	29.431630	O	1.689801	-0.087459	21.592372
Fe	1.607919	-2.463136	21.818636	O	1.046371	1.252377	23.922334
C	-1.381624	-1.740245	23.390232	O	-6.866430	0.073837	20.322592
C	-0.002198	-2.372889	18.770706	H	-7.017699	0.666233	19.571960
C	4.610938	-2.867475	20.200846	H	-7.457171	-0.681195	20.123803
C	3.266226	-1.923563	24.771428	O	-7.422575	-2.308200	26.028767
N	1.033860	-1.962504	23.742236	H	-6.947098	-2.089568	25.186929
C	-0.248071	-1.740555	24.190582	H	-8.279890	-1.873120	25.917248
C	-0.219520	-1.432359	25.608766	O	-5.019496	0.874493	24.227734
C	1.108911	-1.456409	25.993887	H	-4.599862	0.847130	25.128671
C	1.879908	-1.802215	24.813773	H	-5.326505	-0.043145	24.066438
C	1.681761	-1.170273	27.335112	H	-7.369928	-3.356707	20.923388
O	-2.889195	-2.283224	17.604577	H	-2.033048	0.657314	25.298602
C	-1.401715	-1.079661	26.438470	H	-0.901184	1.012055	26.620043
C	-1.766618	0.412310	26.326700	H	-1.198375	-1.307459	27.486138
C	-2.930519	0.734536	27.258681	H	-2.262537	-1.684630	26.139494
O	-2.692651	0.773422	28.498176	H	2.263629	-2.022549	27.702211
O	-4.088505	0.898026	26.743767	H	2.359915	-0.310827	27.295405
N	2.195265	-2.612680	19.858244	H	0.898584	-0.950137	28.061267
C	1.370918	-2.558248	18.752014	H	-2.321294	-1.551793	23.892610
C	2.159205	-2.742021	17.548543	H	3.780284	-1.772531	25.710984
C	3.462514	-2.942769	17.951155	H	5.801254	-2.284386	25.799644
C	3.478125	-2.830993	19.398073	H	8.163913	-1.940444	25.846599
C	1.602451	-2.696360	16.170787	H	8.257747	-1.906050	23.996233
N	3.583717	-2.386650	22.382369	H	7.808303	-3.521486	22.558920
C	4.671434	-2.653048	21.573775	H	7.216482	-3.445913	20.888457
C	5.881526	-2.642178	22.359121	H	7.803131	-1.985061	21.694707
C	5.505871	-2.349421	23.668001	H	5.544870	-3.015857	19.679790
C	4.055609	-2.207749	23.662712	H	4.333988	-3.081646	16.036789
C	7.244767	-2.917451	21.842315	H	4.224434	-5.360611	16.908577
C	6.326678	-2.222877	24.849531	H	5.327093	-4.945864	18.237272
C	7.656703	-2.021435	24.889086	H	2.392819	-2.660199	15.420580
N	-0.358965	-2.168059	21.189507	H	0.979825	-3.575339	15.967887
C	-0.806467	-2.198849	19.893383	H	0.966217	-1.815215	16.042047
C	-2.235102	-1.952497	19.882232	H	-0.514653	-2.354760	17.819372
C	-2.620491	-1.736584	21.201673	H	-4.172685	-1.610112	19.016934
C	-1.436262	-1.899894	22.006454	H	-4.480662	-0.711815	21.060268
C	-3.148574	-1.941491	18.760529	H	-3.866596	-0.916254	22.687197
C	-3.965118	-1.407911	21.723227	H	-4.265683	-3.416635	22.448985
C	-4.834814	-2.654339	21.905775	H	-5.109159	-3.074066	20.938639
C	-6.070781	-2.363742	22.737682	H	5.426756	-1.512852	17.540180
O	-7.197692	-2.793308	22.321924	H	0.713679	0.654788	24.610131
O	-5.921804	-1.738792	23.825816	H	1.423663	0.305338	22.458061
C	4.639279	-3.251999	17.077158	H	2.639574	0.097990	21.561847
O	5.772760	-2.430324	17.376643	H	0.344181	1.911260	23.804013
C	5.053150	-4.712892	17.205798				

Fe<sub>a3</sub><sup>HS,3+</sup>-H<sub>2</sub>O-Cu<sub>B</sub><sup>2+</sup>(b):

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C	1.444534	4.961461	19.788312	C	-10.542964	-1.961514	23.395512
C	2.309683	3.828247	19.391203	N	-9.288173	-1.395909	23.422219
N	1.947204	2.492379	19.583862	C	-11.352105	-1.063148	24.061556
C	3.608517	3.866350	18.973475	C	-9.366785	-0.212576	24.085627
C	3.001490	1.744642	19.269060	N	-10.611528	0.029324	24.492536
N	4.050171	2.549363	18.908147	H	-10.727131	-3.180162	21.643620
H	0.384938	4.701171	19.753303	H	-11.804349	-3.621419	22.983820
H	1.622433	5.835331	19.157339	H	-8.445675	-1.852904	23.042184
H	1.715167	5.225326	20.815386	H	-12.414335	-1.145283	24.253745
H	4.249568	4.693212	18.719108	H	-8.507085	0.423037	24.248623
H	3.069322	0.670916	19.279056	C	-0.036248	-7.415069	24.078531
C	8.746643	3.633333	19.849931	C	0.673475	-6.354037	23.314699
C	7.728949	2.717020	19.247303	N	1.771261	-6.607143	22.506874
C	8.097606	1.464052	18.704239	C	0.424588	-5.011008	23.155705
C	6.374738	3.050050	19.273867	C	2.152737	-5.465994	21.894444
C	7.156384	0.582124	18.230522	N	1.348983	-4.473902	22.270929
C	5.403372	2.176850	18.805360	H	-0.414461	-8.186222	23.397819
C	5.751500	0.884480	18.254545	H	-0.888467	-6.971987	24.597482
O	4.861506	0.083601	17.812564	H	2.215736	-7.506823	22.390366
H	8.423645	4.676429	19.794980	H	-0.341203	-4.403419	23.608450
H	9.716287	3.529072	19.356174	H	2.988522	-5.385257	21.217985
H	9.150339	1.195728	18.674769	C	-7.338003	-2.816517	29.426626
H	6.072886	3.992862	19.714655	N	-6.360328	-1.925984	30.019435
H	7.453577	-0.376661	17.820152	C	-5.662679	-1.026157	29.317364
C	-4.350645	1.084685	17.170148	N	-5.713762	-1.008958	27.991284
C	-2.942422	1.109740	17.622296	N	-4.905432	-0.118672	29.969804
N	-1.865518	1.149988	16.756251	H	-6.865252	-3.468324	28.688621
C	-2.394588	1.185105	18.875600	H	-8.149438	-2.261132	28.946054
C	-0.722809	1.257507	17.475362	H	-6.374440	-1.808138	31.020227
N	-1.017028	1.282017	18.772009	H	-6.402037	-1.542366	27.458626
H	-4.991514	0.692460	17.961677	H	-5.187752	-0.273199	27.507399
H	-4.476680	0.464722	16.279013	H	-4.681687	-0.342540	30.929466
H	-1.924054	1.110320	15.748637	H	-4.130433	0.307203	29.433980
H	-2.894292	1.186833	19.826161	Fe	1.601428	-2.413678	21.821893
H	0.262934	1.320458	17.042075	C	-1.396061	-1.730352	23.380680
C	-4.799394	3.860540	21.633616	C	0.009404	-2.300048	18.760877
C	-3.483652	3.171304	21.727703	C	4.612762	-2.811378	20.214068
N	-3.285249	2.012425	22.457346	C	3.245233	-1.911183	24.784821
C	-2.265607	3.442024	21.144449	N	1.019924	-1.926326	23.737953
C	-2.005495	1.610758	22.297314	C	-0.265942	-1.719970	24.184671
N	-1.347746	2.457924	21.499704	C	-0.244080	-1.431949	25.607059
H	-4.662233	4.836547	21.162660	C	1.082611	-1.461729	25.998498
H	-5.235451	4.014040	22.625615	C	1.859778	-1.785048	24.817513
H	-3.974493	1.553229	23.090470	C	1.652842	-1.202136	27.346296
H	-2.001711	4.248194	20.477915	O	-2.869418	-2.271354	17.587347
H	-1.599290	0.712364	22.728920	C	-1.428323	-1.083589	26.435667
C	-8.411990	-3.794024	17.852618	C	-1.779186	0.412594	26.333075
C	-8.185300	-3.141723	19.191980	C	-2.930210	0.753533	27.274846
O	-8.601895	-2.014375	19.471659	O	-2.678654	0.794982	28.511379
O	-7.481209	-3.889953	20.036299	O	-4.091242	0.935719	26.772201
H	-7.447442	-4.083322	17.424256	N	2.202054	-2.529390	19.858657
H	-8.921153	-3.099457	17.185652	C	1.385046	-2.470485	18.747404
C	-10.802353	-3.266540	22.733722	C	2.179456	-2.658193	17.547808

C	3.477488	-2.877291	17.958234	H	-6.959643	-2.099503	25.200816
C	3.485877	-2.760861	19.404885	H	-8.292273	-1.845049	25.919101
C	1.633808	-2.611367	16.165548	O	-4.993804	0.835806	24.252507
N	3.573704	-2.339875	22.393038	H	-4.584181	0.827620	25.158482
C	4.664784	-2.611799	21.589582	H	-5.298492	-0.083375	24.099461
C	5.867899	-2.638456	22.384720	H	-7.357041	-3.400753	20.942756
C	5.487244	-2.356683	23.695003	H	-2.047786	0.662693	25.306831
C	4.039990	-2.187350	23.678881	H	-0.903931	0.999802	26.622545
C	7.229355	-2.938054	21.876406	H	-1.229788	-1.323170	27.481633
C	6.298345	-2.267618	24.886735	H	-2.291359	-1.679943	26.126864
C	7.635792	-2.127542	24.947701	H	2.222509	-2.067572	27.702069
N	-0.359301	-2.126580	21.180087	H	2.342580	-0.351380	27.321023
C	-0.802083	-2.154372	19.882058	H	0.869928	-0.983700	28.073026
C	-2.236799	-1.942089	19.870245	H	-2.340323	-1.559588	23.880590
C	-2.630277	-1.746063	21.190240	H	3.751542	-1.779420	25.731550
C	-1.444151	-1.887688	21.996212	H	5.757542	-2.304869	25.829298
C	-3.145056	-1.946692	18.744619	H	8.129330	-2.065343	25.913575
C	-3.980360	-1.440706	21.713046	H	8.258028	-2.041899	24.065900
C	-4.819977	-2.702227	21.934264	H	7.762681	-3.586823	22.577145
C	-6.060104	-2.411447	22.761627	H	7.199566	-3.429912	20.903283
O	-7.186301	-2.838357	22.339586	H	7.819834	-2.019628	21.772041
O	-5.915361	-1.784473	23.849177	H	5.548114	-2.970241	19.698595
C	4.651967	-3.216263	17.090810	H	4.351669	-3.052724	16.047620
O	5.799190	-2.411818	17.383149	H	4.204029	-5.320670	16.949499
C	5.043158	-4.681529	17.235577	H	5.318903	-4.905757	18.268430
H	5.892946	-4.900166	16.581986	H	2.431547	-2.564080	15.423686
Cu	0.154636	1.995377	20.249767	H	1.023479	-3.496477	15.951213
H	8.891071	3.392424	20.913364	H	0.990071	-1.735870	16.034648
H	-4.673318	2.104940	16.938341	H	-0.498939	-2.279692	17.807289
H	-5.531463	3.294706	21.032081	H	-4.180249	-1.648656	18.998317
H	-9.006492	-4.710138	17.956795	H	-4.518142	-0.772891	21.038822
H	-10.071120	-4.017666	23.050777	H	-3.886256	-0.923069	22.663770
H	0.595653	-7.919075	24.825693	H	-4.232315	-3.435962	22.496198
H	-7.746921	-3.426171	30.227400	H	-5.087391	-3.153683	20.979567
O	1.592276	0.043117	21.594969	H	5.466913	-1.485035	17.513061
O	1.010200	1.275080	23.994155	H	0.711399	0.647426	24.672054
O	-6.870510	0.052929	20.423122	H	1.371255	0.402222	22.487529
H	-7.014564	0.637980	19.665151	H	2.509543	0.327935	21.472099
H	-7.458040	-0.704159	20.222996	H	0.287306	1.915229	23.916033
O	-7.444533	-2.294901	26.043566				

$\text{Fe}_{\text{a}3}^{\text{HS},3+}\text{-H}_2\text{O-Cu}_{\text{B}}^{2+}(\text{c}):$

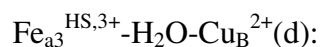
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C	1.369541	4.786186	19.870285	H	4.190059	4.541526	18.794858
C	2.270378	3.659375	19.517004	H	3.105679	0.519529	19.524623
N	1.942352	2.322551	19.742774	C	8.739373	3.578699	19.839445
C	3.565878	3.711714	19.080643	C	7.719281	2.638268	19.276064
C	3.007826	1.588597	19.445371	C	8.092023	1.412124	18.686102
N	4.032417	2.403420	19.044189	C	6.357216	2.929929	19.370622
H	0.340021	4.449155	19.994104	C	7.151664	0.518379	18.223917
H	1.394596	5.570282	19.109346	C	5.390856	2.050012	18.904403
H	1.715167	5.225326	20.815386	C	5.743772	0.786801	18.297785

O	4.856187	-0.018231	17.845955	C	-5.632779	-1.045624	29.360234
H	8.415769	4.618716	19.737547	N	-5.559082	-1.130579	28.034780
H	9.705674	3.454981	19.343840	N	-4.909604	-0.114824	30.014035
H	9.148118	1.167383	18.605169	H	-6.745377	-3.502695	28.766057
H	6.045137	3.854391	19.843348	H	-8.096224	-2.344962	28.860514
H	7.458755	-0.421648	17.778260	H	-6.492919	-1.725313	31.043992
C	-4.305581	1.141437	17.312127	H	-6.268285	-1.623004	27.490498
C	-2.909295	1.247477	17.797582	H	-5.030465	-0.390146	27.556181
N	-1.817806	1.390453	16.959103	H	-4.758397	-0.281663	30.999003
C	-2.381480	1.238599	19.064266	H	-4.103050	0.287812	29.504983
C	-0.689947	1.472424	17.703601	Fe	1.656003	-2.534545	21.763392
N	-1.005555	1.379382	18.992476	C	-1.296974	-1.533970	23.291273
H	-4.953005	0.823602	18.131021	C	0.074092	-2.271023	18.686436
H	-4.385718	0.406470	16.505636	C	4.660170	-2.860681	20.138303
H	-1.856359	1.438635	15.950631	C	3.360055	-1.619235	24.636761
H	-2.891584	1.141910	20.003302	N	1.131858	-1.643599	23.583558
H	0.299112	1.610904	17.296739	C	-0.158694	-1.477364	24.072443
C	-4.840246	3.882958	21.655303	C	-0.117720	-1.188276	25.487644
C	-3.521799	3.214168	21.812549	C	1.215086	-1.168678	25.851956
N	-3.322865	2.118434	22.634913	C	1.980713	-1.476049	24.666735
C	-2.300940	3.445683	21.220072	C	1.793147	-0.907320	27.197038
C	-2.037127	1.723584	22.526572	O	-2.791370	-2.148927	17.510693
N	-1.380898	2.507677	21.669363	C	-1.298094	-0.932740	26.356022
H	-4.700666	4.854866	21.176619	C	-1.644671	0.563926	26.459245
H	-5.320661	4.039257	22.625789	C	-2.847606	0.751187	27.375116
H	-4.025551	1.665867	23.256915	O	-2.640449	0.758351	28.621219
H	-2.040961	4.194495	20.487970	O	-4.003132	0.839496	26.838154
H	-1.614485	0.881828	23.045870	N	2.251189	-2.550778	19.796313
C	-8.430829	-3.786865	17.819241	C	1.437961	-2.502488	18.678298
C	-8.162487	-3.111723	19.140109	C	2.223291	-2.746840	17.484653
O	-8.604113	-2.000062	19.435921	C	3.518280	-2.971843	17.898766
O	-7.386541	-3.826826	19.954683	C	3.529496	-2.820397	19.339355
H	-7.480057	-4.065951	17.355295	C	1.671873	-2.731845	16.104237
H	-8.979085	-3.109410	17.165743	N	3.634578	-2.247321	22.285698
C	-10.663279	-3.200553	22.620050	C	4.721422	-2.581538	21.494976
C	-10.421387	-1.919681	23.334545	C	5.936145	-2.551943	22.271897
N	-9.176096	-1.335050	23.396570	C	5.575318	-2.172101	23.559368
C	-11.247874	-1.069046	24.041152	C	4.130078	-1.992018	23.546050
C	-9.277890	-0.188659	24.119527	C	7.288949	-2.892223	21.767349
N	-10.528337	0.012433	24.531002	C	6.401845	-2.009943	24.733753
H	-10.389496	-3.120357	21.563324	C	7.741570	-1.889741	24.768050
H	-11.720774	-3.464953	22.686400	N	-0.247276	-1.948051	21.098733
H	-8.323900	-1.758337	22.999786	C	-0.713919	-2.039904	19.805995
H	-12.309970	-1.176247	24.221951	C	-2.148469	-1.843211	19.799188
H	-8.430066	0.453313	24.316935	C	-2.536106	-1.620061	21.116601
C	-0.095562	-7.322460	24.215159	C	-1.342553	-1.709534	21.912627
C	0.600409	-6.325789	23.363034	C	-3.066695	-1.870827	18.679292
N	1.466211	-6.679834	22.340108	C	-3.894249	-1.351171	21.645636
C	0.540588	-4.952834	23.315176	C	-4.666156	-2.646478	21.928662
C	1.896574	-5.572139	21.705793	C	-5.925038	-2.357727	22.729764
N	1.349434	-4.500860	22.281187	O	-7.050976	-2.712912	22.250904
H	-0.671691	-8.017626	23.594478	O	-5.785039	-1.779116	23.846603
H	-0.787215	-6.806400	24.883399	C	4.703869	-3.308951	17.045020
H	1.725708	-7.625470	22.096531	O	5.828351	-2.468274	17.325610
H	-0.019743	-4.270672	23.933512	C	5.127356	-4.762616	17.221364
H	2.574877	-5.570076	20.867842	H	5.987540	-4.974193	16.579299
C	-7.303220	-2.838129	29.430318	Cu	0.181095	1.800421	20.564245
N	-6.415788	-1.878380	30.051242	H	8.891070	3.392423	20.913366



H	-4.673319	2.104940	16.938342	H	3.876065	-1.441050	25.570083
H	-5.531463	3.294705	21.032081	H	5.872715	-1.978714	25.683084
H	-9.006492	-4.710139	17.956797	H	8.252604	-1.782588	25.721372
H	-10.071119	-4.017665	23.050779	H	8.351477	-1.870351	23.874237
H	0.595654	-7.919072	24.825695	H	7.820946	-3.510582	22.496249
H	-7.746919	-3.426170	30.227401	H	7.246713	-3.432390	20.821205
O	0.981065	2.200156	24.728435	H	7.887036	-1.986192	21.613688
O	1.271379	0.958497	22.290683	H	5.590161	-3.049442	19.623992
O	-6.834552	0.218256	20.378445	H	4.403992	-3.175397	15.997790
H	-7.048814	0.787616	19.624995	H	4.306182	-5.426612	16.939332
H	-7.391883	-0.565830	20.217061	H	5.399227	-4.964948	18.259588
O	-7.314454	-2.327296	26.027066	H	2.467314	-2.725931	15.358751
H	-6.831150	-2.113964	25.188198	H	1.043570	-3.611890	15.922900
H	-8.154957	-1.858731	25.923360	H	1.045165	-1.848550	15.947044
O	-5.041026	0.867845	24.359381	H	-0.443846	-2.279834	17.737703
H	-4.580901	0.822953	25.237967	H	-4.110589	-1.626168	18.951626
H	-5.292138	-0.058543	24.158449	H	-4.471174	-0.737639	20.952626
H	-7.241989	-3.320831	20.842398	H	-3.818398	-0.789654	22.573741
H	-1.861078	0.968863	25.470876	H	-4.040643	-3.312335	22.530966
H	-0.792590	1.100348	26.880358	H	-4.904261	-3.157342	20.995655
H	-1.097113	-1.313366	27.360093	H	5.471282	-1.551625	17.487349
H	-2.165044	-1.479451	25.977609	H	1.146325	1.474604	23.121283
H	2.370402	-1.769474	27.547488	H	1.158147	0.033652	22.584681
H	2.477802	-0.052460	27.173907	H	1.730389	2.793697	24.891966
H	1.011256	-0.698110	27.927541	H	1.100497	1.488669	25.375155
H	-2.242673	-1.392597	23.796930				



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C	1.397252	4.789940	19.861394	H	9.194166	1.189629	18.487372
C	2.322801	3.685540	19.503265	H	6.121699	3.831087	19.880587
N	1.975929	2.343919	19.633204	H	7.484730	-0.349375	17.602047
C	3.635015	3.750649	19.117215	C	-4.302788	1.129503	17.271879
C	3.045961	1.615057	19.322162	C	-2.901938	1.246492	17.734674
N	4.089374	2.442479	19.009949	N	-1.829895	1.424664	16.878256
H	0.375783	4.422764	19.969948	C	-2.356065	1.246803	18.991235
H	1.405275	5.582060	19.108027	C	-0.693472	1.537562	17.605077
H	1.715167	5.225326	20.815386	N	-0.986704	1.429743	18.898102
H	4.276245	4.589234	18.905104	H	-4.934144	0.784052	18.092048
H	3.128527	0.541547	19.320477	H	-4.390363	0.421026	16.443452
C	8.812428	3.548034	19.828594	H	-1.886991	1.477934	15.871057
C	7.782181	2.634509	19.238879	H	-2.848322	1.134050	19.938390
C	8.140190	1.435406	18.591565	H	0.285118	1.701490	17.182695
C	6.422922	2.928388	19.360775	C	-4.816729	3.852387	21.659357
C	7.187878	0.570221	18.095183	C	-3.495729	3.176006	21.782062
C	5.447211	2.079566	18.856136	N	-3.277604	2.073464	22.591720
C	5.784277	0.843429	18.192427	C	-2.282878	3.420796	21.176892
O	4.885097	0.060147	17.717978	C	-1.990443	1.688327	22.463680
H	8.544899	4.598197	19.674299	N	-1.350304	2.484091	21.605074
H	9.797981	3.366259	19.393967	H	-4.676786	4.836927	21.206844

H	-5.278674	3.988482	22.641930	C	-2.853696	0.737945	27.372464
H	-3.964725	1.613602	23.224576	O	-2.632600	0.768638	28.615138
H	-2.035052	4.175328	20.446656	O	-4.015422	0.844015	26.849886
H	-1.557807	0.847445	22.976391	N	2.264337	-2.458646	19.842546
C	-8.416070	-3.794971	17.835523	C	1.444872	-2.415779	18.729373
C	-8.193763	-3.129114	19.168444	C	2.223163	-2.663923	17.532533
O	-8.695907	-2.046532	19.475812	C	3.519492	-2.893716	17.940591
O	-7.394178	-3.821077	19.978842	C	3.540121	-2.733957	19.381031
H	-7.454096	-4.083305	17.402508	C	1.663020	-2.661042	16.155545
H	-8.939869	-3.112483	17.167165	N	3.652067	-2.226927	22.342434
C	-10.678844	-3.198569	22.646775	C	4.738959	-2.531525	21.540376
C	-10.428880	-1.924879	23.372010	C	5.951439	-2.521911	22.319276
N	-9.180841	-1.346321	23.427149	C	5.587310	-2.183971	23.619157
C	-11.247282	-1.070198	24.083581	C	4.140376	-2.014029	23.612713
C	-9.272191	-0.199901	24.150959	C	7.305714	-2.844892	21.807845
N	-10.519357	0.007687	24.569525	C	6.409704	-2.063915	24.799980
H	-10.427355	-3.100876	21.585763	C	7.751714	-1.970311	24.846908
H	-11.732927	-3.471116	22.730880	N	-0.254815	-1.978245	21.166017
H	-8.333017	-1.778323	23.029961	C	-0.713653	-2.022607	19.870187
H	-12.309397	-1.170484	24.267940	C	-2.148204	-1.830120	19.865824
H	-8.418977	0.436195	24.344281	C	-2.538627	-1.647723	21.188299
C	-0.066741	-7.334318	24.169566	C	-1.346933	-1.765431	21.986942
C	0.642518	-6.319391	23.344845	C	-3.056132	-1.823310	18.737367
N	1.506874	-6.648277	22.311779	C	-3.895981	-1.378519	21.714565
C	0.584120	-4.946173	23.328280	C	-4.693290	-2.666821	21.952027
C	1.937365	-5.523986	21.705354	C	-5.949667	-2.386264	22.758473
N	1.391042	-4.465162	22.304322	O	-7.077607	-2.749665	22.288936
H	-0.595112	-8.042933	23.522606	O	-5.807305	-1.811901	23.876764
H	-0.805213	-6.830531	24.795823	C	4.688588	-3.260594	17.077166
H	1.766979	-7.587378	22.043771	O	5.828115	-2.432672	17.328078
H	0.021613	-4.281267	23.962601	C	5.091709	-4.717381	17.271833
H	2.616264	-5.502100	20.867680	H	5.935684	-4.955059	16.617402
C	-7.303112	-2.838663	29.429406	Cu	0.203991	1.831222	20.459645
N	-6.397170	-1.893222	30.047317	H	8.891071	3.392424	20.913365
C	-5.634629	-1.047059	29.347742	H	-4.673318	2.104940	16.938341
N	-5.571326	-1.129749	28.022590	H	-5.531462	3.294705	21.032081
N	-4.919166	-0.105390	29.995463	H	-9.006491	-4.710139	17.956796
H	-6.757484	-3.505639	28.758197	H	-10.071119	-4.017666	23.050778
H	-8.095231	-2.334530	28.867587	H	0.595655	-7.919073	24.825695
H	-6.501575	-1.708935	31.032538	H	-7.746920	-3.426170	30.227401
H	-6.276949	-1.630911	27.480883	O	0.890989	1.651365	24.505504
H	-5.044723	-0.388907	27.543174	O	1.396133	0.790915	21.982093
H	-4.760076	-0.267608	30.979888	O	-6.895027	0.157463	20.356156
H	-4.118131	0.303370	29.484390	H	-7.096271	0.709678	19.586355
Fe	1.668774	-2.453463	21.820089	H	-7.470143	-0.617852	20.217625
C	-1.294508	-1.617734	23.369492	O	-7.337099	-2.343886	26.035949
C	0.077537	-2.203279	18.743602	H	-6.851137	-2.132519	25.197230
C	4.674267	-2.782211	20.176202	H	-8.175929	-1.872969	25.930456
C	3.363195	-1.695681	24.717396	O	-4.956615	0.807455	24.352812
N	1.129720	-1.775064	23.690630	H	-4.524713	0.783132	25.248513
C	-0.155602	-1.583088	24.156894	H	-5.235027	-0.115695	24.176831
C	-0.121935	-1.281482	25.574966	H	-7.269448	-3.327811	20.876900
C	1.210682	-1.262391	25.944846	H	-1.905693	0.843672	25.438187
C	1.978748	-1.587463	24.759564	H	-0.813067	1.075438	26.811868
C	1.790619	-0.963895	27.281714	H	-1.101945	-1.312263	27.452444
O	-2.770455	-2.086062	17.567727	H	-2.165663	-1.567791	26.078321
C	-1.305123	-0.991955	26.428313	H	2.377371	-1.811038	27.652092
C	-1.668039	0.504532	26.445587	H	2.466837	-0.103476	27.232829

H	1.009717	-0.740020	28.008995	H	1.037453	-3.545357	15.985070
H	-2.237791	-1.464539	23.876812	H	1.031287	-1.781494	15.996633
H	3.881580	-1.522932	25.650563	H	-0.442931	-2.197544	17.796290
H	5.873927	-2.044679	25.745689	H	-4.100549	-1.570026	19.001391
H	8.254771	-1.890330	25.806639	H	-4.455386	-0.735172	21.033457
H	8.370810	-1.945961	23.959823	H	-3.816762	-0.844789	22.658034
H	7.826256	-3.507566	22.505884	H	-4.084757	-3.363418	22.537381
H	7.267058	-3.330215	20.832448	H	-4.935111	-3.145074	21.003093
H	7.913111	-1.937287	21.710032	H	5.487125	-1.502740	17.440040
H	5.601330	-2.964950	19.654495	H	1.217298	1.088993	22.910899
H	4.375594	-3.140560	16.031957	H	2.293806	1.108337	21.807266
H	4.253653	-5.371570	17.017800	H	1.613848	2.239166	24.774799
H	5.380006	-4.905396	18.308245	H	0.976766	0.877523	25.085893
H	2.452886	-2.658022	15.403913				

## Cartesian Coordinates of the Geometry Optimized DNC Clusters Listed in Table 2:

### S1:

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C	1.632904	5.049975	19.740369	H	-1.946114	1.258715	15.707315
C	2.469769	3.876455	19.403964	H	-2.787294	1.174496	19.813186
N	2.034523	2.555830	19.560396	H	0.271508	1.500964	16.937138
C	3.785491	3.855538	19.044025	C	-4.790067	3.841735	21.642925
C	3.062547	1.762769	19.269334	C	-3.450709	3.188131	21.682253
N	4.163245	2.519019	18.966631	N	-3.184805	2.046810	22.419401
H	0.582321	4.889450	19.487013	C	-2.259574	3.499784	21.063394
H	1.993479	5.942086	19.223832	C	-1.893044	1.697792	22.234882
H	1.715167	5.225326	20.815386	N	-1.293313	2.560746	21.409592
H	4.474229	4.655420	18.833998	H	-4.686816	4.843456	21.219396
H	3.075557	0.687600	19.262885	H	-5.204916	3.936641	22.651207
C	8.913892	3.411612	19.815927	H	-3.848815	1.565801	23.061296
C	7.851616	2.518788	19.256322	H	-2.043017	4.309329	20.383286
C	8.155966	1.249140	18.717680	H	-1.433209	0.831545	22.679764
C	6.512468	2.907841	19.309533	C	-8.348167	-3.836882	17.854669
C	7.167538	0.405011	18.268903	C	-8.123159	-3.158057	19.182518
C	5.495692	2.078590	18.860307	O	-8.471914	-1.997447	19.411499
C	5.777993	0.768443	18.309643	O	-7.497143	-3.922332	20.075127
O	4.847685	0.003838	17.883114	H	-7.389809	-4.197563	17.468419
H	8.750732	4.451598	19.515164	H	-8.787768	-3.129253	17.152685
H	9.908914	3.097899	19.493437	C	-10.802554	-3.254726	22.766642
H	9.195021	0.933962	18.671516	C	-10.536242	-1.977120	23.476172
H	6.262368	3.865090	19.751837	N	-9.293640	-1.383427	23.476629
H	7.416772	-0.570296	17.866618	C	-11.335317	-1.132371	24.219698
C	-4.326148	1.101650	17.204643	C	-9.370325	-0.237617	24.204862
C	-2.904844	1.163307	17.611407	N	-10.601538	-0.045573	24.674084
N	-1.857433	1.264268	16.713674	H	-10.737953	-3.128047	21.679708
C	-2.319107	1.218234	18.848219	H	-11.802520	-3.617597	23.013774
C	-0.696164	1.387791	17.400349	H	-8.451050	-1.812951	23.065620
N	-0.949281	1.363012	18.706405	H	-12.386683	-1.248787	24.449955
H	-4.935440	0.736815	18.033467	H	-8.519598	0.411250	24.361629
H	-4.473824	0.440284	16.346949	C	-0.058616	-7.415893	24.099082

C	0.639349	-6.369496	23.306111	C	-3.146803	-1.909023	18.725503
N	1.674759	-6.649341	22.427554	C	-3.964168	-1.411911	21.698682
C	0.440646	-5.013439	23.194281	C	-4.799924	-2.672437	21.946142
C	2.070166	-5.512065	21.820330	C	-6.041248	-2.368350	22.770297
N	1.334517	-4.495539	22.267993	O	-7.170203	-2.789640	22.349926
H	-0.469681	-8.187331	23.438418	O	-5.892519	-1.734123	23.853825
H	-0.885251	-6.958677	24.646221	C	4.627919	-3.312136	17.055679
H	2.067393	-7.564626	22.257628	O	5.761354	-2.483316	17.336738
H	-0.271241	-4.384423	23.703619	C	5.043945	-4.769389	17.214403
H	2.862479	-5.452305	21.091579	H	5.902502	-4.977950	16.569107
C	-7.354593	-2.797064	29.434005	Cu	0.219952	2.094887	20.180807
N	-6.461132	-1.836327	30.046512	H	8.891071	3.392423	20.913366
C	-5.695554	-0.987483	29.355158	H	-4.673318	2.104940	16.938341
N	-5.712515	-0.981680	28.026963	H	-5.531463	3.294707	21.032080
N	-4.911961	-0.106848	30.013814	H	-9.006493	-4.710138	17.956797
H	-6.818886	-3.423496	28.716171	H	-10.071122	-4.017664	23.050778
H	-8.184980	-2.300652	28.923171	H	0.595649	-7.919076	24.825697
H	-6.404016	-1.802522	31.051236	H	-7.746924	-3.426167	30.227402
H	-6.410056	-1.491844	27.483607	O	1.649657	0.130554	21.617714
H	-5.167907	-0.254919	27.547607	O	-6.827213	0.111732	20.585179
H	-4.703706	-0.335526	30.975904	H	-6.954391	0.715030	19.838767
H	-4.116912	0.280436	29.474726	H	-7.371950	-0.658748	20.332603
Fe	1.605912	-2.472518	21.777218	O	-7.425146	-2.246759	26.050565
C	-1.366227	-1.653200	23.344142	H	-6.938362	-2.045306	25.210630
C	-0.001729	-2.333307	18.728112	H	-8.272705	-1.795964	25.927238
C	4.595512	-2.913679	20.172657	O	-4.885753	0.849770	24.203599
C	3.278299	-1.864772	24.727158	H	-4.514757	0.841367	25.125790
N	1.057782	-1.809365	23.669846	H	-5.227192	-0.058354	24.060581
C	-0.229299	-1.617690	24.134697	H	-7.356706	-3.404640	20.961426
C	-0.200925	-1.360924	25.559721	H	-2.010091	0.731100	25.323501
C	1.124521	-1.395405	25.945194	H	-0.889650	1.032920	26.664301
C	1.898625	-1.694218	24.758556	H	-1.187715	-1.320657	27.436734
C	1.695457	-1.168178	27.298415	H	-2.244839	-1.643853	26.071850
O	-2.883684	-2.207443	17.558570	H	2.260025	-2.043282	27.638785
C	-1.386672	-1.049355	26.398605	H	2.389103	-0.320145	27.290690
C	-1.753748	0.445628	26.343881	H	0.912437	-0.959786	28.028156
C	-2.922244	0.724621	27.280606	H	-2.307547	-1.480851	23.848583
O	-2.691073	0.705347	28.522524	H	3.790166	-1.740575	25.671994
O	-4.076954	0.915824	26.767429	H	5.775803	-2.330926	25.771062
N	2.186831	-2.603262	19.822879	H	8.155555	-2.198592	25.848103
C	1.367570	-2.541348	18.712015	H	8.281533	-2.205271	24.000137
C	2.154533	-2.754427	17.514060	H	7.725573	-3.744353	22.527419
C	3.452631	-2.979068	17.922363	H	7.169287	-3.569715	20.853354
C	3.467266	-2.853187	19.367050	H	7.835108	-2.180224	21.722065
C	1.601623	-2.715074	16.134795	H	5.526485	-3.093547	19.656726
N	3.578958	-2.372664	22.346834	H	4.323062	-3.164214	16.012017
C	4.658913	-2.691309	21.543896	H	4.218263	-5.424751	16.925716
C	5.864402	-2.732092	22.333296	H	5.314875	-4.983339	18.250588
C	5.498290	-2.413241	23.639423	H	2.395128	-2.694914	15.387578
C	4.057761	-2.198067	23.625348	H	0.971574	-3.590268	15.937874
C	7.214717	-3.078546	21.825807	H	0.975269	-1.828168	15.996461
C	6.315530	-2.332282	24.827112	H	-0.516801	-2.317089	17.777841
C	7.657735	-2.249657	24.883548	H	-4.178590	-1.612152	18.993936
N	-0.343735	-2.101477	21.146904	H	-4.511927	-0.753891	21.023360
C	-0.799280	-2.146918	19.851681	H	-3.862389	-0.881781	22.641172
C	-2.231314	-1.922344	19.846139	H	-4.208569	-3.392425	22.521829
C	-2.616255	-1.715510	21.167673	H	-5.068415	-3.145052	21.001541
C	-1.424047	-1.841964	21.965132	H	5.414784	-1.569030	17.510193

H 1.463727 0.066390 22.569339

H 2.566396 0.443528 21.593278

**S2:**

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C 1.552756 4.962280 19.764460  
C 2.420456 3.807357 19.434818  
N 2.020011 2.481452 19.620189  
C 3.730922 3.808472 19.052007  
C 3.061707 1.704037 19.339121  
N 4.137642 2.478645 18.999216  
H 0.496151 4.726692 19.618106  
H 1.811260 5.831333 19.155044  
H 1.715167 5.225326 20.815386  
H 4.399892 4.616949 18.812120  
H 3.098842 0.629838 19.381944  
C 8.873165 3.462602 19.817420  
C 7.826435 2.551419 19.260160  
C 8.153655 1.293618 18.708888  
C 6.479395 2.909703 19.330772  
C 7.180222 0.433495 18.258211  
C 5.478190 2.064710 18.878928  
C 5.784273 0.770075 18.305429  
O 4.870269 -0.003571 17.861571  
H 8.658223 4.506959 19.570212  
H 9.867356 3.203471 19.447091  
H 9.198929 1.001982 18.650967  
H 6.210925 3.856461 19.784869  
H 7.446391 -0.531844 17.841637  
C -4.314649 1.099426 17.190942  
C -2.901692 1.162655 17.629631  
N -1.837072 1.262290 16.753218  
C -2.338402 1.209946 18.878177  
C -0.688280 1.378575 17.461496  
N -0.964968 1.349260 18.762333  
H -4.936868 0.705119 17.996185  
H -4.434470 0.456421 16.314990  
H -1.906517 1.262294 15.745187  
H -2.824994 1.162962 19.833893  
H 0.288432 1.487370 17.016863  
C -4.797168 3.857914 21.632755  
C -3.467363 3.191234 21.699547  
N -3.228089 2.050379 22.446871  
C -2.266416 3.479426 21.089558  
C -1.939327 1.682343 22.279456  
N -1.319347 2.529509 21.454185  
H -4.683193 4.845037 21.179150  
H -5.221377 3.985796 22.633514  
H -3.902653 1.581412 23.086804  
H -2.031236 4.278070 20.402961  
H -1.495166 0.812722 22.732466  
C -8.359777 -3.831529 17.839889  
C -8.099255 -3.147522 19.158657  
O -8.381272 -1.965435 19.370030  
O -7.516568 -3.931452 20.062672

H -7.407574 -4.184058 17.430463  
H -8.818166 -3.127130 17.146718  
C -10.801370 -3.257658 22.755404  
C -10.532336 -1.967758 23.442189  
N -9.283829 -1.386097 23.447416  
C -11.332148 -1.100022 24.157946  
C -9.357973 -0.225292 24.150629  
N -10.592969 -0.011272 24.599933  
H -10.738155 -3.150313 21.666079  
H -11.801820 -3.614583 23.009202  
H -8.441852 -1.825222 23.046493  
H -12.387738 -1.200184 24.376184  
H -8.501135 0.415663 24.307905  
C -0.077728 -7.398151 24.133500  
C 0.623427 -6.370875 23.321997  
N 1.638651 -6.676234 22.428716  
C 0.450409 -5.012804 23.209474  
C 2.048013 -5.552368 21.809471  
N 1.338988 -4.519416 22.264584  
H -0.535562 -8.154303 23.486544  
H -0.867481 -6.920057 24.715834  
H 2.009042 -7.600610 22.257517  
H -0.237467 -4.365835 23.729350  
H 2.829069 -5.512216 21.067351  
C -7.361043 -2.794408 29.431488  
N -6.467342 -1.829382 30.037229  
C -5.705250 -0.981034 29.341872  
N -5.710392 -0.993361 28.013543  
N -4.933513 -0.085330 29.995824  
H -6.825628 -3.418562 28.711910  
H -8.196012 -2.301052 28.925054  
H -6.432835 -1.768076 31.041996  
H -6.406239 -1.508588 27.473187  
H -5.172964 -0.262214 27.533336  
H -4.729912 -0.304803 30.961273  
H -4.130673 0.291302 29.460301  
Fe 1.607202 -2.527622 21.772380  
C -1.352798 -1.627547 23.331025  
C -0.006847 -2.343152 18.717195  
C 4.599750 -2.878746 20.145181  
C 3.298704 -1.802059 24.692619  
N 1.075874 -1.757104 23.633857  
C -0.213042 -1.581095 24.113230  
C -0.178564 -1.323157 25.536030  
C 1.149415 -1.344747 25.913072  
C 1.920423 -1.636047 24.723904  
C 1.727351 -1.116907 27.263191  
O -2.914367 -2.246958 17.565029  
C -1.364157 -1.027492 26.383154  
C -1.763382 0.459011 26.326685

C	-2.924989	0.724401	27.277401	O	-6.766743	0.102456	20.581749
O	-2.685808	0.689922	28.517190	H	-6.887418	0.711763	19.838844
O	-4.083261	0.927013	26.775498	H	-7.307628	-0.667259	20.314685
N	2.188734	-2.579512	19.808481	O	-7.419022	-2.293740	26.037383
C	1.363881	-2.539511	18.700199	H	-6.933745	-2.080700	25.199253
C	2.145017	-2.761843	17.500125	H	-8.271249	-1.851473	25.916457
C	3.447376	-2.967805	17.902900	O	-4.933634	0.860776	24.238415
C	3.467505	-2.827005	19.345824	H	-4.542234	0.849212	25.153188
C	1.577659	-2.759057	16.125919	H	-5.250951	-0.054031	24.085285
N	3.584833	-2.331296	22.317607	H	-7.355111	-3.411190	20.943527
C	4.665366	-2.648651	21.513595	H	-2.039364	0.736264	25.309438
C	5.875316	-2.678250	22.296897	H	-0.907947	1.067186	26.631811
C	5.514380	-2.350726	23.600700	H	-1.151907	-1.290839	27.420688
C	4.073272	-2.141012	23.590929	H	-2.213317	-1.640304	26.066284
C	7.223014	-3.027848	21.784588	H	2.299305	-1.989603	27.597153
C	6.336940	-2.263696	24.784716	H	2.415866	-0.264899	27.252606
C	7.679043	-2.176177	24.831507	H	0.947711	-0.915284	27.998333
N	-0.331600	-2.077168	21.133707	H	-2.293082	-1.466554	23.840796
C	-0.798723	-2.145371	19.841653	H	3.811984	-1.669731	25.635509
C	-2.231969	-1.929811	19.841882	H	5.803076	-2.264757	25.732099
C	-2.609061	-1.707157	21.162727	H	8.184168	-2.122793	25.792131
C	-1.412647	-1.818872	21.953301	H	8.295543	-2.130284	23.943221
C	-3.160408	-1.931954	18.731287	H	7.736476	-3.689875	22.487915
C	-3.955290	-1.404926	21.698461	H	7.172698	-3.525165	20.815540
C	-4.793578	-2.666862	21.927636	H	7.843259	-2.130694	21.672426
C	-6.034387	-2.375591	22.756039	H	5.528327	-3.058253	19.624629
O	-7.160239	-2.800276	22.330874	H	4.319276	-3.141842	15.992163
O	-5.889941	-1.750141	23.845116	H	4.177158	-5.412398	16.887362
C	4.621063	-3.306693	17.034417	H	5.286615	-4.998957	18.210726
O	5.768876	-2.500843	17.325354	H	2.362165	-2.756454	15.368996
C	5.014073	-4.772211	17.177538	H	0.949155	-3.641968	15.960278
H	5.866198	-4.988887	16.526250	H	0.945816	-1.878921	15.970481
Cu	0.212207	2.014029	20.270019	H	-0.524699	-2.348104	17.768325
H	8.891071	3.392423	20.913365	H	-4.188171	-1.629455	19.010049
H	-4.673318	2.104939	16.938341	H	-4.501954	-0.737397	21.031464
H	-5.531463	3.294706	21.032080	H	-3.854420	-0.886596	22.647633
H	-9.006491	-4.710139	17.956795	H	-4.203471	-3.397475	22.490949
H	-10.071119	-4.017667	23.050777	H	-5.064080	-3.123936	20.975960
H	0.595652	-7.919075	24.825697	H	5.438244	-1.579357	17.492411
H	-7.746920	-3.426171	30.227400	H	1.271730	-0.023979	22.628715
O	1.466806	0.443843	21.792980	H	2.333138	0.846814	21.944729

### S3:

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C	1.377771	4.772266	19.876456	H	3.110531	0.498647	19.544536
C	2.285209	3.643576	19.549047	C	8.751673	3.566582	19.835734
N	1.954560	2.308365	19.780823	C	7.730100	2.625765	19.275152
C	3.580667	3.691530	19.114159	C	8.100842	1.408015	18.666635
C	3.018750	1.569461	19.478900	C	6.368720	2.909158	19.389804
N	4.043362	2.382257	19.078087	C	7.159174	0.514571	18.206707
H	0.348367	4.434051	19.999644	C	5.401314	2.029302	18.926177
H	1.405699	5.544454	19.103530	C	5.750680	0.774643	18.301512
H	1.715167	5.225326	20.815386	O	4.859494	-0.027682	17.850959
H	4.206025	4.519259	18.825072	H	8.434998	4.607627	19.718360

H	9.721516	3.432011	19.349976	N	-4.905902	-0.110695	30.003019
H	9.157141	1.171898	18.566828	H	-6.754769	-3.489124	28.759601
H	6.057887	3.827481	19.875378	H	-8.107439	-2.335752	28.869823
H	7.466368	-0.416878	17.743287	H	-6.497511	-1.707146	31.039740
C	-4.313153	1.138814	17.310273	H	-6.270464	-1.622799	27.485786
C	-2.915259	1.236896	17.792317	H	-5.025955	-0.395157	27.549806
N	-1.824703	1.375542	16.951231	H	-4.751397	-0.274603	30.987996
C	-2.385864	1.226645	19.057092	H	-4.097438	0.284677	29.491426
C	-0.695995	1.451992	17.694700	Fe	1.656495	-2.520264	21.757133
N	-1.009579	1.361235	18.984840	C	-1.297452	-1.539729	23.287572
H	-4.960393	0.825748	18.131193	C	0.071264	-2.274566	18.682050
H	-4.400695	0.404813	16.503727	C	4.659008	-2.850911	20.134940
H	-1.864289	1.423365	15.942783	C	3.359676	-1.611998	24.636267
H	-2.895868	1.134102	19.997118	N	1.133300	-1.636802	23.577101
H	0.293321	1.583695	17.285929	C	-0.159967	-1.481275	24.069044
C	-4.840002	3.877986	21.661068	C	-0.119992	-1.201026	25.484394
C	-3.520387	3.209916	21.819128	C	1.211610	-1.181125	25.850457
N	-3.316096	2.118469	22.645718	C	1.979939	-1.476823	24.666532
C	-2.301405	3.441698	21.222207	C	1.790332	-0.911703	27.191607
C	-2.030337	1.723368	22.531590	O	-2.780647	-2.159117	17.506440
N	-1.379603	2.504624	21.668467	C	-1.299609	-0.937561	26.350249
H	-4.699470	4.852379	21.187350	C	-1.642736	0.561590	26.443538
H	-5.323357	4.030690	22.630748	C	-2.836427	0.749386	27.372371
H	-4.015723	1.663850	23.270070	O	-2.621236	0.747120	28.617093
H	-2.042721	4.187533	20.486790	O	-3.997314	0.844145	26.846766
H	-1.604230	0.886188	23.055580	N	2.248439	-2.551627	19.792366
C	-8.432397	-3.784510	17.825780	C	1.434883	-2.504520	18.673976
C	-8.160770	-3.116167	19.149763	C	2.220599	-2.748902	17.481855
O	-8.594075	-2.001652	19.447005	C	3.516243	-2.973000	17.895997
O	-7.391966	-3.838876	19.964700	C	3.528295	-2.818852	19.335814
H	-7.482092	-4.058341	17.357619	C	1.670386	-2.732514	16.101319
H	-8.982942	-3.103430	17.177959	N	3.636354	-2.223637	22.282043
C	-10.667013	-3.204235	22.618514	C	4.721999	-2.562454	21.490227
C	-10.424568	-1.920894	23.328204	C	5.936407	-2.534482	22.266494
N	-9.178145	-1.338719	23.389763	C	5.577214	-2.151593	23.554376
C	-11.250012	-1.066853	24.031919	C	4.132645	-1.970138	23.543002
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H	-11.723614	-3.470873	22.689391	N	-0.249926	-1.958983	21.095553
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H	-8.428839	0.449752	24.307158	C	-2.537481	-1.625379	21.112870
C	-0.091128	-7.320333	24.209919	C	-1.343761	-1.716507	21.909052
C	0.605755	-6.321022	23.359056	C	-3.062838	-1.875961	18.672078
N	1.468044	-6.673324	22.331819	C	-3.895981	-1.356108	21.641587
C	0.547617	-4.948926	23.315858	C	-4.666934	-2.651830	21.928490
C	1.899571	-5.564397	21.702282	C	-5.925367	-2.364636	22.731993
N	1.355100	-4.492235	22.280979	O	-7.051645	-2.721241	22.254641
H	-0.665814	-8.014336	23.586768	O	-5.786593	-1.787151	23.849232
H	-0.785248	-6.803592	24.875227	C	4.699287	-3.312410	17.039455
H	1.726429	-7.618235	22.083631	O	5.829116	-2.479828	17.320630
H	-0.011883	-4.268445	23.937539	C	5.115329	-4.768381	17.210889
H	2.576525	-5.560383	20.862706	H	5.970983	-4.983316	16.563974
C	-7.309330	-2.830145	29.431809	Cu	0.169409	1.833783	20.549722
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C	-5.632009	-1.043305	29.353850	H	-4.673319	2.104940	16.938342
N	-5.558759	-1.132568	28.028735	H	-5.531463	3.294706	21.032081

H	-9.006492	-4.710139	17.956798	H	3.873710	-1.440864	25.571959
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H	0.595653	-7.919073	24.825694	H	8.257629	-1.781585	25.714576
H	-7.746919	-3.426170	30.227402	H	8.354342	-1.865679	23.867260
O	1.280747	0.947332	22.347221	H	7.813408	-3.507706	22.493491
O	-6.837749	0.223321	20.402336	H	7.242591	-3.424988	20.817658
H	-7.046861	0.786907	19.642834	H	7.892861	-1.983618	21.611155
H	-7.388957	-0.564728	20.239140	H	5.588571	-3.042516	19.620832
O	-7.322429	-2.327157	26.025847	H	4.398358	-3.173526	15.993153
H	-6.837759	-2.115877	25.187263	H	4.288952	-5.427247	16.932236
H	-8.161089	-1.855572	25.921227	H	5.391725	-4.972620	18.247615
O	-5.030098	0.857303	24.376197	H	2.466529	-2.723015	15.356828
H	-4.567639	0.811981	25.253882	H	1.044419	-3.613675	15.917611
H	-5.280073	-0.068148	24.171066	H	1.041987	-1.850111	15.945985
H	-7.244150	-3.332681	20.851869	H	-0.448100	-2.284068	17.733986
H	-1.873957	0.955952	25.454317	H	-4.107639	-1.627329	18.937574
H	-0.781759	1.101139	26.843175	H	-4.473602	-0.745181	20.946784
H	-1.099340	-1.310813	27.357074	H	-3.820900	-0.791894	22.568207
H	-2.169040	-1.483619	25.976502	H	-4.039469	-3.316870	22.529744
H	2.375200	-1.767726	27.544797	H	-4.906393	-3.164134	20.996597
H	2.465855	-0.050048	27.155556	H	5.477259	-1.561577	17.482192
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H	1.715167	5.225326	20.815386	C	-3.491106	3.172496	21.774983
H	4.340071	4.573879	18.826028	N	-3.283428	2.031824	22.532358
H	3.136922	0.577770	19.524628	C	-2.268813	3.451744	21.205476
C	8.861628	3.486318	19.819285	C	-1.992572	1.654721	22.407993
C	7.816219	2.586160	19.241439	N	-1.340216	2.496396	21.602071
C	8.155307	1.385810	18.579474	H	-4.674263	4.836614	21.218802
C	6.461745	2.898678	19.385043	H	-5.272352	3.973602	22.647288
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C	5.787524	0.813368	18.240221	H	-1.568951	0.785063	22.880625
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H	9.853853	3.241761	19.434734	O	-8.570696	-2.031170	19.487797
H	9.204806	1.133877	18.454542	O	-7.421908	-3.903126	20.002370
H	6.179773	3.805364	19.908980	H	-7.464304	-4.071481	17.386274
H	7.465569	-0.390255	17.601022	H	-8.948732	-3.092593	17.201164
C	-4.294010	1.140705	17.294756	C	-10.810510	-3.245626	22.816574
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N	-10.473058	-0.074322	24.768561	C	6.313235	-2.174147	24.849912
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H	-8.424813	-1.850300	23.045881	C	-0.767650	-2.072262	19.848316
H	-12.288359	-1.240553	24.601337	C	-2.204164	-1.879604	19.835756
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C	0.616262	-6.357396	23.328854	C	-3.111836	-1.873081	18.708125
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C	1.961256	-5.542602	21.742685	C	-6.008202	-2.432703	22.749379
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H	-6.727176	-3.547432	28.779628	H	-10.071119	-4.017666	23.050778
H	-8.090511	-2.401064	28.818504	H	0.595655	-7.919073	24.825695
H	-6.485808	-1.729504	31.008850	H	-7.746920	-3.426170	30.227401
H	-6.317889	-1.643016	27.459284	O	1.474884	0.559954	21.955470
H	-5.108427	-0.377702	27.492228	O	-6.880087	0.142092	20.355768
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C	1.891640	-1.588925	24.755147	H	-1.207348	-1.316498	27.432993
C	1.674368	-1.071706	27.293893	H	-2.265293	-1.610268	26.061806
O	-2.829058	-2.130346	17.536020	H	2.270851	-1.925691	27.632071
C	-1.405589	-1.025064	26.399728	H	2.335438	-0.198153	27.285025
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C	1.655494	-2.639399	16.143291	H	5.547012	-3.044376	19.696818
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**S5:**

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