Supporting Information

DFT Fe_{a3}-O/O-O Vibrational Frequency Calculations over Catalytic Reaction Cycle States in the Dinuclear Center of Cytochrome *c* Oxidase

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Detailed Calculation Methods

The starting geometries of the model clusters for the DNC intermediate states are established based on the *ba*$_3$ C*c*O X-ray crystal structure 3S8G.[1] The calculation method for geometry optimizations using ADF[2-4] is the same (OLYP-D3-BJ[5]/TZP/DZP plus COSMO[6-9] solvation model) as in our recent publication of Ref. 10, and the geometry optimized structures of states **P$_R$**(Fe_{a3}^{4+}=O^{2-}···HO$^-$-Cu_B^{2+}, Tyr-O$^-$), **F**(Fe_{a3}^{4+}=O^{2-}···H_2O-Cu_B^{2+}, Tyr-O$^-$), **F$_H$**(Fe_{a3}^{4+}=O^{2-}···Cu_B^{2+}, Tyr-O$^-$), and **O$_H$**[Fe_{a3}^{3+}-OH$^-$-Cu_B^{2+}, Tyr-O$^-$] are directly taken from Ref. [10] for vibrational frequency calculations in the current paper.

In Ref. 10, the structures for states **P$_R$**, **F**, **F$_H$**, and **O$_H$** were labeled as Fe_{a3}^{4+}=O^{2-}···HO$^-$-Cu_B^{2+}-Y237$^-$-H376$^+$-M**1** (M**1**, M**2**, and M**3** stand for Models **1**, **2**, and **3** in Ref. 10), Fe_{a3}^{4+}=O^{2-}···H_2O-Cu_B^{2+}-Y237$^-$-H376$^+$-M**2**, Fe_{a3}^{4+}=O^{2-}···Cu_B^{2+}-Y237$^-$-H376$^+$-M**3**, and Fe_{a3}^{3+}-OH$^-$-Cu_B^{2+}-Y237$^-$-H376$^+$, respectively. Our DNC models (see Figure 3) include Fe_{a3}, Cu_B, the following residue side chains or part of the residues: His384, His233, His282, His283, Tyr237, Gly232, Arg449, His376, and Asp372, and seven water molecules found in the X-ray crystal structure, which are near (HOH604 and 608) or on the top (HOH583, 589, 607, 609, and 610) of the DNC. The C_α atoms of Tyr237, His282, His283, Asp372, His376, and His384 are each replaced with a link H atom (H_{link}) along the original C_β-C_α direction with the C_β-H_{link} distance 1.09 Å. The C_γ of Arg449, N of Gly232, C of His233, and C_{228} of the geranyl sidechain of the a_3-heme are also replaced with an H_{link} atom. The geometries of the DNC models are optimized in Broken-symmetry (BS)[11-13] state using Amsterdam Density Functional Package ADF2016.104[2-4] with integration grid accuracy parameter 4.0. All calculations in the current paper and in Ref. 10 are performed using the OLYP functional plus Grimme's latest dispersion corrections (D3-BJ)[5] within the conductor like screening (COSMO) solvation model.[6-9] During DNC geometry optimization calculations, H_{link} atoms on Tyr237, His282, His283, Asp372, His376, His384, and Arg449, and the C_α atom of Gly232 are fixed. Since both the cluster and the surrounding protein environment are quite polar and contain many water molecules, to be consistent with Refs. 14, 10, 15, and 16, a large dielectric constant of a simple ketone (ε = 18.5) is applied to the environment in all COSMO calculations. The van der Waals radii 1.86, 1.88, 1.70, 1.52, 1.61, and 1.35 Å are used for atoms Fe, Cu, C, O, N, and H, respectively.[14,16] The triple-ζ plus polarization (TZP) Slater-type basis set is applied to the Fe and Cu atoms and double-ζ plus polarization (DZP) basis set to other atoms. The inner cores of C(1s), N(1s), O(1s), Fe(1s,2s,2p), and Cu(1s,2s,2p) are treated by frozen core approximation.

For comparison, both analytical and numerical vibrational frequency calculations are then performed at the optimized geometries. Because of the large size of our models, Software for Chemistry & Materials (SCM) provided us a development version of ADF package (ADF2017.206.r59320) for the frequency calculations. However, these modifications very recently have been implemented in the current officially released ADF2019 package. By default, when calculating the vibrational frequencies, the derivatives of the energy with respect to all nuclei are calculated. This gives a complete Hessian (second derivative) matrix, from which the vibrational frequencies of the molecule can be calculated. However, calculations of the full spectrum of our DNC models are not practical and unnecessary due to the following reasons: 1) Our DNC models are very large (205-207 atoms, depending on the protonation state of Tyr237 and the presence of oxygen species (O_2/O_2^-, O_2^{2-}, HO_2^-, OH^-, H_2O) binding to Fe_{a3} and Cu_B); 2) The geometries of the DNC clusters were optimized with constraints (fixed H_{link} atoms); and 3) currently, we are only interested in the Fe-O/O-O vibrational modes in each state. Therefore, for each DNC intermediate structure, we compute a partial Hessian (~110 atoms) in analytical frequency calculations, in which all the methyl groups and the atoms in the upper cluster (Arg449, His376, Asp372, HOH583, HOH589, HOH607, HOH610, and the shifted waters HOH604 and HOH608 in states **F**, $\mathbf{F_H}$, and $\mathbf{O_H}$) are excluded from Hessian calculations. In numerical frequency calculations, we applied the mobile block Hessian (MBH) approach built in ADF,[17,18] in which the following groups were treated as individual mobile blocks: each methyl group in the model cluster, each residue side chain of Arg449, His376, and Asp372, and each of the water molecules which are also excluded from analytical Hessian calculations mentioned above. In the MBH method, each mobile block (for example, a methyl group or a water molecule) is treated as a rigid block, which moves as a whole and has only six frequencies related to its rigid motions.

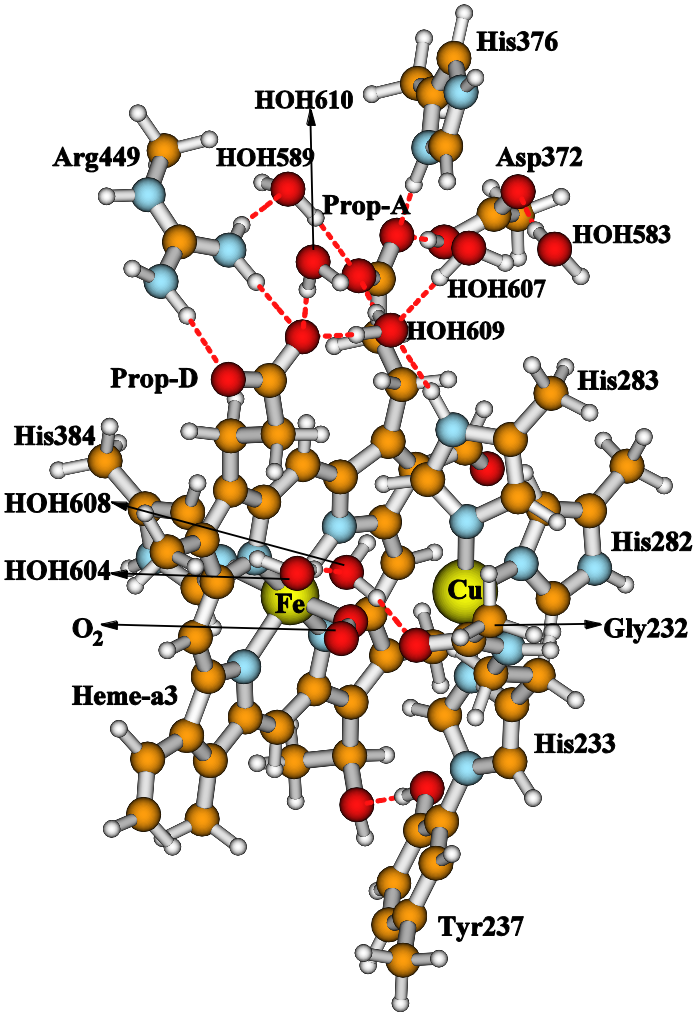

Figure S1. A full picture of **Figure 3**, showing all the H atoms. This is our whole quantum cluster model for state **A** of the DNC, built from the X-ray crystal structure 3S8G of ba_3 C*c*O from *Thermus thermophilus* (*Tt*).[1] A clearer view for both the central Fe_{a3}^{3+}-$O_2^{-\bullet}\cdots Cu_B^{+}$ portion and the top cluster of the model are given in Figure 4.

Spin Projection Corrections and Energy Profile Analysis from A → O_H

The broken-symmetry (BS)[11-13] state obtained from DFT calculations is a mixture of pure spin states. To correct the BS-state energies (E_{BS}) for spin projection effects, a ferromagnetically-coupled single-point energy calculation was performed on each of the BS-optimized geometries of the 8 states to obtain the F-coupled energies E_F. When the following Heisenberg Hamiltonian H (with Heisenberg coupling J) is applicable,

$$H = -2J\boldsymbol{S_1}\bullet\boldsymbol{S_2} \quad \text{(S1)}$$

then the J coupling constant can be calculated by[19]

$$J = (E_{BS} - E_F)/(\langle S^2\rangle_F - \langle S^2\rangle_{BS}) \quad \text{(S2)}$$

where $\langle S^2\rangle_F$ and $\langle S^2\rangle_{BS}$ are the calculated expectation values of the spin squared of the F-coupled and the BS-state, respectively.

The spin projection correction energy to the E_{BS} is then calculated as

$$\Delta E_{corr} = \mathrm{x}J \quad \text{(S3)}$$

where x is the measure of spin contamination in the BS state:

$$\mathrm{x} = \langle S^2\rangle_{BS} - S(S+1) \quad \text{(S4)}$$

in which S is the exact spin of the AF-coupled state. Therefore, the final spin projection corrected AF-state energy is

$$E_0 = E_{BS} + \Delta E_{corr} \quad \text{(S5)}$$

For more accurate calculations, both BS and F-coupled high-spin state geometries need to be optimized. The structure with the minimum E_0 can be obtained by extrapolating the geometries between the optimized BS and F-coupled geometries.

In Table S1, we have listed all the calculated values of E_{BS}, $\langle S^2\rangle_{BS}$, E_F, $\langle S^2\rangle_F$, J, ΔE_{corr}, E_0, and ΔE_0 for the eight DNC states studied here.

We also comment on the effect of spin projection on the wave function and, therefore, on the spin density distribution. There is a significant difference here between the spin density in a pure spin state, and that in the corresponding BS state. The largest difference occurs for states where the true total spin quantum number is $S = 0$. For $S = 0$, the corresponding spin density must be zero everywhere. This is in sharp contrast to the spin density in the related BS state. For two antiferromagnetically spin coupled fragments of equal spin, for example, when $S_1 = S_2 = 1/2$, and total $S = 0$, the BS state spin density is not zero, but shows regions of opposite spin, summing to Ms = 0 (z component of total spin = 0). In Table 3, this result is seen in the Mulliken spin populations (net spin) for states **A**, **Peroxo**, and **Hydroperoxo**. For $\mathbf{P_M}$, similarly, $S_1 = S_2 = 1$, total S for the ground state is $S = 0$, but with a non-zero spin density in the BS state. However, in the true $S = 0$ states of these systems, there is still an effective separation between electrons of opposite spin, as is well known in the electronic wave function of diradicals.[20] For states $\mathbf{P_R}$, **F**, and $\mathbf{F_H}$, the spin coupled states have composition $S_1 = 1$, $S_2 = 1/2$, total $S = 1/2$. For state $\mathbf{O_H}$, the spin coupled state is composed from $S_1 = 5/2$, $S_2 = 1/2$, total $S = 2$. In all these cases, where S is not equal to zero, the effect of spin coupling to attain a pure spin state allows for nonzero spin density throughout the molecule, and opposite but non-equal net spins (see Table 3, main text). However, these spin densities in the pure spin states are less than those in the corresponding BS states in accordance with the Wigner Eckart theorem (to first order).[21,22]

Further, we have also estimated the free energy changes (ΔG) (see Table S1 and Figure 5 in the main text) at pH = 7 along the $\mathbf{A} \rightarrow \mathbf{O_H}$ pathway.

The $\mathbf{A} \rightarrow$ **Peroxo** state energy is –26.5 kcal mol^{-1}. This strong binding energy is the result of an internal electron transfer from Cu_B^+ to $O_2^{-\bullet}$ radical, combined with formation of a O_2^{2-} bond to Cu_B^{2+}. In the subsequent internal proton transfer from Tyr237-OH to the metal bridging peroxide, **Peroxo** $\rightarrow$ **Hydroperoxo**, the calculated energy difference is +13.4 kcal mol^{-1} (we have estimated the zero-point energy (ZPE) difference for proton transfer from Tyr237 to the metal bridging peroxide as

–0.5 kcal mol^{-1} by calculating the ZPE's of the simple HOO^-, H_2O_2, neutral and deprotonated Tyr-OH/Tyr-O^- molecules. The predicted energy cost for the required formation of the Hydroperoxo is larger than found in our earlier work (+7.3 kcal mol^{-1} with an OLYP potential, with no dispersion, or +6.5 kcal mol^{-1} including a small spin projection correction[23]). The following **Hydroperoxo** → $\mathbf{P_M}$ transition involves cleavage of the O-O bond, and changes in the Fe_{a3} and Cu_B oxidation states, as well as generating the Tyr radical. The calculated energy change is –16.2 kcal mol^{-1}, which is less negative than in our earlier work (–18.9 kcal mol^{-1} with OLYP-D3,[24] using an earlier form of the dispersion correction). With OLYP-D3-BJ, the calculated redox potential for the one electron redox process, $\mathbf{P_M}$ + 1e$^-$ → $\mathbf{P_R}$ can be computed from the equation: $E^0 = (E_{ox} - E_{red}) + \Delta E(\text{SHE})$, where the experimental standard hydrogen electrode (SHE) energy is –4.34 V, equivalent to –100.1 kcal mol^{-1} per electron[23] (also see the Supporting Information of Ref. 10). The predicted redox potential with respect to SHE is E^0= +0.052 V. This is less positive than a typical cytochrome *c* redox potential, about +0.22 V referred to SHE, so the predicted ΔE^0 (cytc reference) = –0.17 V, or ΔG = +3.9 kcal mol^{-1}. Compared to our earlier work, some relative energies are altered with the OLYP-D3-BJ potential, but the energy differences between intermediates over this part of the reaction path does not show any large barriers. Beyond $\mathbf{P_R}$, from $\mathbf{P_R}$ → **F** → $\mathbf{F_H}$ → $\mathbf{O_H}$, the energies and pathways are summarized and discussed in Ref. 10. Here we only made the minor ΔE_{corr} corrections for those values.

Table S1. Properties Related to Correcting the Broken-Symmetry (BS) State Energies.[a]

State	E_{BS}	$\langle S^2\rangle_{BS}$	E_F	$\langle S^2\rangle_F$	J	ΔE_{corr}	E_0	ΔE_0	ΔG
A	–28712.3	0.6635	–28708.8	2.0423	–2.5	–1.7	–28714.0	0.0	0.0
Peroxo	–28738.4	0.5896	–28733.4	2.0310	–3.5	–2.1	–28740.5	–26.5	–26.5
Hydroperoxo	–28726.6	0.9649	–28726.6	2.0231	0.0	0.0	–28726.6	–12.6	–13.1
P_M	–28742.7	2.0058	–28742.4	6.0342	–0.1	–0.2	–28742.9	–28.9	–29.3
P_R	–28844.1	1.7582	–28844.0	3.7762	–0.1	–0.1	–28844.2	–130.2	–25.4
F	–28853.5	1.7732	–28853.5	3.7784	0.0	0.0	–28853.5	–139.5	–40.2
F_H	–28859.6	1.7702	–28859.8	3.7809	0.1	0.1	–28859.5	–145.5	–46.2
O_H	–28968.8	6.8805	–28967.0	12.0125	–0.4	–0.4	–28969.2	–255.2	–56.2

[a] Energies are in the unit of kcal mol^{-1}. E_{BS}**:** the calculated broken-symmetry state energies. $\langle S^2\rangle_{BS}$: the calculated expectation value of the spin squared of the broken-symmetry state. E_F**:** the ferromagnetically-coupled (F-coupled) state energy obtained from a single-point energy calculation on the broken-symmetry state optimized geometry. $\langle S^2\rangle_F$: the calculated expectation value of the spin squared of the F-coupled state. J: the calculated Heisenberg coupling constant. ΔE_{corr}: the correction for the BS energy. E_0: the corrected AF-state energy, $E_0 = E_{BS} + \Delta E_{corr}$. ΔE_0: the relative energies of E_0. ΔG: the calculated relative free energies (see Figure 5) at pH = 7 with the corrections of the zero point energy differences (ΔZPE) and with the reference to a typical cytochrome *c* redox potential of $E^0 = +0.22$ eV.

References of Supporting Information

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Cartesian Coordinates of the optimized geometries of the C*c*O dinuclear center states A, Peroxo, Hydroperoxo, P_M, P_R, F, F_H, and O_H:

State A:

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C	0.705000	7.351000	24.202000
C	1.258082	6.127024	23.537897
O	1.784951	5.216086	24.200453
H	1.308282	7.571028	25.085173
H	-0.317621	7.132772	24.529747
H	0.679538	8.218573	23.537918
N	1.129820	6.038144	22.202182
C	1.796293	4.963472	21.496658
C	1.449888	4.885127	20.013579
C	2.271300	3.767358	19.486779
N	1.956737	2.451013	19.809434
C	3.538866	3.795898	18.975521
C	3.003802	1.702150	19.502493
N	3.997246	2.486654	18.991631
H	0.841693	6.859389	21.682448
H	1.523501	4.018644	21.966823
H	0.381340	4.689020	19.880499
H	1.702354	5.819652	19.500361
H	4.161224	4.602778	18.629100
H	3.097528	0.642279	19.632491
H	2.882791	5.080908	21.595366
C	8.727128	3.570275	19.837235
C	7.687706	2.645526	19.273525
C	8.023772	1.418585	18.699231
C	6.336535	2.970220	19.340622
C	7.051323	0.551931	18.216573
C	5.357122	2.113648	18.853329
C	5.698314	0.881521	18.283329
O	4.705194	0.088953	17.819106
H	8.418489	4.614200	19.720061
H	9.684660	3.432602	19.325930
H	9.068710	1.129110	18.628619
H	6.027804	3.899807	19.803682
H	7.341196	-0.392751	17.771585
C	-3.918626	1.430502	16.522856
C	-2.632730	1.532752	17.251361
N	-1.423582	1.634359	16.590492
C	-2.299330	1.478192	18.581149
C	-0.420217	1.645773	17.499035
N	-0.926985	1.544489	18.718196
H	-4.300991	0.405106	16.571178
H	-3.780316	1.691247	15.469448
H	-1.315997	1.719334	15.585187
H	-2.939473	1.409975	19.441847
H	0.622699	1.754010	17.252783
C	-4.828961	3.854520	21.671138
C	-3.507899	3.188845	21.793123
N	-3.276072	2.112385	22.625879
C	-2.307902	3.418097	21.164190
C	-1.992023	1.717453	22.484198
N	-1.373053	2.487605	21.593033
H	-4.695697	4.844670	21.225971
H	-5.290477	3.983599	22.654531
H	-3.950326	1.698481	23.296067
H	-2.071162	4.147835	20.407573
H	-1.557006	0.874313	22.986739
C	-8.632432	-3.687762	17.805954
C	-8.417737	-2.995926	19.117557
O	-9.093967	-2.043146	19.498022
O	-7.420379	-3.519430	19.827853
H	-7.680475	-3.766591	17.271956
H	-9.350408	-3.125560	17.208262
C	-10.657323	-3.293885	22.474737
C	-10.531206	-1.953973	23.078514
N	-9.306712	-1.331263	23.212785
C	-11.452763	-1.097638	23.610000
C	-9.451319	-0.145879	23.794219
N	-10.753551	0.008207	24.043066
H	-10.280940	-3.281015	21.449284
H	-11.703602	-3.605027	22.472214
H	-8.395706	-1.762437	22.875822
H	-12.520418	-1.180302	23.722154
H	-8.676543	0.573593	24.010058
C	0.023021	-7.212119	24.184181
C	0.757528	-6.109417	23.486079
N	1.749502	-6.329169	22.547040
C	0.523936	-4.750299	23.417253
C	2.080362	-5.157771	21.953243

N	1.348560	-4.177497	22.459688
H	-0.488199	-7.823418	23.429150
H	-0.748825	-6.759040	24.812645
H	2.158751	-7.231605	22.328721
H	-0.178579	-4.153035	23.972277
H	2.834257	-5.052926	21.194415
C	-7.126501	-3.012345	29.433783
N	-6.025345	-2.314713	30.060446
C	-5.231575	-1.467212	29.401308
N	-5.443171	-1.196189	28.124582
N	-4.203412	-0.902849	30.045506
H	-6.776320	-3.815062	28.776240
H	-7.728173	-2.304559	28.861668
H	-5.663649	-2.690283	30.929753
H	-6.111489	-1.711613	27.552434
H	-4.950880	-0.404892	27.692330
H	-4.250877	-0.856606	31.056522
H	-3.657578	-0.170345	29.562126
Fe	1.571261	-2.113084	21.885812
C	-1.377631	-1.508654	23.430284
C	-0.037637	-2.347238	18.863662
C	4.529508	-2.778220	20.305778
C	3.250914	-1.502057	24.773716
N	1.044564	-1.669794	23.729673
C	-0.239153	-1.488078	24.195143
C	-0.216096	-1.149781	25.602099
C	1.099737	-1.076399	25.969530
C	1.875891	-1.426341	24.797185
C	1.650485	-0.628267	27.270530
O	-2.799408	-1.901452	17.634297
C	-1.399804	-0.841769	26.435493
C	-1.796095	0.641820	26.380225
C	-2.892285	0.863849	27.398781
O	-2.575272	0.857193	28.610368
O	-4.101224	0.958252	26.974109
N	2.115723	-2.605999	20.002147
C	1.303864	-2.637122	18.890341
C	2.077815	-2.940529	17.703521
C	3.373229	-3.090384	18.115342
C	3.388161	-2.854597	19.544827
C	1.500126	-3.043427	16.342671
N	3.491200	-2.176439	22.443575
C	4.574612	-2.437366	21.637778
C	5.807504	-2.272844	22.368546
C	5.457464	-1.899365	23.648177
C	4.003302	-1.851994	23.676107
C	7.152556	-2.492114	21.789943
C	6.305038	-1.633064	24.785896
C	7.558477	-1.160091	24.740644
N	-0.341913	-2.004778	21.264181
C	-0.794080	-2.029677	19.970244
C	-2.191784	-1.661296	19.932912
C	-2.574463	-1.421804	21.244843
C	-1.418587	-1.662201	22.055729
C	-3.059538	-1.562044	18.791273
C	-3.914049	-1.060285	21.759505
C	-4.813576	-2.292371	21.841509
C	-6.058168	-2.056535	22.665480
O	-7.165988	-2.490965	22.201760
O	-5.948416	-1.488482	23.781127
C	4.544165	-3.456792	17.277232
O	5.578853	-2.445534	17.451051
C	5.097048	-4.831580	17.607288
H	5.937264	-5.068189	16.945352
Cu	0.148298	1.959401	20.436012
H	8.891070	3.392425	20.913367
H	-4.673317	2.104938	16.938340
H	-5.531461	3.294706	21.032081
H	-9.006490	-4.710141	17.956796
H	-10.071120	-4.017668	23.050776
H	0.595656	-7.919075	24.825696
H	-7.746925	-3.426169	30.227401
O	-8.076687	0.558827	20.141334
H	-7.690311	0.746877	19.264959
H	-8.356297	-0.379959	20.057604
O	-7.275888	-2.282262	26.054212
H	-6.878410	-2.003449	25.189511
H	-7.237219	-3.256596	26.016327
O	1.168705	4.027237	27.390896
H	0.925163	3.586218	26.542491
H	1.158162	3.294949	28.035439
O	-7.365109	2.324603	24.248337
H	-6.496736	1.856755	24.357699
H	-7.317377	2.685692	23.344834
O	-4.971553	0.971375	24.471595
H	-4.591492	0.940992	25.402267
H	-5.253178	0.050723	24.251136
O	-5.793587	2.366676	28.692133
H	-5.155591	1.861998	28.125472
H	-5.547804	3.297131	28.522204
O	0.717148	2.791725	24.852072
H	1.043030	3.625067	24.434933
H	-0.100846	2.585153	24.369011
H	-7.333260	-3.040818	20.736258
H	-2.129999	0.908796	25.378195
H	-0.926804	1.249831	26.638170

H	-1.177123	-1.085537	27.478723
H	-2.255389	-1.456371	26.134730
H	2.632454	-1.065206	27.472027
H	1.764099	0.463881	27.270174
H	0.978661	-0.894195	28.091924
H	-2.311119	-1.314717	23.937824
H	3.779692	-1.252252	25.681206
H	5.867777	-1.840640	25.761467
H	8.128156	-1.015705	25.654959
H	8.034186	-0.889100	23.805274
H	7.884898	-2.692262	22.575869
H	7.146937	-3.338358	21.096414
H	7.482683	-1.605950	21.232435
H	5.467879	-2.932151	19.800133
H	4.230054	-3.441764	16.229002
H	4.310373	-5.578311	17.459916
H	5.430747	-4.874624	18.646393
H	2.277139	-3.184433	15.589092
H	0.802705	-3.886869	16.279492
H	0.942567	-2.134315	16.092228
H	-0.547914	-2.343288	17.913019
H	-4.053788	-1.140254	19.028849
H	-4.384018	-0.300359	21.128483
H	-3.823263	-0.634186	22.753814
H	-4.255945	-3.095710	22.339444
H	-5.069220	-2.641745	20.840510
H	6.226086	-2.597267	16.734676
H	5.061392	-0.825465	17.628680
O	1.687639	-0.362603	21.404439
O	2.143037	0.493942	22.263026
H	-11.160876	0.825065	24.487829

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C	0.705000	7.351000	24.202000
C	0.852177	5.924138	23.719494
O	1.038202	4.985802	24.516078
H	1.654554	7.652870	24.653655
H	-0.067917	7.381088	24.973559
H	0.452107	8.046672	23.397174
N	0.785134	5.709707	22.390807
C	1.141184	4.412741	21.836418
C	1.212432	4.438681	20.308260
C	2.129581	3.373898	19.829088
N	1.820092	2.020969	19.846814
C	3.450247	3.509867	19.503245
C	2.923842	1.353419	19.548051
N	3.949822	2.228191	19.330334
H	0.742454	6.506562	21.767825
H	0.406795	3.671070	22.150643
H	0.215349	4.325605	19.875698
H	1.617869	5.401437	19.977620
H	4.075336	4.376306	19.381755
H	3.028488	0.286999	19.495118
H	2.118278	4.121730	22.232911
C	8.706961	3.489104	19.832015
C	7.650254	2.551707	19.318192
C	7.978815	1.462885	18.508880
C	6.300727	2.759693	19.596958
C	7.000820	0.622750	17.991766
C	5.312016	1.934828	19.069090
C	5.652131	0.849597	18.252261
O	4.657771	0.098949	17.719211
H	8.414762	4.528607	19.644107
H	9.654474	3.302382	19.319085
H	9.019815	1.271000	18.263536
H	6.006497	3.578923	20.242674
H	7.275479	-0.203776	17.344075
C	-3.994294	1.366374	16.500040
C	-2.714041	1.308416	17.238926
N	-1.519446	1.007822	16.618020
C	-2.400996	1.413283	18.568673
C	-0.534695	0.946543	17.541799
N	-1.045775	1.191034	18.739839
H	-4.481682	0.384467	16.518331
H	-3.820911	1.641502	15.455492
H	-1.406450	0.851265	15.622259
H	-3.042533	1.626659	19.402559
H	0.497558	0.738310	17.323125
C	-4.782406	3.894721	21.564867
C	-3.516783	3.147002	21.734001
N	-3.363548	2.117883	22.645026
C	-2.323109	3.209618	21.058878
C	-2.132423	1.589454	22.497731
N	-1.476118	2.222767	21.531754
H	-4.595990	4.801044	20.982576

H	-5.209846	4.177328	22.531170
H	-4.080893	1.768877	23.308881
H	-2.042082	3.861781	20.249882
H	-1.743231	0.766943	23.063827
C	-8.676092	-3.670546	17.853897
C	-8.347196	-3.011922	19.160999
O	-8.631089	-1.843810	19.407896
O	-7.693876	-3.794984	20.015115
H	-7.766311	-3.673805	17.241653
H	-9.436852	-3.084207	17.337117
C	-10.745085	-3.390185	22.460898
C	-10.720486	-2.021620	23.007627
N	-9.535626	-1.324785	23.130945
C	-11.695714	-1.201663	23.496736
C	-9.752850	-0.131684	23.671348
N	-11.065063	-0.042795	23.897112
H	-10.398065	-3.397097	21.424249
H	-11.755435	-3.800509	22.507486
H	-8.603792	-1.741643	22.849877
H	-12.758753	-1.339941	23.597630
H	-9.011818	0.634930	23.839311
C	-0.030867	-7.208338	24.242616
C	0.643453	-6.105926	23.484774
N	1.592350	-6.319666	22.499586
C	0.378176	-4.754274	23.409285
C	1.869019	-5.152152	21.873750
N	1.139134	-4.179292	22.399904
H	-0.612547	-7.814540	23.536165
H	-0.739994	-6.754114	24.940350
H	2.001085	-7.219015	22.267772
H	-0.297629	-4.163657	24.001592
H	2.588412	-5.040469	21.083452
C	-7.190131	-2.987760	29.403062
N	-6.270904	-2.037877	29.987271
C	-5.473611	-1.249537	29.265286
N	-5.521222	-1.272684	27.936027
N	-4.605493	-0.456634	29.888208
H	-6.662081	-3.773350	28.851931
H	-7.888959	-2.476875	28.738646
H	-6.024975	-2.162582	30.962234
H	-6.271290	-1.762562	27.445753
H	-5.130942	-0.452069	27.457698
H	-4.657177	-0.363197	30.893549
H	-3.973605	0.171260	29.363543
Fe	1.349869	-2.127733	21.889986
C	-1.600673	-1.548878	23.470599
C	-0.231950	-2.081847	18.863069
C	4.308317	-2.836041	20.273474
C	3.016545	-1.859013	24.809759
N	0.804902	-1.803048	23.760127
C	-0.461927	-1.566143	24.235311
C	-0.421838	-1.292481	25.656519
C	0.896397	-1.347191	26.023532
C	1.647772	-1.686454	24.830724
C	1.513317	-1.091391	27.345566
O	-3.013287	-1.755305	17.677816
C	-1.599568	-0.929379	26.480315
C	-2.093055	0.498620	26.205383
C	-3.107892	0.887299	27.254869
O	-2.721786	0.986991	28.441808
O	-4.333236	1.026947	26.893110
N	1.914930	-2.470942	19.975093
C	1.106898	-2.380518	18.864115
C	1.863141	-2.646896	17.659739
C	3.145278	-2.913166	18.056938
C	3.173640	-2.769188	19.500066
C	1.273596	-2.646861	16.299629
N	3.276044	-2.353097	22.437935
C	4.356228	-2.619151	21.632857
C	5.581748	-2.608776	22.400377
C	5.224707	-2.321292	23.698274
C	3.771973	-2.175534	23.702671
C	6.929139	-2.869594	21.844722
C	6.060183	-2.181479	24.865441
C	7.358152	-1.841779	24.870979
N	-0.535948	-1.905717	21.287568
C	-0.990861	-1.866489	19.991047
C	-2.396386	-1.530776	19.972020
C	-2.786042	-1.370012	21.291600
C	-1.627677	-1.636333	22.093326
C	-3.270756	-1.416437	18.834064
C	-4.127933	-1.049812	21.819733
C	-5.021465	-2.286947	21.856391
C	-6.259071	-2.073732	22.694159
O	-7.361102	-2.546537	22.252952
O	-6.156382	-1.475441	23.794024
C	4.257499	-3.378712	17.185717
O	5.387900	-2.469996	17.286695
C	4.670090	-4.804302	17.495694
H	5.472501	-5.121602	16.819326
Cu	-0.012706	1.214727	20.464909
H	8.891070	3.392424	20.913367
H	-4.673317	2.104938	16.938340
H	-5.531461	3.294705	21.032081
H	-9.006488	-4.710142	17.956795
H	-10.071118	-4.017670	23.050775

H	0.595658	-7.919075	24.825695
H	-7.746922	-3.426171	30.227400
O	-7.095052	0.328278	20.769894
H	-7.114095	0.862127	19.953240
H	-7.588341	-0.479857	20.515237
O	-7.553562	-2.254425	26.019522
H	-7.127376	-1.978461	25.165926
H	-7.578449	-3.227988	25.953928
O	0.940544	2.314721	27.062442
H	1.042049	2.118555	26.095716
H	0.838542	1.434310	27.459998
O	-7.546598	2.023375	23.225173
H	-6.745577	1.763718	23.737905
H	-7.441430	1.517128	22.392857
O	-5.207675	1.035199	24.407975
H	-4.849201	1.021703	25.347925
H	-5.460380	0.104702	24.202808
O	-5.745439	2.869804	28.384391
H	-5.206186	2.183082	27.906181
H	-5.638460	3.665977	27.827865
O	1.408766	2.099882	24.343291
H	1.215096	3.032468	24.115121
H	1.159517	1.556591	23.560871
H	-7.515320	-3.261231	20.883200
H	-2.527457	0.568701	25.211888
H	-1.246002	1.184827	26.264190
H	-1.340754	-0.998794	27.539490
H	-2.422282	-1.634478	26.304151
H	2.030127	-1.983414	27.721189
H	2.260770	-0.293885	27.270653
H	0.761940	-0.798921	28.083361
H	-2.537341	-1.380752	23.980532
H	3.538109	-1.712345	25.744495
H	5.573816	-2.361410	25.822559
H	7.905051	-1.777212	25.807909
H	7.893179	-1.601177	23.960204
H	7.571595	-3.326514	22.602273
H	6.879737	-3.540659	20.982183
H	7.406388	-1.936272	21.517800
H	5.240887	-3.005431	19.762357
H	3.915744	-3.338107	16.146333
H	3.806567	-5.460037	17.345761
H	5.000791	-4.901024	18.532848
H	2.042452	-2.725694	15.529081
H	0.578566	-3.486541	16.177996
H	0.707082	-1.727134	16.124152
H	-0.749758	-2.012749	17.919607
H	-4.263296	-0.993410	19.077564
H	-4.614060	-0.274926	21.224866
H	-4.039662	-0.663890	22.830158
H	-4.464332	-3.112958	22.316859
H	-5.286819	-2.597007	20.845169
H	6.198507	-3.003250	17.372402
H	5.016763	-0.805081	17.516562
O	1.720206	-0.370654	21.742204
O	0.733803	0.509473	22.105616
H	-11.524047	0.769917	24.296157

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C	0.705000	7.351000	24.202000
C	0.946284	5.977350	23.627578
O	1.002263	4.979397	24.369617
H	1.631317	7.669967	24.691040
H	-0.081332	7.288605	24.957658
H	0.433672	8.085381	23.439554
N	1.130337	5.903461	22.294343
C	1.760918	4.751967	21.678489
C	1.430184	4.587188	20.195862
C	2.290100	3.490266	19.689292
N	1.956455	2.149038	19.844862
C	3.596717	3.562290	19.300635
C	3.026054	1.425295	19.540446
N	4.057399	2.258626	19.211352
H	1.207875	6.783328	21.795004
H	1.445104	3.859147	22.209435
H	0.369870	4.352600	20.067088
H	1.646416	5.511353	19.649178
H	4.239820	4.399418	19.090413
H	3.109611	0.355017	19.557246
H	2.850637	4.837905	21.783304
C	8.827562	3.359588	19.812567
C	7.754299	2.444188	19.304664
C	8.069587	1.286152	18.572074

C	6.403663	2.723183	19.515031
C	7.093502	0.446885	18.081444
C	5.408267	1.906110	19.004262
C	5.702034	0.711794	18.259916
O	4.775169	-0.030658	17.788479
H	8.643122	4.386528	19.474086
H	9.803771	3.044600	19.433925
H	9.115158	1.050480	18.389450
H	6.123651	3.598522	20.090231
H	7.362192	-0.440883	17.517910
C	-3.908819	1.470495	16.475192
C	-2.633360	1.481240	17.231104
N	-1.413982	1.333994	16.597583
C	-2.327146	1.543026	18.565420
C	-0.426114	1.326148	17.516579
N	-0.955191	1.451075	18.725877
H	-4.294794	0.447213	16.404375
H	-3.746003	1.843354	15.458779
H	-1.285398	1.271179	15.592955
H	-2.983063	1.643388	19.409369
H	0.622806	1.246216	17.287929
C	-4.810576	3.921055	21.571645
C	-3.522375	3.207950	21.717372
N	-3.384798	2.085612	22.508924
C	-2.300935	3.377329	21.113374
C	-2.135076	1.605947	22.369932
N	-1.446212	2.367863	21.522894
H	-4.661368	4.840389	21.000576
H	-5.237736	4.176558	22.546354
H	-4.106016	1.694269	23.149518
H	-2.004898	4.112749	20.384051
H	-1.768119	0.712838	22.835612
C	-8.383825	-3.841364	17.720084
C	-8.083235	-3.014064	18.932156
O	-8.152346	-1.785904	18.943130
O	-7.709041	-3.738129	19.982337
H	-7.434310	-4.217670	17.321782
H	-8.866223	-3.223062	16.962642
C	-10.816672	-3.295959	22.701086
C	-10.660029	-2.007994	23.396345
N	-9.479516	-1.298174	23.360508
C	-11.523457	-1.263443	24.145393
C	-9.591983	-0.169310	24.051876
N	-10.834117	-0.133608	24.534688
H	-10.678096	-3.168530	21.620433
H	-11.815804	-3.701493	22.881691
H	-8.595526	-1.665102	22.889260
H	-12.553642	-1.429827	24.425077
H	-8.832245	0.583200	24.196653
C	-0.024180	-7.207500	24.242551
C	0.675659	-6.115041	23.500203
N	1.664284	-6.336920	22.556695
C	0.417294	-4.764776	23.411477
C	1.973385	-5.175608	21.940157
N	1.225532	-4.200135	22.436157
H	-0.602591	-7.806725	23.528023
H	-0.734713	-6.746020	24.933737
H	2.081946	-7.237330	22.347190
H	-0.280816	-4.168841	23.970758
H	2.720209	-5.067507	21.175950
C	-7.233246	-2.917111	29.410677
N	-6.106155	-2.200037	29.970508
C	-5.361745	-1.345138	29.262568
N	-5.691788	-1.016313	28.025677
N	-4.259536	-0.826348	29.822318
H	-6.908946	-3.652348	28.667016
H	-7.926729	-2.210386	28.951167
H	-5.670343	-2.591556	30.797920
H	-6.402395	-1.512701	27.485796
H	-5.163497	-0.271590	27.552148
H	-4.210177	-0.824914	30.834611
H	-3.772504	-0.054885	29.340775
Fe	1.433071	-2.206227	21.911400
C	-1.496613	-1.571350	23.517825
C	-0.189321	-2.195419	18.908855
C	4.370215	-2.929687	20.274824
C	3.136898	-1.891443	24.811470
N	0.915103	-1.828245	23.781896
C	-0.343798	-1.563211	24.261739
C	-0.282614	-1.246297	25.671620
C	1.037631	-1.310696	26.030058
C	1.772115	-1.693460	24.839817
C	1.664645	-1.039732	27.344262
O	-2.980008	-1.727129	17.730797
C	-1.448769	-0.850194	26.493998
C	-1.860912	0.610783	26.258698
C	-2.994504	0.934880	27.206040
O	-2.723380	1.082687	28.418903
O	-4.186945	0.952955	26.731465
N	1.962544	-2.602395	20.006758
C	1.145821	-2.514884	18.902118
C	1.903056	-2.761105	17.691141
C	3.195492	-2.992165	18.076788
C	3.222954	-2.869054	19.520190
C	1.312053	-2.742836	16.331549
N	3.366366	-2.422240	22.445903

C	4.436011	-2.704095	21.630012
C	5.667436	-2.700166	22.385769
C	5.323876	-2.411811	23.688273
C	3.874579	-2.241445	23.702788
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C	6.165275	-2.306882	24.855409
C	7.474434	-2.015087	24.864506
N	-0.476810	-2.005460	21.332236
C	-0.938273	-1.959914	20.040699
C	-2.343544	-1.614929	20.033227
C	-2.724485	-1.467515	21.357604
C	-1.554565	-1.722827	22.147092
C	-3.230996	-1.454922	18.906877
C	-4.055751	-1.114683	21.892859
C	-5.019462	-2.298451	21.883234
C	-6.285147	-1.987858	22.645504
O	-7.394685	-2.358849	22.136178
O	-6.197912	-1.402712	23.755100
C	4.361492	-3.340261	17.209777
O	5.534848	-2.582532	17.517288
C	4.709594	-4.813900	17.336243
H	5.543768	-5.055154	16.668316
Cu	0.101676	1.618089	20.435750
H	8.891071	3.392424	20.913367
H	-4.673317	2.104938	16.938341
H	-5.531461	3.294705	21.032081
H	-9.006488	-4.710142	17.956796
H	-10.071118	-4.017669	23.050776
H	0.595658	-7.919074	24.825696
H	-7.746921	-3.426171	30.227401
O	1.815246	-0.481984	21.674948
O	0.683425	0.421137	22.073003
O	-6.388322	0.272042	19.902960
H	-6.315488	0.730259	19.045025
H	-6.969844	-0.492174	19.696724
O	-7.616059	-2.016437	26.041140
H	-7.183414	-1.802703	25.175401
H	-7.674857	-2.989432	26.030250
O	1.626669	2.495282	26.939819
H	1.367720	2.316882	26.005294
H	1.238677	1.744493	27.424867
O	-7.540591	2.439941	24.395871
H	-6.669220	1.962599	24.380544
H	-7.632192	2.770127	23.484193
O	-5.165150	1.042718	24.288934
H	-4.727753	0.985591	25.191851
H	-5.483188	0.128039	24.087156
O	-5.615383	2.955143	28.004490
H	-5.104456	2.202520	27.612765
H	-4.976440	3.337374	28.637009
O	0.861311	2.244993	24.194303
H	0.943467	3.234739	24.114776
H	-0.099923	2.109893	24.232514
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H	-2.163858	0.758034	25.222931
H	-1.010472	1.259424	26.478437
H	-1.213877	-0.971075	27.554547
H	-2.305827	-1.501009	26.279300
H	2.199962	-1.922614	27.713788
H	2.395608	-0.228564	27.259569
H	0.915343	-0.758050	28.087740
H	-2.421786	-1.376597	24.040553
H	3.668566	-1.739271	25.739630
H	5.673643	-2.483151	25.810544
H	8.023100	-1.980145	25.801565
H	8.019028	-1.784302	23.956572
H	7.657088	-3.431042	22.554120
H	6.947656	-3.604102	20.935015
H	7.481024	-2.015311	21.503279
H	5.287582	-3.086303	19.731301
H	4.064466	-3.147670	16.168328
H	3.841618	-5.422543	17.066336
H	4.993894	-5.042703	18.367147
H	2.085711	-2.780935	15.562639
H	0.642932	-3.599833	16.186274
H	0.720053	-1.834274	16.179017
H	-0.710649	-2.117303	17.967313
H	-4.221795	-1.051160	19.180419
H	-4.498250	-0.301115	21.315894
H	-3.957965	-0.771329	22.918339
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H	1.102457	0.987227	22.768251
H	-11.208600	0.618662	25.103148

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C	0.705000	7.351000	24.202000	H	-1.432532	1.378808	15.942901
C	1.114891	5.976922	23.732901	H	-3.046146	1.189697	19.808220
O	1.646487	5.164416	24.512865	H	0.514860	1.395736	17.589536
H	1.616836	7.919649	24.402774	C	-4.858459	4.000972	21.521458
H	0.146096	7.252151	25.133377	C	-3.566318	3.329151	21.751534
H	0.108258	7.890391	23.460079	N	-3.402010	2.341942	22.704693
N	0.904792	5.670254	22.439087	C	-2.374443	3.389571	21.078011
C	1.490206	4.467710	21.869056	C	-2.156792	1.841417	22.599193
C	1.333828	4.396971	20.350022	N	-1.511976	2.459116	21.618995
C	2.217686	3.310086	19.857954	H	-4.723054	4.859942	20.860043
N	1.868727	1.962981	19.936910	H	-5.315434	4.337012	22.456282
C	3.533453	3.393508	19.508951	H	-4.112650	1.989111	23.373623
C	2.939349	1.247175	19.648402	H	-2.106688	3.992509	20.226832
N	3.994511	2.089237	19.378607	H	-1.737236	1.063327	23.204262
H	0.564321	6.391667	21.814614	C	-8.189953	-4.012494	17.746401
H	1.034724	3.583988	22.311233	C	-7.944064	-3.098816	18.908397
H	0.292591	4.205353	20.078990	O	-8.054359	-1.875490	18.839646
H	1.643275	5.343775	19.892571	O	-7.584988	-3.745146	20.012970
H	4.173680	4.239459	19.335192	H	-7.291581	-4.611516	17.563872
H	3.011619	0.176938	19.668808	H	-8.428862	-3.425309	16.859557
H	2.557947	4.452159	22.114147	C	-10.776387	-3.278302	22.660305
C	8.778769	3.226685	19.822149	C	-10.608442	-1.980327	23.342781
C	7.699300	2.264536	19.441514	N	-9.423468	-1.272175	23.298727
C	8.022840	1.020314	18.847876	C	-11.474222	-1.226771	24.082983
C	6.343932	2.583108	19.615930	C	-9.539703	-0.136810	23.977840
C	7.052334	0.150784	18.438562	N	-10.783084	-0.095284	24.460336
C	5.340971	1.731825	19.204886	H	-10.593941	-3.169857	21.586363
C	5.651227	0.460876	18.559813	H	-11.793640	-3.645371	22.809887
O	4.749831	-0.292810	18.113219	H	-8.532054	-1.629318	22.836198
H	8.561172	4.207344	19.381832	H	-12.500117	-1.393199	24.364741
H	9.742888	2.880171	19.441773	H	-8.783631	0.622663	24.102040
H	9.069090	0.761893	18.714882	C	-0.154657	-7.332289	24.278004
H	6.089204	3.519423	20.096146	C	0.447243	-6.317123	23.381740
H	7.304905	-0.798129	17.976934	N	1.324702	-6.642710	22.364603
C	-4.047962	1.195509	16.887472	C	0.274365	-4.959860	23.274539
C	-2.752543	1.282827	17.618111	C	1.654640	-5.523174	21.683922
N	-1.540303	1.335869	16.951012	N	1.026536	-4.486451	22.213750
C	-2.410854	1.244022	18.946699	H	-0.768378	-8.035215	23.702166
C	-0.529548	1.340777	17.843517	H	-0.799617	-6.831788	25.004235
N	-1.030905	1.286030	19.071502	H	1.662746	-7.576618	22.159492
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H	-3.857894	0.990833	15.830420	H	2.339047	-5.488758	20.856815

C	-7.280012	-2.843020	29.428861
N	-6.219868	-2.044451	30.010786
C	-5.506029	-1.145908	29.334857
N	-5.689792	-0.967639	28.035921
N	-4.617164	-0.374103	29.980984
H	-6.884827	-3.525192	28.669625
H	-8.034797	-2.192200	28.979611
H	-5.952491	-2.223838	30.970506
H	-6.384710	-1.481799	27.496650
H	-5.200644	-0.185702	27.584780
H	-4.354858	-0.656922	30.915120
H	-3.869700	0.071191	29.421293
Fe	1.453188	-2.493953	21.708599
C	-1.438295	-1.563992	23.282682
C	-0.199283	-2.613666	18.729717
C	4.340715	-3.403712	20.134609
C	3.112851	-2.336014	24.669702
N	0.932937	-2.049001	23.592088
C	-0.306787	-1.680632	24.053765
C	-0.260744	-1.426175	25.476184
C	1.041081	-1.617015	25.862384
C	1.768705	-2.017886	24.674384
C	1.658273	-1.440199	27.196611
O	-2.977480	-2.084351	17.533858
C	-1.423420	-1.065529	26.324563
C	-1.996946	0.333669	26.082935
C	-2.930380	0.721543	27.213308
O	-2.503341	0.643318	28.386099
O	-4.124999	1.092046	26.912513
N	1.942640	-3.050210	19.835586
C	1.126818	-2.965821	18.733003
C	1.892878	-3.230608	17.527814
C	3.184357	-3.439470	17.922025
C	3.207146	-3.314637	19.368922
C	1.306175	-3.259151	16.166351
N	3.337131	-2.900139	22.308040
C	4.402580	-3.202127	21.499264
C	5.624457	-3.243405	22.264522
C	5.278895	-2.951394	23.567346
C	3.837045	-2.733256	23.569473
C	6.962751	-3.542125	21.707572
C	6.115330	-2.856559	24.736344
C	7.418683	-2.534145	24.743312
N	-0.458393	-2.185505	21.122980
C	-0.931216	-2.244396	19.841663
C	-2.317124	-1.829309	19.817760
C	-2.664909	-1.509754	21.122243
C	-1.496809	-1.750585	21.920811
C	-3.210724	-1.734915	18.694207
C	-3.979748	-1.070153	21.645004
C	-4.922113	-2.262811	21.825813
C	-6.172507	-1.902566	22.595860
O	-7.294579	-2.264668	22.101534
O	-6.062104	-1.301308	23.693482
C	4.363574	-3.751549	17.062868
O	5.505886	-2.931229	17.370990
C	4.781978	-5.206354	17.193919
H	5.634805	-5.409811	16.536937
Cu	0.035722	1.442157	20.785587
H	8.891071	3.392426	20.913366
H	-4.673317	2.104936	16.938341
H	-5.531461	3.294704	21.032081
H	-9.006486	-4.710145	17.956797
H	-10.071115	-4.017670	23.050778
H	0.595660	-7.919073	24.825699
H	-7.746918	-3.426168	30.227401
O	1.877750	-0.933101	21.363030
O	0.707033	1.173151	22.540667
O	-6.373830	0.273574	19.709987
H	-6.220936	0.654916	18.827809
H	-6.933003	-0.515284	19.520570
O	-7.542925	-1.976442	25.952724
H	-7.095764	-1.740959	25.100624
H	-7.802856	-2.906734	25.829894
O	1.257586	2.015517	27.246998
H	0.969833	2.156451	26.302376
H	0.603429	1.381235	27.589188
O	-7.521113	2.521121	24.072344
H	-6.665894	2.060069	24.273424
H	-7.459768	2.702496	23.115688
O	-5.147131	1.175546	24.490701
H	-4.719149	1.110338	25.402938
H	-5.381517	0.256714	24.220769
O	-4.636663	3.522346	28.182492
H	-4.458181	2.635143	27.778197
H	-4.451288	4.140580	27.450609
O	0.409157	2.601531	24.726631
H	0.891005	3.435163	24.533089
H	0.541870	2.025949	23.911457
H	-7.437483	-3.081087	20.790768
H	-2.532029	0.383086	25.139177
H	-1.185615	1.063345	26.035791
H	-1.129141	-1.122467	27.373677
H	-2.225426	-1.801962	26.179270
H	2.239786	-2.322799	27.484942
H	2.332255	-0.576630	27.186773

H	0.899508	-1.263364	27.961369
H	-2.348824	-1.287327	23.788943
H	3.639767	-2.231539	25.606425
H	5.629047	-3.055499	25.689762
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H	7.596380	-4.011018	22.465059
H	6.892021	-4.212435	20.846708
H	7.458465	-2.620343	21.376049
H	5.264861	-3.582322	19.609979
H	4.069447	-3.573070	16.019546
H	3.946438	-5.851999	16.907415
H	5.059329	-5.430848	18.227060
H	2.078662	-3.386910	15.405939
H	0.594351	-4.088125	16.071753
H	0.762468	-2.331854	15.955925
H	-0.723497	-2.585084	17.786115
H	-4.193584	-1.304548	18.953319
H	-4.457931	-0.356304	20.971193
H	-3.856101	-0.576849	22.606532
H	-4.403466	-3.039747	22.401184
H	-5.175956	-2.685283	20.852950
H	5.173572	-2.026774	17.580059
H	1.242924	0.359092	22.431562
H	-11.160387	0.666277	25.015813

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C	0.705000	7.351000	24.202000
C	1.238108	6.046850	23.662821
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H	0.034016	7.130577	25.036831
H	0.174970	7.939096	23.444135
N	1.068277	5.790935	22.351368
C	1.742242	4.657779	21.737231
C	1.429777	4.499743	20.250640
C	2.270047	3.381353	19.743908
N	1.897607	2.049083	19.850465
C	3.587977	3.426331	19.376671
C	2.964024	1.304440	19.567118
N	4.023173	2.113797	19.281365
H	0.731591	6.536031	21.752266
H	1.449934	3.743269	22.249860
H	0.367032	4.288190	20.105295
H	1.673059	5.421692	19.708827
H	4.247992	4.254651	19.187563
H	3.021891	0.232688	19.565547
H	2.825611	4.778456	21.857377
C	8.826550	3.212512	19.822600
C	7.737231	2.261960	19.394328
C	8.031899	1.046164	18.763312
C	6.384625	2.565330	19.550829
C	7.041311	0.188900	18.310393
C	5.378686	1.718778	19.091314
C	5.651867	0.473973	18.435533
O	4.718064	-0.298273	17.995628
H	8.689281	4.192348	19.348770
H	9.799840	2.825539	19.502951
H	9.073883	0.767223	18.615418
H	6.105658	3.485549	20.052847
H	7.314678	-0.741937	17.821983
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C	-2.690672	1.386702	17.511996
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C	-0.472744	1.501097	17.761930
N	-0.987341	1.429819	18.983056
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H	-3.763182	1.256884	15.685727
H	-1.358825	1.517974	15.851207
H	-3.005724	1.289430	19.700885
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C	-4.866674	4.007664	21.522624
C	-3.559925	3.355171	21.727509
N	-3.368651	2.352293	22.660323
C	-2.374993	3.449718	21.045304
C	-2.115568	1.876366	22.532878
N	-1.491448	2.523961	21.559368
H	-4.755834	4.878143	20.870908
H	-5.320059	4.322983	22.467047
H	-4.069650	1.972254	23.323455
H	-2.121134	4.078497	20.207737
H	-1.675600	1.088127	23.110965

C	-8.240617	-3.954680	17.751003
C	-7.955031	-3.071732	18.929721
O	-7.870970	-1.848587	18.842062
O	-7.765694	-3.743273	20.062640
H	-7.317586	-4.489546	17.495656
H	-8.539288	-3.339260	16.901715
C	-10.808444	-3.314563	22.656493
C	-10.666212	-2.006141	23.322031
N	-9.474638	-1.307042	23.328656
C	-11.561988	-1.239766	24.010305
C	-9.617530	-0.162111	23.987275
N	-10.882638	-0.107599	24.407032
H	-10.646223	-3.219271	21.578108
H	-11.809308	-3.713729	22.832124
H	-8.568086	-1.661217	22.894417
H	-12.600182	-1.398905	24.248238
H	-8.863598	0.594605	24.138190
C	-0.139659	-7.344196	24.246805
C	0.479494	-6.316808	23.377199
N	1.360324	-6.625229	22.357672
C	0.315805	-4.956299	23.299170
C	1.699884	-5.492140	21.702866
N	1.074971	-4.464335	22.254502
H	-0.718332	-8.055253	23.645728
H	-0.821214	-6.855050	24.946938
H	1.690081	-7.557298	22.131038
H	-0.274726	-4.304312	23.917088
H	2.382954	-5.441888	20.875676
C	-7.283671	-2.828229	29.436568
N	-6.167789	-2.106070	30.015457
C	-5.417426	-1.232329	29.334410
N	-5.696189	-0.927354	28.075812
N	-4.388381	-0.643002	29.941887
H	-6.954878	-3.490950	28.629721
H	-8.021416	-2.120711	29.050809
H	-5.756254	-2.482461	30.861602
H	-6.382235	-1.435106	27.518001
H	-5.173842	-0.165352	27.627832
H	-4.251594	-0.774178	30.935052
H	-3.741107	-0.032185	29.417365
Fe	1.470048	-2.465376	21.773700
C	-1.427255	-1.562004	23.364903
C	-0.201017	-2.610057	18.806811
C	4.364417	-3.283238	20.185536
C	3.144247	-2.249029	24.728221
N	0.950983	-2.026577	23.663007
C	-0.292715	-1.665890	24.125646
C	-0.235814	-1.377892	25.543633
C	1.070001	-1.534489	25.921881
C	1.795767	-1.957118	24.737922
C	1.696569	-1.295729	27.243024
O	-2.970733	-2.017218	17.606547
C	-1.397947	-0.994278	26.382347
C	-1.897257	0.435221	26.146751
C	-2.892083	0.810180	27.226129
O	-2.506360	0.785668	28.418087
O	-4.093566	1.096888	26.873461
N	1.953427	-3.012916	19.900874
C	1.129644	-2.953023	18.803430
C	1.895952	-3.188682	17.593245
C	3.200794	-3.334226	17.977556
C	3.222245	-3.220697	19.422624
C	1.301777	-3.238609	16.235709
N	3.360098	-2.836363	22.371171
C	4.425340	-3.107780	21.549259
C	5.654933	-3.122972	22.308202
C	5.314418	-2.839127	23.612434
C	3.867891	-2.651789	23.627516
C	6.992981	-3.394741	21.736674
C	6.162060	-2.722294	24.774132
C	7.460320	-2.387270	24.768887
N	-0.454865	-2.184161	21.200759
C	-0.926836	-2.233537	19.918858
C	-2.307616	-1.798218	19.894532
C	-2.655577	-1.490902	21.202385
C	-1.492620	-1.748742	21.998247
C	-3.191908	-1.664473	18.768188
C	-3.972381	-1.054170	21.724784
C	-4.938484	-2.236372	21.842729
C	-6.185706	-1.902913	22.632699
O	-7.309917	-2.273680	22.151232
O	-6.063812	-1.317305	23.738100
C	4.396309	-3.571223	17.111864
O	5.510056	-2.750957	17.458959
C	4.835286	-5.027358	17.183397
H	5.696877	-5.188105	16.525340
Cu	0.086633	1.590823	20.698543
H	8.891071	3.392426	20.913366
H	-4.673317	2.104936	16.938341
H	-5.531461	3.294704	21.032081
H	-9.006486	-4.710145	17.956797
H	-10.071115	-4.017670	23.050778
H	0.595660	-7.919073	24.825699
H	-7.746918	-3.426168	30.227401
O	1.876828	-0.903581	21.416845
O	0.756875	1.281814	22.455148

O	-6.293883	0.394006	19.800154
H	-6.119639	0.781348	18.923658
H	-6.806446	-0.416360	19.586314
O	-7.553092	-1.896526	26.004768
H	-7.095702	-1.700145	25.147981
H	-7.777234	-2.841909	25.933940
O	1.293124	2.382601	27.304200
H	1.097961	2.385284	26.326734
H	0.509444	1.952130	27.688262
O	-7.522889	2.395483	24.082515
H	-6.644541	1.965416	24.252698
H	-7.495107	2.597270	23.128940
O	-5.084694	1.146447	24.438368
H	-4.666562	1.094890	25.354489
H	-5.338346	0.225572	24.192017
O	-4.865313	3.388503	28.299462
H	-4.583976	2.553372	27.843442
H	-4.529956	4.087673	27.705453
O	0.719013	2.635969	24.666167
H	1.144777	3.488441	24.437238
H	0.728649	2.087212	23.814000
H	-7.535249	-3.090084	20.826785
H	-2.355138	0.531751	25.166370
H	-1.048189	1.120710	26.182945
H	-1.125137	-1.078420	27.436340
H	-2.228179	-1.692392	26.210298
H	2.295817	-2.155004	27.562271
H	2.355759	-0.422063	27.193374
H	0.939830	-1.098580	28.004082
H	-2.335611	-1.280236	23.873592
H	3.679796	-2.113849	25.656996
H	5.684979	-2.918554	25.733146
H	8.021399	-2.336921	25.698511
H	7.981780	-2.131805	23.854151
H	7.645798	-3.845862	22.488925
H	6.925943	-4.070172	20.879970
H	7.463624	-2.464017	21.393594
H	5.287510	-3.404798	19.642430
H	4.092216	-3.361787	16.074557
H	4.014427	-5.678738	16.867223
H	5.112478	-5.284394	18.209801
H	2.072934	-3.356220	15.472383
H	0.606145	-4.082429	16.150728
H	0.737049	-2.324579	16.020835
H	-0.726326	-2.583084	17.863960
H	-4.155962	-1.192460	19.027100
H	-4.426218	-0.301243	21.077461
H	-3.850797	-0.605017	22.707542
H	-4.434926	-3.050653	22.379953
H	-5.199573	-2.608052	20.851261
H	5.172612	-1.814261	17.665079
H	1.254791	0.443239	22.343642
H	-11.281489	0.661987	24.935574

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C	0.705000	7.351000	24.202000
C	1.184819	6.042240	23.640631
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H	1.549890	7.843414	24.694189
H	-0.057051	7.149251	24.960472
H	0.293360	8.019435	23.442061
N	1.133326	5.912008	22.295945
C	1.799367	4.798671	21.657477
C	1.500593	4.703162	20.163983
C	2.323699	3.583050	19.648413
N	1.962926	2.257782	19.871141
C	3.616786	3.604195	19.212894
C	3.002109	1.493396	19.568120
N	4.043338	2.284807	19.168952
H	0.953905	6.740921	21.740963
H	1.488012	3.880226	22.155212
H	0.434366	4.525389	19.993639
H	1.776421	5.634764	19.656857
H	4.269827	4.416313	18.945299
H	3.063842	0.424647	19.650513
H	2.885513	4.890672	21.787330
C	8.805507	3.353190	19.814687
C	7.737978	2.406909	19.355626
C	8.050489	1.158653	18.789351
C	6.388792	2.739411	19.472207
C	7.072014	0.288010	18.363048
C	5.390556	1.887551	19.028963
C	5.680953	0.602470	18.446140
O	4.755430	-0.171386	18.028755
H	8.588919	4.371394	19.472000

H	9.779407	3.053670	19.417376
H	9.095082	0.876146	18.686570
H	6.116404	3.684506	19.927548
H	7.339673	-0.670408	17.931028
C	-4.003414	1.240966	16.836963
C	-2.705381	1.405713	17.540289
N	-1.510036	1.486626	16.851125
C	-2.343919	1.428831	18.863922
C	-0.486261	1.561464	17.726090
N	-0.966736	1.523528	18.961697
H	-4.526810	0.360010	17.213630
H	-3.825334	1.083781	15.769537
H	-1.423421	1.501214	15.839902
H	-2.963550	1.384298	19.738311
H	0.550854	1.655019	17.453665
C	-4.875708	3.943054	21.622973
C	-3.569266	3.275643	21.788451
N	-3.427122	2.135152	22.550807
C	-2.340191	3.488086	21.216630
C	-2.160374	1.694324	22.438640
N	-1.472484	2.493917	21.631802
H	-4.752841	4.888945	21.090605
H	-5.352263	4.138415	22.587943
H	-4.138830	1.731506	23.192324
H	-2.040196	4.246139	20.512402
H	-1.789171	0.802776	22.902370
C	-8.602618	-3.697032	17.825497
C	-8.306983	-3.025551	19.134468
O	-8.766923	-1.932605	19.455726
O	-7.474909	-3.719598	19.909809
H	-7.666507	-3.793835	17.264662
H	-9.304733	-3.089579	17.253797
C	-10.676529	-3.286116	22.504735
C	-10.548576	-1.958766	23.135868
N	-9.338895	-1.298723	23.189732
C	-11.450744	-1.143497	23.759909
C	-9.478710	-0.135554	23.820440
N	-10.759848	-0.023829	24.170496
H	-10.323763	-3.249364	21.470387
H	-11.719618	-3.607844	22.519335
H	-8.443668	-1.721170	22.829278
H	-12.505964	-1.263267	23.940013
H	-8.710859	0.599319	23.994830
C	-0.085673	-7.232232	24.294661
C	0.587586	-6.194643	23.471554
N	1.507130	-6.493297	22.482889
C	0.414022	-4.833815	23.383981
C	1.859828	-5.360673	21.838350
N	1.205656	-4.335628	22.363988
H	-0.734300	-7.844551	23.656267
H	-0.716558	-6.737688	25.037535
H	1.858975	-7.421096	22.272143
H	-0.209214	-4.186830	23.974615
H	2.570308	-5.310227	21.034566
C	-7.240112	-2.911006	29.410094
N	-6.157034	-2.144487	29.988203
C	-5.392813	-1.300758	29.290320
N	-5.615732	-1.082165	28.004469
N	-4.380891	-0.684513	29.908293
H	-6.870129	-3.647406	28.689225
H	-7.949574	-2.241353	28.918848
H	-5.784350	-2.454546	30.877844
H	-6.282891	-1.623211	27.453461
H	-5.118028	-0.313015	27.542751
H	-4.411416	-0.609763	30.917258
H	-3.799849	-0.005689	29.390325
Fe	1.534523	-2.343938	21.802077
C	-1.393370	-1.541348	23.396273
C	-0.118107	-2.486812	18.830005
C	4.440636	-3.160657	20.219820
C	3.234329	-1.883875	24.705288
N	1.014734	-1.854027	23.673010
C	-0.244662	-1.557059	24.144114
C	-0.183281	-1.204156	25.545513
C	1.137991	-1.259463	25.905233
C	1.871235	-1.682012	24.728778
C	1.760883	-0.950381	27.212612
O	-2.865033	-1.911997	17.617155
C	-1.357981	-0.858175	26.382491
C	-1.861499	0.577867	26.187409
C	-2.938971	0.861361	27.215694
O	-2.602875	0.878232	28.421530
O	-4.148248	1.010372	26.810258
N	2.026174	-2.924613	19.935121
C	1.211806	-2.829948	18.831828
C	1.982845	-3.051642	17.622990
C	3.278113	-3.253485	18.014694
C	3.293982	-3.148541	19.460614
C	1.405688	-3.016321	16.258195
N	3.442960	-2.607252	22.384971
C	4.508464	-2.881000	21.564064
C	5.749963	-2.765674	22.294780
C	5.414517	-2.405659	23.580591
C	3.960809	-2.303848	23.613848
C	7.092826	-2.980367	21.713017
C	6.274124	-2.157383	24.712952

C	7.542247	-1.726874	24.655139
N	-0.403190	-2.141994	21.233563
C	-0.860740	-2.158379	19.944460
C	-2.248390	-1.749976	19.919580
C	-2.616139	-1.491742	21.231008
C	-1.456101	-1.747023	22.031819
C	-3.119347	-1.609055	18.782943
C	-3.944313	-1.107009	21.759858
C	-4.859131	-2.326335	21.846329
C	-6.115856	-2.067712	22.642016
O	-7.207012	-2.549473	22.190550
O	-6.037384	-1.438932	23.727258
C	4.468758	-3.513138	17.149525
O	5.585929	-2.678008	17.470748
C	4.922652	-4.959712	17.256565
H	5.780118	-5.125782	16.595100
Cu	0.150194	1.861430	20.632302
H	8.891071	3.392424	20.913364
H	-4.673318	2.104938	16.938342
H	-5.531461	3.294704	21.032082
H	-9.006489	-4.710142	17.956797
H	-10.071117	-4.017669	23.050779
H	0.595657	-7.919074	24.825695
H	-7.746917	-3.426173	30.227402
O	1.873711	-0.770847	21.382366
O	1.124997	1.311717	22.593461
O	-7.080768	0.276423	20.646003
H	-7.023114	0.712561	19.776350
H	-7.577637	-0.540064	20.440888
O	-7.428536	-2.228624	25.964337
H	-7.005064	-1.944722	25.113600
H	-7.365889	-3.201685	25.928888
O	-11.581697	2.054778	25.820277
H	-10.849942	2.722038	25.700285
H	-12.383759	2.519958	25.508405
O	-7.509137	2.421676	24.182677
H	-6.643300	1.953775	24.341031
H	-7.405085	2.820968	23.300784
O	-5.156399	1.051364	24.375771
H	-4.717810	1.007704	25.281178
H	-5.423928	0.127236	24.145713
O	-5.513337	2.767903	28.485003
H	-5.008935	2.124092	27.925325
H	-5.624981	3.533144	27.888501
O	-9.501794	3.833705	25.514309
H	-8.747170	3.321961	25.128821
H	-9.194497	4.056368	26.415016
H	-7.339809	-3.208563	20.798947
H	-2.245554	0.724670	25.180474
H	-1.026348	1.268822	26.346928
H	-1.097864	-0.976904	27.436713
H	-2.179196	-1.556011	26.175225
H	2.356468	-1.795335	27.574029
H	2.431074	-0.087269	27.123068
H	1.001356	-0.714728	27.960098
H	-2.311511	-1.301041	23.910853
H	3.776285	-1.669841	25.614926
H	5.833348	-2.333193	25.693069
H	8.118256	-1.584586	25.565736
H	8.023387	-1.486108	23.714675
H	7.793867	-3.315208	22.481911
H	7.064726	-3.725778	20.914112
H	7.477961	-2.045091	21.286554
H	5.364672	-3.297042	19.683121
H	4.163721	-3.327794	16.109441
H	4.106038	-5.626517	16.964030
H	5.212672	-5.186985	18.286002
H	2.188811	-3.054148	15.498853
H	0.730713	-3.865639	16.098174
H	0.825586	-2.099444	16.108527
H	-0.632082	-2.430134	17.882487
H	-4.106340	-1.180828	19.039188
H	-4.420978	-0.346750	21.138093
H	-3.844315	-0.684391	22.755827
H	-4.320863	-3.132803	22.360523
H	-5.103381	-2.683729	20.845985
H	5.238261	-1.760162	17.661479
H	0.473295	1.031752	23.261818
H	1.474256	0.425092	22.227302
H	-11.145958	0.770019	24.725670

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C	0.705000	7.351000	24.202000
C	1.023715	5.932082	23.805188
O	1.480070	5.112108	24.617832
H	1.572242	7.764781	24.725604

H	-0.136262	7.335770	24.902717
H	0.451590	7.988622	23.351575
N	0.781820	5.600929	22.520696
C	1.159612	4.307209	21.982475
C	1.270089	4.363433	20.458047
C	2.179374	3.301821	19.969076
N	1.863468	1.941077	19.985782
C	3.484586	3.434768	19.606098
C	2.943942	1.274731	19.618397
N	3.970423	2.150272	19.384292
H	0.434056	6.309428	21.887223
H	0.437213	3.542559	22.279505
H	0.282323	4.281752	19.997879
H	1.699586	5.328749	20.168968
H	4.100215	4.305669	19.473159
H	3.047004	0.210706	19.550883
H	2.131138	4.040701	22.404629
C	8.695212	3.425401	19.831849
C	7.655620	2.431107	19.430501
C	8.009403	1.183260	18.878155
C	6.301794	2.714769	19.603377
C	7.055466	0.281931	18.478488
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H	1.979835	0.448839	21.743343
H	4.389484	1.166901	21.405770
H	-11.124053	0.824296	24.793069