

Supporting Information

Synchronous and Basic Asynchronous Hydrogen Atom Abstraction of Benzylic Substrates by High-Valent Iron-Oxo Porphyrin Species

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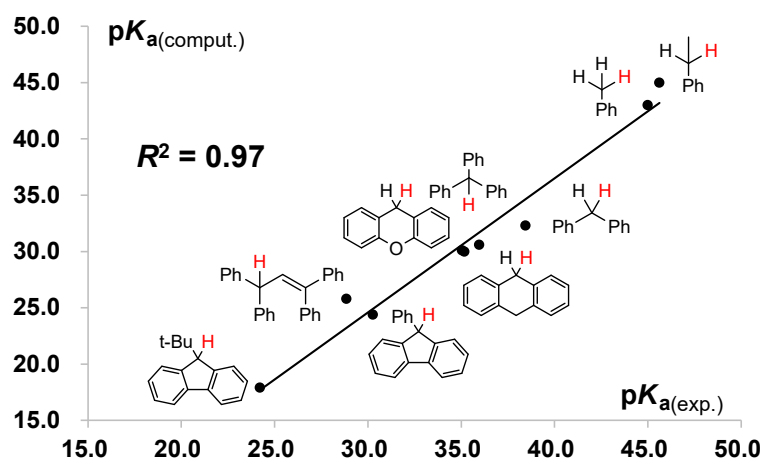


Figure S1. Plot of computational pK_a ($pK_{a(\text{comput.})}$) versus experimental pK_a ($pK_{a(\text{exp.})}$). Experimental pK_a data taken from the literature.¹

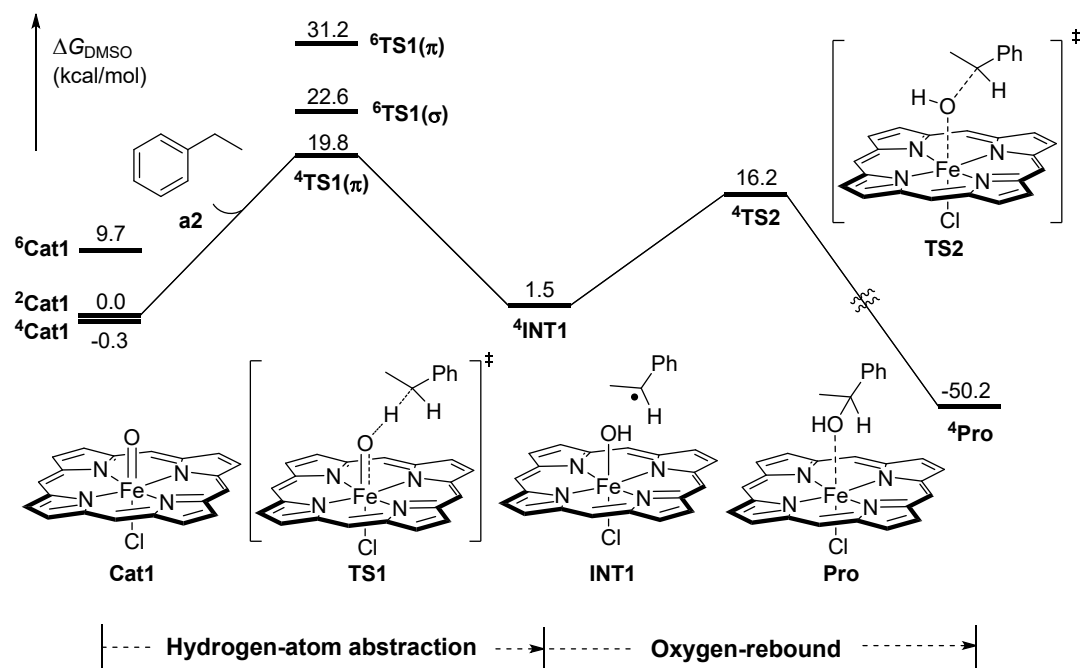


Figure S2. Gibbs free energy profiles for ethylbenzene benzylic C–H hydroxylation with **Cat1**.

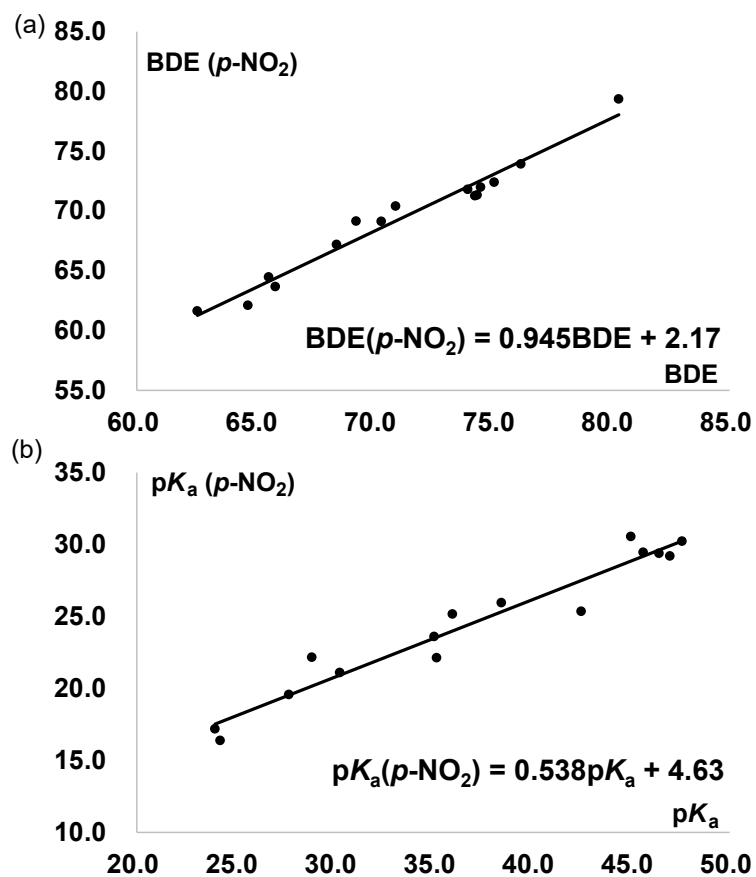


Figure S3. (a) Plot of BDE of unsubstituted substrates versus BDE of substrates bearing an electron-withdrawing group $-NO_2$. (b) Plot of pK_a of unsubstituted substrates versus pK_a of substrates bearing an electron-withdrawing group $-NO_2$.

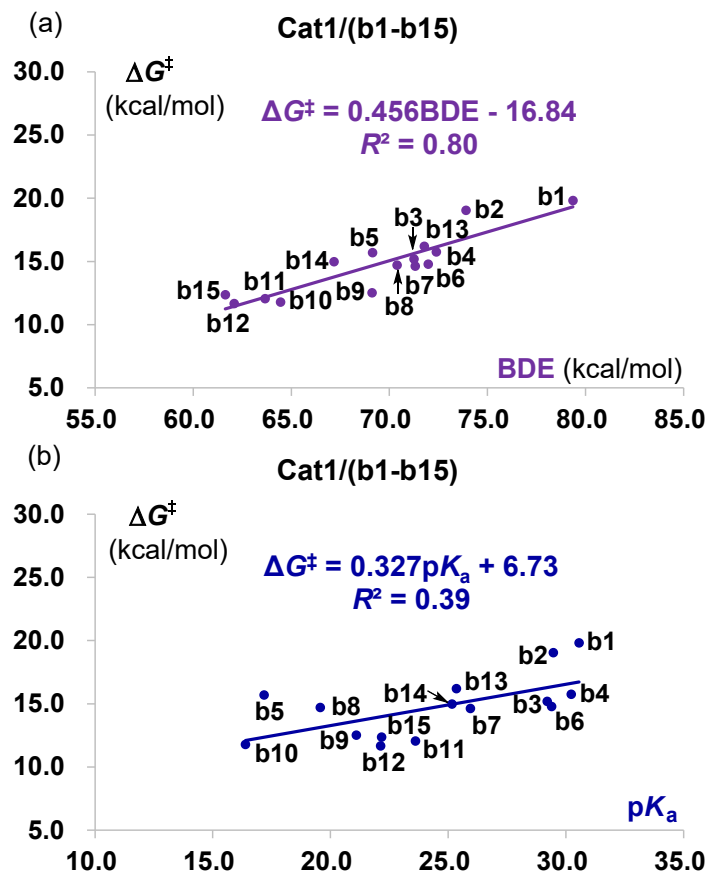


Figure S4. Activation free energy ΔG^\ddagger versus BDE (a) and $\text{p}K_a$ (b) in the system of **Cat1** with **b1-b15**.

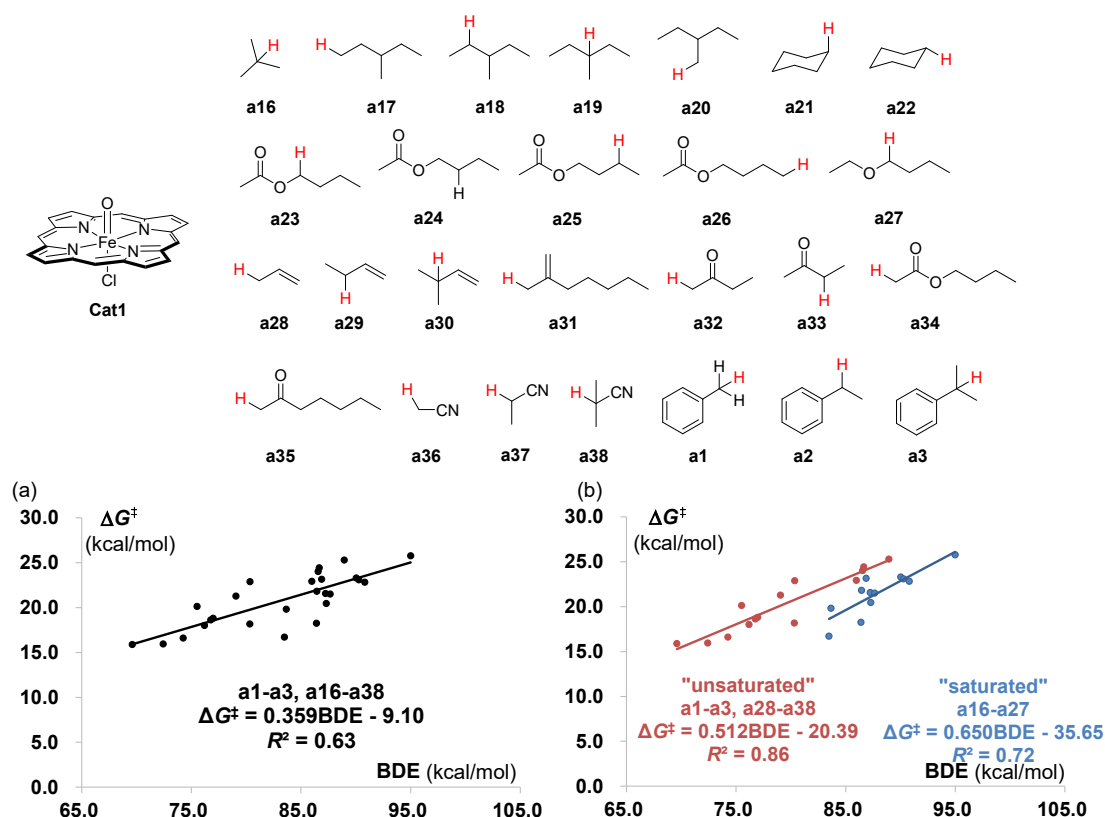


Figure S5. Activation free energy of hydroxylation by **Cat1** versus BDE. (a) All the substrates investigated in this study. (b) Red dots are C–H bonds in the “unsaturated group”; blue dots are C–H bonds in the “saturated group”.

The electron-donating mesitylene substituents are anticipated to augment the electron density at the iron center. Therefore, Mulliken charge and natural population analysis (NPA) charge of **Cat1** and **Cat2** were calculated to confirm their electronic nature. The results showed that substituting electron-donating groups at the *meso*-positions of the porphyrin ring increases the electron density around the central metal.

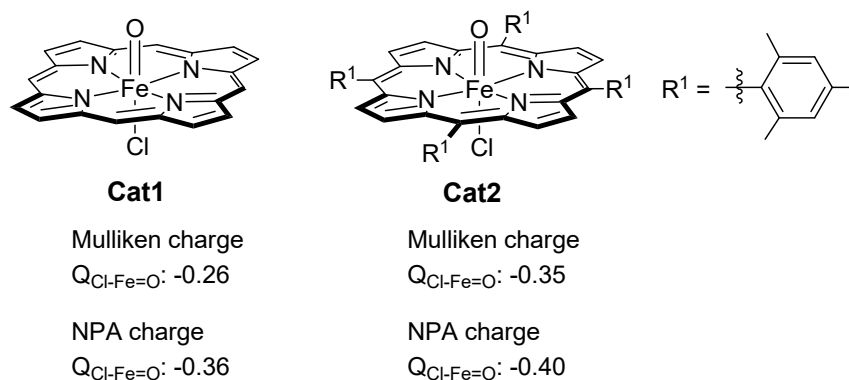


Figure S6. Mulliken charge and natural population analysis (NPA) charge (Q in e) of **Cat1** and **Cat2**.

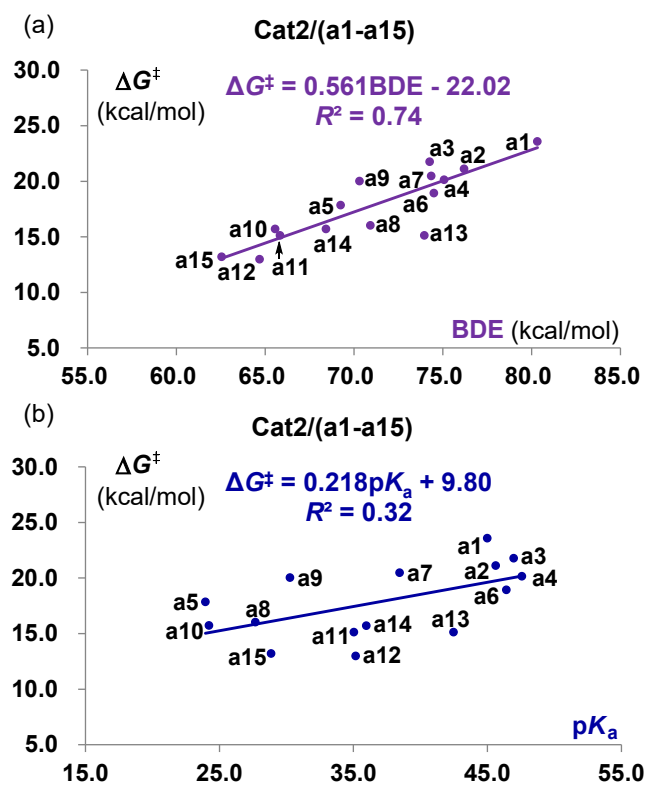


Figure S7. Activation free energy ΔG^\ddagger versus BDE (a) and $\text{p}K_a$ (b) in the system of **Cat2** with **a1-a15**.

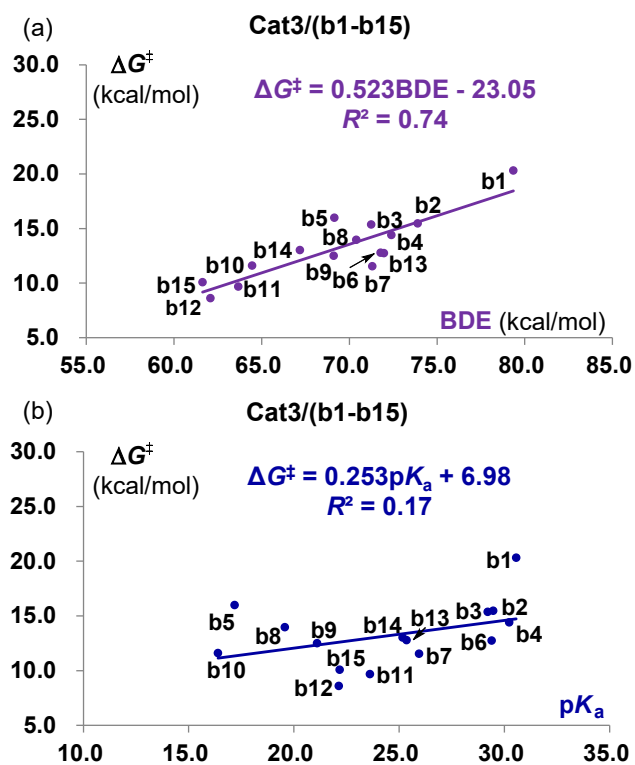


Figure S8. Activation free energy ΔG^\ddagger versus BDE (a) and $\text{p}K_a$ (b) in the system of **Cat3** with **b1-b15**.

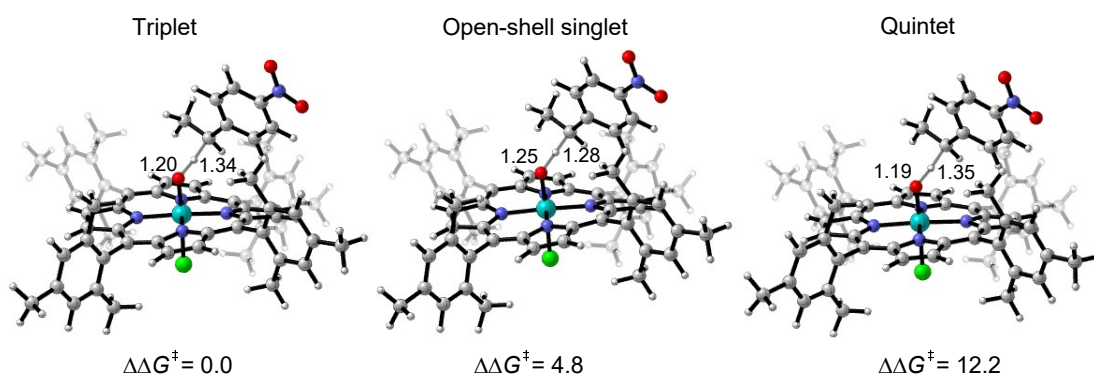


Figure S9. Optimized geometries and Gibbs free energy for transition states of **Cat4** with **b2**. The distances are shown in Å. The energies are shown in kcal/mol.

The potential positions for K^+ on **Cat4** were analyzed using electrostatic potential (ESP). The ESP surface analysis of **Cat4** demonstrates that areas with more negative ESP values (indicated by red surface) are prominently located around the central metal. These regions, which have a stronger propensity to attract protons, are the most probable sites for interaction with the cations. Consequently, K^+ is situated within the negative ESP area, aligning with O (**[Cat4]K**) or with Cl (**[Cat4]K-cf2**) on respective sides. Although ${}^3[\text{Cat4}]\text{K}$ is 1.4 kcal/mol higher than ${}^3[\text{Cat4}]\text{K-cf2}$, ${}^3\text{TS2}[\text{K}]$ is 6.0 kcal/mol lower than ${}^3\text{TS2}[\text{K}]\text{-cf2}$. Therefore, K^+ was placed on the O side for further investigations.

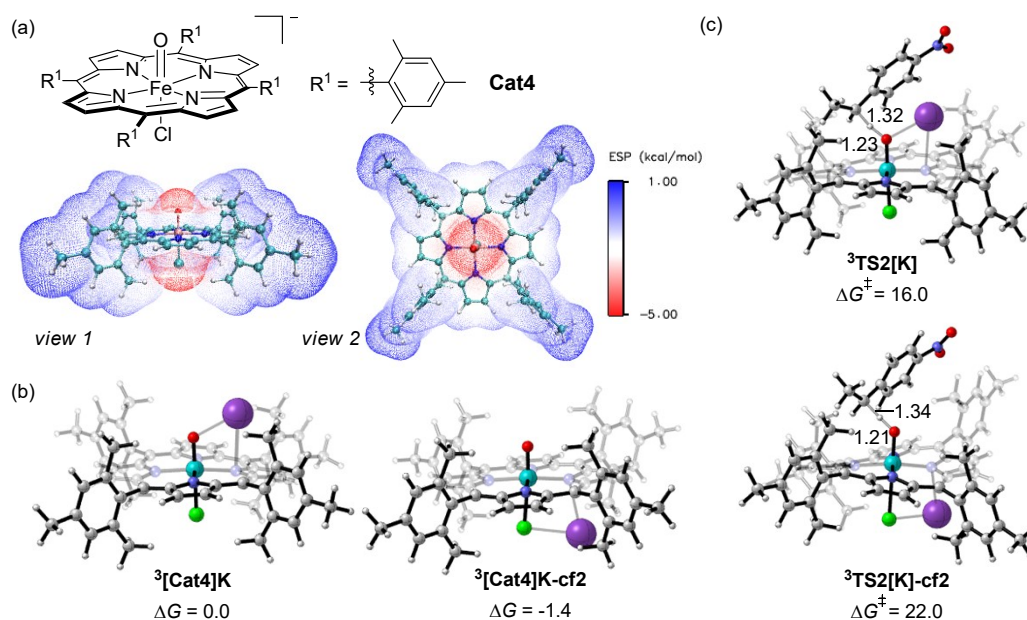


Figure S10. (a) Electrostatic potential (ESP) surface of **Cat4**, optimized geometries and Gibbs free energy for ${}^3[\text{Cat4}]\text{K}$, ${}^3[\text{Cat4}]\text{K-cf2}$ (b), ${}^3\text{TS2}[\text{K}]$ and ${}^3\text{TS2}[\text{K}]\text{-cf2}$ (c). The distances are shown in Å. The energies are shown in kcal/mol.

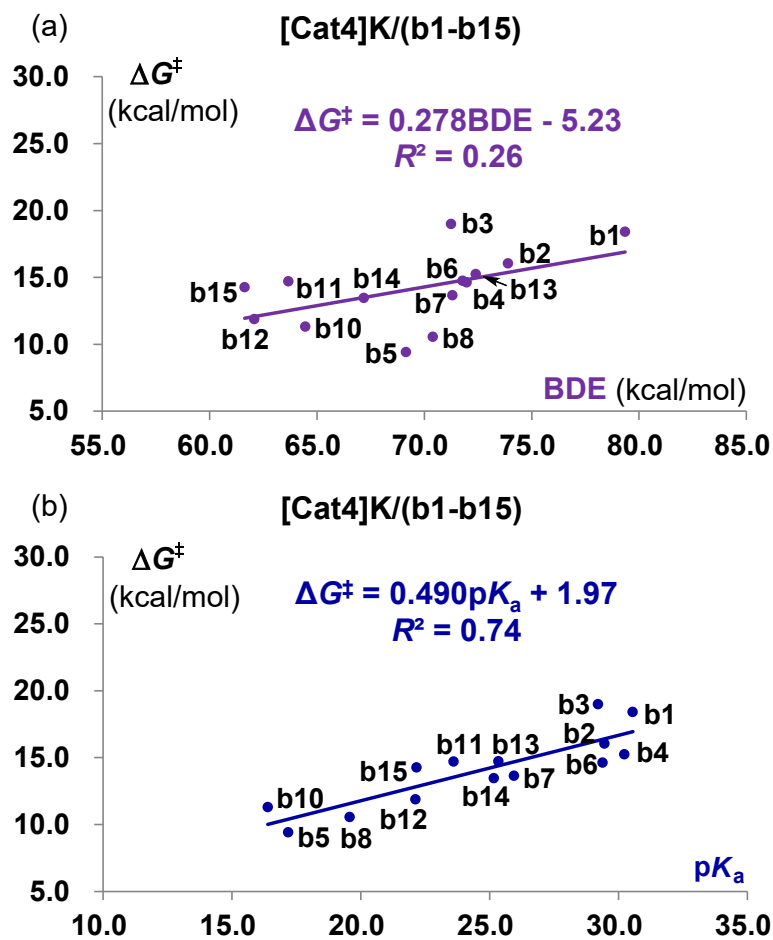


Figure S11. Activation free energy (ΔG^\ddagger) versus BDE (a) and pK_a (b) in the system of [Cat4]K with **b1-b15**, with exception of anomalous result for substrate **b9** (not shown), potentially attributed to steric effects.

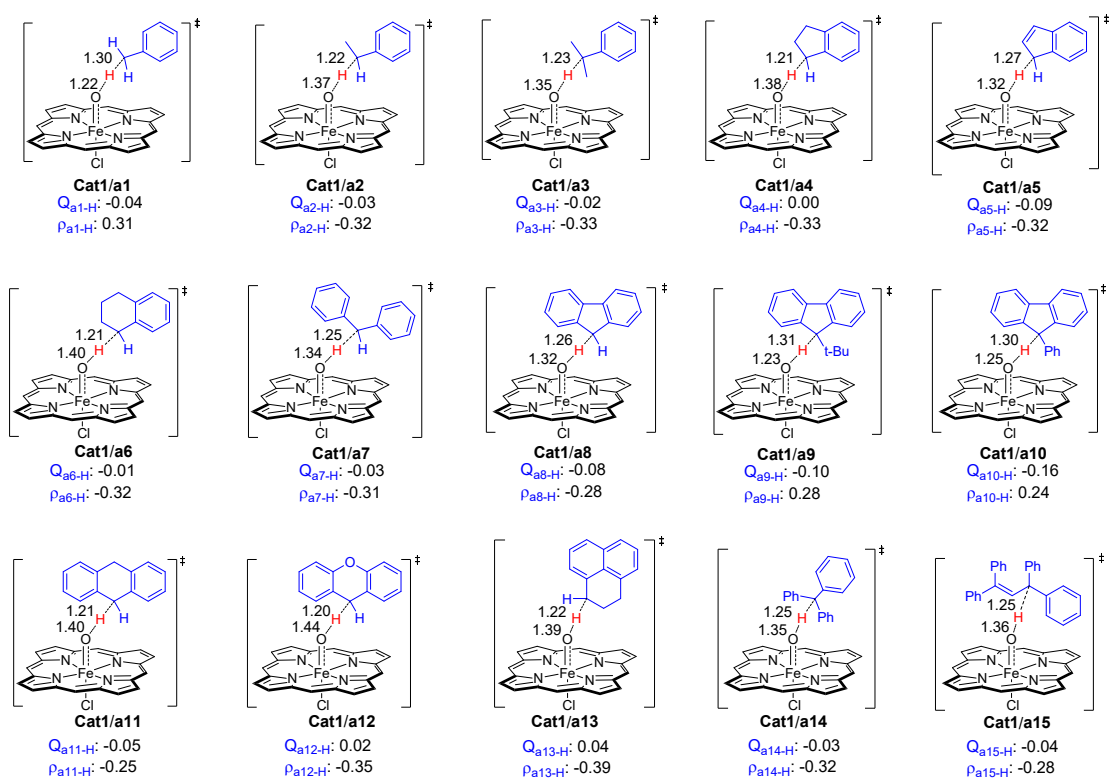


Figure S12. Geometric parameters (bond length in Å) along with NPA charges (Q) and spin densities (ρ) on the hydrogen-atom-abstracted substrate moiety.

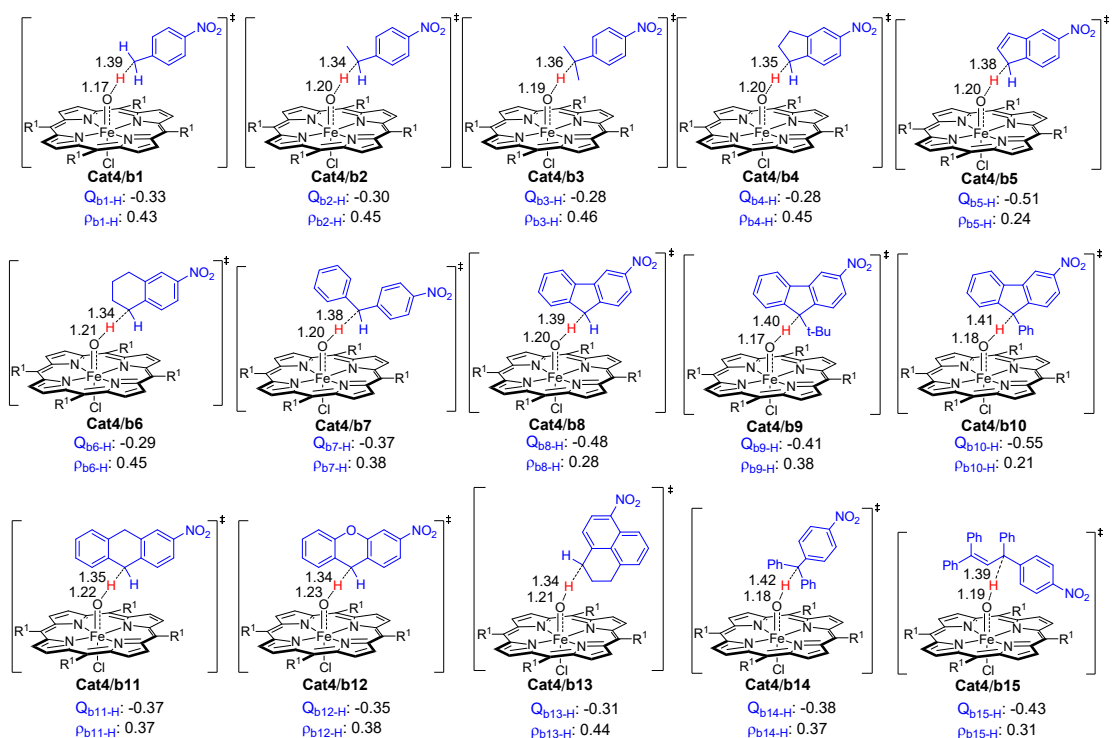


Figure S13. Geometric parameters (bond length in Å) along with NPA charges (Q) and spin densities (ρ) on the hydrogen-atom-abstracted substrate moiety.

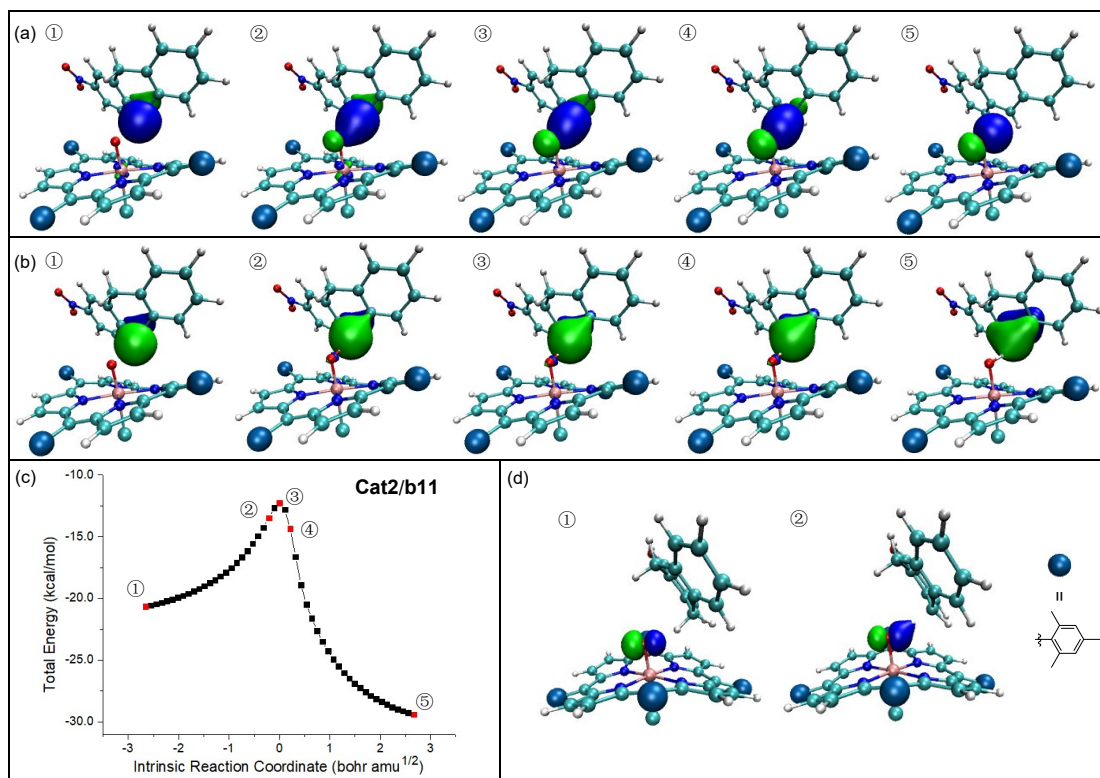


Figure S14. (a) α -LMO and (b) β -LMO analysis along the intrinsic reaction coordinate (IRC) between **Cat2** and **b11**. (c) Plots of the change in electronic energies along the IRC for **Cat2/b11** case. (d) α -LMO of the oxo group in the **Cat2/b11** case.

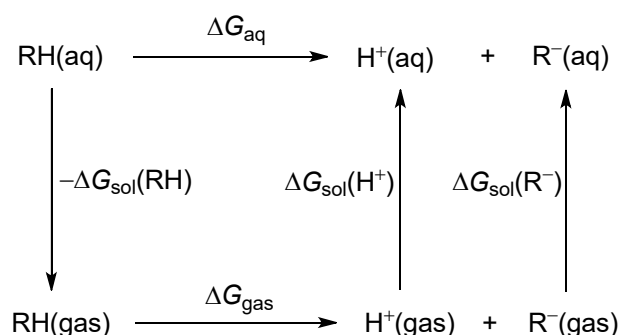
Thermodynamic Cycle for pK_a Calculations

The pK_a for a reaction $RH(aq) \rightleftharpoons H^+(aq) + R^-(aq)$ is given by:

$$pK_a = -\lg K_a = \Delta G_{aq}/(2.303RT)$$

where K_a is the equilibrium constant for the deprotonation of the acid, R is the universal gas constant (0.00198 kcal/(mol*K)), T refers to the temperature.

The Gibbs free energy change (ΔG_{aq}) is calculated according to the following thermodynamic cycle and equation:



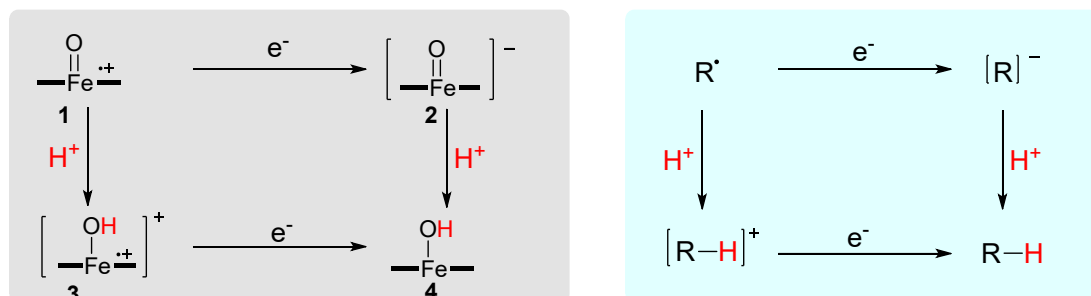
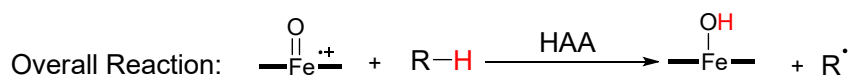
$$\begin{aligned}
 \Delta G_{aq} &= \Delta G_{gas} + \Delta \Delta G_{sol} \\
 \Delta G_{gas} &= G_{gas}(H^+) + G_{gas}(R^-) + G_{gas}(RH) \\
 \Delta \Delta G_{sol} &= \Delta G_{sol}(H^+) + \Delta G_{sol}(R^-) - \Delta G_{sol}(RH)
 \end{aligned}$$

It should be noted that computational methods poorly reproduce the energies of H^+ . In this work, we have used $G_{gas}(H^+) = -6.28$ kcal/mol and $\Delta G_{sol}(H^+) = -265.9$ kcal/mol, on the basis of the recommendation of Tissandier and Kelly.² It should be emphasized that the calculated gas-phase energies are for a standard state of 1 atm but solvation energies use a standard state of 1 mol/L. The free energy change of 1 mol of an ideal gas from 1 atm to 1 mol/L at 298 K is $RT \ln(24.4654) = 1.89$ kcal/mol.³ $\Delta G_{sol}(H^+) = -265.9$ kcal/mol + 1.89 kcal/mol = -264.01 kcal/mol.

Table S1. The doublet and quartet transition state and Gibbs free energy of the HAA step for benzylic C–H hydroxylation (a1-a15) by Cat1

Transition state	² TS(π)	⁴ TS(π)
Cat1/a1	18.2	20.6
Cat1/a2	18.0	19.8
Cat1/a3	16.6	18.9
Cat1/a4	16.2	18.2
Cat1/a5	16.4	17.1
Cat1/a6	16.0	17.9
Cat1/a7	17.1	19.0
Cat1/a8	15.9	17.1
Cat1/a9	12.5	15.5
Cat1/a10	11.4	13.2
Cat1/a11	12.1	13.9
Cat1/a12	10.3	12.0
Cat1/a13	14.3	16.3
Cat1/a14	15.7	17.3
Cat1/a15	12.5	14.0

Asynchronicity Factor (η)



$$\text{Asynchronicity Factor } (\eta) = (1/\sqrt{2}) * [G(\text{R}^\cdot) + G(\mathbf{3}) - G(\mathbf{2}) - G(\text{R-H}^+)]$$

Scheme S1. The two thermodynamic cycles for computing asynchronicity factor. [R·] means the structure for the radical product expected from HAA step; [R-H]⁺ means the structure that was oxidized by one electron; [R]⁻ means the structure after deprotonating the acidic C-H bond.

Table S2. Calculated asynchronicity factors (η) in mV

Reaction	η (mV)	Reaction	η (mV)	Reaction	η (mV)
Cat1/a1	749	Cat2/b1	-517	Cat4/b1	-2199
Cat1/a2	728	Cat2/b2	-582	Cat4/b2	-2265
Cat1/a3	814	Cat2/b3	-570	Cat4/b3	-2252
Cat1/a4	1000	Cat2/b4	-328	Cat4/b4	-2010
Cat1/a5	232	Cat2/b5	-548	Cat4/b5	-2230
Cat1/a6	937	Cat2/b6	-374	Cat4/b6	-2056
Cat1/a7	474	Cat2/b7	-409	Cat4/b7	-2091
Cat1/a8	381	Cat2/b8	-415	Cat4/b8	-2097
Cat1/a9	529	Cat2/b9	-306	Cat4/b9	-1988
Cat1/a10	215	Cat2/b10	-564	Cat4/b10	-2246
Cat1/a11	502	Cat2/b11	-350	Cat4/b11	-2032
Cat1/a12	745	Cat2/b12	-222	Cat4/b12	-1904
Cat1/a13	1178	Cat2/b13	-57	Cat4/b13	-1739
Cat1/a14	425	Cat2/b14	-354	Cat4/b14	-2036
Cat1/a15	347	Cat2/b15	-211	Cat4/b15	-1893

Table S3. Electronic Energies and Free Energies (in Hartree) of the Structures Calculated at the (U)B3LYP-D3/def2-TZVP (SMD: DMSO)//(U)B3LYP-D3/6-31G(d)-LANL2DZ Level

Structures	ZPVE	TCE	TCH	TCG	E	G(E+TCG)	Imaginary Frequenc y	ΔG^\ddagger (kcal/mol)
Cat1/a1	0.402649	0.429994	0.430938	0.343801	-3059.741955	-3059.398154	1641.87i	18.2
Cat1/a2	0.433122	0.461832	0.462776	0.373202	-3099.075220	-3098.702018	2243.10i	18.0
Cat1/a3	0.461541	0.491528	0.492472	0.400500	-3138.408885	-3138.008385	1689.22i	16.6
Cat1/a4	0.440736	0.469117	0.470061	0.381022	-3137.197736	-3136.816714	1849.39i	16.2
Cat1/a5	0.415630	0.443663	0.444607	0.355611	-3135.970106	-3135.614495	2141.91i	16.4
Cat1/a6	0.470469	0.499810	0.500754	0.410168	-3176.535921	-3176.125753	2391.09i	16.0
Cat1/a7	0.485964	0.517758	0.518703	0.421228	-3290.895691	-3290.474463	2721.99i	17.1
Cat1/a8	0.463490	0.494059	0.495003	0.401154	-3289.693377	-3289.292223	2303.72i	15.9
Cat1/a9	0.576534	0.612427	0.613371	0.509981	-3447.022344	-3446.512363	1769.08i	12.5
Cat1/a10	0.543402	0.578843	0.579787	0.475861	-3520.848881	-3520.373020	1773.08i	11.4
Cat1/a11	0.493179	0.524796	0.525740	0.430124	-3329.032264	-3328.602140	2177.94i	12.1
Cat1/a12	0.469278	0.500611	0.501555	0.406194	-3364.952010	-3364.545816	1338.54i	10.3
Cat1/a13	0.488852	0.519535	0.520480	0.426673	-3290.913657	-3290.486984	1601.63i	14.3
Cat1/a14	0.567356	0.603749	0.604693	0.497443	-3522.040257	-3521.542814	1886.92i	15.7
Cat1/a15	0.681865	0.725094	0.726039	0.603226	-3830.630236	-3830.027010	1923.62i	12.5
Cat1/b1	0.405094	0.434891	0.435835	0.343224	-3264.338712	-3263.995488	1824.61i	19.8
Cat1/b2	0.433820	0.465277	0.466221	0.369597	-3303.670142	-3303.300545	1727.57i	19.0
Cat1/b3	0.462167	0.494932	0.495876	0.397658	-3343.008412	-3342.610754	1820.41i	15.2
Cat1/b4	0.441401	0.472518	0.473462	0.377414	-3341.795593	-3341.418179	1695.01i	15.7
Cat1/b5	0.417170	0.447870	0.448815	0.353569	-3340.569056	-3340.215487	1821.94i	15.7
Cat1/b6	0.471177	0.503298	0.504242	0.406071	-3381.134659	-3380.728588	1691.41i	14.8
Cat1/b7	0.487115	0.521613	0.522557	0.418438	-3495.493739	-3495.075301	1828.18i	14.6
Cat1/b8	0.464720	0.498051	0.498995	0.398055	-3494.291458	-3493.893403	1719.33i	14.7
Cat1/b9	0.579102	0.617643	0.618588	0.508351	-3651.619975	-3651.111624	1843.67i	12.5
Cat1/b10	0.546330	0.584325	0.585269	0.474461	-3725.445640	-3724.971179	1845.68i	11.8
Cat1/b11	0.495415	0.529652	0.530596	0.427985	-3533.630194	-3533.202209	3229.14i	12.0
Cat1/b12	0.471708	0.505578	0.506522	0.405175	-3569.546784	-3569.141609	1818.49i	11.7
Cat1/b13	0.490944	0.524298	0.525242	0.424204	-3495.501797	-3495.077593	2193.53i	16.2
Cat1/b14	0.568592	0.607734	0.608678	0.494407	-3726.637910	-3726.143503	1854.48i	15.0
Cat1/b15	0.684420	0.730165	0.731109	0.602468	-4035.229003	-4034.626535	2312.76i	12.4
Cat2/a1	1.059223	1.126815	1.127759	0.950772	-4456.346132	-4455.395360	1828.35i	23.6
Cat2/a2	1.088294	1.157484	1.158428	0.978162	-4495.681048	-4494.702886	1791.52i	21.1
Cat2/a3	1.116665	1.187292	1.188236	1.004642	-4535.010630	-4534.005988	1437.53i	21.8
Cat2/a4	1.095755	1.164595	1.165540	0.986202	-4533.802510	-4532.816308	1901.91i	20.1
Cat2/a5	1.071352	1.139831	1.140775	0.961227	-4532.579278	-4531.618051	1763.94i	17.8
Cat2/a6	1.125695	1.195467	1.196411	1.014112	-4573.140968	-4572.126856	1745.06i	18.9

Cat2/a7	1.141324	1.213542	1.214486	1.026323	-4687.501196	-4686.474873	1856.06i	20.5
Cat2/a8	1.119340	1.190339	1.191284	1.003115	-4686.300946	-4685.297831	1874.96i	16.0
Cat2/a9	1.233161	1.309637	1.310581	1.115974	-4843.622227	-4842.506253	1645.74i	20.0
Cat2/a10	1.200288	1.276180	1.277124	1.081446	-4917.453415	-4916.371969	1974.9i	15.7
Cat2/a11	1.149281	1.220974	1.221918	1.036907	-4725.640053	-4724.603146	1680.94i	15.1
Cat2/a12	1.126206	1.197418	1.198362	1.012730	-4761.560039	-4760.547309	3701.39i	13.0
Cat2/a13	1.143589	1.214986	1.215930	1.029344	-4687.520933	-4686.491589	1760.25i	15.1
Cat2/a14	1.223271	1.299933	1.300877	1.104568	-4918.653190	-4917.548622	2060.16i	15.7
Cat2/a15	1.337829	1.421490	1.422434	1.209865	-5227.241596	-5226.031731	1903.88i	13.2
Cat2/b1	1.062662	1.132286	1.133230	0.952667	-4660.944427	-4659.991760	1925.13i	25.8
Cat2/b2	1.090752	1.162540	1.163484	0.975529	-4700.281483	-4699.305954	1863.34i	19.3
Cat2/b3	1.120292	1.192682	1.193626	1.008377	-4739.609309	-4738.600932	1952.85i	25.0
Cat2/b4	1.099317	1.170213	1.171157	0.987844	-4738.400344	-4737.412500	1916.33i	23.0
Cat2/b5	1.074408	1.145414	1.146358	0.960715	-4737.181582	-4736.220867	1619.58i	16.0
Cat2/b6	1.129177	1.201034	1.201978	1.015905	-4777.739508	-4776.723603	1930.6i	21.6
Cat2/b7	1.145761	1.219646	1.220590	1.030649	-4892.097792	-4891.067143	1977.75i	23.4
Cat2/b8	1.122584	1.195802	1.196746	1.006203	-4890.899255	-4889.893052	1964.81i	18.6
Cat2/b9	1.236078	1.315018	1.315962	1.115766	-5048.222977	-5047.107211	1944.05i	19.0
Cat2/b10	1.203227	1.281579	1.282523	1.080992	-5122.055622	-5120.974630	1995.03i	13.3
Cat2/b11	1.152683	1.226355	1.227299	1.039897	-4930.237104	-4929.197207	1878.73i	18.9
Cat2/b12	1.128542	1.201892	1.202836	1.015476	-4966.152341	-4965.136865	1808.35i	18.3
Cat2/b13	1.146672	1.220279	1.221223	1.030789	-4892.110258	-4891.079469	1919.13i	18.7
Cat2/b14	1.22657	1.305293	1.306237	1.106090	-5123.248522	-5122.142432	2164.53i	19.3
Cat2/b15	1.341458	1.427001	1.427945	1.212733	-5431.837374	-5430.624641	2064.96i	17.2
Cat3/b1	0.564238	0.631915	0.632859	0.455058	-6174.396136	-6173.941078	1817.17i	20.3
Cat3/b2	0.595169	0.664416	0.665360	0.484523	-6213.737133	-6213.252610	2235.34i	15.4
Cat3/b3	0.62385	0.694116	0.695060	0.513347	-6253.070215	-6252.556868	2684.89i	15.3
Cat3/b4	0.602756	0.671602	0.672546	0.492232	-6251.858912	-6251.366680	2214.82i	14.4
Cat3/b5	0.578134	0.646357	0.647301	0.469558	-6250.630935	-6250.161377	1906.63i	16.0
Cat3/b6	0.632439	0.702276	0.703221	0.520165	-6291.19838	-6290.678215	2558.43i	12.7
Cat3/b7	0.648524	0.720672	0.721616	0.533417	-6405.560019	-6405.026602	2358.54i	11.5
Cat3/b8	0.625556	0.696414	0.697358	0.512835	-6404.353787	-6403.840952	2482.78i	14.0
Cat3/b9	0.740336	0.816494	0.817438	0.624795	-6561.682825	-6561.058030	1914.08i	12.5
Cat3/b10	0.706807	0.782553	0.783498	0.590220	-6635.50805	-6634.917830	2411.27i	11.6
Cat3/b11	0.655365	0.727198	0.728142	0.543745	-6443.696117	-6443.152372	2389.75i	9.7
Cat3/b12	0.631487	0.702974	0.703918	0.520252	-6479.613109	-6479.092857	1764.63i	8.6
Cat3/b13	0.650631	0.721772	0.722716	0.539291	-6405.568684	-6405.029393	1526.62i	12.8
Cat3/b14	0.729793	0.806407	0.807351	0.612044	-6636.70503	-6636.092986	1791.16i	13.0
Cat3/b15	0.845110	0.928382	0.929326	0.720794	-6945.297346	-6944.576552	1507.71i	10.1
Cat4/b1	1.062759	1.132154	1.133098	0.952661	-4661.115975	-4660.163314	1871.49i	25.5

Cat4/b2	1.090996	1.162448	1.163392	0.976581	-4700.453007	-4699.476426	1906.01i	19.6
Cat4/b3	1.120429	1.192513	1.193457	1.009213	-4739.779081	-4738.769868	1987.74i	26.3
Cat4/b4	1.099259	1.169952	1.170896	0.987366	-4738.571028	-4737.583662	1643.73i	22.9
Cat4/b5	1.074849	1.145639	1.146583	0.961170	-4737.358593	-4736.397423	1942.91i	12.5
Cat4/b6	1.129393	1.200876	1.201820	1.016889	-4777.90873	-4776.891841	1993.00i	23.3
Cat4/b7	1.145274	1.219225	1.220169	1.027828	-4892.270748	-4891.242920	2025.30i	20.4
Cat4/b8	1.122337	1.195566	1.196510	1.004615	-4891.076112	-4890.071497	1763.84i	13.9
Cat4/b9	1.235859	1.314698	1.315642	1.115436	-5048.395574	-5047.280138	1843.45i	17.8
Cat4/b10	1.203868	1.281797	1.282741	1.083904	-5122.231497	-5121.147593	1568.38i	12.1
Cat4/b11	1.152531	1.226136	1.227080	1.038199	-4930.409370	-4929.371171	1980.92i	17.0
Cat4/b12	1.128178	1.201520	1.202464	1.013776	-4966.323168	-4965.309392	2035.49i	17.4
Cat4/b13	1.146735	1.220032	1.220976	1.030447	-4892.280339	-4891.249892	1983.34i	19.0
Cat4/b14	1.226680	1.305072	1.306016	1.107396	-5123.420104	-5122.312708	2103.01i	19.8
Cat4/b15	1.341393	1.426699	1.427643	1.212722	-5432.008482	-5430.795760	2019.49i	17.2
[Cat4]K/b1	1.063916	1.135767	1.136711	0.948907	-5261.016557	-5260.067650	1916.06i	18.4
[Cat4]K/b2	1.092946	1.166341	1.167286	0.976338	-5300.351573	-5299.375235	1865.91i	16.0
[Cat4]K/b3	1.121218	1.195847	1.196791	1.004731	-5339.679370	-5338.674639	1964.07i	19.0
[Cat4]K/b4	1.100010	1.173263	1.174207	0.983298	-5338.472212	-5337.488914	1877.56i	15.2
[Cat4]K/b5	1.076640	1.149338	1.150282	0.961197	-5337.256604	-5336.295407	1417.94i	9.4
[Cat4]K/b6	1.130333	1.204307	1.205251	1.013564	-5377.812333	-5376.798769	1881.23i	14.6
[Cat4]K/b7	1.145855	1.222295	1.223239	1.025299	-5492.172102	-5491.146803	1891.33i	13.7
[Cat4]K/b8	1.123753	1.199331	1.200275	1.003173	-5490.973123	-5489.969950	1655.69i	10.6
[Cat4]K/b10	1.206649	1.285931	1.286875	1.087046	-5722.128904	-5721.041858	1553.79i	11.3
[Cat4]K/b11	1.154294	1.229832	1.230776	1.037833	-5530.305737	-5529.267904	1924.60i	14.7
[Cat4]K/b12	1.129848	1.205379	1.206323	1.012083	-5566.223272	-5565.211189	1907.32i	11.9
[Cat4]K/b13	1.148579	1.223902	1.224846	1.031350	-5492.181191	-5491.149841	1951.45i	14.7
[Cat4]K/b14	1.227273	1.308243	1.309187	1.104045	-5723.319898	-5722.215853	2172.40i	13.5
[Cat4]K/b15	1.342920	1.430406	1.431351	1.210998	-6031.904429	-6030.693431	2264.97i	14.3

ZPVE = zero-point vibrational energy; TCE = thermal correction to energy; TCH = thermal correction to enthalpy; TCG = thermal correction to Gibbs free energy.

Table S4. Electronic Energies and Free Energies (in Hartree) of the Structures Calculated at the (U)B3LYP-D3/def2-TZVP (SMD: DMSO)//(U)B3LYP-D3/6-31G(d)-LANL2DZ Level

Structures	ZPVE	TCE	TCH	TCG	E	G(E+TCG)	Imaginary Frequenc y	ΔG^\ddagger (kcal/mol)
Cat1/a1(quartet)	0.401841	0.429324	0.430269	0.341936	-3059.736265	-3059.394329	1923.95i	20.6
Cat1/a2(quartet)	0.432252	0.460924	0.461868	0.371972	-3099.071131	-3098.699159	2081.61i	19.8
Cat1/a2(sextet, σ)	0.429522	0.459009	0.459953	0.367131	-3099.061822	-3098.694691	1336.88i	22.6
Cat1/a2(sextet, π)	0.428473	0.458004	0.458949	0.366180	-3099.047086	-3098.680906	19.7.05i	31.2
Cat1/a3(quartet)	0.458969	0.489340	0.490285	0.396744	-3138.401426	-3138.004682	1960.37i	18.9
Cat1/a4(quartet)	0.439848	0.468197	0.469141	0.379607	-3137.193171	-3136.813564	1873.33i	18.2
Cat1/a5(quartet)	0.415146	0.443116	0.444060	0.354700	-3135.968140	-3135.613440	1923.87i	17.1
Cat1/a6(quartet)	0.469756	0.499043	0.499987	0.408959	-3176.531675	-3176.122716	1877.75i	17.9
Cat1/a7(quartet)	0.485203	0.516987	0.517931	0.419912	-3290.891300	-3290.471388	2117.01i	19.0
Cat1/a8(quartet)	0.463069	0.493548	0.494492	0.400541	-3289.690806	-3289.290265	1992.94i	17.1
Cat1/a9(quartet)	0.575963	0.611914	0.612858	0.509185	-3447.016827	-3446.507642	2000.66i	15.5
Cat1/a10(quartet)	0.542814	0.578361	0.579305	0.474235	-3520.844406	-3520.370171	1983.71i	13.2
Cat1/a11(quartet)	0.492878	0.524420	0.525364	0.429217	-3329.028415	-3328.599198	1702.39i	13.9
Cat1/a12(quartet)	0.468906	0.500176	0.501120	0.405327	-3364.948296	-3364.542969	1454.77i	12.0
Cat1/a13(quartet)	0.488023	0.518685	0.519630	0.425526	-3290.909397	-3290.483871	1729.13i	16.3
Cat1/a14(quartet)	0.566672	0.603108	0.604052	0.495968	-3522.036155	-3521.540187	2071.25i	17.3
Cat1/a15(quartet)	0.681563	0.724773	0.725717	0.601764	-3830.626410	-3830.024646	1864.01i	14.0

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Cartesian coordinates of the structures

cat1/a1

C	0.63441600	-2.99035300	-0.55417300
C	1.28071600	-4.20754200	-0.12613000
C	2.30451900	-3.83642500	0.69114100
C	2.28909200	-2.39341500	0.74491300
N	1.25317700	-1.90051000	-0.00556500
H	0.97931600	-5.20371800	-0.42337100
H	3.02394500	-4.46427100	1.20093300
C	2.94463500	1.86242500	0.94220400
C	4.15333400	1.82841500	1.73576400
C	4.39385300	0.52021300	2.01945300
C	3.33803500	-0.23925900	1.38538100
N	2.47452200	0.59431500	0.73776100
H	4.72235700	2.70066800	2.03060400
H	5.20554700	0.09003800	2.59194400
C	-1.70788400	0.33200600	-1.92638000
C	-2.65654200	-0.41528400	-2.71721200
C	-2.29020800	-1.72518600	-2.63212000
C	-1.12971000	-1.77256800	-1.77664600
N	-0.79329600	-0.50872100	-1.35596800
H	-3.47905500	0.02200100	-3.26841500
H	-2.75018700	-2.58787400	-3.09665700
C	-0.72299300	2.49157200	-1.21214200
C	-0.70044300	3.93746200	-1.20520600
C	0.45548800	4.30300300	-0.58835800
C	1.12434500	3.07877000	-0.20699100
N	0.39384000	1.99502900	-0.59780700
H	-1.46902900	4.56881600	-1.63206500
H	0.83440200	5.29852900	-0.39627200
C	-0.46824500	-2.93400700	-1.40196200
C	2.32863000	3.02138600	0.48958800
C	3.24003900	-1.62734900	1.40914300
C	-1.70867600	1.72129900	-1.81364300
H	4.00415200	-2.16553200	1.96251600
H	2.80943000	3.96557400	0.72778400
H	-2.52747000	2.25166200	-2.29080500
H	-0.84689200	-3.87391900	-1.79223600
Fe	0.80260100	0.03803000	-0.26545300
Cl	2.09518000	0.05773900	-2.22121300
O	-0.03077400	0.17897800	1.23323700

H	-0.91658300	-0.64314500	1.41383500
C	-4.64767400	0.73139900	2.92573700
C	-5.45348400	0.79687600	1.78301100
C	-5.08026100	0.09651100	0.63114200
C	-3.91256200	-0.66017100	0.61901200
C	-3.09257100	-0.74296500	1.76418000
C	-3.48156500	-0.02705300	2.91652200
H	-4.93281200	1.27392900	3.82320600
H	-6.36426500	1.38957400	1.79132300
H	-5.70184700	0.14223900	-0.25953800
H	-3.62420000	-1.19941600	-0.27751600
H	-2.85292100	-0.07141900	3.80244300
C	-1.84141400	-1.49562400	1.73532700
H	-1.74303800	-2.24439900	0.94902500
H	-1.46527800	-1.83711600	2.70150700

cat1/a2

C	-0.21623400	-2.59110000	1.47866900
C	-0.56418200	-3.98502200	1.36235400
C	-1.50758700	-4.07514400	0.38352300
C	-1.75340600	-2.73313200	-0.08408900
N	-0.94181800	-1.84891900	0.58206700
H	-0.13083300	-4.77763100	1.95867000
H	-2.01669900	-4.95629100	0.01467400
C	-3.15265300	1.07956900	-1.48792300
C	-4.21291300	0.58307800	-2.33503600
C	-4.15391600	-0.77487400	-2.28247700
C	-3.07082100	-1.10864700	-1.38609300
N	-2.48093700	0.03209800	-0.91818800
H	-4.89447800	1.20978200	-2.89572100
H	-4.78204500	-1.49993100	-2.78391200
C	1.34748800	1.37732100	1.93651900
C	2.34621900	1.06661900	2.92937100
C	2.21560400	-0.25913300	3.21891400
C	1.15147500	-0.76338400	2.38721600
N	0.64222300	0.24775200	1.61129800
H	3.03535400	1.78607400	3.35272600
H	2.78001500	-0.85653300	3.92335600
C	0.06351900	3.00723800	0.60836100
C	-0.23611800	4.35929300	0.19585800
C	-1.37365300	4.29793000	-0.54726900
C	-1.75752000	2.90589000	-0.60788500
N	-0.87317300	2.14576600	0.10621600
H	0.35195600	5.22781000	0.46321400

H	-1.91339400	5.10452000	-1.02659800
C	0.74776200	-2.09001100	2.34284000
C	-2.84031700	2.42123900	-1.32782100
C	-2.71856900	-2.40099700	-1.02404400
C	1.11434800	2.65346100	1.44053900
H	-3.28022300	-3.21583100	-1.46991500
H	-3.46306800	3.14535600	-1.84343800
H	1.77276500	3.44696400	1.77960900
H	1.24197300	-2.79062900	3.00808300
Fe	-0.87926400	0.13428600	0.30812100
Cl	-2.36396800	0.41201400	2.06671500
O	0.09433000	0.05941500	-1.04076800
H	1.15565000	-0.80787700	-0.94355500
C	4.83501100	0.12608100	-2.94186300
C	5.46422000	0.85289300	-1.92554600
C	4.98963500	0.76089100	-0.61214500
C	3.89875500	-0.04980000	-0.32024900
C	3.25604100	-0.79591500	-1.33297800
C	3.74091800	-0.68477800	-2.65147800
H	5.19959600	0.19434600	-3.96336900
H	6.31568200	1.48749200	-2.15598100
H	5.47213400	1.32363100	0.18268700
H	3.52815200	-0.11480400	0.69879400
H	3.25999000	-1.24045300	-3.45024700
C	2.07512100	-1.60785100	-0.98252100
C	1.59913400	-2.70269900	-1.92171400
H	1.30681700	-2.30130200	-2.89795000
H	0.72707400	-3.20566800	-1.49499900
H	2.38541200	-3.45213600	-2.08663700
H	2.09359700	-1.92881300	0.06341900

cat1/a3

C	-0.13085400	-2.60526100	-1.23003200
C	-1.25747600	-3.23612100	-1.86780600
C	-2.16952800	-2.25557800	-2.12131000
C	-1.59677000	-1.02024000	-1.65465500
N	-0.36326000	-1.25510700	-1.09444400
H	-1.32339500	-4.29425500	-2.08650600
H	-3.13955000	-2.33892600	-2.59393700
C	-0.22593800	2.91583500	-0.64562300
C	-1.38171700	3.63937400	-1.12183300
C	-2.25477300	2.71314100	-1.60290900
C	-1.63165600	1.42422600	-1.42367100
N	-0.40176100	1.57132600	-0.84456600

H	-1.48866200	4.71597700	-1.08451800
H	-3.23384000	2.86390100	-2.03830600
C	3.45643000	-1.19438700	0.65252700
C	4.10890000	-2.47514200	0.78781900
C	3.26503900	-3.40391000	0.26102500
C	2.09617600	-2.68982700	-0.19329000
N	2.23375700	-1.35204200	0.05607500
H	5.08784200	-2.62102600	1.22620200
H	3.40328100	-4.47408800	0.17520400
C	3.41667200	1.25157200	0.92410100
C	4.01667500	2.49672800	1.34334200
C	3.13835600	3.48401900	1.02073700
C	1.99872200	2.84345100	0.40637100
N	2.19174100	1.48949400	0.35934900
H	4.98680400	2.58140800	1.81601800
H	3.23372400	4.55153500	1.17271900
C	0.99816000	-3.28253700	-0.79918300
C	0.88149400	3.51540700	-0.06542000
C	-2.20697800	0.21659100	-1.78683900
C	4.01181000	0.00825200	1.06441700
Fe	0.88425100	0.09985100	-0.34037000
Cl	1.88813000	0.35483800	-2.40538900
O	0.32146200	0.06039600	1.23561300
H	-0.78638500	-0.66923000	1.49094300
C	-5.10878500	-0.41580200	0.44450700
C	-5.14543400	0.97752400	0.53075600
C	-4.06230200	1.66048300	1.09333300
C	-2.96707700	0.95490100	1.57991300
C	-2.92369800	-0.45358300	1.52662700
C	-4.00632500	-1.12269700	0.92563400
H	-5.94156200	-0.95675900	0.00239500
H	-4.06174200	2.74580700	1.13298000
C	-1.74219400	-1.17555500	2.08322400
H	-3.20209200	0.24136400	-2.21666000
H	1.02776400	-4.35614800	-0.95523900
H	4.99473600	-0.02695500	1.52345700
H	0.87208300	4.59679800	0.02777000
C	-1.39411700	-0.81474600	3.52936400
H	-0.42776700	-1.24803600	3.80520700
H	-1.33639800	0.26549400	3.68372900
H	-2.16163100	-1.21517100	4.20668200
C	-1.65154400	-2.67128300	1.82820100
H	-1.87221500	-2.93102400	0.79133800
H	-0.64133200	-3.02786800	2.05544100

H	-2.35067000	-3.21662700	2.47921400
H	-3.99808300	-2.20457900	0.85025200
H	-2.10902800	1.49486900	1.96841100
H	-6.00325800	1.52729400	0.15266300

cat1/a4

C	0.92818400	-0.49181600	2.59772000
C	1.91970900	0.12038600	3.44634000
C	2.03777300	1.41691300	3.04164700
C	1.10164500	1.60373300	1.96065200
N	0.44912900	0.42684500	1.69693400
H	2.44775800	-0.39060900	4.24121600
H	2.67740400	2.19384900	3.44050800
C	-1.88866800	2.79656400	-0.88151100
C	-1.55327200	4.20173900	-0.92024800
C	-0.46190100	4.36677000	-0.12503600
C	-0.14477900	3.06633300	0.41905200
N	-1.02354100	2.13243000	-0.05678000
H	-2.08960300	4.94495100	-1.49615800
H	0.08246800	5.27552000	0.09748800
C	-1.72233600	-2.77541400	0.11468100
C	-1.47435300	-4.06137500	0.71979900
C	-0.62064400	-3.84964200	1.75947600
C	-0.32436300	-2.43843200	1.77417400
N	-0.99772300	-1.80604200	0.76140300
H	-1.92407900	-4.99021500	0.39310900
H	-0.21462900	-4.56945600	2.45857700
C	-2.99718000	-1.31764500	-1.40960100
C	-4.02716600	-1.10318000	-2.40029800
C	-4.13841100	0.24288800	-2.56343900
C	-3.16032200	0.85087800	-1.69051900
N	-2.48882900	-0.11848400	-0.99582400
H	-4.58906700	-1.89238300	-2.88318900
H	-4.80449300	0.79268600	-3.21592400
C	0.55979500	-1.82828100	2.65387900
C	-2.90842500	2.21279700	-1.62050400
C	0.86517600	2.82207700	1.33762200
C	-2.62260600	-2.56128600	-0.91942500
H	1.47853400	3.66419400	1.64231500
H	-3.52254500	2.86776400	-2.23039400
H	-3.11926600	-3.43225400	-1.33546300
H	1.02058800	-2.44733100	3.41688200
Fe	-0.97979800	0.14851600	0.31861700
Cl	-2.58873800	0.51141200	1.94916600

O	0.07770400	-0.01981700	-0.95556900
H	1.19605300	-0.77260200	-0.64688900
C	2.08257900	-2.44407100	-1.75486800
C	2.79057500	-1.66559500	-2.89370100
C	2.16444700	-1.49922400	-0.55205700
C	3.33050700	-0.64100900	-0.79457700
C	4.00649300	0.20925600	0.09158800
C	5.08470700	0.95123800	-0.38606000
C	5.47434600	0.85768900	-1.73146800
C	4.78817300	0.02190300	-2.62218700
C	3.71262800	-0.72292400	-2.15276600
H	3.69317000	0.27926500	1.12927000
H	6.31893300	1.44240400	-2.08654100
H	5.09646400	-0.04120200	-3.66284100
H	5.63107800	1.60735100	0.28623200
H	3.31487600	-2.31515800	-3.60380500
H	1.05308600	-2.72426700	-1.99629000
H	2.03752000	-1.92757000	0.44486600
H	2.05446300	-1.08591600	-3.46847900
H	2.63581200	-3.36679100	-1.53013400

cat1/a5

C	0.94376400	-0.29895000	2.62456600
C	1.88716700	0.39921500	3.46188400
C	1.92824000	1.68694200	3.01696300
C	0.99653900	1.77766600	1.91914000
N	0.42056500	0.55686100	1.68861400
H	2.43808600	-0.05265000	4.27660600
H	2.51443500	2.51440800	3.39559100
C	-1.97443300	2.67982700	-1.04992600
C	-1.71467100	4.09832500	-1.14466300
C	-0.66092200	4.35879400	-0.32496500
C	-0.29148300	3.10275100	0.28619500
N	-1.10209900	2.10015000	-0.17224400
H	-2.27176300	4.78416500	-1.76982700
H	-0.17399800	5.30517800	-0.12796800
C	-1.56525100	-2.82596100	0.22410100
C	-1.26626200	-4.06755600	0.89432300
C	-0.43318300	-3.76554200	1.92879300
C	-0.20282300	-2.34338700	1.87534400
N	-0.89143800	-1.79250600	0.82575800
H	-1.67053800	-5.03099300	0.61156000
H	-0.00131400	-4.43043300	2.66565900
C	-2.88515300	-1.50405100	-1.38590300

C	-3.90586500	-1.38868500	-2.40233700
C	-4.06909000	-0.05961600	-2.64150000
C	-3.13329200	0.63459500	-1.78670800
N	-2.43409500	-0.26502500	-1.02869900
H	-4.42487800	-2.22620200	-2.85043400
H	-4.74477300	0.42551000	-3.33407900
C	0.64435500	-1.65014300	2.73094200
C	-2.94361700	2.00852800	-1.78392500
C	0.70248600	2.95514000	1.24171000
C	-2.46357600	-2.70331700	-0.82664600
H	1.25833900	3.84337600	1.52523600
H	-3.57265200	2.60131900	-2.44055100
H	-2.91638500	-3.61543500	-1.20278300
H	1.12945700	-2.21235600	3.52242500
Fe	-0.96169200	0.13907300	0.29188500
Cl	-2.61837300	0.48879600	1.88633300
O	0.15127700	-0.02484400	-0.93949900
H	1.16694300	-0.83496200	-0.71856300
C	2.21777600	-2.48200300	-1.65102700
C	3.16351500	-2.10318900	-2.56601200
C	2.20416000	-1.54196800	-0.53142100
C	3.32908400	-0.61051300	-0.79361400
C	3.81710800	0.46286500	-0.06395000
C	4.87692500	1.21773200	-0.60244900
C	5.41599900	0.90356200	-1.85077400
C	4.91889200	-0.17967100	-2.59490000
C	3.87695000	-0.93689100	-2.06167100
H	3.39149600	0.71831000	0.90178300
H	6.23004800	1.50088400	-2.25235200
H	5.34733400	-0.42408600	-3.56374200
H	5.27518600	2.05781900	-0.03977600
H	3.36484200	-2.58660900	-3.51615700
H	1.52945100	-3.31329200	-1.74855300
H	2.00625600	-1.89398300	0.48178900

cat1/a6

C	-0.47138200	3.15753900	-0.19037400
C	-0.84700100	4.27824000	-1.02166900
C	-1.86042700	3.84918400	-1.82114600
C	-2.08867600	2.45965500	-1.49539500
N	-1.23882400	2.06794900	-0.49831900
H	-0.39187200	5.25912100	-0.97293400
H	-2.40796000	4.40097500	-2.57438200
C	-2.84370100	-1.75530400	-1.16526800

C	-3.81231300	-1.85086400	-2.23338900
C	-4.00938000	-0.58683100	-2.69612900
C	-3.14449400	0.27827000	-1.92681600
N	-2.45533900	-0.45538900	-0.99972000
H	-4.27844700	-2.77167800	-2.55979600
H	-4.66485400	-0.25101000	-3.48937600
C	0.72623100	0.25420500	2.75889100
C	1.61365900	1.11706800	3.49850000
C	1.65625000	2.30381200	2.82905500
C	0.77650700	2.17398900	1.69343900
N	0.23391900	0.91579000	1.66215000
H	2.13078600	0.83352000	4.40621200
H	2.20966200	3.20033600	3.07749400
C	-0.31543300	-1.92685600	2.31740300
C	-0.50235700	-3.32873500	2.59691700
C	-1.27137800	-3.83130900	1.59122200
C	-1.57595200	-2.73119000	0.70936100
N	-0.96863400	-1.58636900	1.16060300
H	-0.08722600	-3.84469500	3.45312100
H	-1.62748400	-4.84428400	1.45432800
C	0.48723600	3.20646900	0.81054800
C	-2.41590600	-2.82529300	-0.39166300
C	-3.00229600	1.64089200	-2.14421000
C	0.46010800	-1.06818600	3.08435700
H	-3.61758700	2.09154400	-2.91647800
H	-2.81621400	-3.80577300	-0.62978300
H	0.91861100	-1.46889400	3.98266000
H	1.01160900	4.14580600	0.95503600
Fe	-1.06862900	0.22146500	0.30303300
Cl	-2.81343800	0.78339400	1.72691000
O	0.09436900	-0.10158200	-0.84022100
H	1.22469200	-0.74628000	-0.33277600
C	4.79762600	1.33056800	-0.17042200
C	3.77033600	0.50405500	0.26297500
C	4.97078900	0.02287300	-2.20135700
C	5.40213500	1.08990200	-1.41110800
H	5.12649500	2.16178100	0.44737900
H	3.28552200	0.68938400	1.21764300
H	6.20220000	1.73558600	-1.76345200
C	3.93923300	-0.82083100	-1.78104600
C	3.33204200	-0.58338600	-0.52294500
H	5.44177800	-0.15743400	-3.16546200
C	2.10318100	-2.51112600	-2.29602900
C	1.97089400	-2.72470800	-0.78361600

C	2.20142900	-1.40707900	-0.05964600
C	3.50817500	-1.99541000	-2.63895800
H	1.90454000	-3.44159600	-2.84070200
H	0.98136200	-3.11596200	-0.52555500
H	4.23236800	-2.81344500	-2.49685500
H	3.57055700	-1.71861500	-3.69882300
H	2.12085000	-1.46732300	1.02994600
H	1.34844200	-1.77890400	-2.61011300
H	2.71135700	-3.46681400	-0.44378900

cat1/a7

C	-1.11081800	-2.59975300	0.74962700
C	-1.69453500	-3.78254900	0.16398900
C	-0.97016100	-4.06159600	-0.95358900
C	0.05652200	-3.05018800	-1.04671000
N	-0.05047300	-2.17338000	-0.00187500
H	-2.55123500	-4.30661600	0.56648900
H	-1.09976300	-4.87164500	-1.65981000
C	3.35782900	-0.37532100	-1.71028800
C	3.87118100	-1.01278900	-2.90120600
C	3.04427000	-2.05744100	-3.17347300
C	2.03032300	-2.06389700	-2.14396800
N	2.24158600	-1.03184000	-1.26959300
H	4.74960300	-0.68506300	-3.44219400
H	3.10069600	-2.77276000	-3.98395300
C	0.16846700	0.97953400	2.77480200
C	-0.82585500	0.95388700	3.81632600
C	-1.57682600	-0.16671100	3.61774800
C	-1.05019100	-0.82103800	2.44830800
N	0.00339000	-0.10333100	1.94068500
H	-0.91310100	1.69588100	4.59966000
H	-2.41197600	-0.53320800	4.20075600
C	2.15031800	1.96233000	1.69232600
C	3.19218800	2.95858500	1.60619600
C	3.98228400	2.60505400	0.55619800
C	3.41522400	1.40065400	-0.00408600
N	2.30671400	1.02798200	0.70737800
H	3.29318700	3.80301600	2.27592100
H	4.86706200	3.10069800	0.17784800
C	-1.57753900	-1.98159300	1.89866200
C	3.91832500	0.74785600	-1.11981500
C	1.01311400	-3.00124800	-2.05190300
C	1.14738400	1.95360700	2.65302700
H	0.97288700	-3.77097500	-2.81625700

H	4.81062200	1.16093900	-1.57972100
H	1.14569500	2.75645700	3.38361900
H	-2.43330200	-2.42581700	2.39496800
Fe	1.09161700	-0.54257400	0.32572000
Cl	2.50512900	-1.85705900	1.61655500
O	0.18316000	0.38367300	-0.72156300
H	-0.95341000	0.87622000	-0.20469500
C	-2.66337900	3.96087100	-2.71616000
C	-1.71934200	4.93245800	-2.37451000
C	-0.90800500	4.74417100	-1.24884100
C	-1.04454000	3.59751300	-0.47585900
C	-1.99405100	2.60845400	-0.80957100
C	-2.79745700	2.80629800	-1.94609100
H	-3.30147200	4.10443300	-3.58419600
H	-1.61563900	5.82986100	-2.97835900
H	-0.16801800	5.49301200	-0.97926700
H	-0.40268300	3.43891200	0.38773600
H	-3.53993800	2.06103700	-2.21212300
C	-2.05927300	1.39337700	0.04400600
H	-1.98465700	1.63942900	1.10644200
C	-3.02514200	0.30143400	-0.22760300
C	-2.95877600	-0.42917800	-1.43003100
C	-3.97445200	-0.07876300	0.73680700
C	-3.83040900	-1.48694400	-1.66680600
H	-2.18470700	-0.18043500	-2.14985600
C	-4.85892600	-1.13004500	0.49256400
H	-4.01483600	0.46086900	1.67916000
C	-4.78972000	-1.83736500	-0.70914800
H	-3.75249100	-2.05332300	-2.59057500
H	-5.59501900	-1.40227900	1.24460300
H	-5.46872500	-2.66509100	-0.89556800

cat1/a8

C	-0.14043200	1.23013500	2.71201900
C	0.18343400	2.50400900	3.30354200
C	-0.17676800	3.45896300	2.40036900
C	-0.73485700	2.76767000	1.26374900
N	-0.68831200	1.41274000	1.46767200
H	0.62822400	2.63209100	4.28190900
H	-0.09718000	4.53503800	2.48665100
C	-2.87016900	1.23171500	-2.13477400
C	-3.17874100	2.50388600	-2.74750300
C	-2.59331000	3.46071500	-1.97843900
C	-1.94399800	2.77324200	-0.88561700

N	-2.12584000	1.42346300	-1.00383200
H	-3.76027400	2.62454100	-3.65238700
H	-2.59821900	4.53468400	-2.11305900
C	-0.73473100	-2.76794900	1.26322100
C	-0.17662300	-3.45943600	2.39971400
C	0.18355000	-2.50463800	3.30306300
C	-0.14036100	-1.23066400	2.71177900
N	-0.68823400	-1.41305900	1.46739500
H	-0.09699700	-4.53552300	2.48579600
H	0.62834500	-2.63288500	4.28140700
C	-1.94386600	-2.77317100	-0.88615100
C	-2.59314500	-3.46046500	-1.97910400
C	-3.17861900	-2.50351500	-2.74798600
C	-2.87010700	-1.23144700	-2.13501200
N	-2.12577000	-1.42337500	-1.00411100
H	-2.59800700	-4.53440800	-2.11393000
H	-3.76014600	-2.62402400	-3.65289400
C	0.10808900	-0.00031700	3.30597900
C	-3.24376100	0.00017700	-2.65377500
C	-1.27913300	3.40407800	0.15591700
C	-1.27897900	-3.40417200	0.15526500
H	-1.22528200	4.48792900	0.12940100
H	-3.84023100	0.00025000	-3.56066200
H	-1.22508600	-4.48801700	0.12854800
H	0.54660900	-0.00040100	4.29875800
Fe	-1.35847100	-0.00005500	0.20950200
Cl	-3.38876500	-0.00023400	1.34062800
O	0.01483000	0.00007000	-0.73515900
H	1.16984000	0.00007100	-0.08920000
C	4.54475500	-3.02657000	-1.48387900
C	3.57940300	-3.45844900	-0.56657500
C	2.79646700	-2.53327700	0.13308900
C	3.00518800	-1.17302700	-0.09275700
C	3.98543400	-0.73442600	-1.02067700
C	4.75590000	-1.65971200	-1.71728700
H	5.14071600	-3.75935600	-2.02135800
H	2.04118300	-2.86408200	0.83973600
H	5.51370600	-1.33475700	-2.42563000
C	2.29951300	0.00012300	0.46169100
C	3.00507300	1.17331700	-0.09281100
C	2.79620700	2.53355800	0.13295600
C	3.57904300	3.45877300	-0.56676200
C	4.54443800	3.02694500	-1.48404400
C	4.75572600	1.66009500	-1.71737700

C	3.98536000	0.73476800	-1.02071300
H	2.04088400	2.86432300	0.83958000
H	5.14032100	3.75976300	-2.02156700
H	5.51356200	1.33518200	-2.42570700
H	3.43503100	-4.52238300	-0.39925200
H	3.43455900	4.52270200	-0.39950200
H	1.99627900	0.00012800	1.51037400

cat1/a9

C	-0.66435700	1.02874100	-1.98853300
C	-1.05014100	2.12121700	-2.84733900
C	-0.00254200	2.99257100	-2.85996400
C	1.02077700	2.42102100	-2.01774900
N	0.58942800	1.23010200	-1.49100000
H	-1.99945800	2.19527200	-3.36192100
H	0.09094800	3.92978500	-3.39344900
C	4.45371900	1.08652100	0.21205700
C	5.33079000	2.18826300	-0.11409600
C	4.61295400	3.03449500	-0.90169900
C	3.30482600	2.43954900	-1.05885000
N	3.23308800	1.25821200	-0.37791000
H	6.35367300	2.28465800	0.22658300
H	4.92274200	3.97117400	-1.34707500
C	-0.05793300	-2.34832600	0.60382500
C	-1.31891600	-3.00513200	0.35181300
C	-1.98828500	-2.23208400	-0.54475700
C	-1.13884900	-1.10044100	-0.82909800
N	0.02951000	-1.18472900	-0.11428400
H	-1.62981300	-3.93191000	0.81464600
H	-2.96961900	-2.38417200	-0.97315900
C	2.20343700	-2.31128600	1.60875300
C	3.23248700	-2.88582600	2.44176400
C	4.32774000	-2.08652000	2.31026100
C	3.95688800	-1.02329300	1.40643000
N	2.66080400	-1.18257400	0.99408500
H	3.11707000	-3.78533800	3.03260900
H	5.30066500	-2.19084800	2.77313200
C	-1.47256500	-0.06643000	-1.69086700
C	4.79680600	0.01933600	1.03405200
C	2.27162100	2.98869900	-1.81116400
C	0.93122600	-2.85120100	1.43910100
H	2.46839100	3.93790700	-2.30120000
H	5.80484000	0.00972600	1.43828000
H	0.70047300	-3.75997600	1.98437000

H	-2.44967500	-0.10665900	-2.15967700
Fe	1.60396900	0.04877400	-0.21190300
Cl	2.42313900	-1.14410400	-2.04630100
O	1.20702000	1.03845300	1.13289600
H	0.09870100	0.92811300	1.64584100
C	-4.64401300	0.55042900	0.34065400
C	-3.85265900	1.64532800	-0.01922800
C	-2.61992000	1.87854400	0.60520500
C	-2.18348300	1.01418700	1.61199900
C	-2.97068100	-0.12218400	1.93286200
C	-4.19709400	-0.34986100	1.31351600
H	-5.59986700	0.38714400	-0.15001600
H	-4.18762500	2.32112600	-0.80168100
H	-2.00149500	2.70244900	0.27177200
H	-4.79411800	-1.21985000	1.57487900
C	-0.93880600	1.01706400	2.44198300
C	-0.99695900	-0.29403100	3.16310900
C	-0.03529600	-0.95975900	3.92624300
C	-0.34119600	-2.20971700	4.48110200
C	-1.58717100	-2.80641000	4.26388500
C	-2.53601000	-2.17683300	3.45152700
C	-2.23150900	-0.93665600	2.89449900
H	0.95401500	-0.54062300	4.06056200
H	0.40803900	-2.72394800	5.07714200
H	-1.81020700	-3.77337400	4.70702100
H	-3.49040400	-2.65496400	3.24626400
C	-0.58885900	2.31012400	3.24721000
C	-1.74899100	2.59769900	4.22850600
H	-1.52446400	3.49349800	4.82066000
H	-2.68862200	2.76846300	3.69242500
H	-1.89644700	1.76002400	4.91931200
C	-0.40858900	3.52142200	2.30750300
H	0.30046900	3.29200300	1.50604800
H	-1.35703400	3.83877800	1.86635500
H	-0.02114700	4.37319500	2.87865300
C	0.71338500	2.13754900	4.05571100
H	0.98924800	3.09677600	4.50915700
H	0.59052800	1.42017700	4.87184400
H	1.53453500	1.81159500	3.41077100
cat1/a10			
C	1.05511500	3.14504100	0.47320100
C	1.63180400	4.13140200	1.35645500
C	2.80183000	3.60529600	1.81304500

C	2.92006300	2.29043300	1.22594200
N	1.85403800	2.03815500	0.41048500
H	1.19337300	5.09697200	1.57304100
H	3.52242700	4.04523500	2.49038000
C	3.48605300	-1.82034200	0.11741100
C	4.68881500	-2.06098600	0.88230900
C	5.02349400	-0.87547600	1.46096800
C	4.01221000	0.07689700	1.06273800
N	3.09666600	-0.51938400	0.23887400
H	5.19988400	-3.01302700	0.94616200
H	5.86231200	-0.65078800	2.10702100
C	-0.88064000	0.69450700	-2.49921500
C	-1.86691200	1.66420600	-2.91117700
C	-1.71838600	2.74155500	-2.09409600
C	-0.62352900	2.43741500	-1.20239900
N	-0.13103300	1.18909500	-1.45959900
H	-2.58554800	1.50789600	-3.70412200
H	-2.28220500	3.66443500	-2.07907300
C	0.15256000	-1.54527000	-2.59823000
C	0.19724200	-2.90251300	-3.08327000
C	1.18003900	-3.53384200	-2.38144000
C	1.74599400	-2.55174500	-1.48769300
N	1.09085900	-1.35239800	-1.62950400
H	-0.45094100	-3.30349500	-3.85141100
H	1.51725000	-4.55912300	-2.46376600
C	-0.11579600	3.32210800	-0.25428700
C	2.83918400	-2.77682800	-0.66257300
C	3.94592800	1.39167100	1.50485300
C	-0.75385000	-0.57738300	-3.03246400
H	4.73742100	1.73385900	2.16505100
H	3.25742600	-3.77924700	-0.66129600
H	-1.44457700	-0.85923400	-3.81959800
H	-0.65289900	4.25438400	-0.11408300
Fe	1.44421600	0.32519900	-0.57975400
Cl	2.81642500	1.08355000	-2.31953400
O	0.60882900	-0.23597500	0.78663900
H	-0.63024800	-0.39335800	0.73285700
C	-3.52814000	3.26962500	1.39452000
C	-2.54464700	2.92988400	2.33296100
C	-1.95735000	1.65884800	2.32501400
C	-2.37351200	0.73250700	1.37023400
C	-3.34521600	1.08576600	0.40366600
C	-3.93044600	2.35103700	0.41891000
H	-3.97720500	4.25913300	1.41992100

H	-2.23319200	3.66040900	3.07478300
H	-1.18373800	1.39516400	3.04001900
H	-4.68126500	2.62280400	-0.31863500
C	-1.85826000	-0.63536600	1.09577400
C	-2.63179700	-1.08047700	-0.09937500
C	-2.59004600	-2.28190700	-0.80341300
C	-3.43145300	-2.45073100	-1.91015000
C	-4.30844100	-1.43357800	-2.30543100
C	-4.35638900	-0.22472000	-1.60227800
C	-3.51788100	-0.04948000	-0.50307100
H	-1.91237300	-3.07442400	-0.50228400
H	-3.40340600	-3.38467700	-2.46517100
H	-4.95912800	-1.58515600	-3.16266100
H	-5.04024500	0.56352100	-1.90661800
C	-1.61828000	-1.61552600	2.20375900
C	-0.69871600	-2.66465300	2.03044800
C	-2.32124300	-1.52944600	3.41505800
C	-0.50623600	-3.61199900	3.03378000
H	-0.10868100	-2.70651800	1.12031900
C	-2.12510300	-2.47785100	4.41994200
H	-3.03188500	-0.72143600	3.56037000
C	-1.21976500	-3.52406400	4.23258400
H	0.21295700	-4.41355900	2.88556400
H	-2.68333500	-2.39916800	5.34938100
H	-1.06512100	-4.26069400	5.01656900

cat1/a11

C	-0.70226200	-2.76572000	1.27130300
C	-0.13825700	-3.45901000	2.40355500
C	0.22010500	-2.50573100	3.30922900
C	-0.10345500	-1.23045800	2.71818300
N	-0.65904600	-1.41233300	1.47740100
H	-0.05415400	-4.53500200	2.48547500
H	0.66500500	-2.63510600	4.28752900
C	-0.70205700	2.76567200	1.27146900
C	-0.13799800	3.45884900	2.40376300
C	0.22030400	2.50548600	3.30937200
C	-0.10335500	1.23027400	2.71825100
N	-0.65893400	1.41226700	1.47747900
H	-0.05381800	4.53483000	2.48575200
H	0.66521600	2.63476700	4.28767900
C	-2.96647000	-1.23240900	-2.04454300
C	-3.28740300	-2.50449000	-2.65188800
C	-2.66023300	-3.45955300	-1.91384700

C	-1.97503400	-2.77166700	-0.84289800
N	-2.17655300	-1.42336500	-0.94538200
H	-3.90469900	-2.62651000	-3.53262400
H	-2.66003100	-4.53273700	-2.05493100
C	-2.96638300	1.23273000	-2.04446500
C	-3.28723800	2.50487200	-2.65172200
C	-2.66000000	3.45984500	-1.91362300
C	-1.97483800	2.77184200	-0.84272500
N	-2.17644500	1.42356100	-0.94529600
H	-3.90453300	2.62699100	-3.53244500
H	-2.65972800	4.53303800	-2.05463600
C	-1.26769800	-3.40061900	0.17194700
C	-1.26745300	3.40068100	0.17215800
C	0.14892700	-0.00011900	3.31013100
C	-3.36403700	0.00019000	-2.54484400
H	0.59178200	-0.00016400	4.30113600
H	-1.20361800	4.48379000	0.13781700
H	-3.99663600	0.00024100	-3.42704200
H	-1.20393600	-4.48373000	0.13753700
Fe	-1.36697400	0.00003300	0.23716200
Cl	-3.36568700	0.00007600	1.44338300
O	-0.04020700	-0.00001900	-0.75711300
H	1.20013700	0.00001100	-0.10570500
C	4.01061200	-3.63560600	-1.17562800
C	4.08735100	-2.45687600	-1.92108200
C	2.84000900	-2.44971600	0.57138400
C	3.38013200	-3.63112500	0.07345500
H	4.44088300	-4.55325200	-1.56775100
H	4.57486600	-2.46198700	-2.89355200
H	3.31402800	-4.54575600	0.65663400
C	2.33065000	-0.00002200	0.33822500
C	2.92285700	-1.25826500	-0.16787100
C	3.54027200	-1.26796200	-1.43575200
C	3.54424500	-0.00009400	-2.26081100
H	2.14266300	-0.00000800	1.41598000
H	4.38539200	-0.00013700	-2.96459400
H	2.63142600	-0.00005800	-2.88068700
H	2.34611700	-2.43985000	1.53839000
C	2.92296500	1.25816100	-0.16788900
C	2.84022100	2.44963000	0.57135000
C	3.38045600	3.63098300	0.07340900
C	4.01094000	3.63539000	-1.17567200
C	4.08757200	2.45664500	-1.92111100
C	3.54038500	1.26778600	-1.43576900

H	2.34632500	2.43981900	1.53835500
H	3.31443500	4.54562700	0.65657700
H	4.44129700	4.55299200	-1.56780500
H	4.57508900	2.46170000	-2.89358100

cat1/a12

C	-2.06010300	2.77664400	-0.85912900
C	-2.70955100	3.46317600	-1.95319200
C	-3.24685200	2.50245500	-2.75134500
C	-2.91585900	1.22986700	-2.14996900
N	-2.19909500	1.42413200	-1.00230800
H	-2.74524200	4.53876400	-2.06952800
H	-3.81425600	2.62050200	-3.66556800
C	-2.05458200	-2.77968900	-0.85972800
C	-2.70263600	-3.46727200	-1.95395600
C	-3.24180100	-2.50744100	-2.75192400
C	-2.91334800	-1.23433200	-2.15026000
N	-2.19622200	-1.42742500	-1.00262900
H	-2.73620900	-4.54290300	-2.07051500
H	-3.80894400	-2.62641200	-3.66619000
C	-0.16346300	1.23143700	2.69044200
C	0.12447800	2.50522300	3.30305800
C	-0.29841400	3.46345100	2.43062600
C	-0.84996200	2.77324100	1.29000600
N	-0.74751200	1.41784500	1.46386600
H	0.58382900	2.63045100	4.27520200
H	-0.26139600	4.53989700	2.53876700
C	-0.16116100	-1.23146200	2.69024800
C	0.12892500	-2.50479900	3.30277800
C	-0.29207100	-3.46368600	2.43015200
C	-0.84461800	-2.77434500	1.28949600
N	-0.74460100	-1.41878300	1.46350400
H	0.58828800	-2.62931600	4.27500800
H	-0.25315400	-4.54007600	2.53818500
C	-1.42563100	3.41080600	0.19860500
C	-1.41897100	-3.41282400	0.19793900
C	-3.26546000	-0.00252500	-2.68345600
C	0.12132600	0.00020300	3.26664700
H	-3.84257400	-0.00300700	-3.60286200
H	-1.40318600	-4.49827200	0.19249700
H	0.58467900	0.00055700	4.24829200
H	-1.41187600	4.49628200	0.19332400
Fe	-1.41248000	-0.00100300	0.19898000
Cl	-3.44573500	-0.00314700	1.35597900

O	-0.05337100	0.00071900	-0.74550800
H	1.22790900	0.00046100	-0.09032700
C	4.12357000	-3.57650400	-1.17802700
C	4.45940200	-2.33957700	-1.71614000
C	2.66044000	-2.50330300	0.42240900
C	3.22494600	-3.65866600	-0.10214900
H	4.56288400	-4.47918300	-1.59276100
H	5.15661800	-2.24159100	-2.54170800
H	2.96564700	-4.62602000	0.31808200
C	2.33780800	0.00151400	0.37399000
C	2.97805800	-1.23984100	-0.10366600
C	3.88674500	-1.18505700	-1.17673200
H	2.10101800	0.00145500	1.44463800
H	1.95927600	-2.56134400	1.24807300
C	2.97547200	1.24406200	-0.10404800
C	2.65510100	2.50701900	0.42156400
C	3.21715600	3.66340600	-0.10336700
C	4.11602400	3.58279400	-1.17915900
C	4.45451800	2.34640500	-1.71684000
C	3.88427800	1.19085500	-1.17708000
H	1.95375600	2.56383500	1.24715600
H	2.95574000	4.63034900	0.31649800
H	4.55343200	4.48626800	-1.59417700
H	5.15196700	2.24963000	-2.54235500
O	4.27127000	0.00321300	-1.74307100

cat1/a13

C	1.20160600	-0.89416600	2.87391600
C	1.36288500	-2.11189200	3.62953400
C	1.77647200	-3.06791300	2.75157200
C	1.89405400	-2.42849100	1.46336800
N	1.52136100	-1.11191900	1.55904100
H	1.17447000	-2.20514300	4.69138500
H	2.00868900	-4.10746700	2.94445600
C	2.85299100	-0.88145200	-2.43059800
C	3.41076600	-2.09786900	-2.97646400
C	3.27008500	-3.05695500	-2.02181900
C	2.64757800	-2.42135000	-0.88290900
N	2.40644100	-1.10407500	-1.15665600
H	3.83776400	-2.18661800	-3.96718300
H	3.56606200	-4.09754800	-2.05903700
C	0.21177400	2.81163600	0.95318400
C	-0.30419700	3.48831200	2.11787900
C	-0.13233500	2.64287200	3.17369300

C	0.46487200	1.43931400	2.65017200
N	0.65915000	1.56258900	1.29691000
H	-0.71736700	4.48893100	2.11356100
H	-0.38356800	2.80124800	4.21468900
C	0.93718900	2.82193700	-1.40106500
C	1.12831600	3.48393900	-2.67145000
C	1.85768800	2.63745100	-3.44723800
C	2.09138400	1.44773800	-2.66026600
N	1.53106800	1.59005500	-1.42123200
H	0.75741100	4.47215400	-2.91143600
H	2.20453600	2.77948700	-4.46274000
C	0.73525000	0.30346600	3.39988900
C	2.73897400	0.31252900	-3.12762000
C	2.38275800	-3.05312600	0.32418600
C	0.29496500	3.38589000	-0.30882000
H	2.63412200	-4.10622400	0.40269800
H	3.13957300	0.34396500	-4.13588400
H	-0.11900000	4.38182500	-0.43127900
H	0.52792500	0.34007100	4.46452500
Fe	1.48578600	0.21822800	0.05741800
Cl	3.59009300	0.96375300	0.69815400
O	0.03125400	-0.32183200	-0.54493300
C	-5.69117500	-1.74192000	-2.11987100
C	-5.92723200	-0.46053300	-1.66793200
C	-5.03766400	0.14708700	-0.74541000
C	-3.90090500	-0.58974900	-0.28332300
C	-3.66023200	-1.90366800	-0.77832000
C	-4.55761100	-2.45693800	-1.67734600
C	-5.23792000	1.47307600	-0.27518100
C	-3.01475000	0.01548700	0.67248300
C	-3.24217600	1.33137700	1.08362300
C	-4.35084300	2.05405300	0.61375400
C	-1.86710000	-0.73909200	1.17558300
C	-1.98009900	-2.25336900	1.07077100
C	-2.40831100	-2.63999000	-0.35034500
H	-2.55904400	-3.72240400	-0.43542600
H	-1.02066400	-2.71639900	1.32159100
H	-6.09936600	2.03054600	-0.63505600
H	-6.37595700	-2.20691900	-2.82387200
H	-6.79327000	0.09870900	-2.01314900
H	-4.38026400	-3.46174100	-2.05370400
H	-4.51298700	3.07201400	0.95712800
H	-2.54945200	1.79187800	1.78306500
H	-0.95713600	-0.45148600	0.42103900

H	-1.49078200	-0.37762900	2.13567900
H	-1.59025900	-2.37309400	-1.03518700
H	-2.72196700	-2.61394200	1.79990900

cat1/a14

C	-0.34779500	0.07287900	-3.01278900
C	-1.05015800	0.99141300	-3.87227500
C	-0.85937800	2.23860000	-3.35610000
C	-0.00349500	2.08678000	-2.20589900
N	0.28471800	0.75822800	-2.00840400
H	-1.62690300	0.69991300	-4.74064900
H	-1.23253500	3.18649500	-3.72186200
C	3.01847000	2.19608700	0.83609500
C	3.05971800	3.63042200	1.00372800
C	2.09778800	4.14878800	0.19116600
C	1.48732300	3.03214900	-0.49156100
N	2.05855100	1.86078000	-0.08145800
H	3.73688900	4.15157400	1.66827300
H	1.82586500	5.18553300	0.03942200
C	1.34351500	-3.02657900	-0.57928300
C	0.71844200	-4.14535300	-1.24458700
C	0.00158800	-3.63459600	-2.28378500
C	0.17179700	-2.20303000	-2.24068000
N	0.98156800	-1.85697100	-1.19208400
H	0.84060500	-5.18028100	-0.95166200
H	-0.59731700	-4.15980800	-3.01632000
C	2.93212200	-2.09375700	1.06010900
C	3.92670200	-2.24087500	2.09859100
C	4.39830900	-0.99384000	2.36799500
C	3.67608500	-0.08082000	1.51033900
N	2.80589000	-0.77459100	0.71730400
H	4.21760900	-3.18472800	2.54167700
H	5.15225000	-0.69596800	3.08530600
C	-0.41308400	-1.30951400	-3.12450500
C	3.80187300	1.30120000	1.55093300
C	0.50132500	3.14371400	-1.46349700
C	2.23232400	-3.14291300	0.48352400
Fe	1.49272200	-0.00368600	-0.61774200
Cl	3.22253900	-0.02831600	-2.16406900
O	0.40928800	-0.01435100	0.64884800
H	-0.93241300	-0.03623400	0.53513500
C	-2.12131300	-0.01884700	0.92645600
C	-2.42253000	1.45894300	0.98684600
C	-3.69688100	1.97575000	0.69706400

C	-1.41184700	2.35266700	1.38725700
C	-3.95197200	3.34323900	0.80236000
H	-4.49133400	1.29899200	0.39814200
C	-1.66551400	3.71934500	1.48083400
H	-0.42142500	1.96428600	1.59902400
C	-2.93651100	4.22148800	1.18955500
H	-4.94723300	3.72208800	0.58454300
H	-0.86184300	4.39102700	1.77093100
C	-2.86500700	-0.80685200	-0.10770600
C	-3.05640600	-0.25237500	-1.39033100
C	-3.37347800	-2.09864100	0.13186900
C	-3.74599700	-0.94579100	-2.38084700
H	-2.65485600	0.73125400	-1.60591500
C	-4.05187500	-2.79626400	-0.86483900
H	-3.25286500	-2.54902100	1.11024400
C	-4.24662000	-2.22404000	-2.12565000
H	-3.87713000	-0.48849400	-3.35798700
H	-4.44306900	-3.78747700	-0.65122600
H	-4.78207500	-2.76916600	-2.89838900
H	-3.13525400	5.28752500	1.26310100
H	0.14462700	4.13986800	-1.70393800
H	4.53122600	1.71614900	2.23949700
H	2.42994500	-4.14195300	0.85962000
H	-1.00784300	-1.71907700	-3.93376100
C	-1.93586100	-0.67150500	2.27441200
C	-1.13024300	-1.82131500	2.38976600
C	-2.53968700	-0.15604800	3.43140100
C	-0.95022000	-2.44232600	3.62221600
H	-0.62780100	-2.20471700	1.50771200
C	-2.36253400	-0.78305500	4.66543700
H	-3.15580500	0.73452800	3.35935500
C	-1.56721700	-1.92623700	4.76642100
H	-0.31575800	-3.32193500	3.69262800
H	-2.84617000	-0.37545200	5.54933000
H	-1.42325400	-2.40837900	5.72972400

cat1/a15

C	-2.92045700	-2.11580300	-1.48969100
C	-3.60487800	-3.37359800	-1.31147200
C	-4.18393700	-3.33100500	-0.08010800
C	-3.85596900	-2.04498100	0.48904900
N	-3.08619500	-1.32632000	-0.38850000
H	-3.62541100	-4.17000200	-2.04404600
H	-4.78598900	-4.08434000	0.41164100

C	-3.25642800	1.66447900	2.58117900
C	-3.99150600	1.32130500	3.77706000
C	-4.45206700	0.05361000	3.60177300
C	-3.99925800	-0.37527500	2.29812600
N	-3.27826300	0.61874400	1.69847400
H	-4.12672100	1.97980900	4.62547700
H	-5.04622600	-0.55037000	4.27550100
C	-0.74863500	1.45627100	-2.50548800
C	-0.30081600	1.02758600	-3.80802200
C	-0.77280100	-0.23604300	-3.98889300
C	-1.50734500	-0.58077500	-2.79719000
N	-1.46140700	0.45326700	-1.89620300
H	0.28876100	1.63424600	-4.48320500
H	-0.64811700	-0.89154600	-4.84044300
C	-0.95832400	3.16092400	-0.73894500
C	-0.71128500	4.47974200	-0.20608600
C	-1.30275900	4.52160600	1.01981900
C	-1.91498000	3.23109200	1.22944500
N	-1.69090200	2.42196400	0.14769000
H	-0.16581800	5.25866000	-0.72265400
H	-1.34031100	5.34156200	1.72549700
C	-2.17420500	-1.78079500	-2.61247800
C	-2.63055300	2.88324000	2.36733300
C	-4.27344500	-1.61649500	1.74035400
C	-0.49871700	2.71196800	-1.97046300
Fe	-2.32172000	0.51252200	-0.09039700
Cl	-4.25859000	1.38399300	-1.05438500
O	-1.02918300	-0.08510700	0.77479900
H	0.08255800	-0.65997900	0.23602100
C	1.22159500	-1.11775800	0.01707500
C	1.59259600	-1.57929400	1.40216600
C	2.09051400	-2.86127000	1.68411000
C	1.43837000	-0.67116700	2.46773500
C	2.44733900	-3.21616500	2.98411900
H	2.23255700	-3.56956200	0.87533500
C	1.78957300	-1.02755800	3.76518200
H	1.02380500	0.31013000	2.26198700
C	2.30006800	-2.30256000	4.02974200
H	2.85415700	-4.20529700	3.17739500
H	1.66000800	-0.31321500	4.57390300
C	0.96826100	-2.17447100	-1.01469800
C	0.10094300	-3.24531800	-0.72392200
C	1.56892400	-2.13381600	-2.28454700
C	-0.10682500	-4.26934100	-1.64533200

H	-0.41320600	-3.26050000	0.23251000
C	1.35053200	-3.15247100	-3.21210100
H	2.21910500	-1.30173300	-2.53617000
C	0.52243100	-4.23165800	-2.89273500
H	-0.77784900	-5.08617700	-1.39430400
H	1.83687400	-3.10687800	-4.18312700
C	1.89921400	0.12551400	-0.45326600
C	3.15189900	0.57077000	-0.16910200
H	1.28215100	0.76105500	-1.08267200
C	4.19944500	-0.27017500	0.47065400
C	4.90564100	0.19771900	1.59054000
C	4.52828700	-1.52851300	-0.05538300
C	5.88869100	-0.58738800	2.18934600
H	4.66423900	1.17564000	1.99709100
C	5.52393300	-2.30771600	0.53348100
H	3.99423600	-1.89516100	-0.92645300
C	6.20251700	-1.84293100	1.66127500
H	6.41187000	-0.21943700	3.06794800
H	5.76636700	-3.27988400	0.11226600
H	6.97383500	-2.45232100	2.12471000
C	3.54079500	1.94805200	-0.55714900
C	4.82462000	2.22280800	-1.06478000
C	2.63394000	3.01484500	-0.41666800
C	5.17648700	3.51417500	-1.45080000
H	5.53974200	1.41158000	-1.16373600
C	2.99073600	4.30776600	-0.79720300
H	1.65999800	2.82894800	0.02215400
C	4.26000900	4.56253900	-1.32116900
H	6.16817200	3.70487100	-1.85261200
H	2.28060200	5.11932700	-0.66337300
H	4.53917200	5.57125300	-1.61382000
H	0.36185400	-5.03053900	-3.61186100
H	2.57885100	-2.58120500	5.04254900
H	-4.87305200	-2.30526300	2.32742200
H	-2.71228300	3.63020900	3.15094500
H	0.09361800	3.39982900	-2.56478800
H	-2.09898600	-2.51990500	-3.40207100

cat1/b1

C	-1.55677100	0.04689600	-1.40747000
C	-2.65840200	0.91150300	-1.75812200
C	-2.28635000	2.17207700	-1.40131500
C	-0.95317300	2.07012800	-0.85393700
N	-0.53360500	0.76858200	-0.85705700

H	-3.59507900	0.57686700	-2.18524300
H	-2.84758800	3.09245600	-1.49642800
C	3.13214100	2.38480500	0.46225200
C	3.17859300	3.82395400	0.59844500
C	1.93070500	4.28010200	0.30662600
C	1.13473800	3.11753900	-0.02056500
N	1.88450400	1.98038600	0.08535200
H	4.05665200	4.38952800	0.88223200
H	1.56876200	5.30002300	0.29449200
C	1.32660800	-2.95161500	-0.29677000
C	0.55808600	-4.10524300	-0.69752700
C	-0.60021900	-3.63233300	-1.23806600
C	-0.54248000	-2.19415800	-1.14262000
N	0.62506500	-1.79808300	-0.55223700
H	0.88819700	-5.13136600	-0.59974300
H	-1.42175000	-4.18956400	-1.66967400
C	3.44639800	-1.90896300	0.45324700
C	4.82392700	-1.99789700	0.87867200
C	5.27650300	-0.71893100	0.99238600
C	4.16831000	0.14218800	0.65061700
N	3.07171000	-0.60411100	0.31687600
H	5.35834500	-2.92274600	1.05328000
H	6.25921600	-0.37311500	1.28571100
C	-1.55580700	-1.33368800	-1.56023100
C	4.20414600	1.53115200	0.70525200
C	-0.19171600	3.15858400	-0.43640300
C	2.62484100	-3.00410100	0.19470100
Fe	1.24155000	0.07608900	-0.20241300
Cl	2.03233500	0.23509800	-2.40226600
O	0.78166500	0.09864500	1.45890800
H	0.04394800	-0.76573800	1.80946600
C	-4.12316800	-1.38178100	0.59166300
C	-4.48572900	-0.06117400	0.85237300
C	-3.73060800	0.75432600	1.70382400
C	-2.57390500	0.24426500	2.26521300
C	-2.14406000	-1.07559000	1.98610900
C	-2.95541500	-1.88010100	1.15576000
H	-4.73874400	-1.98328700	-0.06598400
H	-4.04654800	1.77514800	1.87846800
H	-1.95149100	0.87748500	2.89028900
C	-0.84905200	-1.53536400	2.46180800
H	-0.58280100	-2.56865100	2.23992600
H	-0.55938700	-1.21494000	3.46377500
H	-0.66376800	4.13559400	-0.48548900

H	-2.43221500	-1.78226900	-2.01658500
H	3.05540600	-3.98993100	0.34481500
H	5.14627800	1.98949100	0.99150500
H	-2.64628200	-2.89865400	0.94263800
N	-5.64019000	0.50890400	0.16360400
O	-6.15635500	-0.15733900	-0.73997200
O	-6.02060700	1.63112700	0.50262700

cat1/b2

C	-1.58341000	-2.73861100	1.02778100
C	-2.23049900	-3.96727100	0.63713100
C	-3.01615800	-3.66849200	-0.43510800
C	-2.86086100	-2.25390300	-0.67947500
N	-1.96946500	-1.71195000	0.20859400
H	-2.09115100	-4.92182400	1.12781000
H	-3.66265100	-4.32552300	-1.00236800
C	-3.11474800	1.95996800	-1.54787400
C	-4.14094400	1.88047700	-2.56373100
C	-4.41693200	0.55930100	-2.73282200
C	-3.57102400	-0.15937300	-1.80517000
N	-2.79307000	0.71029100	-1.09743400
H	-4.57202800	2.73233000	-3.07345900
H	-5.12787500	0.09751000	-3.40571500
C	0.79235800	0.58708700	2.33183300
C	1.52413800	-0.09436500	3.37314700
C	1.04104100	-1.36847600	3.41939700
C	0.03301400	-1.46305900	2.39173000
N	-0.09880800	-0.26264200	1.73934000
H	2.28889600	0.36063300	3.98926600
H	1.33093800	-2.17757100	4.07721200
C	0.14507500	2.67587200	1.16045400
C	0.24980600	4.10449600	0.95932600
C	-0.74818400	4.44791400	0.10157300
C	-1.44362500	3.22429800	-0.23233000
N	-0.88838000	2.16532500	0.42401500
H	0.98626000	4.74203000	1.43101900
H	-1.00046700	5.42664200	-0.28540500
C	-0.66757700	-2.61900700	2.06960800
C	-2.50289300	3.13652900	-1.13179500
C	-3.58056700	-1.54027400	-1.63340700
C	0.94194800	1.94025200	2.02754300
H	-4.25320100	-2.11027800	-2.26783800
H	-2.85314800	4.06288000	-1.57736200
H	1.71635000	2.48030900	2.56436600

H	-0.46222500	-3.50816100	2.65813900
Fe	-1.40286200	0.21243500	0.28561900
Cl	-3.02924800	0.61040300	1.92890100
O	-0.26863800	0.06881100	-0.99951100
H	0.45975800	-0.92398900	-0.92926300
C	4.50396900	-0.43222200	-2.15049900
C	5.07014900	-0.12921800	-0.91068800
C	4.41682000	-0.43530200	0.28601600
C	3.17772500	-1.05397300	0.23046300
C	2.56984700	-1.37545700	-1.00408200
C	3.25979900	-1.04866000	-2.19035200
H	5.04147300	-0.18013200	-3.05635000
H	4.88650900	-0.18718000	1.22979000
H	2.65999300	-1.29327400	1.15365300
H	2.81653300	-1.27829000	-3.15328500
C	1.22323500	-1.96376600	-1.00709200
C	0.69899900	-2.69150300	-2.22817200
H	0.67249400	-2.04023600	-3.10827600
H	-0.32186800	-3.03842500	-2.04374200
H	1.32092200	-3.56436000	-2.47233000
H	0.97823500	-2.45963900	-0.06601300
N	6.37897400	0.52756500	-0.86222100
O	6.94061100	0.77246500	-1.93173600
O	6.84429000	0.79956000	0.24703000

cat1/b3

C	0.93249200	-2.72720800	-1.10900000
C	-0.00686500	-3.64535200	-1.70644200
C	-1.12471500	-2.92297200	-1.99832500
C	-0.86032000	-1.56817300	-1.57954300
N	0.38488600	-1.47057800	-1.02130000
H	0.18482200	-4.69573300	-1.88377600
H	-2.04265500	-3.25516100	-2.46563100
C	-0.52850200	2.60430200	-0.61712700
C	-1.82849600	3.01553800	-1.09395100
C	-2.43435900	1.90062900	-1.58659500
C	-1.50254700	0.81327500	-1.40023200
N	-0.35116300	1.26291700	-0.81042700
H	-2.21158000	4.02681400	-1.05101900
H	-3.42517200	1.80634900	-2.01075000
C	4.16635000	-0.38356800	0.50108900
C	5.12988300	-1.45227400	0.62341800
C	4.50947300	-2.58570900	0.19437600
C	3.17196300	-2.20025300	-0.18998000

N	2.98514700	-0.86170300	0.00302400
H	6.14171700	-1.33181300	0.98828100
H	4.90509500	-3.59117200	0.13092100
C	3.50580000	1.99000800	0.75595600
C	3.78750400	3.35643800	1.13892700
C	2.65568200	4.06829400	0.89141600
C	1.69128000	3.13292600	0.35468100
N	2.22970800	1.87840400	0.28469000
H	4.73201200	3.70369300	1.53743500
H	2.47374200	5.12459200	1.04178600
C	2.21435900	-3.07200300	-0.70158500
C	0.40889900	3.47057900	-0.05845700
C	-1.74730500	-0.50759400	-1.74856600
C	4.41212800	0.93931100	0.85176600
Fe	1.28745400	0.18560700	-0.33366100
Cl	2.10908300	0.62873000	-2.48465300
O	0.82821800	0.00756900	1.32058700
H	-0.01604900	-0.83318400	1.60580800
C	-4.29038900	-1.31716500	0.50943300
C	-4.51867800	0.05408800	0.60219300
C	-3.61298900	0.90176700	1.24619700
C	-2.46193100	0.35981100	1.79373900
C	-2.18285500	-1.02270900	1.70830500
C	-3.12169200	-1.84361500	1.05124400
H	-5.01396600	-1.94611600	0.00507900
H	-3.80561900	1.96612500	1.27456800
C	-0.90455600	-1.54890400	2.25006100
H	-2.70888300	-0.73265100	-2.19830200
H	2.50589300	-4.11173100	-0.81857900
H	5.40051400	1.17205200	1.23718200
H	0.11639700	4.51200200	0.03970500
C	-0.57251500	-1.13536100	3.68093800
H	0.46584200	-1.39019300	3.91463800
H	-0.69708800	-0.06266400	3.84627600
H	-1.22544900	-1.66712300	4.38840800
C	-0.56199400	-3.00033200	1.96953300
H	-0.74447500	-3.28242800	0.93064100
H	0.49735500	-3.17961600	2.18193400
H	-1.14635000	-3.67242500	2.61663100
H	-2.94071900	-2.90844900	0.96197100
H	-1.72822700	1.02042700	2.24205600
N	-5.69706200	0.62658900	-0.04837400
O	-6.53444600	-0.14906200	-0.51442600
O	-5.77584800	1.85676300	-0.11304500

cat1/b4

C	-0.14217000	-1.42130900	2.50351100
C	0.80777200	-1.30384700	3.58271200
C	1.28623400	-0.02798700	3.54176800
C	0.61218200	0.63116200	2.44843400
N	-0.24294900	-0.23276100	1.82329000
H	1.06272300	-2.09956400	4.27069400
H	2.01335600	0.44207500	4.19129100
C	-1.47794400	3.21380800	-0.28927200
C	-0.79736600	4.44298800	0.05355200
C	0.15038600	4.11773200	0.97338500
C	0.03031800	2.69463300	1.20130600
N	-0.96268900	2.16917700	0.42081300
H	-1.02471000	5.41298900	-0.36925700
H	0.86177700	4.76465600	1.47012800
C	-2.90808700	-2.26629000	-0.66877400
C	-3.08569500	-3.67313900	-0.39651800
C	-2.34672400	-3.95200200	0.71295200
C	-1.70486400	-2.71905900	1.09986800
N	-2.05031000	-1.70921100	0.24322700
H	-3.71432700	-4.33854300	-0.97405500
H	-2.23538100	-4.89533100	1.23177200
C	-3.54837200	-0.19666900	-1.87893100
C	-4.34419000	0.50282700	-2.86392300
C	-4.06476500	1.82605900	-2.71810300
C	-3.08666500	1.92595300	-1.65762300
N	-2.79631200	0.68591800	-1.15999700
H	-5.02777200	0.02810200	-3.55593600
H	-4.46485300	2.66686100	-3.26977300
C	-0.83010700	-2.58219500	2.17426000
C	-2.48922300	3.10893600	-1.24082100
C	0.77713500	1.97805400	2.12682700
C	-3.57917500	-1.57263400	-1.67067900
H	1.52005400	2.52995100	2.69516800
H	-2.81104400	4.02587700	-1.72555900
H	-4.22901200	-2.15376800	-2.31860400
H	-0.65461500	-3.45909800	2.79017800
Fe	-1.47880600	0.21565300	0.30269400
Cl	-3.18135500	0.65621200	1.85155200
O	-0.29103200	0.03299500	-0.92728700
H	0.46081800	-0.93565000	-0.73679900
C	1.23165300	-2.38773600	-2.21471200
C	2.22729600	-1.43504400	-2.92788100

C	1.27272600	-1.93167800	-0.75746900
C	2.58558600	-1.31590100	-0.55959200
C	3.24286700	-0.97906900	0.63147700
C	4.48352800	-0.35389900	0.56544500
C	5.03956000	-0.06909500	-0.68707100
C	4.39536200	-0.38677400	-1.88959900
C	3.16085400	-1.01116700	-1.81483600
H	2.79245300	-1.20482700	1.59232700
H	4.86962500	-0.14249500	-2.83258900
H	5.03262500	-0.08442500	1.45901500
H	2.74529800	-1.89854500	-3.77414600
H	0.22297800	-2.34844100	-2.63629300
H	0.86722700	-2.58457900	0.01595100
H	1.69269300	-0.55511900	-3.31019200
H	1.58428000	-3.42688700	-2.28631900
N	6.34999200	0.58921300	-0.74224000
O	6.89556400	0.87944900	0.32487000
O	6.83234300	0.81729000	-1.85348900

cat1/b5

C	-0.12885100	-1.04347000	2.67195500
C	0.77632500	-0.74405500	3.75394500
C	1.16663700	0.55120400	3.58597500
C	0.48673800	1.03740200	2.40920700
N	-0.28741800	0.05341800	1.86282600
H	1.06472200	-1.44191900	4.52915600
H	1.83939500	1.13878000	4.19705600
C	-1.60785800	3.12682100	-0.71634800
C	-1.01541200	4.42890400	-0.50486900
C	-0.10307100	4.28144200	0.49280800
C	-0.15537100	2.89350000	0.89479200
N	-1.07415400	2.21283200	0.14378000
H	-1.27335900	5.32181800	-1.05924200
H	0.54361200	5.02813000	0.93482600
C	-2.76170300	-2.42674100	-0.42842000
C	-2.87134500	-3.79652800	0.01274800
C	-2.14108500	-3.89633200	1.15817500
C	-1.57547700	-2.59171500	1.39944000
N	-1.95477500	-1.71454200	0.41916500
H	-3.45144400	-4.56119500	-0.48734600
H	-1.98953900	-4.76152200	1.79038500
C	-3.46713000	-0.56214300	-1.90494700
C	-4.25876500	-0.03545800	-2.99426900
C	-4.03528100	1.30600500	-3.02087700

C	-3.09763400	1.58795500	-1.95742500
N	-2.77464800	0.44003500	-1.28922600
H	-4.89952500	-0.62761000	-3.63464700
H	-4.44904500	2.04792000	-3.69136100
C	-0.73513200	-2.27616300	2.46367500
C	-2.56834200	2.84353400	-1.68396900
C	0.58317100	2.34539800	1.93454900
C	-3.44218600	-1.89951700	-1.52185600
H	1.26436600	3.00851000	2.45951800
H	-2.91156000	3.67081300	-2.29805100
H	-4.04623200	-2.58974200	-2.10354900
H	-0.52110300	-3.06389500	3.17978700
Fe	-1.47632400	0.23086600	0.24962200
Cl	-3.25430200	0.76140200	1.68748000
O	-0.23042000	-0.03657200	-0.87925200
H	0.49706000	-1.02258800	-0.70911800
C	1.38833400	-2.60671100	-1.92527300
C	2.52707900	-2.21224700	-2.56124100
C	1.33654300	-2.02415200	-0.57855600
C	2.63039300	-1.33785100	-0.40416900
C	3.16633000	-0.64794000	0.67906000
C	4.40791800	-0.02287600	0.53666000
C	5.07611100	-0.09626200	-0.68921100
C	4.56099800	-0.78545300	-1.79470600
C	3.33063500	-1.41270800	-1.64135900
H	2.63502600	-0.59265400	1.62305800
H	5.12348200	-0.81672100	-2.71990400
H	4.86535800	0.52028900	1.35384500
H	2.80957600	-2.44365000	-3.58210000
H	0.59229000	-3.20551400	-2.35198200
H	0.87448700	-2.55982600	0.24947700
N	6.37448700	0.57482700	-0.82263300
O	6.95336200	0.49885100	-1.90850700
O	6.81707600	1.17962000	0.15682200

cat1/b6

C	-0.12089100	3.04985900	0.40025800
C	-0.03016300	4.33821900	-0.25107400
C	-0.94567100	4.32806300	-1.25680400
C	-1.57580300	3.02648000	-1.22729500
N	-1.06401500	2.27194700	-0.21128900
H	0.64133800	5.13368900	0.04494000
H	-1.18053100	5.11140100	-1.96573300
C	-3.45715700	-0.79679700	-1.76909900

C	-4.21494600	-0.47112100	-2.95725200
C	-3.98527700	0.84497300	-3.21383600
C	-3.07317700	1.31063400	-2.19289500
N	-2.77442300	0.29895000	-1.32452500
H	-4.84245500	-1.16654000	-3.49957900
H	-4.37846600	1.45643600	-4.01562900
C	-0.25039300	-0.46127700	2.91284000
C	0.66882700	0.00851100	3.92053800
C	1.12400200	1.22140300	3.49598900
C	0.46461900	1.49384300	2.24085100
N	-0.35468300	0.45446200	1.89675900
H	0.92254300	-0.52942500	4.82475600
H	1.82459100	1.88790000	3.98224100
C	-1.71887600	-2.18609800	1.93049100
C	-2.30651800	-3.50347900	1.92059500
C	-2.98907500	-3.61560800	0.74708600
C	-2.83311300	-2.35715500	0.05639400
N	-2.04285900	-1.50845800	0.78517400
H	-2.19942200	-4.23333600	2.71255700
H	-3.56609700	-4.45403100	0.37894800
C	0.60859300	2.68001400	1.52319100
C	-3.46125300	-2.03984400	-1.14497200
C	-2.53427600	2.59119600	-2.13732400
C	-0.90055400	-1.68954400	2.94057300
H	-2.85761100	3.29953300	-2.89428500
H	-4.05451400	-2.82211400	-1.60958900
H	-0.73090500	-2.32552000	3.80416300
H	1.31722700	3.40544200	1.91194800
Fe	-1.52398300	0.35987300	0.26512600
Cl	-3.31474800	1.19354800	1.52611600
O	-0.26141800	-0.13821900	-0.78867400
H	3.29366700	-3.39642500	-2.40255600
C	5.01788400	-0.08250700	-0.47172000
C	4.52197100	-0.87442500	-1.50682000
C	3.11236700	-0.57584300	0.88057900
C	4.32590300	0.07537400	0.73203600
H	4.74212000	0.69814000	1.51384900
C	2.58178300	-1.38387900	-0.14766000
C	3.30229700	-1.53223100	-1.35940100
C	0.85905400	-3.07593900	-0.96973500
C	1.26208200	-2.65868900	-2.39005500
C	2.77778900	-2.42578100	-2.46847200
C	1.25392900	-1.99018100	0.01300200
H	-0.21947800	-3.25534900	-0.90365500

H	0.96609300	-3.42226900	-3.11854700
H	0.47703000	-1.02113900	-0.30141300
H	0.96197800	-2.16744400	1.04969700
H	3.05357100	-2.00216900	-3.44168000
H	1.35963300	-4.02024900	-0.69973000
H	0.72779700	-1.73465200	-2.64200000
H	5.09708700	-0.96581000	-2.42128700
H	2.55019300	-0.46104700	1.80243400
N	6.29863100	0.60815100	-0.65362500
O	6.89093100	0.45359200	-1.72356000
O	6.71130900	1.30632500	0.27541000

cat1/b7

C	-2.69949500	1.95550600	0.07161300
C	-3.40476900	2.86031500	-0.80386000
C	-3.54292400	2.21602700	-1.99491500
C	-2.92152300	0.92171900	-1.83830400
N	-2.41586700	0.78452700	-0.57664000
H	-3.73195500	3.85374000	-0.52798400
H	-4.01725700	2.56627700	-2.90253000
C	-1.32307100	-3.07451400	-1.89572400
C	-1.68891800	-3.40690000	-3.25528900
C	-2.29753900	-2.30625300	-3.77169400
C	-2.30410200	-1.31012700	-2.72262500
N	-1.70479300	-1.79912900	-1.59538800
H	-1.49710900	-4.36031700	-3.73020600
H	-2.71401400	-2.16414600	-4.76051400
C	-0.55099100	-0.33009400	3.02416800
C	-0.58413000	0.65421800	4.07773100
C	-1.27312600	1.72409500	3.58950800
C	-1.64995500	1.39042500	2.23838100
N	-1.19295100	0.14527200	1.90530400
H	-0.14779800	0.52225400	5.05940200
H	-1.51675400	2.65487200	4.08518000
C	0.04218500	-2.57340000	2.15839900
C	0.63575000	-3.88029000	2.31857800
C	0.42472500	-4.54598800	1.15019300
C	-0.28959400	-3.63903300	0.28230300
N	-0.51508000	-2.44875400	0.91809700
H	1.13710800	-4.22585500	3.21339300
H	0.71970900	-5.55225700	0.88254300
C	-2.34822600	2.24045000	1.38364400
C	-0.66892100	-3.93622300	-1.02164300
C	-2.86314900	-0.04432800	-2.84008900

C	0.03546900	-1.58364700	3.13774500
H	-3.31172900	0.21097200	-3.79572300
H	-0.42340900	-4.92645200	-1.39385400
H	0.51376300	-1.82097500	4.08361800
H	-2.62955700	3.21317200	1.77276200
Fe	-1.41642200	-0.80722000	0.15402200
Cl	-3.46170600	-1.69261000	0.87387200
O	0.06819300	-0.26759000	-0.50017400
H	0.63072400	0.62463900	0.14547300
C	4.69901000	1.21663300	-1.15502000
C	5.17317300	0.05992800	-0.53609700
C	4.43998200	-0.58939000	0.46164000
C	3.21507000	-0.06239500	0.83763100
C	2.70152700	1.10613000	0.23199100
C	3.46583300	1.73124200	-0.77136100
H	5.29942000	1.69546300	-1.91875900
H	4.83803800	-1.48736000	0.91762400
H	2.62257000	-0.56479900	1.59772500
H	3.09528800	2.63524700	-1.24205500
C	1.36452000	1.57711100	0.65582500
H	1.20871800	1.45164600	1.72947700
C	0.75991600	2.81911700	0.11908100
C	0.44591300	2.93348100	-1.24847900
C	0.41655100	3.87912000	0.97572900
C	-0.16852000	4.08032500	-1.74273500
H	0.65049700	2.09195700	-1.90366400
C	-0.19122900	5.03340000	0.47790100
H	0.63514500	3.79319100	2.03693800
C	-0.48463100	5.13834300	-0.88259600
H	-0.41887400	4.14483300	-2.79797900
H	-0.43892400	5.84741900	1.15438800
H	-0.96511100	6.03226400	-1.27097000
N	6.47170900	-0.48678200	-0.93902300
O	7.09390100	0.10099700	-1.82618300
O	6.86884100	-1.50461200	-0.36750700

cat1/b8

C	-1.62877700	1.26962500	2.60084700
C	-1.99156700	2.58346000	3.07139000
C	-2.53912300	3.23914100	2.00935700
C	-2.52356100	2.31481100	0.90066000
N	-1.95168500	1.12918100	1.27606300
H	-1.83977200	2.94144400	4.08134400
H	-2.93915900	4.24406200	1.96930200

C	-3.13112100	-0.16100300	-2.56945100
C	-3.83847700	0.81123600	-3.37266700
C	-3.87473500	1.96084400	-2.64680400
C	-3.20514900	1.67869300	-1.39652600
N	-2.76398900	0.38613000	-1.37294100
H	-4.23772000	0.62155500	-4.36054000
H	-4.31592000	2.91353200	-2.90953100
C	-0.16560800	-2.63775900	1.58651300
C	0.41507100	-2.96273500	2.86757400
C	0.15430600	-1.90912000	3.69235900
C	-0.56981100	-0.94116100	2.90614000
N	-0.74707100	-1.40032900	1.62637800
H	0.93354100	-3.88549100	3.09379700
H	0.41992100	-1.78445300	4.73405400
C	-0.83244600	-3.28211300	-0.71265300
C	-0.90627100	-4.24121900	-1.79249300
C	-1.68603400	-3.67998200	-2.75494400
C	-2.06899200	-2.37417700	-2.26538800
N	-1.54483300	-2.15772300	-1.02365500
H	-0.42774500	-5.21190800	-1.78966200
H	-1.97835200	-4.08979800	-3.71296900
C	-0.99708400	0.29808000	3.37043200
C	-2.82886500	-1.45432200	-2.98068800
C	-3.07111800	2.58454900	-0.35087400
C	-0.17081100	-3.49694000	0.48962600
H	-3.47678200	3.58003700	-0.50527800
H	-3.18531700	-1.75974700	-3.95985500
H	0.34918800	-4.44333200	0.60507100
H	-0.79805000	0.53706100	4.41075600
Fe	-1.70473800	-0.48932400	0.11172400
Cl	-3.72909500	-1.34697600	0.92086200
O	-0.28078500	0.08155100	-0.62175700
H	0.52697600	0.65695700	0.12347000
C	4.99220100	-0.67348800	-0.32650400
C	4.18927700	-1.38903900	0.56874600
C	3.00002200	-0.82119400	1.02427100
C	2.64552700	0.45368800	0.58149600
C	3.47871500	1.16748500	-0.32300300
C	4.66050800	0.60580100	-0.78667300
H	2.36155400	-1.36487600	1.71335400
H	5.32224600	1.11818700	-1.47438800
C	1.43365600	1.24789200	0.84775500
C	1.65630900	2.53857000	0.17157800
C	0.86300600	3.68573400	0.13747000

C	1.27963000	4.76695800	-0.64511400
C	2.46480500	4.69853400	-1.38991600
C	3.26466000	3.54971400	-1.36157600
C	2.85925600	2.47246300	-0.57830500
H	-0.05862300	3.73419300	0.71043500
H	2.76871900	5.54836300	-1.99491900
H	4.18621000	3.50553100	-1.93619300
H	4.50710100	-2.37320300	0.88897400
H	0.67755600	5.67105400	-0.67854400
H	0.96025500	1.20946900	1.82769500
N	6.23792700	-1.28942000	-0.80061800
O	6.93560100	-0.64476200	-1.58619200
O	6.51832700	-2.41686800	-0.38808200

cat1/b9

C	1.43792400	2.32649400	-1.69286700
C	2.16268400	3.57255900	-1.72111200
C	3.29913600	3.37646900	-0.99517100
C	3.26780600	2.00697500	-0.54046700
N	2.11894800	1.39241000	-0.96699700
H	1.82965100	4.46743100	-2.23037100
H	4.10025600	4.07526300	-0.79149000
C	3.79445900	-2.03418100	0.85535100
C	5.10565500	-1.86351000	1.43852500
C	5.44027900	-0.55602600	1.26272100
C	4.33543800	0.06014700	0.56390300
N	3.35203700	-0.85691000	0.32347000
H	5.67521100	-2.64915200	1.91790200
H	6.34439100	-0.04264800	1.56358200
C	-1.17869900	-1.08552400	-1.72940800
C	-2.21960600	-0.51474100	-2.55225200
C	-1.81547800	0.74472600	-2.87152500
C	-0.53731200	0.94223300	-2.23204400
N	-0.16820600	-0.17983400	-1.53587600
H	-3.13116500	-1.02596100	-2.83241500
H	-2.32467100	1.48958100	-3.46788500
C	-0.15253400	-3.01191000	-0.55772900
C	-0.17705600	-4.38588600	-0.11492100
C	1.03394500	-4.62795300	0.45953800
C	1.78458000	-3.39725700	0.37377000
N	1.04132200	-2.42932300	-0.24816600
H	-1.01349100	-5.06045600	-0.24477900
H	1.40058600	-5.54452400	0.90332500
C	0.20232500	2.11520200	-2.29921600

C	3.07026600	-3.22216500	0.87075200
C	4.28833500	1.39630900	0.17988700
C	-1.19492100	-2.38489100	-1.23740300
H	5.14216800	2.01453800	0.44167100
H	3.54300200	-4.08388200	1.33285500
H	-2.08538500	-2.97527900	-1.42927900
H	-0.22902500	2.94313100	-2.85117400
Fe	1.56171600	-0.49828800	-0.56630600
Cl	2.54092600	-1.16640000	-2.58011400
O	1.01667000	-0.09233600	1.00836100
H	0.04440200	0.63221600	1.14381800
C	-2.60513700	4.25206800	-0.95750300
C	-1.35626000	4.51294000	-0.38207300
C	-0.74924300	3.58875600	0.47574100
C	-1.40520800	2.39040500	0.77670200
C	-2.65082100	2.12083500	0.15208700
C	-3.25489400	3.04193800	-0.70146500
H	-3.06269500	4.98448900	-1.61686400
H	-0.84088100	5.44201600	-0.61066200
H	0.24020400	3.79677900	0.86199500
H	-4.21236100	2.81874300	-1.16467400
C	-1.01368300	1.24185900	1.64844100
C	-2.08022100	0.22613100	1.38938100
C	-2.14755400	-1.12754600	1.73532500
C	-3.19612600	-1.91294300	1.25612700
C	-4.16453900	-1.33981400	0.42694600
C	-4.11505600	0.00123900	0.04196900
C	-3.05871200	0.76853100	0.51485300
H	-1.36410200	-1.59302900	2.31741800
H	-3.25639100	-2.96818800	1.49025500
H	-4.85917700	0.39469500	-0.63940800
C	-0.53095300	1.53025700	3.10517100
C	-1.63027800	2.33845700	3.83183200
H	-1.33057100	2.53235700	4.86903700
H	-1.80764000	3.30101400	3.34113100
H	-2.57622000	1.78470700	3.84954800
C	0.78618700	2.33720500	3.10354400
H	1.53954900	1.85128800	2.47571500
H	0.64027100	3.36307000	2.75701800
H	1.17661600	2.40023700	4.12592400
C	-0.27768300	0.22691000	3.88987300
H	0.15552200	0.47141600	4.86663500
H	-1.20621700	-0.31982800	4.07785900
H	0.42245600	-0.42270800	3.35634600

N	-5.20864200	-2.19691600	-0.13881000
O	-6.05416600	-1.67165200	-0.86720300
O	-5.17314700	-3.40161200	0.12556900

cat1/b10

C	1.30141200	1.62963500	-2.53856800
C	2.04631400	2.77797700	-2.99384300
C	3.26647400	2.71031700	-2.39343800
C	3.25624000	1.52443800	-1.56865900
N	2.05525700	0.88641200	-1.66729900
H	1.67020900	3.52051100	-3.68520200
H	4.10623900	3.38631800	-2.48988800
C	3.73253500	-1.80574100	1.11220800
C	5.09765700	-1.54078500	1.50812200
C	5.48841100	-0.42815200	0.82964300
C	4.35909400	-0.01939500	0.02592100
N	3.30824200	-0.88024300	0.20957400
H	5.66359900	-2.13870200	2.21072800
H	6.44218000	0.08253700	0.85859100
C	-1.30984800	-1.63867300	-1.50228000
C	-2.36562000	-1.32866300	-2.43766900
C	-1.98877200	-0.19240300	-3.08450200
C	-0.70454700	0.18395100	-2.54402900
N	-0.30488800	-0.70022600	-1.58550200
H	-3.27867700	-1.89946000	-2.54654300
H	-2.51854700	0.35870000	-3.84992300
C	-0.28324100	-3.07834100	0.22655100
C	-0.32606700	-4.20992300	1.12144400
C	0.88012600	-4.24918700	1.75296800
C	1.65144000	-3.14295300	1.23820400
N	0.91386600	-2.43956900	0.31551800
H	-1.17158900	-4.87656600	1.23127400
H	1.23478000	-4.95823300	2.48979800
C	0.01970000	1.30475200	-2.95176000
C	2.95664700	-2.85692700	1.60335000
C	4.33488300	1.09920000	-0.79173400
C	-1.32236500	-2.71650100	-0.63623900
H	5.23627600	1.70375700	-0.83073800
H	3.42112600	-3.51334300	2.33336100
H	-2.20824300	-3.34383900	-0.63276400
H	-0.46061500	1.97266500	-3.65857200
Fe	1.46974500	-0.74614400	-0.63974200
Cl	2.30094900	-2.07210500	-2.37671500
O	1.05410800	0.19751100	0.71060500

H	0.02731300	0.87492200	0.79667400
C	-2.28466500	3.96674900	-2.04138800
C	-1.11205200	4.37474500	-1.38681900
C	-0.61968200	3.66349600	-0.28935800
C	-1.31783500	2.53895100	0.15515700
C	-2.48926400	2.11642500	-0.52143000
C	-2.97734000	2.83005900	-1.61717800
H	-2.65467500	4.53843500	-2.88827200
H	0.29202700	3.97405900	0.21244200
H	-3.87985300	2.50790700	-2.12990800
C	-0.99149100	1.58990900	1.24618800
C	-2.08898900	0.58640900	1.19774500
C	-2.29074300	-0.56078500	1.96548400
C	-3.33537900	-1.42372300	1.63674100
C	-4.16917300	-1.11487000	0.55521300
C	-4.01568400	0.04884600	-0.20267000
C	-2.96341900	0.89416600	0.12149700
H	-1.62972200	-0.79549600	2.79253700
H	-4.68121000	0.24233400	-1.03404900
C	-0.47669100	2.06982600	2.56892600
C	0.26803700	1.21558300	3.40205200
C	-0.75949700	3.36915900	3.02207900
C	0.70356400	1.64721300	4.65393000
H	0.53591600	0.22818100	3.04242300
C	-0.32027000	3.79900200	4.27438600
H	-1.33911700	4.03851200	2.39383000
C	0.41121300	2.93967500	5.09677700
H	1.28266700	0.97450500	5.28130300
H	-0.55561600	4.80597000	4.60928500
H	-0.58006900	5.25490000	-1.73770600
H	-3.50256000	-2.34065600	2.18752500
H	0.75406900	3.27528100	6.07187200
N	-5.17874400	-2.08926500	0.14413800
O	-5.84617500	-1.83879900	-0.86457400
O	-5.29020900	-3.12473500	0.80600000

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C	0.60600000	-2.43862500	1.58994100
C	1.30424800	-2.56840500	2.84516900
C	0.82032700	-1.59355400	3.66611700
C	-0.15356200	-0.85400800	2.90150800
N	-0.26542000	-1.38321600	1.64066200
H	2.04868000	-3.32431200	3.05929700
H	1.08864200	-1.37938100	4.69266800

C	-2.92315200	1.76462500	0.92871400
C	-3.10751900	2.69266700	2.01703600
C	-2.37291100	2.22144800	3.06408300
C	-1.72164100	1.01941100	2.60562200
N	-2.06530700	0.76359700	1.30197800
H	-3.73721900	3.57195800	1.97481400
H	-2.26923000	2.63615600	4.05853600
C	-1.58120000	-2.83992300	-2.08898100
C	-0.91141100	-4.02623600	-2.57249600
C	0.06458700	-4.31894500	-1.67154100
C	-0.02545100	-3.32487500	-0.62606100
N	-1.03052800	-2.43965700	-0.90362400
H	-1.16362300	-4.54397500	-3.48889600
H	0.77826300	-5.13248600	-1.68666300
C	-3.16354800	-0.97119200	-2.37874000
C	-4.12671300	-0.22967700	-3.16103400
C	-4.37001500	0.92687600	-2.48761000
C	-3.57318800	0.87984000	-1.28263500
N	-2.85200900	-0.28073000	-1.24056600
H	-4.54027700	-0.56328900	-4.10394700
H	-5.03228100	1.73981700	-2.75593000
C	0.75749700	-3.31325000	0.51954100
C	-3.58761100	1.84938600	-0.28942300
C	-0.84128400	0.25994100	3.36476100
C	-2.59802100	-2.17891800	-2.76570000
H	-0.66012000	0.57318500	4.38807400
H	-4.22079700	2.71651200	-0.44905000
H	-2.94206300	-2.61519200	-3.69825500
H	1.50939400	-4.09019800	0.61677700
Fe	-1.51587800	-0.80575600	0.17694200
Cl	-3.19978800	-2.06779800	1.16666500
O	-0.35417500	0.03059300	-0.67642700
H	0.39108900	0.86480300	0.05656700
C	4.90925700	-0.19148500	-0.30503500
C	4.34629200	0.70848700	-1.21069500
C	3.08138500	0.10586200	1.20834900
C	4.28852900	-0.50736800	0.90531100
H	4.86303200	0.91787500	-2.14012900
C	1.18812100	1.64352900	0.61189100
C	2.49336100	1.02104500	0.31835100
C	3.12877400	1.31065700	-0.90930200
C	2.43542100	2.22345500	-1.89625100
H	0.87718800	1.56968100	1.65677500
H	3.16532000	2.69757600	-2.56242300

H	1.79807400	1.59294600	-2.53890500
H	2.57794600	-0.12838300	2.14054300
C	0.91916300	2.94877500	-0.02031600
C	0.01864500	3.86386500	0.55097000
C	-0.23557500	5.08386300	-0.06729700
C	0.40713200	5.40260500	-1.26866100
C	1.29322100	4.49156600	-1.84947100
C	1.54870900	3.26115500	-1.24395000
H	-0.47845900	3.60630000	1.48173200
H	-0.92879300	5.78755800	0.38545700
H	0.21838900	6.35692500	-1.75266600
H	1.78687300	4.73904800	-2.78647300
H	4.75578000	-1.21359100	1.57998700
N	6.18840200	-0.82884800	-0.63778900
O	6.65226800	-1.63912500	0.16711100
O	6.72568700	-0.52033100	-1.70309700

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C	-3.54399200	1.07399500	-1.38281300
C	-4.27615300	1.17484900	-2.62513800
C	-4.02932900	0.03028800	-3.31632200
C	-3.13620300	-0.76251400	-2.50152900
N	-2.86148800	-0.10990800	-1.33214300
H	-4.89837500	2.01484300	-2.90578700
H	-4.40144500	-0.26739800	-4.28809600
C	-0.32455800	-3.37757900	-0.56827300
C	-0.25787200	-4.37743300	-1.61017000
C	-1.12178800	-3.98340200	-2.58322100
C	-1.70510600	-2.73666200	-2.14098200
N	-1.20795100	-2.39265500	-0.91475300
H	0.36696900	-5.26049700	-1.57560200
H	-1.35431700	-4.47174400	-3.52071700
C	-1.74977700	1.16104800	2.53708200
C	-2.35191500	2.39546900	2.97680800
C	-3.08105700	2.87061900	1.92740900
C	-2.93075900	1.92051500	0.85267100
N	-2.10826400	0.89544000	1.23987200
H	-2.22718700	2.82376800	3.96304400
H	-3.68281600	3.76879400	1.87419200
C	-0.32602700	-0.81569600	2.90004300
C	0.54333400	-1.62701200	3.71593100
C	0.92043400	-2.68966000	2.94923500
C	0.27333200	-2.52943900	1.67017600
N	-0.46962900	-1.37800600	1.65701600

H	0.81361100	-1.40192900	4.73960300
H	1.56257700	-3.51988200	3.21388200
C	-3.56966100	2.02824800	-0.37669400
C	0.37681600	-3.44100200	0.62644900
C	-2.61635300	-1.99315200	-2.87796900
C	-0.91608200	0.37054200	3.31741900
H	-2.92616300	-2.39342000	-3.83822300
H	1.02848700	-4.29598600	0.77710300
H	-0.71680100	0.70042200	4.33214700
H	-4.17414200	2.91399200	-0.54543500
Fe	-1.61416600	-0.71553200	0.13841200
Cl	-3.42365800	-1.85152100	1.06981200
O	-0.36981300	0.03895800	-0.66316400
H	0.48520400	0.82521600	0.07976400
C	4.94535400	-0.48810200	-0.29966100
C	4.60037400	0.65906600	-1.00463600
C	2.99664700	-0.31305600	1.08058300
C	4.16244200	-0.98584100	0.74758300
H	5.22439500	1.03446800	-1.80487600
H	4.47336400	-1.88117500	1.27018400
C	1.31700400	1.51994700	0.65394200
C	2.59892800	0.84502800	0.39123400
C	3.42514300	1.31571200	-0.64863600
H	0.96166300	1.43944300	1.68627900
H	2.36931000	-0.68444000	1.88317900
C	1.19431300	2.86226700	0.05919200
C	0.16813600	3.75495900	0.41080500
C	0.04095200	4.98255200	-0.22714700
C	0.93955800	5.34312900	-1.24318000
C	1.96655700	4.47912700	-1.61026500
C	2.08446000	3.25105000	-0.95867900
H	-0.52937900	3.46536100	1.19009800
H	-0.75840900	5.66013300	0.05804600
H	0.83973200	6.30062500	-1.74595300
H	2.68178500	4.73271200	-2.38563000
O	3.12513900	2.44675100	-1.35926400
N	6.17996000	-1.19574700	-0.66857300
O	6.85392500	-0.73168300	-1.58834800
O	6.46588500	-2.21210600	-0.03424200

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C	-2.03853100	0.90540400	2.77414500
C	-2.51730400	2.09936300	3.42484200
C	-3.06348900	2.88458700	2.45454600

C	-2.94436100	2.15839600	1.21397400
N	-2.30002700	0.96606300	1.42958600
H	-2.43303800	2.29645500	4.48580400
H	-3.53082600	3.85575600	2.55493700
C	-3.27673000	0.19142000	-2.59341100
C	-4.05646100	1.21115500	-3.25676800
C	-4.19260300	2.23759400	-2.37413000
C	-3.51807800	1.83489900	-1.16140900
N	-2.97267000	0.59142000	-1.32045500
H	-4.42895800	1.13656100	-4.27027900
H	-4.70952000	3.17936800	-2.50634700
C	-0.10323700	-2.57789000	1.19000500
C	0.45077300	-3.05987200	2.43093800
C	0.01049400	-2.22095800	3.41185000
C	-0.79045700	-1.21064900	2.76713500
N	-0.84153000	-1.44515500	1.41438200
H	1.07406500	-3.93993100	2.52422700
H	0.20379500	-2.26538900	4.47599200
C	-0.62859700	-2.88712100	-1.19742200
C	-0.57485000	-3.64966100	-2.42370300
C	-1.43022000	-3.04954200	-3.29455200
C	-1.98630700	-1.90421100	-2.61045100
N	-1.48984600	-1.83314800	-1.33861600
H	0.03209100	-4.53354000	-2.57148300
H	-1.66688300	-3.33090500	-4.31254500
C	-1.36173400	-0.12475900	3.41430500
C	-2.84921100	-0.98490700	-3.19135800
C	-3.47854400	2.58521600	0.00578100
C	0.04480100	-3.22218100	-0.03245600
H	-3.95999300	3.55799200	-0.00932700
H	-3.16735600	-1.17253800	-4.21189000
H	0.68322300	-4.09956000	-0.05862300
H	-1.23566700	-0.05411400	4.48982800
Fe	-1.86473200	-0.40705100	0.03726600
Cl	-3.77497000	-1.57653700	0.61320200
O	-0.52833000	0.42336900	-0.53176700
C	4.82441400	2.71036500	-2.04176600
C	5.27240200	1.53644400	-1.47489500
C	4.46831900	0.84718200	-0.52862800
C	3.19627900	1.41473200	-0.16299900
C	2.74296600	2.61171200	-0.79488400
C	3.56132700	3.23983700	-1.71510800
C	4.84329300	-0.36914300	0.12891800
C	2.38207500	0.78135100	0.83877600

C	2.81165300	-0.40791200	1.42775400
C	4.04116600	-0.97106200	1.08411900
C	1.09590200	1.36152200	1.21585700
C	0.92707900	2.84515600	0.94656400
C	1.36028700	3.15054300	-0.49066800
H	1.32678400	4.22747100	-0.69041700
H	-0.11542900	3.13860900	1.10609200
H	5.45412800	3.23020000	-2.75850300
H	6.23421500	1.13247300	-1.75304300
H	3.22215100	4.15572000	-2.19289400
H	4.38333800	-1.88427100	1.55493000
H	2.18422600	-0.89711100	2.16606500
H	0.29407000	0.82218800	0.42910700
H	0.72110900	1.01892800	2.18265400
N	6.09763000	-1.07512600	-0.17372800
O	6.58333700	-0.96681500	-1.30191200
O	6.58483500	-1.77023100	0.72076800
H	0.64011900	2.67301400	-1.17062800
H	1.54313900	3.41606200	1.65867500

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C	2.78830000	1.47484400	-1.25645600
C	3.63746900	2.55267500	-0.81281700
C	3.86561700	2.34682400	0.51482400
C	3.18551700	1.12311000	0.86586500
N	2.52474700	0.61812100	-0.22480900
H	3.98750000	3.36047400	-1.44234000
H	4.45534100	2.94207900	1.19981500
C	1.86321800	-2.72961300	2.24759300
C	2.41455100	-2.65014000	3.58093800
C	2.97214900	-1.41343700	3.69846200
C	2.77963900	-0.75309700	2.42764300
N	2.10537200	-1.56899400	1.56541300
H	2.36241500	-3.44095200	4.31804200
H	3.48284400	-0.97963100	4.54854100
C	0.01641500	-1.34159000	-2.93427100
C	-0.17297900	-0.68620500	-4.20679700
C	0.64229300	0.40502600	-4.20937200
C	1.31128400	0.42153500	-2.93191300
N	0.90782600	-0.63970300	-2.16791800
H	-0.83324500	-1.03838500	-4.98879400
H	0.78171200	1.14441900	-4.98667500
C	-0.33309000	-3.26281100	-1.40861700
C	-0.89582400	-4.55984400	-1.10298400

C	-0.37864600	-4.93258800	0.09840500
C	0.48095500	-3.85243100	0.53112700
N	0.50031100	-2.85753000	-0.40362200
H	-1.58520300	-5.09930600	-1.73951300
H	-0.55928000	-5.83988300	0.66015800
C	2.22204300	1.38773800	-2.52475000
C	1.13743800	-3.80873600	1.75675700
C	3.25883400	0.51547800	2.11319500
C	-0.58114300	-2.54726200	-2.57365000
H	3.78840400	1.05260100	2.89412800
H	1.02943100	-4.67105600	2.40781900
H	-1.26896000	-2.98920300	-3.28867300
H	2.47357900	2.16539800	-3.23754400
Fe	1.48050000	-1.08479300	-0.29876000
Cl	3.35850900	-2.18138000	-1.14669900
O	0.05427800	-0.47771500	0.40929400
H	-0.34178000	0.70092400	0.23026200
C	-1.54201800	3.37031700	-3.09503900
C	-0.40301700	4.17827300	-3.15515700
C	0.49215300	4.17084600	-2.08422200
C	0.25393300	3.36563500	-0.97255200
C	-0.90297900	2.56186400	-0.88241100
C	-1.79161000	2.57857500	-1.97636600
H	-2.25199200	3.36804800	-3.91777500
H	-0.21849300	4.80475600	-4.02358300
H	1.38878600	4.78475900	-2.11396800
H	0.96898000	3.35888200	-0.15769800
H	-2.69867400	1.98680500	-1.94341500
C	-1.13186400	1.73808600	0.34450600
C	-2.43278000	0.98079000	0.42704900
C	-3.39261500	1.26894300	1.41088600
C	-2.69153700	-0.06816900	-0.47925400
C	-4.58440100	0.55248200	1.48157000
H	-3.20454900	2.06357100	2.12444200
C	-3.87260400	-0.79350300	-0.41989100
H	-1.93974600	-0.32802000	-1.21485300
C	-4.80992600	-0.47141100	0.56363200
H	-5.33399500	0.77329500	2.23143100
H	-4.07234500	-1.60805700	-1.10486700
C	-0.68719600	2.35422000	1.65123700
C	-0.13636600	1.54463000	2.66024700
C	-0.85652500	3.72522600	1.91045900
C	0.24764200	2.09462800	3.88253600
H	0.00624700	0.48747600	2.46518700

C	-0.48216500	4.27123000	3.13870700
H	-1.28762700	4.36313300	1.14470100
C	0.07652100	3.45892800	4.12846800
H	0.68622100	1.45153600	4.64141100
H	-0.62925400	5.33246200	3.32181600
H	0.37387800	3.88645800	5.08239000
N	-6.06147900	-1.23601100	0.63550800
O	-6.86632000	-0.94050000	1.52012100
O	-6.23613200	-2.12954600	-0.19520800

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C	3.14778200	-1.10565800	2.37043000
C	3.65286700	-2.32245800	2.95911500
C	4.01135900	-3.13440800	1.92700800
C	3.72425500	-2.41121200	0.71037400
N	3.20000300	-1.18022800	1.00853800
H	3.71597500	-2.50910100	4.02321000
H	4.43546500	-4.12961200	1.96392300
C	3.07385100	-0.69457600	-3.17940000
C	3.53868000	-1.82064300	-3.95648500
C	3.92152200	-2.77639700	-3.06796900
C	3.68908100	-2.23331500	-1.74911500
N	3.17770800	-0.96925900	-1.84229300
H	3.56212800	-1.85312500	-5.03811700
H	4.32583100	-3.76096500	-3.26467100
C	1.61336400	2.71476900	1.11595400
C	1.38551400	3.25446100	2.43361000
C	1.73612000	2.28376100	3.32111500
C	2.18130200	1.15252600	2.54688500
N	2.07823400	1.42534700	1.20553700
H	1.01124300	4.25061800	2.63111200
H	1.70706200	2.31046800	4.40225000
C	1.61753200	2.91693800	-1.33914200
C	1.37779100	3.65404200	-2.55652500
C	1.70912200	2.82521700	-3.58523600
C	2.15670000	1.58740400	-2.99314400
N	2.08728400	1.66558700	-1.62757800
H	1.01232700	4.67203000	-2.59660400
H	1.67032800	3.01882000	-4.64944300
C	2.65852400	-0.02657400	3.09558400
C	2.60223900	0.49149400	-3.72076100
C	3.95014400	-2.90845600	-0.56439500
C	1.38511500	3.41152200	-0.06216100
Fe	2.57841100	0.21559500	-0.30561700

C1	4.73179700	1.08730700	-0.28080300
O	1.09082400	-0.53164900	-0.48112400
H	0.07390200	-0.35552600	0.32935600
C	-1.06932600	-0.34128300	0.89628700
C	-1.76229400	-1.40386900	0.08596700
C	-2.50670200	-2.44780500	0.65953400
C	-1.68945200	-1.31999200	-1.31943900
C	-3.19945300	-3.35244800	-0.13675500
H	-2.58479200	-2.52002700	1.73781700
C	-2.36403600	-2.22263900	-2.12747600
H	-1.08640000	-0.53816300	-1.76715300
C	-3.12366300	-3.22631400	-1.52286000
H	-3.80840100	-4.13601600	0.29618200
H	-2.31670500	-2.16421000	-3.20766700
C	-0.73175400	-0.66367500	2.31629800
C	-0.08767000	-1.87673400	2.62863100
C	-1.02957900	0.21986200	3.36836300
C	0.18697300	-2.22208700	3.94987900
H	0.20197300	-2.54210100	1.82053000
C	-0.74370900	-0.12099300	4.69007500
H	-1.49843300	1.17238900	3.14295100
C	-0.14752000	-1.34900300	4.98903700
H	0.68151100	-3.16537400	4.16393600
H	-0.99689300	0.57113900	5.48894500
C	-1.50545700	1.05157100	0.59604600
C	-2.74989600	1.47425800	0.24739000
H	-0.72020400	1.80060700	0.64900300
C	-3.95636900	0.60966600	0.37973500
C	-4.75623400	0.31710000	-0.73579300
C	-4.31546300	0.07962500	1.62775400
C	-5.85937200	-0.52573200	-0.61428800
H	-4.48796800	0.73127600	-1.70341800
C	-5.43488700	-0.74363500	1.75454500
H	-3.70355700	0.30461400	2.49571700
C	-6.20295400	-1.05791500	0.63227200
H	-6.45181300	-0.76884600	-1.49208300
H	-5.70005100	-1.14689800	2.72832600
H	-7.06564300	-1.71179900	0.72559900
C	-2.95661900	2.85894000	-0.23381200
C	-4.11503300	3.57910300	0.11336000
C	-2.00187600	3.48248700	-1.05920100
C	-4.29322200	4.89126300	-0.31929400
H	-4.86797800	3.10370800	0.73492700
C	-2.18492800	4.79354100	-1.49491900

H	-1.13314100	2.92123600	-1.38401600
C	-3.32735000	5.50593300	-1.12224400
H	-5.18827900	5.43626700	-0.03145200
H	-1.44291800	5.25106800	-2.14436300
H	-3.47238700	6.52649500	-1.46612300
H	0.06369400	-1.61856300	6.02035600
H	4.36624100	-3.90811500	-0.64193400
H	2.58991700	0.57529000	-4.80305900
H	0.99663100	4.42121600	0.02083800
H	2.64697700	-0.11379800	4.17620600
N	-3.87167400	-4.16418900	-2.36663100
O	-3.80682500	-4.01551300	-3.58852400
O	-4.52723500	-5.04552300	-1.80702700

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C	1.51361200	-2.70170500	0.12655500
C	1.22697600	-4.11261000	0.00165100
C	-0.04465400	-4.21243600	-0.47771700
C	-0.55333200	-2.86576000	-0.58573300
N	0.40817100	-1.96600500	-0.21182200
H	1.93046400	-4.90445200	0.21628100
H	-0.60442000	-5.10310800	-0.72541400
C	-2.57828900	0.89832800	-0.41339200
C	-3.91021000	0.40927000	-0.68888300
C	-3.78693300	-0.91319800	-0.99721900
C	-2.39081800	-1.24481100	-0.84381600
N	-1.67706200	-0.12531400	-0.49356400
H	-4.80475500	1.01488000	-0.66654400
H	-4.55972400	-1.61736400	-1.27173900
C	3.06030000	1.28840200	-0.25674300
C	4.45332600	0.97070000	-0.03156200
C	4.50114500	-0.34473100	0.31595500
C	3.14271400	-0.84004200	0.24919900
N	2.29075200	0.17026800	-0.09180000
H	5.26563600	1.67941400	-0.10876300
H	5.36293400	-0.94499000	0.57081300
C	1.21293900	2.91048700	-0.48516700
C	0.70479700	4.26530000	-0.49489800
C	-0.64247000	4.17637400	-0.32257200
C	-0.95922600	2.76534600	-0.26091800
N	0.18554000	2.02276700	-0.35734500
H	1.31624100	5.15031300	-0.59901900
H	-1.37120900	4.97284400	-0.26993300
C	2.78461800	-2.18653800	0.41737200

C	-2.26142700	2.25535400	-0.21515700
C	-1.86801100	-2.53802100	-0.95128900
C	2.57640700	2.57838100	-0.50557100
Fe	0.29551300	0.02460600	-0.23684300
Cl	0.55817000	-0.03353500	-2.59549400
O	0.20358800	0.18908900	1.48876000
H	-0.52692800	-0.60709600	2.02701700
C	-4.63168700	0.07768400	3.24846300
C	-4.46948800	0.65089400	4.51359800
C	-3.24540500	0.51825200	5.17848100
C	-2.19836300	-0.18521200	4.58908900
C	-2.34895100	-0.78296400	3.32016100
C	-3.58509600	-0.62574900	2.65886100
H	-5.57260700	0.18730200	2.71560800
H	-3.10899400	0.96612200	6.15949900
H	-3.71228600	-1.04959100	1.66893500
C	-1.24367900	-1.49854700	2.68335000
H	-1.51728900	-2.18986800	1.88844400
H	-0.48656000	-1.90505000	3.35670800
C	-2.75164200	-3.62078000	-1.48419700
C	-3.45682400	-4.47925500	-0.61997500
C	-2.84928400	-3.76645100	-2.88408100
C	-4.25394300	-5.48545000	-1.17677000
C	-3.65462600	-4.78854200	-3.39459700
C	-4.36599800	-5.65633100	-2.55939400
H	-4.79959400	-6.15197800	-0.51183500
H	-3.72597900	-4.91077600	-4.47368500
C	3.84299500	-3.14552000	0.86264500
C	4.69555600	-3.75414800	-0.07868300
C	3.96202300	-3.43401000	2.23556000
C	5.66783700	-4.64868900	0.37965700
C	4.95025000	-4.33215100	2.64988800
C	5.81452200	-4.94675300	1.73838300
H	6.32594000	-5.12588700	-0.34388100
H	5.04547500	-4.55812400	3.71014900
C	3.56561300	3.67315700	-0.74697400
C	3.97669700	3.93261200	-2.06905800
C	4.07171500	4.42681900	0.32853600
C	4.89968700	4.95891800	-2.29181000
C	4.99386400	5.44336300	0.05915800
C	5.41683600	5.72686000	-1.24331600
H	5.22296800	5.16258700	-3.31082200
H	5.39070500	6.02699100	0.88756000
C	-3.38588800	3.21763300	-0.00178800

C	-4.11111100	3.72999600	-1.09515600
C	-3.69552100	3.60634600	1.31726000
C	-5.17278900	4.60498000	-0.84304200
C	-4.76939400	4.47849700	1.52099700
C	-5.52539300	4.98072500	0.45716100
H	-5.73446000	5.00623500	-1.68435600
H	-5.01707200	4.77646800	2.53802600
C	-2.10653600	-2.83073000	-3.81055800
H	-2.51486100	-1.81445700	-3.75501800
H	-1.04790400	-2.73834700	-3.54443200
H	-2.17664100	-3.16840800	-4.84905900
C	-3.36209600	-4.32428300	0.88093400
H	-2.33166600	-4.44904500	1.23345400
H	-3.68816000	-3.32888700	1.20349700
H	-3.98528100	-5.06271000	1.39429700
C	-5.25305000	-6.73229500	-3.14155100
H	-5.44414100	-7.53175200	-2.41787700
H	-6.22640800	-6.32181300	-3.44183500
H	-4.80361300	-7.18227300	-4.03397700
C	-3.73761900	3.36008200	-2.51317800
H	-2.67335900	3.54193600	-2.70276900
H	-3.91115300	2.29610200	-2.71219800
H	-4.31843000	3.93916800	-3.23748300
C	-2.86267300	3.12232600	2.48191300
H	-2.70578600	2.04034700	2.45370300
H	-1.86795900	3.58558200	2.46561500
H	-3.33717900	3.36688200	3.43601700
C	-6.70433300	5.89216500	0.70807000
H	-6.88200100	6.56286600	-0.13959700
H	-7.62457700	5.31299300	0.86357500
H	-6.55334300	6.50693100	1.60218800
C	3.43159900	3.11184600	-3.21541000
H	3.68260700	2.05055300	-3.10350400
H	2.33726400	3.15748000	-3.25848900
H	3.82886700	3.45897900	-4.17407000
C	6.38659600	6.85339900	-1.51595200
H	7.02568200	6.63269100	-2.37796600
H	5.85361400	7.78778900	-1.73770500
H	7.03375600	7.04481500	-0.65315500
C	3.62514900	4.14095300	1.74422500
H	2.54387000	4.28678000	1.85606500
H	3.83137200	3.10128500	2.02515100
H	4.13262200	4.79531100	2.45948400
C	3.03023000	-2.78926500	3.23692700

H	3.06174100	-1.69553100	3.16733300
H	1.98893700	-3.08133400	3.05228700
H	3.28834500	-3.07650300	4.26077400
C	4.55470900	-3.45144800	-1.55297000
H	3.54031800	-3.66690100	-1.90860700
H	4.73894400	-2.39077700	-1.76109400
H	5.25848400	-4.04220300	-2.14700900
C	6.89781500	-5.88865000	2.21064700
H	7.11192200	-6.66085900	1.46366000
H	7.83568300	-5.34870700	2.39808200
H	6.61760800	-6.38763800	3.14462400
H	-1.24781000	-0.28158100	5.10828700
H	-5.28518900	1.20169800	4.97406500

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C	-1.24426100	2.67451500	-0.32811500
C	-1.07302900	4.10997500	-0.39473500
C	0.26238800	4.33681900	-0.52698600
C	0.90698000	3.04213300	-0.49073200
N	-0.02703200	2.05318400	-0.38339900
H	-1.88158300	4.82674000	-0.37163500
H	0.78175700	5.27985400	-0.62180700
C	3.21044000	-0.49331400	0.25594500
C	4.51333900	0.13571500	0.30728100
C	4.32656100	1.44465400	-0.01508700
C	2.90636000	1.62054900	-0.22321200
N	2.25460500	0.42886000	-0.05881600
H	5.43638100	-0.37740700	0.53650200
H	5.06158900	2.23316500	-0.09331000
C	-2.24627900	-1.46814900	-0.88666800
C	-3.66581500	-1.28358900	-1.07177200
C	-3.92911300	0.02367900	-0.79003300
C	-2.65981500	0.65150900	-0.49860700
N	-1.65694200	-0.27650300	-0.54216100
H	-4.35624400	-2.06763400	-1.34909600
H	-4.88107800	0.53464300	-0.79377500
C	-0.26239000	-2.89157700	-0.55460700
C	0.36925200	-4.18076400	-0.40520800
C	1.62636000	-3.94791900	0.06594200
C	1.78108500	-2.51321200	0.14888000
N	0.60618200	-1.89502900	-0.20146200
H	-0.10543800	-5.12684200	-0.62330600
H	2.39969000	-4.66454200	0.30311800
C	-2.48918700	2.03534800	-0.31330000

C	2.99950900	-1.87259300	0.41092100
C	2.29661400	2.85317400	-0.48117900
C	-1.59603900	-2.70419300	-0.95158200
Fe	0.28554200	0.07580900	-0.24643200
Cl	0.61251000	0.03627000	-2.59597300
O	0.13302300	0.22706000	1.47261300
C	4.18416400	-2.71830700	0.76334200
C	4.55111400	-2.87564700	2.11350100
C	4.93882500	-3.32415700	-0.26152800
C	5.66605600	-3.66206000	2.42029800
C	6.04714900	-4.10055400	0.09120800
C	6.42298900	-4.28777800	1.42517300
H	5.95203100	-3.78481000	3.46312500
H	6.63519500	-4.56527700	-0.69779800
C	-2.35623300	-3.88173500	-1.47554400
C	-3.02080100	-4.76943700	-0.60809000
C	-2.39130300	-4.07740300	-2.87190400
C	-3.71204300	-5.85430200	-1.15800200
C	-3.09279000	-5.17661600	-3.37608800
C	-3.75599300	-6.07780500	-2.53727800
H	-4.22961100	-6.54070900	-0.49071700
H	-3.12149700	-5.33161400	-4.45285500
C	-3.70926200	2.88504900	-0.15032700
C	-4.08160100	3.28760200	1.14837200
C	-4.45718300	3.29097700	-1.27360700
C	-5.23901300	4.05726900	1.30281900
C	-5.60294200	4.06666500	-1.07054000
C	-6.01783400	4.44825200	0.20953100
H	-5.53432400	4.36412600	2.30433100
H	-6.18160000	4.38620600	-1.93506700
C	3.17301100	4.04140900	-0.71661000
C	3.58523300	4.84766900	0.36103700
C	3.57895100	4.33156800	-2.03371100
C	4.40664800	5.94849400	0.09866200
C	4.40005700	5.44282300	-2.24978400
C	4.82117600	6.26439600	-1.19935600
H	4.73137000	6.57307500	0.92869000
H	4.71928600	5.67047700	-3.26492600
C	-3.00398500	-4.55590600	0.88839100
H	-1.98002600	-4.52252600	1.27763900
H	-3.47814600	-3.60635800	1.16347200
H	-3.53729400	-5.35785800	1.40773600
C	-1.70029900	-3.10769600	-3.80333900
H	-2.18728900	-2.12536100	-3.78389600

H	-0.65958900	-2.92779200	-3.51245100
H	-1.71485200	-3.47418600	-4.83429900
C	-4.47672600	-7.27756900	-3.10687700
H	-4.91182900	-7.05586100	-4.08761400
H	-3.78921100	-8.12351400	-3.24090400
H	-5.28264100	-7.61433400	-2.44586200
C	-4.01624900	2.92251400	-2.67262800
H	-2.96978700	3.20063800	-2.84345100
H	-4.08321600	1.84266700	-2.84833100
H	-4.63133300	3.42625100	-3.42446500
C	-3.22797700	2.93596400	2.34513000
H	-2.94020600	1.88125800	2.35095900
H	-2.29735100	3.51771600	2.34009400
H	-3.75436000	3.14366900	3.28050900
C	-7.28409500	5.24902500	0.40633100
H	-8.15284300	4.58886700	0.53266600
H	-7.22495100	5.88180800	1.29862400
H	-7.48955300	5.89425500	-0.45484600
C	3.13949100	3.45247100	-3.18216900
H	3.49170700	2.42207300	-3.05530000
H	2.04707000	3.38933600	-3.24607600
H	3.51905800	3.82988600	-4.13655200
C	3.15059600	4.52319500	1.77195700
H	2.05790400	4.53854300	1.86434500
H	3.47555400	3.51803700	2.06639500
H	3.56369400	5.23940900	2.48873900
C	5.67973700	7.47983300	-1.46291600
H	6.30849100	7.34274200	-2.34933300
H	5.06044700	8.36999800	-1.63742500
H	6.33432600	7.70154100	-0.61284300
C	4.56768900	-3.12762800	-1.71391700
H	3.59663000	-3.58184200	-1.94362900
H	4.47923300	-2.06378300	-1.96277500
H	5.31616500	-3.57364700	-2.37573700
C	3.76084100	-2.19970800	3.21039000
H	3.73515700	-1.11252800	3.07098200
H	2.71821100	-2.53575600	3.21723000
H	4.19165400	-2.40858200	4.19436400
C	7.60405000	-5.16029300	1.78194800
H	7.29748000	-6.20764000	1.90604200
H	8.37081900	-5.13721400	0.99991400
H	8.06782400	-4.84369900	2.72243900
C	-4.57109300	0.43452700	4.52865700
C	-3.31903700	0.37630700	5.14920200

C	-3.67436400	-0.78647000	2.64433900
C	-4.74230800	-0.14844200	3.26983200
H	-5.70680000	-0.09900600	2.77118400
C	-2.40895000	-0.86935100	3.26168200
C	-2.25118000	-0.26485300	4.52481200
C	-0.23090200	-2.26314600	3.36470300
C	-1.29967700	-1.54322400	2.56409400
H	0.48373400	-2.73438900	2.68413200
H	-0.63383700	-0.60643100	1.96658800
H	-1.64108400	-2.12186600	1.70711800
H	-0.67130900	-3.04554100	3.99902400
H	-3.17490900	0.83477500	6.12424000
H	0.32781400	-1.58004900	4.01326200
H	-1.28366800	-0.29523000	5.01666900
H	-3.81107600	-1.22327600	1.66025800
H	-5.40176800	0.93560700	5.01840200

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C	0.15494200	-2.88792800	-0.56046200
C	-0.53339700	-4.14890500	-0.43680500
C	-1.78060800	-3.86932300	0.03513800
C	-1.87188400	-2.43129900	0.14602000
N	-0.66675200	-1.85881100	-0.18456200
H	-0.09906600	-5.11052100	-0.67146600
H	-2.58753800	-4.55428000	0.25340000
C	-2.84033800	1.73107400	-0.28324700
C	-4.26490800	1.61507300	-0.06074500
C	-4.50136200	0.31970300	0.28434200
C	-3.22604700	-0.36239200	0.22967900
N	-2.23747900	0.51563200	-0.10902600
H	-4.96855500	2.43132000	-0.14283700
H	-5.44209700	-0.15165700	0.53093500
C	2.68293600	0.55575400	-0.48529000
C	3.92703800	-0.11818800	-0.77922400
C	3.61643300	-1.41342200	-1.06793800
C	2.19344200	-1.55070100	-0.87510400
N	1.64829800	-0.33995000	-0.51760200
H	4.89579100	0.35988300	-0.79278500
H	4.27714700	-2.21763500	-1.35897500
C	1.34618800	2.63409800	-0.36741400
C	1.22731000	4.07438800	-0.45212400
C	-0.09757100	4.34717800	-0.60200000
C	-0.78938700	3.07633600	-0.55928500
N	0.10888100	2.05715900	-0.43286100

H	2.06032000	4.76251300	-0.42610000
H	-0.58186500	5.30722000	-0.71104900
C	1.49176600	-2.75699600	-0.96288700
C	-2.18444100	2.93792500	-0.55265600
C	-3.06679600	-1.74684500	0.39861400
C	2.56505100	1.94774500	-0.32925800
Fe	-0.27100900	0.08379800	-0.25750500
Cl	-0.55744900	0.03373400	-2.60380800
O	-0.16899300	0.37394000	1.45480300
H	0.45081900	-0.45549300	2.22581900
C	3.96624900	0.29156900	4.86209200
C	4.92934500	-0.00550000	3.89649100
C	4.53973800	-0.65130600	2.71952700
C	3.20770000	-1.00326500	2.52428700
C	2.22159400	-0.72036400	3.48868600
C	2.62833400	-0.05166300	4.65726700
H	4.25399100	0.79808600	5.77996600
H	5.26741100	-0.86760000	1.94237800
H	2.91600300	-1.47531300	1.59519700
C	0.79935000	-1.11490500	3.23746800
C	-4.28262300	-2.55205300	0.74085700
C	-4.60328500	-2.79530600	2.08940200
C	-5.10560000	-3.04338200	-0.29228400
C	-5.75047100	-3.53761800	2.38656900
C	-6.24274600	-3.78207500	0.04973900
C	-6.58074500	-4.04291000	1.38148200
H	-6.00270200	-3.72251800	3.42898700
H	-6.88216800	-4.16027800	-0.74546500
C	2.17843100	-3.94589100	-1.56068800
C	1.96696300	-4.20189000	-2.93274300
C	3.01042500	-4.78609600	-0.79612800
C	2.61800400	-5.29189500	-3.51862400
C	3.63863000	-5.86643400	-1.42500800
C	3.46182200	-6.13179500	-2.78583500
H	2.45940100	-5.48943300	-4.57700800
H	4.27929300	-6.51806200	-0.83406900
C	3.81885900	2.75241900	-0.19038400
C	4.56078900	3.12496600	-1.32911900
C	4.23112900	3.14434100	1.09860700
C	5.73805500	3.85838400	-1.15106700
C	5.41791900	3.87276200	1.22859800
C	6.18970000	4.23098000	0.11932600
H	6.31299300	4.15074400	-2.02762600
H	5.74308600	4.17180000	2.22323300

C	-3.01688300	4.15705500	-0.79207700
C	-3.41265200	4.45902700	-2.10938800
C	-3.39185300	4.98581100	0.28244300
C	-4.18726000	5.60247900	-2.32933400
C	-4.16713100	6.11870100	0.01668300
C	-4.57657400	6.44230900	-1.28112300
H	-4.49284600	5.84235300	-3.34587800
H	-4.45731100	6.76424000	0.84349800
C	-4.76929200	-2.77016500	-1.74049200
H	-4.73048100	-1.69350600	-1.94344800
H	-3.78343700	-3.17120300	-2.00342800
H	-5.51031900	-3.21789200	-2.40950000
C	-3.72301300	-2.26143800	3.19548600
H	-2.72559700	-2.71571400	3.16148200
H	-3.57828100	-1.17876100	3.10242400
H	-4.15293100	-2.46649300	4.18063500
C	-7.79715500	-4.87106300	1.72516500
H	-8.22602900	-4.57363500	2.68833100
H	-8.57687700	-4.77561600	0.96176800
H	-7.54131100	-5.93667700	1.79802900
C	-3.00484200	3.56212800	-3.25576700
H	-1.91504800	3.46546000	-3.32341000
H	-3.38890000	2.54396500	-3.12240000
H	-3.37619600	3.94677800	-4.21052200
C	-2.96012000	4.65514100	1.69283200
H	-3.31684100	3.66293100	1.99420300
H	-1.86704600	4.63417200	1.77915500
H	-3.34519300	5.38873000	2.40767400
C	-5.44336800	7.65313700	-1.53891400
H	-5.29103700	8.04838600	-2.54904400
H	-6.50872000	7.40335200	-1.44398100
H	-5.23393600	8.45674700	-0.82428500
C	4.08176400	2.76335900	-2.71709700
H	4.07412800	1.67856900	-2.87358400
H	3.05435600	3.10821100	-2.88259100
H	4.72069200	3.21205200	-3.48374900
C	7.48774000	4.98597300	0.28830200
H	8.33636300	4.29541600	0.38565200
H	7.69228300	5.63135000	-0.57305800
H	7.47419600	5.61262000	1.18671700
C	3.38874800	2.82156100	2.31068400
H	2.47061500	3.42307900	2.31532800
H	3.07806300	1.77373100	2.32629700
H	3.93339300	3.02405600	3.23679100

C	3.20360000	-4.55644100	0.68495300
H	3.58277300	-3.55136100	0.89797300
H	2.25580500	-4.66003000	1.22596200
H	3.90982400	-5.27735700	1.10783300
C	1.03590500	-3.33590000	-3.75052300
H	-0.00789900	-3.49093500	-3.45053700
H	1.22593900	-2.26677900	-3.61034100
H	1.11942300	-3.56875800	-4.81652300
C	4.18124900	-7.28047100	-3.45388700
H	3.58705500	-7.70454600	-4.27074500
H	5.13620500	-6.95049800	-3.88455500
H	4.40449700	-8.08342500	-2.74305100
C	0.60620800	-2.57431100	2.84060900
H	-0.43042800	-2.76139600	2.54766200
H	1.24202000	-2.85906300	2.00148300
H	0.85300300	-3.23112500	3.68759800
C	-0.22734200	-0.64295100	4.25618100
H	-0.10139100	-1.16047700	5.21848600
H	-0.15618100	0.43518800	4.42826100
H	-1.23473200	-0.85280000	3.88765800
H	1.90038100	0.19258500	5.42334000
H	5.96791400	0.27362700	4.05198300

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C	-2.30292100	-1.33049100	-0.97981400
C	-3.70520400	-1.06316200	-1.19099200
C	-3.89670300	0.25782200	-0.91515000
C	-2.59926800	0.80926700	-0.59682500
N	-1.65016900	-0.17402500	-0.62728800
H	-4.43552300	-1.80561300	-1.48028300
H	-4.81658200	0.82420300	-0.93703600
C	1.09139400	3.00260700	-0.51792400
C	0.51847900	4.33112200	-0.54064900
C	-0.82880900	4.17549800	-0.42780100
C	-1.07894800	2.75064800	-0.38799100
N	0.10402000	2.06460000	-0.44102800
H	1.08978600	5.24571600	-0.61288100
H	-1.59725400	4.93507700	-0.40177300
C	1.66052100	-2.60076400	0.04182500
C	1.44129100	-4.02309200	-0.08868000
C	0.17071900	-4.18300400	-0.55283700
C	-0.40035200	-2.86172900	-0.65963000
N	0.51701500	-1.91674200	-0.28564900
H	2.18461100	-4.78054200	0.11507500

H	-0.34865100	-5.09867700	-0.79748200
C	3.19175400	-0.66208500	0.21623100
C	4.52183600	-0.09908300	0.31830200
C	4.41013200	1.22216800	0.01273600
C	3.00666700	1.47326900	-0.23052300
N	2.29147700	0.31349200	-0.10416400
H	5.41100100	-0.66094500	0.56664700
H	5.18520700	1.97419700	-0.02984300
C	-1.72270400	-2.60016600	-1.04777200
C	2.46856100	2.73947500	-0.48397600
C	-2.35567300	2.17989900	-0.39529600
C	2.90762300	-2.03140400	0.33009900
Fe	0.30628700	0.07110300	-0.31840300
Cl	0.65174400	0.02867800	-2.66159800
O	0.14800100	0.23492300	1.39646200
H	-0.66667900	-0.57278300	1.88297100
C	-0.39328300	-1.64342300	3.78707100
C	-0.85925000	-0.52958100	4.76080000
C	-1.29557600	-1.46294400	2.56595100
C	-2.52485300	-0.83411400	3.06540300
C	-3.78089700	-0.70856900	2.45886200
C	-4.80323800	-0.05251400	3.14640700
C	-4.57383000	0.48446100	4.41947900
C	-3.31367800	0.37344500	5.02318400
C	-2.29351700	-0.28417500	4.34559400
H	-3.95477200	-1.10504700	1.46487700
H	-3.14120200	0.79209000	6.01196900
H	-5.78280600	0.04813100	2.68669000
H	-0.26453900	0.38018400	4.59850200
H	0.66695300	-1.57140200	3.53246500
H	-1.37363100	-2.28137500	1.85093000
C	-3.53038600	3.09123800	-0.23143900
C	-4.23025400	3.57036400	-1.35589600
C	-3.91561900	3.46473100	1.07225200
C	-5.33859000	4.39897200	-1.15197800
C	-5.03373900	4.28984500	1.22750400
C	-5.75918500	4.76498700	0.13044300
H	-5.88393900	4.77025800	-2.01749300
H	-5.34242700	4.57101400	2.23258900
C	3.41117600	3.88270600	-0.68475500
C	3.85279500	4.17253300	-1.99048600
C	3.84766500	4.64890700	0.41221500
C	4.73511100	5.24156200	-2.17530800
C	4.73058900	5.70855400	0.18110900

C	5.18245100	6.02249000	-1.10475900
H	5.08210100	5.46839400	-3.18152300
H	5.07397200	6.30187400	1.02641200
C	4.03524200	-2.95533900	0.67252500
C	4.88807000	-3.42503400	-0.34652300
C	4.23191300	-3.34651000	2.00978300
C	5.93693200	-4.28230000	-0.00026700
C	5.29555800	-4.20293600	2.31207000
C	6.15748600	-4.68302400	1.32170700
H	6.59900400	-4.64551600	-0.78391500
H	5.45359700	-4.50165500	3.34653200
C	-2.55008100	-3.73105100	-1.57222000
C	-2.61390300	-3.91624900	-2.96914600
C	-3.24220000	-4.59210300	-0.70022500
C	-3.37617800	-4.97596600	-3.46901800
C	-3.99571600	-5.63723800	-1.24581100
C	-4.07662500	-5.84474900	-2.62564000
H	-3.42253400	-5.12696700	-4.54581700
H	-4.53191100	-6.30509000	-0.57447800
C	3.37196500	4.32711600	1.81049700
H	2.27997100	4.39724200	1.88397500
H	3.63984600	3.30267200	2.09583900
H	3.80804800	5.01120100	2.54486000
C	3.38437600	3.33750600	-3.16023000
H	3.67798700	2.28744300	-3.04596500
H	2.29121700	3.33531900	-3.24103400
H	3.79863700	3.70913800	-4.10238600
C	6.10895400	7.19396500	-1.33550800
H	6.75910100	7.02679600	-2.20115200
H	5.54119800	8.11427800	-1.52796900
H	6.74519400	7.38119100	-0.46357800
C	3.30275600	-2.85575300	3.09596000
H	3.22641300	-1.76200500	3.09465100
H	2.28688600	-3.24088900	2.94629200
H	3.64358400	-3.17509200	4.08556600
C	4.67401100	-3.00807600	-1.78366200
H	3.65238400	-3.22685600	-2.11529600
H	4.81642900	-1.92831600	-1.90998600
H	5.36979100	-3.52378800	-2.45230600
C	7.28053400	-5.63485700	1.66300000
H	7.60298000	-5.51991200	2.70340900
H	6.96649300	-6.67906200	1.53150300
H	8.15152800	-5.47532400	1.01777000
C	-3.17390000	-4.40133700	0.79787700

H	-2.14913100	-4.52269300	1.16887600
H	-3.49966900	-3.39717600	1.09134100
H	-3.80801900	-5.12558000	1.31808300
C	-1.87998300	-2.98219500	-3.90426400
H	-2.31089700	-1.97425700	-3.87549400
H	-0.82769300	-2.86273600	-3.62391300
H	-1.92641300	-3.34240000	-4.93650300
C	-4.92048600	-6.96055600	-3.19686200
H	-5.90520600	-6.58931300	-3.51095800
H	-4.44847900	-7.40884600	-4.07837600
H	-5.08971900	-7.75450800	-2.46170200
C	-3.11974500	3.01164300	2.27475800
H	-2.92067800	1.93658500	2.25462500
H	-2.14396300	3.51306400	2.30378300
H	-3.64692300	3.23672300	3.20577500
C	-3.78561400	3.20920400	-2.75542500
H	-2.72345800	3.43597700	-2.90397200
H	-3.90513400	2.13766800	-2.95371500
H	-4.36144400	3.75890600	-3.50615500
C	-6.94267200	5.68424800	0.32555400
H	-7.65466300	5.60526700	-0.50314000
H	-7.47701400	5.45901800	1.25516700
H	-6.62254600	6.73342400	0.38138800
H	-0.75475400	-0.80319200	5.81677000
H	-0.56761500	-2.63295900	4.23495700
H	-5.37942900	0.99254000	4.94318800

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C	-2.40216100	-1.10545400	-1.01524200
C	-3.77437900	-0.72044400	-1.24194000
C	-3.85825300	0.61008000	-0.95835400
C	-2.52418900	1.04673800	-0.61671300
N	-1.65943200	-0.00900800	-0.65071600
H	-4.56136300	-1.39740600	-1.54246900
H	-4.72728000	1.25137000	-0.98665800
C	1.32599400	2.93237500	-0.47219900
C	0.86371700	4.30334600	-0.46163400
C	-0.49186700	4.25496300	-0.35350300
C	-0.85591300	2.85460500	-0.34998700
N	0.26703100	2.07551700	-0.41821100
H	1.50823200	5.16933200	-0.51123100
H	-1.19670800	5.07304200	-0.30895000
C	1.44701300	-2.71071900	-0.00801700
C	1.10980500	-4.10860800	-0.14294500

C	-0.17590000	-4.15908300	-0.59009700
C	-0.63620000	-2.79444500	-0.68268300
N	0.36146000	-1.93145400	-0.31691800
H	1.79067900	-4.92619200	0.04588700
H	-0.77159800	-5.02674300	-0.83487900
C	3.13419500	-0.90543800	0.16184500
C	4.50531800	-0.45343200	0.25837700
C	4.49652600	0.87853900	-0.01991000
C	3.11558800	1.24558800	-0.24031400
N	2.31122700	0.14396000	-0.13149900
H	5.34804500	-1.08975200	0.48766700
H	5.32888400	1.56676200	-0.05630800
C	-1.93366000	-2.42143100	-1.06813400
C	2.67832600	2.55790300	-0.45262500
C	-2.17361500	2.38932800	-0.37842200
C	2.74057000	-2.24816600	0.26845500
Fe	0.30977900	0.06808200	-0.31724800
Cl	0.63588600	0.02536600	-2.66906400
O	0.15654400	0.21588100	1.38333400
H	-0.56017500	-0.60432000	1.98207800
C	-0.42547400	-1.52278500	3.94234800
C	-1.06291400	-0.84794700	4.93838900
C	-1.22262600	-1.47059700	2.70667400
C	-2.48493600	-0.80114500	3.09575400
C	-3.64545100	-0.52538100	2.38162100
C	-4.68755400	0.16795500	3.01504800
C	-4.55821600	0.59141000	4.34118300
C	-3.39039700	0.31987900	5.06846300
C	-2.35855600	-0.38371900	4.44871400
H	-3.74502600	-0.82420800	1.34524800
H	-3.29886000	0.64339200	6.10261300
H	-5.59594700	0.39031000	2.46149500
H	-0.68621700	-0.67568700	5.94110400
H	0.55799000	-1.97174300	4.00476000
H	-1.23692100	-2.31749400	2.02033100
C	-3.27537400	3.38188100	-0.18941300
C	-3.92297900	3.95592500	-1.30031100
C	-3.64277100	3.73251400	1.12567800
C	-4.96659100	4.85880800	-1.07278100
C	-4.69526800	4.63575900	1.30351800
C	-5.37445400	5.20237400	0.22011900
H	-5.46949100	5.30736500	-1.92722800
H	-4.98820800	4.90587500	2.31623600
C	3.70771100	3.62902500	-0.62114400

C	4.16374900	3.93095100	-1.91906200
C	4.20793800	4.31727000	0.50004200
C	5.12597200	4.93384500	-2.07165100
C	5.16972800	5.31270600	0.30021500
C	5.63830000	5.63764700	-0.97681900
H	5.48482500	5.16962000	-3.07162100
H	5.56228300	5.84601300	1.16379300
C	3.78872900	-3.26177900	0.60712200
C	4.61572700	-3.78472900	-0.40725000
C	3.93469700	-3.68227900	1.94201600
C	5.59173800	-4.72238900	-0.05706200
C	4.92665900	-4.61927400	2.24807500
C	5.76411300	-5.15152200	1.26339800
H	6.23436300	-5.12744000	-0.83634500
H	5.04683400	-4.94036200	3.28083500
C	-2.85979500	-3.48363300	-1.56875600
C	-3.00074700	-3.64386600	-2.96316100
C	-3.56497800	-4.31037800	-0.67299600
C	-3.85114800	-4.64642800	-3.43797400
C	-4.40914900	-5.29643600	-1.19531800
C	-4.56619000	-5.48022500	-2.57198700
H	-3.95553200	-4.78036700	-4.51296500
H	-4.95705500	-5.93672200	-0.50693700
C	3.71494600	3.98311700	1.88946200
H	2.63389400	4.14557400	1.97768600
H	3.89372400	2.92895000	2.13270100
H	4.21402100	4.59706700	2.64522100
C	3.62604400	3.17805200	-3.11449900
H	3.83619900	2.10458500	-3.03974400
H	2.53592200	3.26626200	-3.18875600
H	4.06511100	3.54906700	-4.04552300
C	6.65256800	6.74071100	-1.17266700
H	7.29878600	6.54287300	-2.03480800
H	6.15746600	7.70455900	-1.35195300
H	7.29020400	6.86166600	-0.29027500
C	3.02330300	-3.14096800	3.01942800
H	2.99538900	-2.04510200	3.01216100
H	1.99257700	-3.48263300	2.86259200
H	3.34142800	-3.47107800	4.01298900
C	4.44890400	-3.34154500	-1.84285800
H	3.41468800	-3.47096200	-2.18234300
H	4.68403300	-2.27726900	-1.96205700
H	5.10273700	-3.91087100	-2.51023600
C	6.80933700	-6.18698000	1.60805100

H	7.11043900	-6.12003400	2.65890000
H	6.42808400	-7.20325900	1.44083700
H	7.70646000	-6.07224400	0.98960600
C	-3.41619700	-4.15018100	0.82322400
H	-2.39668400	-4.38552600	1.15155000
H	-3.62158600	-3.12414000	1.14621600
H	-4.10124800	-4.81305000	1.36013300
C	-2.25427200	-2.74625200	-3.92414300
H	-2.65182500	-1.72435800	-3.89925400
H	-1.19243500	-2.66051800	-3.66890500
H	-2.33629400	-3.11593200	-4.95078000
C	-5.50349900	-6.53374600	-3.11498000
H	-6.47505400	-6.09733600	-3.38275800
H	-5.09921200	-7.00113100	-4.01990800
H	-5.69109700	-7.32330300	-2.37964300
C	-2.89082600	3.17788200	2.31402100
H	-2.74717900	2.09612500	2.24368500
H	-1.89118300	3.62605600	2.38119600
H	-3.42001900	3.38277200	3.24855000
C	-3.48440600	3.62110500	-2.70827700
H	-2.41526600	3.82072300	-2.84776300
H	-3.63456000	2.55959000	-2.93696800
H	-4.04026800	4.20877300	-3.44504900
C	-6.53257900	6.14723700	0.44286000
H	-6.66381300	6.82961900	-0.40381600
H	-7.47390800	5.59494000	0.56612400
H	-6.39042100	6.75000100	1.34662400
H	-5.37191500	1.13468800	4.81493700

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C	-1.15443700	2.74709100	-0.47356200
C	-0.93625000	4.17696400	-0.51907300
C	0.40711300	4.36208400	-0.63740300
C	1.00934900	3.04675100	-0.61006900
N	0.04225500	2.08787600	-0.52818100
H	-1.72158700	4.91913000	-0.49313400
H	0.95772600	5.28889500	-0.71470000
C	3.17629400	-0.56711900	0.17241400
C	4.49694200	0.01953800	0.25970900
C	4.36085300	1.33509000	-0.06163400
C	2.95297100	1.55864000	-0.30332600
N	2.25862000	0.38809800	-0.15879900
H	5.39708300	-0.52366000	0.50943800
H	5.12293100	2.09939600	-0.11821900

C	-2.28269900	-1.35416600	-1.09593500
C	-3.69472000	-1.12292700	-1.28593800
C	-3.91901900	0.18835500	-0.98780000
C	-2.63220200	0.77348700	-0.68450700
N	-1.65862900	-0.18478400	-0.73844200
H	-4.40826300	-1.88170700	-1.57466100
H	-4.85562800	0.72701700	-0.98578500
C	-0.35250600	-2.84371100	-0.74418300
C	0.23578700	-4.15404700	-0.59937100
C	1.48994400	-3.96676700	-0.10139400
C	1.68648500	-2.53890900	0.00684100
N	0.53920500	-1.87928800	-0.35912900
H	-0.26416900	-5.08176600	-0.83913400
H	2.23673500	-4.70976000	0.13989600
C	-2.41867000	2.14708600	-0.47008500
C	2.91807500	-1.94101400	0.30491900
C	2.39106900	2.81170000	-0.57241100
C	-1.67169100	-2.61034100	-1.16238400
Fe	0.28555900	0.10147500	-0.40111800
Cl	0.67299000	0.06673600	-2.73913500
O	0.07818800	0.26126200	1.30886100
H	-1.18409000	-1.55897600	5.89738300
C	4.07341000	-2.83009600	0.65078200
C	4.39750800	-3.07944400	1.99734100
C	4.84811500	-3.38642800	-0.38866600
C	5.49702200	-3.89593700	2.28492200
C	5.93596000	-4.19808500	-0.05495500
C	6.27470500	-4.46860700	1.27515000
H	5.75256600	-4.08543500	3.32575300
H	6.53862800	-4.62386900	-0.85481900
C	-2.46219500	-3.75935400	-1.70471400
C	-3.20145000	-4.60342200	-0.85521300
C	-2.44908900	-3.97288900	-3.09897900
C	-3.91919500	-5.66371800	-1.41976900
C	-3.17967500	-5.04535800	-3.61834700
C	-3.91748500	-5.90385000	-2.79661400
H	-4.49434700	-6.31632300	-0.76590300
H	-3.17278000	-5.21332000	-4.69358300
C	-3.60969200	3.02641700	-0.26101600
C	-3.93665200	3.40860500	1.05639900
C	-4.37777600	3.47513900	-1.35394300
C	-5.07472700	4.19598700	1.25968800
C	-5.50127900	4.26869200	-1.10219300
C	-5.87504200	4.62657600	0.19742600

H	-5.33666800	4.48562600	2.27554300
H	-6.09524600	4.62151400	-1.94309700
C	3.31117800	3.97094000	-0.78446200
C	3.73820000	4.75192500	0.30584500
C	3.74160300	4.26044300	-2.09399600
C	4.60049900	5.82603500	0.06416400
C	4.60369800	5.34407600	-2.28926400
C	5.04121100	6.13981500	-1.22564900
H	4.93644000	6.43106700	0.90414400
H	4.94237000	5.57061200	-3.29835900
C	-3.23081900	-4.37119900	0.63798100
H	-2.22517900	-4.42653700	1.07111200
H	-3.62643000	-3.37814400	0.88145100
H	-3.85634600	-5.11417800	1.14187000
C	-1.67181600	-3.05110600	-4.01058600
H	-2.07252000	-2.03106200	-3.98091500
H	-0.62257200	-2.96556900	-3.70686600
H	-1.70542200	-3.40154400	-5.04664100
C	-4.67103600	-7.07458800	-3.38387900
H	-5.11038900	-6.82137400	-4.35526700
H	-4.00439000	-7.93250000	-3.54422500
H	-5.47821300	-7.40694900	-2.72241700
C	-3.97988700	3.13429700	-2.77295700
H	-2.92750800	3.37918900	-2.95757200
H	-4.09069400	2.06384000	-2.98093900
H	-4.59115100	3.68371000	-3.49538800
C	-3.05332200	3.02545300	2.22238400
H	-2.72068700	1.98569900	2.16826100
H	-2.14828200	3.64665500	2.23693700
H	-3.57451700	3.16047900	3.17391200
C	-7.12019100	5.44557000	0.44693900
H	-7.99899600	4.79886700	0.57333500
H	-7.02838000	6.04980100	1.35606000
H	-7.33190100	6.12039800	-0.38972200
C	3.28263900	3.41033300	-3.25656700
H	3.58468800	2.36386000	-3.13246400
H	2.18964600	3.39786300	-3.33881900
H	3.69477000	3.77720400	-4.20151900
C	3.27464000	4.43036100	1.70824500
H	2.18149200	4.47431400	1.78472800
H	3.56863200	3.41524500	2.00116600
H	3.69609700	5.13095900	2.43553200
C	5.94511300	7.32659500	-1.46747900
H	6.58792600	7.17010000	-2.34053300

H	5.35967800	8.23713300	-1.65336300
H	6.58817700	7.52493000	-0.60300500
C	4.51558600	-3.10190600	-1.83579700
H	3.52481200	-3.48909800	-2.10111100
H	4.49091300	-2.02439400	-2.03559800
H	5.25024200	-3.55801200	-2.50613900
C	3.56801300	-2.49912400	3.12023000
H	3.30057200	-1.45360800	2.93537800
H	2.62666600	-3.04965500	3.23596700
H	4.10252200	-2.55353800	4.07385800
C	7.43776800	-5.37397600	1.60842500
H	7.12252100	-6.42561300	1.63990200
H	8.23381400	-5.29661600	0.85975000
H	7.86685400	-5.13345500	2.58710600
C	-4.50893000	0.50998100	4.42953500
C	-3.29784100	0.26883800	5.08107500
C	-3.65835900	-0.60379100	2.46941400
C	-4.69104000	0.06503500	3.11575800
H	-5.62594800	0.25433700	2.59531100
C	-2.43174800	-0.85460000	3.11684400
C	-2.25230500	-0.41205800	4.44944500
C	-0.23764000	-2.12977200	3.24585300
C	0.20552600	-1.11118400	4.30372900
C	-0.97431200	-0.72516900	5.20875200
C	-1.33974400	-1.52714700	2.39696700
H	0.59863400	-2.41551700	2.60147200
H	1.02512400	-1.51142200	4.91274800
H	-0.71635200	-0.59158700	1.77966700
H	-1.66863900	-2.14388600	1.56152200
H	-0.70537300	0.12779400	5.84499900
H	-0.60237300	-3.04856200	3.73461100
H	0.58484300	-0.22461400	3.78174900
H	-3.16041100	0.61189900	6.10480900
H	-3.78539800	-0.93253600	1.44298200
H	-5.30430200	1.04443100	4.94253300

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C	-0.30462200	-2.68020200	-0.95526000
C	-1.24272200	-3.77763000	-0.93763700
C	-2.44037200	-3.26119200	-0.54747900
C	-2.24334400	-1.84024300	-0.37400500
N	-0.92577300	-1.51731900	-0.58576500
H	-0.99911700	-4.79912300	-1.19273600
H	-3.38501600	-3.76998600	-0.42018400

C	-2.28564800	2.46782700	-0.42289100
C	-3.71908000	2.63692000	-0.33891300
C	-4.24951800	1.39315200	-0.19093600
C	-3.13974500	0.46426900	-0.21447500
N	-1.96149400	1.13820000	-0.34912800
H	-4.22871300	3.58912900	-0.37793300
H	-5.28721400	1.10897900	-0.09128300
C	2.87749200	0.16688500	-0.66289700
C	3.96137900	-0.72374100	-1.00943200
C	3.39470500	-1.90990500	-1.36979900
C	1.97156300	-1.76110100	-1.18238200
N	1.68163600	-0.48410600	-0.76556300
H	5.00804100	-0.45687800	-0.98891200
H	3.87991300	-2.81861500	-1.69679300
C	2.00210600	2.45549700	-0.31349900
C	2.19186100	3.88712600	-0.22254000
C	0.95903400	4.45069500	-0.34087000
C	0.01643000	3.35958700	-0.45969700
N	0.67073800	2.16439400	-0.45167200
H	3.15018600	4.37432600	-0.11182000
H	0.69025000	5.49743400	-0.33647300
C	1.04875200	-2.80338300	-1.30586900
C	-1.37661900	3.52558500	-0.50915200
C	-3.29074600	-0.93145500	-0.18326600
C	3.04789000	1.53048000	-0.35352100
Fe	-0.12857700	0.31771400	-0.47754300
Cl	-0.34721100	0.50844800	-2.83263800
O	0.00111000	0.33604000	1.24693100
H	0.37750600	-0.72245700	1.76496000
C	3.49431100	-0.89331900	4.82441900
C	4.61688100	-1.09537200	4.01699400
C	4.44084200	-1.52704000	2.69933000
C	3.16010000	-1.75249600	2.20462700
C	2.01594700	-1.55834000	3.00422400
C	2.21099100	-1.11910700	4.32784300
H	3.61765800	-0.56199900	5.85245900
H	5.29949300	-1.67990500	2.05095100
H	3.03616900	-2.07560100	1.17889000
H	1.35541500	-0.97612800	4.97854700
C	0.67979900	-1.81261500	2.40632200
H	0.73747800	-2.52452500	1.58152800
C	-0.49282300	-2.05751900	3.29177500
C	-1.03468200	-1.03156100	4.08635000
C	-1.07214000	-3.33490000	3.36518900

C	-2.07596900	-1.29333900	4.97572700
H	-0.63873200	-0.02550500	3.98392500
C	-2.11765200	-3.59681000	4.25188600
C	-2.61236600	-2.58056600	5.07248400
H	-2.47839800	-0.48881200	5.58575800
H	-2.54441600	-4.59521700	4.30265400
C	-4.68109400	-1.47321000	-0.05986700
C	-5.41670500	-1.77211900	-1.22407100
C	-5.24649700	-1.65272400	1.21579400
C	-6.71841100	-2.26363300	-1.08409500
C	-6.55058600	-2.14904300	1.30865900
C	-7.30103300	-2.46382700	0.17168800
H	-7.29267200	-2.49225800	-1.97982300
H	-6.99013200	-2.28969100	2.29428000
C	1.52201200	-4.10496600	-1.87241500
C	1.86590300	-5.18553500	-1.03700800
C	1.60318900	-4.22577100	-3.27532100
C	2.28867600	-6.38161400	-1.62590500
C	2.02862500	-5.44193500	-3.81902700
C	2.37869900	-6.52949600	-3.01338600
H	2.55348900	-7.21896300	-0.98322600
H	2.08456500	-5.54138500	-4.90123600
C	-1.91469900	4.91568100	-0.62775700
C	-2.08690500	5.47026600	-1.91106600
C	-2.24261600	5.65052200	0.52680900
C	-2.59655700	6.76819300	-2.01472100
C	-2.74689300	6.94629100	0.37611600
C	-2.92946700	7.52270700	-0.88492700
H	-2.73736700	7.19969000	-3.00384600
H	-3.00414900	7.51789900	1.26576000
C	4.43472700	2.02445000	-0.09151700
C	4.84782900	2.18574600	1.24660100
C	5.30347900	2.32995100	-1.15763800
C	6.15892200	2.60509400	1.49359500
C	6.60308200	2.75323300	-0.86181200
C	7.05414100	2.88256400	0.45593000
H	6.48566600	2.72311600	2.52499800
H	7.27726300	2.99267500	-1.68182000
C	3.88394800	1.96131000	2.38936400
H	3.15933900	2.78375300	2.44670400
H	3.30682300	1.04045800	2.26968000
H	4.41084300	1.90407600	3.34542400
C	4.83323600	2.23024400	-2.59158000
H	4.60874100	1.19537400	-2.87436600

H	3.90986100	2.80105800	-2.74471500
H	5.59073100	2.61329600	-3.28205500
C	8.47732500	3.29602600	0.75072800
H	9.13296700	2.41894100	0.83643400
H	8.88511200	3.92981800	-0.04426000
H	8.54812100	3.84713600	1.69489000
C	-2.05473600	5.04637900	1.89976700
H	-2.67254700	4.14922100	2.02675700
H	-1.01488800	4.73594700	2.05801900
H	-2.32217600	5.75860400	2.68626500
C	-1.72479000	4.67484700	-3.14439000
H	-0.65297900	4.44414400	-3.16733000
H	-2.24174800	3.70878800	-3.16939900
H	-1.97532000	5.22432000	-4.05685700
C	-3.44619800	8.93597800	-1.02431900
H	-2.61834600	9.65617100	-1.07236600
H	-4.03580100	9.05887900	-1.93946500
H	-4.07557000	9.21981100	-0.17392000
C	-4.45568100	-1.30509700	2.45271800
H	-3.48887800	-1.81696000	2.47002400
H	-4.23947500	-0.23053100	2.49670300
H	-4.99562200	-1.57989400	3.36297600
C	-4.81466200	-1.56019200	-2.59446400
H	-4.44542000	-0.53532000	-2.71637200
H	-3.95427000	-2.22003400	-2.75741300
H	-5.54809400	-1.75682200	-3.38228600
C	-8.69672400	-3.02981100	0.29621800
H	-8.67531800	-4.12708400	0.34045200
H	-9.19302300	-2.67762400	1.20709900
H	-9.32075300	-2.75174000	-0.56016700
C	1.24515300	-3.06352400	-4.17394100
H	0.28122500	-2.61667000	-3.90731000
H	1.98155500	-2.25546200	-4.08778900
H	1.20572100	-3.37551100	-5.22206700
C	1.78093000	-5.06930800	0.46813700
H	2.41447200	-4.26075100	0.84955400
H	0.75753700	-4.85087000	0.79508200
H	2.09722600	-5.99742900	0.95363000
C	2.86813300	-7.82199800	-3.62429800
H	3.95963500	-7.81229700	-3.74623100
H	2.61952000	-8.68353000	-2.99497300
H	2.43211000	-7.98789100	-4.61539400
H	5.61465700	-0.91636700	4.40841500
H	-0.68241700	-4.13106300	2.73558300

H	-3.42450500	-2.78405400	5.76533600
cat2/a8			
C	2.75456500	-0.89335500	-0.58830200
C	3.42996500	-2.14789400	-0.83308600
C	2.47156000	-3.04686200	-1.19218100
C	1.20816000	-2.35443100	-1.11899000
N	1.40112400	-1.05160700	-0.73739700
H	4.49743600	-2.29672900	-0.75770000
H	2.58834000	-4.08572700	-1.46584600
C	-2.77400600	-0.83395600	-0.58888400
C	-3.47662600	-2.07290600	-0.83643700
C	-2.53770100	-2.99244300	-1.19487100
C	-1.25939200	-2.32830400	-1.11871300
N	-1.42428700	-1.02181700	-0.73596600
H	-4.54731900	-2.19794600	-0.76368500
H	-2.67705400	-4.02795800	-1.47051100
C	1.26762500	3.13751000	-0.36442000
C	2.54814300	3.80285100	-0.27938900
C	3.49033500	2.82438700	-0.21893100
C	2.78301400	1.56386100	-0.28920700
N	1.43626600	1.78068300	-0.37479900
H	2.68370500	4.87475500	-0.26305900
H	4.56414200	2.92425800	-0.15273000
C	-1.20104600	3.16441100	-0.36414500
C	-2.46734100	3.85692800	-0.28198700
C	-3.43007000	2.89877600	-0.22032800
C	-2.74972300	1.62338900	-0.28853200
N	-1.39850900	1.81151000	-0.37280000
H	-2.58061000	4.93145000	-0.26874600
H	-4.50155600	3.02162500	-0.15545500
C	3.42023600	0.31719500	-0.33848700
C	-3.41344100	0.39076600	-0.33920600
C	-0.03225400	-2.96080900	-1.35712400
C	0.04054700	3.80995700	-0.39186900
Fe	0.00339600	0.36580300	-0.48958500
Cl	0.00460700	0.70405100	-2.83775600
O	0.00254900	0.25161100	1.22581000
H	-0.00677500	-0.89707100	1.70524500
C	2.99622900	-2.37199400	5.16270800
C	3.42875600	-2.40728700	3.83158300
C	2.50888700	-2.33177700	2.77903800
C	1.15132300	-2.23112300	3.07730300
C	0.71113600	-2.22156200	4.42700400

C	1.63238800	-2.28301400	5.46960500
H	2.84530100	-2.35554900	1.74724300
H	1.30133700	-2.27787200	6.50520600
C	-0.01719000	-2.11747200	2.18163800
C	-1.19116600	-2.21227300	3.07237300
C	-2.54896900	-2.29094800	2.76853700
C	-3.47425100	-2.35202100	3.81730600
C	-3.04675700	-2.32380600	5.15022500
C	-1.68295400	-2.25659700	5.46269100
C	-0.75653400	-2.20982100	4.42389800
H	-2.88176800	-2.30929700	1.73549200
H	-3.77995000	-2.36511300	5.95147300
H	-1.35609100	-2.25676500	6.49963300
C	-0.04700800	-4.34434100	-1.92771900
C	-0.03429900	-4.47804400	-3.33162300
C	-0.06793300	-5.47958300	-1.09559800
C	-0.04570300	-5.76325300	-3.88112500
C	-0.07862600	-6.74588400	-1.69091400
C	-0.07108700	-6.90890600	-3.07922500
H	-0.03304800	-5.87109200	-4.96393400
H	-0.09188800	-7.62636700	-1.05161100
C	-4.90408200	0.39872200	-0.20252100
C	-5.48359900	0.53299000	1.07577900
C	-5.71524600	0.30557200	-1.35287200
C	-6.87801400	0.51916700	1.18413200
C	-7.10463700	0.30531400	-1.19537200
C	-7.70551500	0.39661200	0.06408600
H	-7.32788900	0.61488000	2.17047100
H	-7.73319100	0.23931900	-2.08127600
C	0.05713200	5.30513100	-0.42960100
C	0.03410400	6.04048400	0.77045900
C	0.09053100	5.95718700	-1.67730400
C	0.04505700	7.43698600	0.70061800
C	0.09919300	7.35541400	-1.69968300
C	0.07978000	8.11226100	-0.52374600
H	0.02447500	8.01057600	1.62523600
H	0.12070000	7.86540700	-2.66080200
C	4.91029700	0.29279700	-0.19833800
C	5.48970000	0.41736300	1.08098100
C	5.72209300	0.17823900	-1.34641800
C	6.88318200	0.37109600	1.19299900
C	7.11062100	0.14605300	-1.18534400
C	7.71039200	0.22622100	0.07549000
H	7.33256200	0.45883800	2.18029400

H	7.73972200	0.06342800	-2.06947400
C	-0.07270400	-5.34299000	0.40956700
H	0.81490600	-4.80807700	0.76768600
H	-0.94521700	-4.77932400	0.76050200
H	-0.09072900	-6.32318500	0.89522100
C	-0.00282200	-3.25550400	-4.22053500
H	-0.85877400	-2.59728100	-4.03291100
H	0.88838000	-2.64524300	-4.03398600
H	-0.01075700	-3.53699900	-5.27782200
C	-0.11759800	-8.28594600	-3.69970200
H	0.30389700	-9.04328700	-3.03006500
H	-1.15130300	-8.58397200	-3.92068800
H	0.43778300	-8.31949800	-4.64347900
C	4.63658700	0.64374200	2.30822200
H	4.26939300	1.67753800	2.33917300
H	3.75494500	-0.00182600	2.32879300
H	5.20712300	0.46301000	3.22438000
C	5.11466400	0.11446300	-2.73062700
H	4.64227800	-0.85659400	-2.92017900
H	4.33294000	0.87085100	-2.86194700
H	5.87746100	0.27225500	-3.49920300
C	9.21135700	0.14306700	0.22645100
H	9.72649400	0.54629600	-0.65224000
H	9.55805600	0.69462800	1.10707100
H	9.53788900	-0.89884900	0.34533600
C	-0.00597500	5.33060500	2.10446000
H	-0.90393100	4.70781000	2.19698700
H	0.85329100	4.65985500	2.22426100
H	0.00032000	6.04432100	2.93379000
C	0.12517600	9.62199900	-0.57403900
H	-0.34583300	10.00756900	-1.48477200
H	-0.38386500	10.06842400	0.28714300
H	1.16141000	9.98587900	-0.56433900
C	0.11669700	5.15749200	-2.95967600
H	1.01267600	4.52823000	-3.01862300
H	-0.73782100	4.47421800	-3.02602800
H	0.10151800	5.81367300	-3.83515700
C	-4.62793400	0.73445700	2.30557000
H	-5.20755200	0.57539300	3.22005300
H	-3.76848200	0.05962500	2.33087200
H	-4.22620300	1.75534500	2.33531000
C	-5.10565500	0.23067800	-2.73555500
H	-4.30735000	0.97013100	-2.86357700
H	-4.65376600	-0.75009200	-2.92519500

H	-5.86270700	0.40599600	-3.50600300
C	-9.20838700	0.34855100	0.21150400
H	-9.54464200	0.91369300	1.08758800
H	-9.71209100	0.75750600	-0.67112800
H	-9.55883900	-0.68483700	0.33663400
H	-0.01939500	-2.66152300	1.24216800
H	-4.53564800	-2.41554900	3.59247500
H	4.48990900	-2.48781600	3.61114900
H	3.72535600	-2.42484400	5.96698600

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C	2.63607800	-0.11727300	-0.75881000
C	3.74816700	-1.03790900	-0.81225000
C	3.22219200	-2.28858100	-0.76548500
C	1.78860800	-2.13533700	-0.67097800
N	1.45165000	-0.80414400	-0.61538900
H	4.78434900	-0.74224500	-0.88878500
H	3.73553500	-3.23876100	-0.79451400
C	-2.49611500	-2.20897100	-0.38922300
C	-2.66225200	-3.64174300	-0.42863500
C	-1.42099500	-4.17628400	-0.59453000
C	-0.49522700	-3.07059200	-0.61883600
N	-1.16894300	-1.88337300	-0.49947500
H	-3.61186300	-4.15228100	-0.35686000
H	-1.14180600	-5.21607600	-0.68258800
C	-0.33119400	2.99392000	-0.93979000
C	0.57260100	4.09685000	-1.16851000
C	1.82664000	3.57198000	-1.21722900
C	1.68785300	2.15066400	-1.00206500
N	0.37260000	1.81902700	-0.84235000
H	0.26763900	5.12748300	-1.27929600
H	2.76596600	4.08106500	-1.37696600
C	-2.61039800	2.08003800	-0.64879400
C	-4.03588300	2.24576900	-0.46335100
C	-4.55262700	0.99892700	-0.29485300
C	-3.44245900	0.07616000	-0.38666000
N	-2.27555200	0.75783200	-0.60729100
H	-4.55007500	3.19636100	-0.46200900
H	-5.58080800	0.71006900	-0.12974600
C	2.76836400	1.25612100	-0.97746000
C	-3.56850400	-1.31189100	-0.29146600
C	0.89486300	-3.21080500	-0.72746000
C	-1.71636100	3.14262600	-0.83369200
Fe	-0.38866300	-0.02809700	-0.60185500

C1	-0.48336600	-0.21451700	-2.94216000
O	-0.60462200	0.23492900	1.09893600
H	0.29640600	-0.05884300	1.94212300
C	4.88509700	-1.57441100	3.09085400
C	3.90913400	-2.45949600	2.62413700
C	2.56330700	-2.08003800	2.57658200
C	2.19060100	-0.80687300	3.00132800
C	3.18929300	0.09668300	3.44080400
C	4.52905500	-0.28349300	3.49608900
H	5.92655500	-1.88287400	3.12325900
H	1.82949500	-2.75825800	2.16758100
H	5.28776300	0.41535700	3.83909500
C	0.84048200	-0.15663500	3.08977800
C	1.17052500	1.26590300	3.44693500
C	0.36699100	2.40745600	3.45148700
C	0.93193800	3.63981500	3.79980500
C	2.28886900	3.74041900	4.12804000
C	3.11279300	2.61234300	4.07611800
C	2.55429000	1.38798900	3.71360000
H	-0.67184500	2.35238800	3.15126100
H	4.17556500	2.69467200	4.28849500
C	-0.26113100	-0.90049700	3.91961900
C	-0.65187400	-2.23321800	3.24698400
C	0.29819100	-1.18287100	5.33243100
C	-1.54078300	-0.05118200	4.05742200
H	-0.94633800	-2.07070800	2.20588200
H	0.16122000	-2.96231000	3.27789100
H	-1.49954000	-2.68004800	3.78014700
H	0.59335300	-0.25132200	5.82866700
H	-0.46844200	-1.66891900	5.94842400
H	1.17252200	-1.84042000	5.29192400
H	-2.31514600	-0.64208000	4.56109200
H	-1.36834700	0.84311700	4.66276200
H	-1.91646300	0.24780400	3.07554100
C	1.44249600	-4.56633300	-1.05914600
C	1.77578400	-4.82103500	-2.41105700
C	1.59900000	-5.57270500	-0.08800100
C	2.26875200	-6.08128700	-2.75532900
C	2.09879300	-6.82077400	-0.48165100
C	2.43927700	-7.09579500	-1.80656500
H	2.52089700	-6.27904300	-3.79546100
H	2.22065400	-7.59686400	0.27163400
C	-4.93931500	-1.88100800	-0.09853400
C	-5.38166400	-2.20146100	1.19938200

C	-5.76803100	-2.09769700	-1.21609600
C	-6.66316000	-2.73728300	1.35865900
C	-7.04108900	-2.63951200	-1.01110900
C	-7.50817000	-2.96206300	0.26690300
H	-7.00894300	-2.98660400	2.36004200
H	-7.68223500	-2.81558400	-1.87263900
C	-2.28371400	4.52547000	-0.90798700
C	-2.35414900	5.31194500	0.25777000
C	-2.75167300	5.02006200	-2.14024800
C	-2.89952200	6.59624500	0.16965500
C	-3.28734900	6.31112000	-2.18372500
C	-3.36802500	7.11478000	-1.04196000
H	-2.96200600	7.20518200	1.06951700
H	-3.65156500	6.69752700	-3.13362300
C	4.11775900	1.78838000	-1.35381600
C	4.93054700	2.43665100	-0.40567700
C	4.54508300	1.64900700	-2.69174200
C	6.17268000	2.93562800	-0.81172600
C	5.79338500	2.16506000	-3.05261200
C	6.62096500	2.81278300	-2.12972600
H	6.80436400	3.43229600	-0.07778700
H	6.12598200	2.06043200	-4.08361500
C	1.27584600	-5.34078300	1.37158700
H	2.14837400	-4.95187300	1.91188700
H	0.45960700	-4.62673900	1.50705700
H	0.98758500	-6.27701000	1.86089100
C	1.61507100	-3.75513600	-3.47296000
H	0.66566400	-3.21659500	-3.38447100
H	2.40242200	-2.99550800	-3.39062400
H	1.67412300	-4.19225100	-4.47449800
C	2.94649500	-8.45796000	-2.21891400
H	3.30185600	-9.03346400	-1.35779000
H	2.15419700	-9.04411100	-2.70313900
H	3.77092100	-8.37668400	-2.93661500
C	4.47723200	2.57183800	1.02651300
H	3.51214100	3.08380700	1.10505500
H	4.34530300	1.58891100	1.48915200
H	5.20408500	3.13161800	1.62333800
C	3.68187600	0.94769700	-3.71661600
H	3.63812100	-0.13133500	-3.52405500
H	2.64572800	1.30278300	-3.69422500
H	4.07572400	1.09450500	-4.72696700
C	7.95020500	3.39108800	-2.55679500
H	7.82454800	4.39382800	-2.98691900

H	8.63940200	3.48306600	-1.71047500
H	8.43110100	2.76987400	-3.32064400
C	-1.85586200	4.76880900	1.57732600
H	-2.37557100	3.84072700	1.84527000
H	-0.78846700	4.52440900	1.53078700
H	-2.00750600	5.49076700	2.38599900
C	-3.92078100	8.51912000	-1.12072000
H	-4.66927300	8.61225000	-1.91511800
H	-4.38784400	8.82066400	-0.17676400
H	-3.12517800	9.24489500	-1.33660600
C	-2.67639400	4.16778300	-3.38627700
H	-1.64848600	3.84365100	-3.58690100
H	-3.27190700	3.25336400	-3.27913200
H	-3.04155800	4.71282200	-4.26197700
C	-4.48317600	-1.97219900	2.39293000
H	-3.57407800	-2.58141700	2.32994200
H	-4.15049600	-0.92935800	2.44972500
H	-4.99455400	-2.21915800	3.32838900
C	-5.28743500	-1.75489100	-2.60769900
H	-5.12766800	-0.67545800	-2.71715700
H	-4.32670500	-2.23365700	-2.82953900
H	-6.01151700	-2.07006300	-3.36507600
C	-8.90088100	-3.51336100	0.46722200
H	-8.94563400	-4.18754300	1.32961300
H	-9.62280500	-2.70564600	0.64817800
H	-9.24503900	-4.06548500	-0.41400000
H	4.19754800	-3.44749200	2.27491100
H	0.30884700	4.52976800	3.80581800
H	2.70940100	4.70460600	4.40105300

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C	3.01764400	0.95549800	-0.73399000
C	4.33023700	0.35395500	-0.72143200
C	4.14286500	-0.99446300	-0.73780600
C	2.71737000	-1.21295700	-0.75057300
N	2.05099500	-0.01945500	-0.74560500
H	5.25920800	0.90563300	-0.70324500
H	4.88406200	-1.78040900	-0.72974400
C	-1.41253500	-2.38379900	-0.92184300
C	-1.20235200	-3.81271300	-0.90624300
C	0.13947600	-4.00917400	-0.80481900
C	0.74560700	-2.70018400	-0.74290200
N	-0.22261500	-1.72311600	-0.77200600
H	-1.98903400	-4.54904000	-0.98271500

H	0.68674800	-4.94063500	-0.78832400
C	-0.62902700	3.24220600	-0.78938800
C	-0.02973000	4.55420600	-0.68206600
C	1.31670100	4.36611200	-0.67898300
C	1.53403500	2.93758300	-0.76069300
N	0.34098600	2.27816200	-0.84157000
H	-0.58390100	5.48044500	-0.62949700
H	2.10247700	5.10554500	-0.62070900
C	-2.58484200	1.74923700	-1.01708900
C	-3.99675700	1.54119800	-1.24135900
C	-4.17513000	0.19990000	-1.37955200
C	-2.87831800	-0.41001600	-1.19737900
N	-1.92418800	0.55363400	-1.00415100
H	-4.73243100	2.33054700	-1.29762800
H	-5.08916400	-0.34371500	-1.56950700
C	2.79959000	2.33773000	-0.72731800
C	-2.66087500	-1.79033100	-1.16856700
C	2.12560400	-2.48474400	-0.76805100
C	-2.00613500	3.01603500	-0.85493400
Fe	0.05702500	0.26719000	-0.78492100
Cl	0.19623100	0.19888700	-3.14485300
O	-0.06259200	0.52910300	0.90638200
H	-0.11697500	-0.34633100	1.77420800
C	-2.37925700	2.11647700	4.98946700
C	-1.09391200	2.49321900	4.57649200
C	-0.25322500	1.57810900	3.93463500
C	-0.71483900	0.28232700	3.71904200
C	-2.00865100	-0.10293500	4.14230400
C	-2.84528900	0.81434800	4.77664300
H	-3.01981300	2.84282000	5.48285700
H	-0.74962100	3.50886000	4.75279800
H	0.73909500	1.86756300	3.60215600
H	-3.84123600	0.52532300	5.10314400
C	-0.06042900	-0.85021400	2.99714100
C	-1.04487800	-1.95739900	3.10023700
C	-0.96098100	-3.26904600	2.63687300
C	-2.01696600	-4.14934700	2.89617700
C	-3.14313100	-3.72014600	3.60968200
C	-3.24835000	-2.39570300	4.05098700
C	-2.20304200	-1.51247000	3.78770500
H	-0.08863500	-3.59594400	2.08106700
H	-1.96142300	-5.17450800	2.54041500
H	-3.95167400	-4.41850500	3.80883100
H	-4.12969200	-2.06555200	4.59509400

C	3.02455300	-3.66945600	-0.94334800
C	3.47995000	-3.97454300	-2.24474200
C	3.40803500	-4.45951600	0.15501800
C	4.31985500	-5.07771500	-2.41755000
C	4.25795400	-5.54965800	-0.06521300
C	4.72068500	-5.87779500	-1.34171700
H	4.67283800	-5.31687500	-3.41885200
H	4.56562100	-6.15466700	0.78564600
C	-3.81640200	-2.68889200	-1.47734300
C	-4.78508100	-2.96353800	-0.49348400
C	-3.92042300	-3.24654200	-2.76882300
C	-5.84614100	-3.81563000	-0.81621900
C	-5.00373100	-4.08527900	-3.04823400
C	-5.97489300	-4.38378600	-2.08705100
H	-6.58933500	-4.04084900	-0.05359300
H	-5.08995500	-4.51719200	-4.04346900
C	-2.92432400	4.19036700	-0.73541500
C	-3.45199100	4.51456800	0.53012000
C	-3.25412600	4.95031000	-1.87366100
C	-4.31217400	5.61246300	0.63225000
C	-4.12098200	6.03736300	-1.72446600
C	-4.66182600	6.38260300	-0.48153100
H	-4.71896200	5.87174100	1.60778700
H	-4.37978000	6.62810000	-2.60110100
C	3.99628500	3.23493100	-0.67405400
C	4.45140300	3.71957300	0.56778600
C	4.65312300	3.58436000	-1.86938700
C	5.57359600	4.55308100	0.59122800
C	5.77137600	4.42152500	-1.79869200
C	6.24582000	4.91708800	-0.58034000
H	5.93187900	4.92662300	1.54857900
H	6.28334400	4.69310200	-2.71973200
C	2.90438600	-4.15619900	1.54518000
H	2.82978600	-3.08287500	1.73129700
H	1.90329600	-4.57937400	1.69990900
H	3.56015200	-4.58405600	2.30904300
C	3.07976300	-3.12222200	-3.42816200
H	1.99993300	-2.93915700	-3.45507000
H	3.55405700	-2.13430600	-3.38436400
H	3.37328600	-3.59611600	-4.36980300
C	5.60896200	-7.08016800	-1.56257500
H	6.17405200	-7.33392500	-0.65926800
H	5.01636300	-7.96337400	-1.83651400
H	6.32461400	-6.90668700	-2.37388800

C	3.73914500	3.34758800	1.84880900
H	2.69461100	3.68162800	1.83341100
H	3.71689400	2.26224600	1.99845400
H	4.22769600	3.79748400	2.71828600
C	4.16189200	3.05741400	-3.19834800
H	4.25430900	1.96605800	-3.25236300
H	3.10045500	3.28359400	-3.35212400
H	4.72886900	3.48875500	-4.02877900
C	7.43587000	5.84722800	-0.53151900
H	7.11689100	6.89775600	-0.56147000
H	8.01471800	5.71042700	0.38852900
H	8.10658700	5.68622500	-1.38228600
C	-3.09040000	3.69775200	1.74957900
H	-3.42518200	2.65792500	1.65457900
H	-2.00653400	3.65233100	1.90313100
H	-3.54132100	4.11356200	2.65524100
C	-5.62405900	7.54057200	-0.35148600
H	-6.65869500	7.21501300	-0.52447300
H	-5.58586500	7.98419100	0.64932500
H	-5.40601600	8.32835800	-1.08092000
C	-2.68046700	4.59383300	-3.22591800
H	-1.58787900	4.68696300	-3.23094100
H	-2.90475700	3.55436000	-3.49314900
H	-3.08141300	5.24299500	-4.01013600
C	-4.69022600	-2.34152300	0.87895500
H	-3.66514000	-2.34413500	1.25689800
H	-5.01925600	-1.29463700	0.86219200
H	-5.31355200	-2.87725000	1.60039600
C	-2.87981400	-2.96100500	-3.82898700
H	-2.59825300	-1.90277000	-3.85680400
H	-1.95543300	-3.51892000	-3.63401300
H	-3.24259300	-3.24901100	-4.82050400
C	-7.14951500	-5.27278100	-2.42405200
H	-7.52145400	-5.79975600	-1.53862200
H	-7.98500900	-4.68603900	-2.82906500
H	-6.88324000	-6.02111300	-3.17849500
C	1.39743900	-1.11151000	3.24437900
C	2.39158900	-0.37288200	2.58415800
C	1.79261200	-2.06518700	4.19802000
C	3.74229900	-0.58447600	2.86729400
H	2.09205100	0.34798900	1.83267700
C	3.14181200	-2.26512900	4.49041900
H	1.03352400	-2.64385400	4.71587300
C	4.12347500	-1.52755800	3.82390800

H	4.49579100	-0.02415900	2.32108100
H	3.42596200	-3.00306400	5.23645700
H	5.17527200	-1.69351300	4.04141200

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C	2.69542200	-1.00368600	-0.57912500
C	3.32962500	-2.27401500	-0.84935800
C	2.35656500	-3.10910300	-1.31216100
C	1.11745400	-2.37085000	-1.25668500
N	1.34901000	-1.09581900	-0.80899800
H	4.38295000	-2.47559200	-0.71837600
H	2.44606900	-4.13633500	-1.63622800
C	-2.78104100	-0.73068700	-0.59550400
C	-3.53664300	-1.93209500	-0.86902200
C	-2.64855900	-2.85969400	-1.32677300
C	-1.34290700	-2.24749300	-1.26561800
N	-1.44953700	-0.95554200	-0.81904300
H	-4.60549800	-2.02810100	-0.74407800
H	-2.83765200	-3.87363400	-1.65000000
C	1.38881500	3.08824200	-0.55540500
C	2.69305400	3.69691700	-0.41504000
C	3.57777700	2.68083300	-0.22037700
C	2.81756500	1.45121900	-0.28935800
N	1.49512000	1.72760900	-0.48783300
H	2.88050300	4.76088700	-0.44379800
H	4.64673000	2.73484500	-0.07059700
C	-1.07528400	3.21251100	-0.56424800
C	-2.31428100	3.94714900	-0.43495000
C	-3.29616700	3.02370400	-0.24464900
C	-2.66081600	1.72504000	-0.30758800
N	-1.31636000	1.86899700	-0.49742100
H	-2.39636400	5.02424200	-0.46752500
H	-4.35555700	3.18300100	-0.10189000
C	3.39107800	0.17277400	-0.25427800
C	-3.35810700	0.50963300	-0.27448800
C	-0.14223600	-2.91473900	-1.54024400
C	0.19018400	3.80747900	-0.64987900
Fe	0.01859900	0.37706700	-0.59505200
Cl	0.04580700	0.67501400	-2.95150600
O	0.00460200	0.30300200	1.12250900
H	-0.05484700	-0.88271600	1.58928100
C	3.42184600	-2.41629100	4.50492300
C	2.30513200	-1.72464900	4.98406800
C	2.25778900	-2.84674000	2.43292000

C	3.39878700	-2.97258600	3.22327400
H	2.32412300	-1.28725300	5.97993700
H	4.26793500	-3.49933600	2.83877600
C	-0.11323800	-2.04786000	2.11632700
C	1.12755100	-2.16821100	2.91264500
C	1.16085800	-1.58826400	4.19816100
C	-0.05951100	-0.81956100	4.65937500
H	-0.14165100	-2.68307200	1.23226300
H	-0.05633800	-0.69373800	5.74804800
H	-0.00792100	0.19199600	4.22353700
H	2.23777100	-3.27126600	1.43457500
C	-1.36409800	-2.04670100	2.90635600
C	-2.55277200	-2.61214300	2.42129200
C	-3.70570000	-2.62187700	3.20454200
C	-3.68148500	-2.06211600	4.48457100
C	-2.50436400	-1.48410100	4.96968100
C	-1.34737000	-1.46405200	4.19094800
H	-2.56874800	-3.04024600	1.42433300
H	-4.62043900	-3.06084800	2.81567100
H	-4.57543200	-2.07123500	5.10257800
H	-2.48590200	-1.04473900	5.96471900
C	-0.20726200	-4.27010500	-2.17074500
C	-0.21799800	-4.34133000	-3.57942500
C	-0.24967400	-5.44096500	-1.39070900
C	-0.26856800	-5.60016000	-4.18496700
C	-0.30066600	-6.67916400	-2.04061600
C	-0.31282800	-6.77975500	-3.43471500
H	-0.27212700	-5.65978300	-5.27160000
H	-0.33044300	-7.58669200	-1.44086300
C	4.84182600	0.06960500	0.09202800
C	5.21350000	0.13213500	1.45039100
C	5.81666400	-0.06204400	-0.91763300
C	6.56661900	0.00007100	1.77899200
C	7.15806100	-0.18066300	-0.54113400
C	7.55141600	-0.16793600	0.80127200
H	6.85740000	0.03730600	2.82707500
H	7.91527000	-0.27785700	-1.31676400
C	-4.81249400	0.54867800	0.06930600
C	-5.17670400	0.64108000	1.42823500
C	-5.79498100	0.51037800	-0.94027300
C	-6.53592900	0.63194600	1.75690500
C	-7.14181900	0.51350000	-0.56367900
C	-7.53215800	0.55686100	0.77880100
H	-6.82210100	0.69186600	2.80522700

H	-7.90461700	0.48793100	-1.33943400
C	0.26720000	5.29409200	-0.79037300
C	0.34379300	5.84988200	-2.08256100
C	0.27131900	6.11698200	0.35142900
C	0.42078800	7.24021400	-2.20792900
C	0.35023200	7.50271200	0.17888700
C	0.42207200	8.08293000	-1.09138900
H	0.48259600	7.67521400	-3.20358900
H	0.35731400	8.14319500	1.05867500
C	-0.17663300	-3.08108900	-4.41288500
H	-1.04373800	-2.44069400	-4.21445200
H	0.70114500	-2.46819200	-4.17947100
H	-0.16018800	-3.31605500	-5.48144400
C	-0.23854000	-5.37242800	0.11907800
H	0.66737400	-4.88207600	0.49359500
H	-1.08997800	-4.79756800	0.50146500
H	-0.28473900	-6.37208700	0.56124500
C	-0.40086900	-8.12566800	-4.11611000
H	-1.44180800	-8.37671800	-4.36031700
H	0.16319100	-8.13711300	-5.05536200
H	-0.01336300	-8.92640000	-3.47715400
C	4.18430300	0.38626600	2.52807300
H	3.85946200	1.43464400	2.50891500
H	3.28756200	-0.22525900	2.39697900
H	4.59145600	0.17422500	3.51997900
C	5.42886600	-0.04151800	-2.37954400
H	4.86528800	-0.93736000	-2.66443700
H	4.78439800	0.81575800	-2.60598800
H	6.31446800	0.01755000	-3.01956500
C	9.00279800	-0.34498900	1.18270600
H	9.22620100	0.12761000	2.14527900
H	9.25955800	-1.40900200	1.27425600
H	9.67159000	0.08549200	0.42916200
C	0.19955700	5.51176800	1.73492200
H	-0.72027300	4.92939400	1.86678300
H	1.03487200	4.82325700	1.91091600
H	0.22669400	6.28580500	2.50790800
C	0.35009100	4.95544500	-3.30094800
H	1.21637500	4.28349100	-3.29865900
H	-0.53254100	4.30623000	-3.32843400
H	0.37467400	5.54362900	-4.22329600
C	0.47171300	9.58422900	-1.25735400
H	-0.53468700	9.99837100	-1.40558400
H	0.89835800	10.07288900	-0.37477100

H	1.07126500	9.87175200	-2.12814100
C	-5.40640100	0.49911300	-2.40208300
H	-4.69304700	1.30023800	-2.62782100
H	-4.91892600	-0.44027700	-2.68721000
H	-6.28359600	0.63186500	-3.04267500
C	-4.12716000	0.79573200	2.50518900
H	-3.29462600	0.09901900	2.37484200
H	-3.70099700	1.80708200	2.48329700
H	-4.55229600	0.62671000	3.49772300
C	-8.99308500	0.50969000	1.16188400
H	-9.62580100	0.96185700	0.39029000
H	-9.33268000	-0.52643800	1.29468800
H	-9.17866900	1.03539200	2.10487000
H	4.30641800	-2.51567600	5.12845200

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C	2.74450000	-0.86735100	-0.62855500
C	3.42065000	-2.11108100	-0.91499400
C	2.47312000	-2.98638100	-1.35669500
C	1.20511200	-2.30275900	-1.27918800
N	1.39632200	-1.01814800	-0.83410800
H	4.48387500	-2.27016900	-0.80671000
H	2.59861400	-4.00928300	-1.68273900
C	-2.76234000	-0.81260900	-0.63178000
C	-3.46216000	-2.04421800	-0.91414300
C	-2.53151700	-2.93877300	-1.35315900
C	-1.25069400	-2.27921500	-1.27820200
N	-1.41717000	-0.99019300	-0.83620900
H	-4.52835500	-2.18239100	-0.80630800
H	-2.67666300	-3.95997900	-1.67632400
C	1.25886200	3.15189400	-0.52532100
C	2.53786200	3.81143600	-0.38798700
C	3.46825800	2.83296200	-0.22082700
C	2.76543400	1.57147700	-0.30253800
N	1.42834500	1.79436100	-0.48113300
H	2.67796700	4.88300000	-0.40138200
H	4.53579100	2.93156300	-0.08365500
C	-1.19693000	3.17745900	-0.53238200
C	-2.46372900	3.86233500	-0.40635500
C	-3.41411000	2.90291500	-0.24133300
C	-2.73575900	1.62759200	-0.31413700
N	-1.39366300	1.82339500	-0.48521400
H	-2.58304000	4.93631500	-0.42507800
H	-4.48035200	3.02292900	-0.11134100

C	3.39967500	0.32607400	-0.29776400
C	-3.39465500	0.39486500	-0.30769900
C	-0.02873400	-2.90566300	-1.54221200
C	0.03798400	3.82643200	-0.60465500
Fe	0.00312100	0.38925100	-0.58861300
Cl	0.00872200	0.71541900	-2.92193500
O	-0.00040400	0.27767800	1.07805700
H	-0.01243700	-0.95920900	1.60111800
C	3.52699800	-2.22126300	4.51137400
C	2.31585500	-1.81955100	5.06856500
C	2.44171200	-2.60824400	2.38562400
C	3.58863100	-2.62751300	3.17033000
H	2.23341900	-1.51888600	6.10786000
H	4.53548800	-2.93403000	2.73607700
C	-0.02550800	-2.10414600	2.12158500
C	1.20796200	-2.19855900	2.91761400
C	1.16877000	-1.82254000	4.27406600
H	-0.03635800	-2.71559700	1.21838400
H	2.48680600	-2.90279400	1.34343100
C	-1.25654300	-2.16457800	2.92471700
C	-2.50435100	-2.53936200	2.39974800
C	-3.64696100	-2.52552300	3.19084100
C	-3.56635600	-2.12007800	4.53114100
C	-2.34123700	-1.75266500	5.08137000
C	-1.19905300	-1.78909100	4.28069500
H	-2.56338100	-2.83293100	1.35788800
H	-4.60462000	-2.80486600	2.76196900
H	-4.45961300	-2.09712300	5.14884200
H	-2.24464800	-1.45370800	6.11993900
C	-0.04193700	-4.27085400	-2.15742700
C	-0.03739300	-4.36393200	-3.56484800
C	-0.05314900	-5.43386800	-1.36404400
C	-0.04543300	-5.63157900	-4.15450600
C	-0.06103600	-6.68206000	-1.99643200
C	-0.06036200	-6.80194400	-3.38911900
H	-0.03861100	-5.70582000	-5.24025500
H	-0.06670400	-7.58219300	-1.38475200
C	4.85841300	0.27912400	0.03053200
C	5.25024400	0.37741900	1.38186400
C	5.82641900	0.16026100	-0.98859800
C	6.61050900	0.28063800	1.69524700
C	7.17499200	0.07730800	-0.62853500
C	7.58602900	0.11678200	0.70809300
H	6.91457700	0.34546600	2.73837300

H	7.92444700	-0.01119100	-1.41281300
C	-4.85552300	0.37781700	0.01431200
C	-5.25167700	0.48902900	1.36334800
C	-5.82102900	0.27197300	-1.00872700
C	-6.61484700	0.41728100	1.67102100
C	-7.17240200	0.21426300	-0.65442900
C	-7.58865800	0.26621100	0.68019700
H	-6.92230300	0.49165800	2.71251300
H	-7.91978800	0.13565500	-1.44173300
C	0.05483300	5.31847600	-0.71723700
C	0.09620000	5.90462800	-1.99745800
C	0.03702600	6.11960400	0.44023900
C	0.11546100	7.29946200	-2.09593000
C	0.05812300	7.51056000	0.29605300
C	0.09359900	8.11895400	-0.96273500
H	0.14988700	7.75653500	-3.08303900
H	0.04799700	8.13315000	1.18869400
C	-0.01981400	-3.11522400	-4.41648300
H	-0.88502800	-2.47521200	-4.20977500
H	0.86162200	-2.49827900	-4.20796900
H	-0.02193100	-3.36472000	-5.48194800
C	-0.05261300	-5.34609000	0.14477300
H	0.83339300	-4.81681500	0.51516900
H	-0.92835900	-4.79936100	0.51421100
H	-0.06276200	-6.34113300	0.59985000
C	-0.10390400	-8.15941300	-4.05170500
H	-1.13772500	-8.45874700	-4.27066300
H	0.44107300	-8.15952900	-5.00216000
H	0.33066500	-8.93412200	-3.41073200
C	4.23790800	0.64627300	2.47300400
H	3.95259300	1.70626900	2.47618800
H	3.31766300	0.07301900	2.33611600
H	4.64528500	0.40280100	3.45831100
C	5.42443700	0.15954300	-2.44704300
H	4.91479500	-0.76801500	-2.73161000
H	4.72622500	0.97576000	-2.66424400
H	6.29945300	0.27466000	-3.09420500
C	9.04615700	-0.02291900	1.07127600
H	9.26536000	0.43577300	2.04146500
H	9.33779500	-1.07994100	1.13598000
H	9.69292400	0.44483800	0.32054700
C	0.00175900	5.48486000	1.81179700
H	-0.89275700	4.86336200	1.93888700
H	0.86471500	4.82620700	1.96685500

H	0.00495800	6.24375600	2.60027900
C	0.12751800	5.03703600	-3.23476500
H	1.01903900	4.39913100	-3.25212500
H	-0.73006900	4.35543500	-3.26924600
H	0.12250700	5.64494300	-4.14470300
C	0.07962600	9.62426100	-1.09668700
H	-0.94761300	10.00365200	-1.18220500
H	0.53395100	10.10982900	-0.22610000
H	0.62168100	9.95272600	-1.99030400
C	-5.41266700	0.25836700	-2.46533500
H	-4.70321100	1.06455700	-2.68364600
H	-4.91355700	-0.67702400	-2.74270700
H	-6.28324400	0.38126300	-3.11703400
C	-4.23987800	0.74544800	2.45802600
H	-3.32686300	0.15980000	2.32544300
H	-3.94046600	1.80157400	2.46088300
H	-4.65418500	0.50888200	3.44215200
C	-9.05261400	0.15315700	1.03711000
H	-9.68750100	0.63216800	0.28332800
H	-9.36361900	-0.89838600	1.10093100
H	-9.26777700	0.61622100	2.00611600
O	-0.00857000	-1.46233200	4.88435500
H	4.42391900	-2.22440800	5.12415100

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C	-0.00284400	-2.90656700	-0.92187400
C	-0.67830200	-4.16132600	-0.69004800
C	-1.87620300	-3.86038200	-0.11404000
C	-1.95650500	-2.41847400	-0.04835100
N	-0.78960500	-1.86473000	-0.51429500
H	-0.26813500	-5.13290400	-0.92692000
H	-2.65775900	-4.53450200	0.20660500
C	-2.91535400	1.75379000	-0.44908900
C	-4.32217100	1.65005800	-0.13130600
C	-4.54209800	0.36167700	0.24909800
C	-3.27696100	-0.33033100	0.12024100
N	-2.30829300	0.53652600	-0.29478600
H	-5.02554500	2.46913000	-0.18126200
H	-5.46708600	-0.09957600	0.56441100
C	2.56299900	0.50454100	-1.04655300
C	3.78122900	-0.19076000	-1.39885900
C	3.43346100	-1.47947100	-1.67646900
C	2.01740400	-1.59020000	-1.41910200
N	1.51215000	-0.36875600	-1.04619800

H	4.75967100	0.26541200	-1.44349500
H	4.06649800	-2.29700100	-1.99159400
C	1.26242600	2.59696500	-0.81978100
C	1.15831000	4.03860200	-0.89104600
C	-0.16943200	4.32996300	-0.96694500
C	-0.87462200	3.06921200	-0.88566800
N	0.01464600	2.03746300	-0.81652900
H	2.00095900	4.71525400	-0.90932300
H	-0.64608100	5.29676800	-1.04542800
C	1.30207600	-2.79112500	-1.42813500
C	-2.26863600	2.94862700	-0.78310700
C	-3.11595400	-1.71432900	0.30055200
C	2.47242400	1.89491400	-0.84587900
Fe	-0.38209600	0.08393000	-0.62578500
Cl	-0.88930000	0.02640400	-2.93909200
O	-0.08005900	0.25228500	1.06820400
C	2.10548300	0.70945800	6.60908500
C	3.31942700	0.78247400	5.96241900
C	3.47291700	0.23531800	4.66162500
C	2.34833100	-0.38869600	4.03114200
C	1.09700400	-0.44955500	4.71457200
C	0.99915700	0.09125900	5.98396200
C	4.71147800	0.29519800	3.96607300
C	2.50244100	-0.94536900	2.71494900
C	3.73453100	-0.85184900	2.07395100
C	4.83626200	-0.23592800	2.69861800
C	1.35196700	-1.57838600	2.06948500
C	0.30892100	-2.14602000	3.01425000
C	-0.10343300	-1.07076200	4.02896900
H	-0.64657100	-0.28762200	3.48213100
H	-0.55817300	-2.48972400	2.44265100
H	1.99244800	1.12524200	7.60692200
H	4.17443100	1.25660000	6.43858400
H	0.04876100	0.04137800	6.51079900
H	5.78461500	-0.17533300	2.17176200
H	3.84151400	-1.25639400	1.07269500
H	0.71229800	-0.62563800	1.49311600
H	1.60626900	-2.21835100	1.22674700
C	-4.30521600	-2.49164400	0.77493600
C	-5.18887700	-3.05641000	-0.16753100
C	-4.55119200	-2.62136700	2.15505100
C	-6.30542400	-3.75884900	0.29593000
C	-5.68093700	-3.33180600	2.57373900
C	-6.56681100	-3.91209800	1.66137500

H	-6.99257300	-4.19043400	-0.42919500
H	-5.87467800	-3.43019900	3.64013700
C	-3.09946700	4.17537100	-0.98443300
C	-3.56039400	4.47402200	-2.28127000
C	-3.41475100	5.00989400	0.10470900
C	-4.33760100	5.62186400	-2.46603800
C	-4.19474200	6.14720400	-0.12622000
C	-4.66210500	6.47188200	-1.40406200
H	-4.69909300	5.85594400	-3.46540900
H	-4.44324600	6.79464300	0.71257200
C	3.73932100	2.67214300	-0.68458900
C	4.51641000	3.03398700	-1.80292200
C	4.13205100	3.04502200	0.61827500
C	5.71453800	3.72394000	-1.59149300
C	5.34225700	3.72642000	0.78053300
C	6.15256600	4.06450900	-0.30774100
H	6.31649800	4.00803500	-2.45241400
H	5.65458500	4.00662100	1.78475900
C	1.95702600	-4.01109300	-1.99481200
C	1.79313500	-4.27061100	-3.37119200
C	2.70659100	-4.88349100	-1.18315000
C	2.39414100	-5.41075800	-3.91320600
C	3.28943200	-6.01241800	-1.76867800
C	3.14761000	-6.29170500	-3.13116800
H	2.26706400	-5.61658000	-4.97421700
H	3.86675700	-6.69056100	-1.14324000
C	2.87684500	-4.61653000	0.29487200
H	3.37647200	-3.65741600	0.47508000
H	1.90803600	-4.57070100	0.80633300
H	3.47347600	-5.39965500	0.77233000
C	0.97645400	-3.33940800	-4.23756200
H	-0.05715700	-3.26116800	-3.88152700
H	1.37197200	-2.31769200	-4.21935000
H	0.95739200	-3.68332400	-5.27616600
C	3.81285100	-7.49980500	-3.74887000
H	4.81298400	-7.24946300	-4.12752300
H	3.93397300	-8.30865600	-3.02012100
H	3.23385100	-7.88752900	-4.59411300
C	-3.60877600	-2.01644500	3.17047700
H	-2.65346200	-2.55377600	3.19002600
H	-3.37548800	-0.97191400	2.93694000
H	-4.03489300	-2.05607000	4.17777100
C	-4.94263700	-2.89283100	-1.65012700
H	-4.84668900	-1.83571700	-1.92398800

H	-4.00850800	-3.37850400	-1.95572800
H	-5.75907300	-3.32585800	-2.23578300
C	-7.76357200	-4.70262900	2.13681900
H	-7.51539800	-5.76702100	2.24526000
H	-8.11655900	-4.35018800	3.11210800
H	-8.59684400	-4.63441600	1.42891600
C	-2.92095500	4.67730400	1.49419000
H	-3.29350200	3.70023500	1.82481100
H	-1.82616400	4.62142700	1.52374300
H	-3.24406100	5.42936800	2.22035300
C	-3.22411600	3.56553200	-3.44158200
H	-2.14045500	3.46878100	-3.57536000
H	-3.59677300	2.54810200	-3.27534500
H	-3.65368200	3.94108800	-4.37529800
C	-5.47258400	7.72635300	-1.63492100
H	-4.81968300	8.58562500	-1.83924100
H	-6.14514600	7.61817900	-2.49270300
H	-6.07824900	7.98052600	-0.75805100
C	3.24582100	2.76607300	1.81120800
H	2.39402100	3.45819400	1.82612100
H	2.82752800	1.75648200	1.79109200
H	3.79554600	2.88307100	2.74865700
C	4.04970500	2.71893400	-3.20690600
H	4.02908500	1.64030300	-3.39906100
H	3.02942100	3.08374600	-3.37362000
H	4.70392700	3.18230700	-3.95165600
C	7.47357600	4.76806900	-0.09968500
H	8.28034300	4.04612100	0.08587500
H	7.75912200	5.35607600	-0.97862000
H	7.43792800	5.44224100	0.76325700
H	0.72695800	-3.02016700	3.53825200
H	-0.79252700	-1.48035700	4.77713400
H	5.55957300	0.77484700	4.44916900

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C	1.63997700	-2.28147800	-1.17125000
C	1.69854500	-3.72266300	-1.19105600
C	0.43563200	-4.16711100	-0.94231100
C	-0.39685100	-2.99614600	-0.79922100
N	0.36042900	-1.85972000	-0.93818300
H	2.59855000	-4.29818800	-1.35219500
H	0.08026600	-5.18519800	-0.87042800
C	-3.35265000	0.12634100	-0.76746700
C	-4.51692700	-0.71895500	-0.61515200

C	-4.05796900	-1.99269100	-0.49542400
C	-2.61557800	-1.92270400	-0.59620600
N	-2.21141800	-0.62800000	-0.75886700
H	-5.53696900	-0.36273000	-0.59743200
H	-4.62161200	-2.90522900	-0.36507200
C	2.00778000	1.99749100	-0.94343200
C	3.44107600	2.06795300	-1.11417300
C	3.87721400	0.79320600	-1.30455500
C	2.71642500	-0.06001100	-1.20895000
N	1.59066600	0.69432200	-0.97710700
H	4.01630800	2.98224300	-1.10774700
H	4.88328100	0.44357300	-1.48628100
C	-0.21873000	3.07382200	-0.85919000
C	-1.06828200	4.24325700	-0.90131100
C	-2.35024000	3.79127800	-0.94234700
C	-2.28120100	2.34772900	-0.91063900
N	-0.97889400	1.93516900	-0.87253200
H	-0.71063700	5.26286700	-0.91104600
H	-3.26696800	4.36171200	-0.98571600
C	2.75940100	-1.45154800	-1.32784000
C	-3.41026000	1.51857400	-0.87167500
C	-1.77940700	-3.04637100	-0.58323400
C	1.17850900	3.12794400	-0.84735800
Fe	-0.29361900	0.03517700	-0.82245700
Cl	-0.45027700	0.03816700	-3.18575400
O	-0.38898600	0.05096900	0.89647700
H	0.50286600	0.03106700	1.75849600
C	2.90341800	2.95532400	4.37922700
C	3.92041700	3.09203600	3.43273400
C	3.96044300	2.22295100	2.33802600
C	2.99760800	1.22728400	2.20151200
C	1.96452500	1.07766300	3.14414300
C	1.93142700	1.96312800	4.23511400
H	2.86414700	3.62203700	5.23698700
H	4.67013200	3.87105300	3.54156000
H	4.73308600	2.32432300	1.58155300
H	3.03115300	0.55356600	1.35395500
H	1.15033600	1.86129200	4.98146000
C	1.00320000	-0.06383800	2.99251800
C	-0.30677300	0.04589000	3.71208600
C	-1.08778000	1.20775800	3.53966800
C	-0.83261400	-0.99510700	4.49488400
C	-2.33698400	1.32697000	4.13934700
C	-2.09004100	-0.87786100	5.08964300

H	-0.25240000	-1.89989400	4.64057000
C	-2.84812000	0.28118300	4.91562800
H	-2.92066200	2.23122200	3.99084700
H	-2.47472600	-1.69530200	5.69426400
H	-3.82782400	0.37054100	5.37761100
C	-2.41673300	-4.38538900	-0.37569300
C	-2.77812200	-5.16453800	-1.49376100
C	-2.66485600	-4.84594700	0.93223600
C	-3.37359000	-6.41088800	-1.28004400
C	-3.26523000	-6.09922700	1.09740100
C	-3.62590200	-6.89610800	0.00747600
H	-3.65153700	-7.01537600	-2.14127100
H	-3.45564500	-6.46035900	2.10624100
C	4.06767300	-2.09563300	-1.66275800
C	5.01711200	-2.35013000	-0.65536500
C	4.32851800	-2.44067300	-3.00530000
C	6.22479700	-2.96044800	-1.01244300
C	5.55154400	-3.04125100	-3.31583100
C	6.51025300	-3.31445100	-2.33377800
H	6.95982600	-3.16265400	-0.23576000
H	5.76050000	-3.30253200	-4.35150000
C	-4.75852500	2.16598200	-0.90265200
C	-5.42281900	2.32324200	-2.13418100
C	-5.34914900	2.60457900	0.29761000
C	-6.68277400	2.92956700	-2.14142100
C	-6.61169100	3.20341300	0.24409000
C	-7.29216600	3.37852200	-0.96509400
H	-7.20128000	3.05292000	-3.09029700
H	-7.07421700	3.54016100	1.16985400
C	1.82305800	4.47685500	-0.78142100
C	1.88433800	5.15278900	0.45412400
C	2.34053300	5.06993300	-1.95171300
C	2.51556900	6.39974500	0.50530700
C	2.95437200	6.32230600	-1.85312900
C	3.06541600	6.99664900	-0.63281300
H	2.57225600	6.91941900	1.45987100
H	3.34975000	6.78552400	-2.75505600
C	1.24756600	4.56992900	1.69409000
H	0.15541700	4.67283900	1.65327900
H	1.46404100	3.50458700	1.80160800
H	1.60231800	5.07538600	2.59575600
C	2.21784000	4.38324900	-3.29404500
H	2.88934300	3.51984400	-3.36944800
H	1.20378300	4.00211900	-3.45842200

H	2.46236900	5.07128200	-4.10911000
C	3.77364800	8.32857200	-0.54605300
H	4.84848000	8.19287700	-0.36498000
H	3.67104000	8.89908700	-1.47563400
H	3.38077500	8.94021000	0.27341000
C	-4.62892500	2.42709500	1.61444900
H	-4.38518900	1.37564600	1.80489000
H	-3.67540800	2.96883400	1.61881700
H	-5.23371400	2.79363100	2.44990100
C	-4.78440700	1.83934700	-3.41581100
H	-3.79872500	2.29377600	-3.56969000
H	-4.62091000	0.75534500	-3.39389700
H	-5.40972200	2.07350200	-4.28265400
C	-8.63969500	4.06132800	-1.00524700
H	-8.53094600	5.13847800	-1.19029300
H	-9.27039500	3.65760900	-1.80496100
H	-9.17721300	3.94629900	-0.05781300
C	-2.27536600	-4.02508900	2.14162000
H	-1.19185900	-4.04585700	2.30543400
H	-2.55517000	-2.97202400	2.03498500
H	-2.75183400	-4.41249700	3.04760600
C	-2.53207300	-4.65803200	-2.89672900
H	-3.00477400	-3.68167500	-3.05547900
H	-1.46211700	-4.51943200	-3.09123400
H	-2.92660200	-5.35446000	-3.64271800
C	-4.30310500	-8.23156400	0.21163600
H	-4.04096900	-8.67088500	1.18008500
H	-5.39619700	-8.12813500	0.18478800
H	-4.02620200	-8.94571400	-0.57175000
C	3.30455400	-2.17132100	-4.08487600
H	2.42435200	-2.81443900	-3.96459200
H	2.93400400	-1.14087700	-4.04831600
H	3.72361900	-2.35344700	-5.07918600
C	4.75264700	-1.95782800	0.77904600
H	4.86989800	-0.87636000	0.92115800
H	3.73562000	-2.20832400	1.09212100
H	5.44546100	-2.45794900	1.46183400
C	7.80786500	-4.00047200	-2.69312400
H	8.58545500	-3.80735700	-1.94643700
H	7.67529800	-5.08902600	-2.75407700
H	8.18182800	-3.66598700	-3.66737000
C	1.66301100	-1.41746700	3.03045000
C	1.12587000	-2.48499600	2.29464300
C	2.78585700	-1.65941400	3.83907500

C	1.68721200	-3.75937200	2.37037500
H	0.27165400	-2.29213400	1.65684200
C	3.34308400	-2.93643300	3.92186000
H	3.21467000	-0.84303100	4.41191700
C	2.79674000	-3.99155500	3.18818300
H	1.26719200	-4.56366100	1.77434400
H	4.20719900	-3.10507400	4.55949200
H	3.23702300	-4.98353000	3.24452300
H	-0.71051300	2.00382800	2.90573900

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C	1.41550100	3.16564600	-0.43730700
C	2.44774900	4.07939500	0.00444100
C	3.59878800	3.35982000	0.07509800
C	3.26024200	2.00022100	-0.29037200
N	1.93493700	1.90955900	-0.60269000
H	2.29288400	5.12954000	0.20694300
H	4.58783200	3.69194000	0.35659400
C	2.64094000	-2.23225500	-0.74643100
C	4.00491000	-2.64511300	-0.50295700
C	4.73312800	-1.50737700	-0.34190600
C	3.80940800	-0.40219200	-0.46372200
N	2.54835700	-0.86827900	-0.72192500
H	4.34073500	-3.67189800	-0.47864900
H	5.79142000	-1.40421700	-0.14909100
C	-1.87909900	0.91912600	-2.07580800
C	-2.73605300	2.04684300	-2.34861600
C	-2.10840200	3.14514300	-1.84092000
C	-0.85487500	2.68950600	-1.28859400
N	-0.73413700	1.33580600	-1.44523600
H	-3.69641300	1.98382600	-2.83979300
H	-2.44008400	4.17356600	-1.84153500
C	-1.39315400	-1.49742400	-2.04120800
C	-1.75472800	-2.87353300	-2.28436300
C	-0.71282100	-3.63405000	-1.85131100
C	0.30211000	-2.72033500	-1.38144700
N	-0.14532000	-1.42716500	-1.47128000
H	-2.68733500	-3.19351100	-2.72645100
H	-0.61081400	-4.70942800	-1.86262600
C	0.10523200	3.54920700	-0.73182300
C	1.59360200	-3.12178700	-1.01434100
C	4.17040900	0.93661800	-0.27245800
C	-2.20839900	-0.40805200	-2.36953600
Fe	0.87897200	0.22461500	-0.99832400

C1	1.51783600	0.43359300	-3.26916200
O	0.60745900	0.23500500	0.68608500
H	-0.21133400	-0.40495400	1.41268100
C	-0.87620100	-0.65172900	2.51059400
C	-1.20498800	-2.11320000	2.46782100
C	-0.92651800	-2.98619200	3.53248100
C	-1.83607900	-2.63678400	1.32770100
C	-1.29654700	-4.32915300	3.46926400
H	-0.44271600	-2.60126000	4.42381900
C	-2.19644100	-3.97928500	1.25835300
H	-2.03340500	-1.97504700	0.49205500
C	-1.93322000	-4.83297400	2.33374100
H	-1.08835000	-4.98271400	4.31251700
H	-2.66986100	-4.35926100	0.35802400
C	0.18688000	-0.21524600	3.47554700
C	1.45162200	-0.83415800	3.44597800
C	-0.02070400	0.83563900	4.38193100
C	2.46309900	-0.42934200	4.31045300
H	1.63428500	-1.62109000	2.72056100
C	0.99847200	1.24964600	5.24259600
H	-0.99022500	1.32454900	4.41343200
C	2.24250800	0.61830800	5.21232000
H	3.43153500	-0.92038000	4.27432900
H	0.81623300	2.06365900	5.93956600
C	-1.97334300	0.32868600	2.30262300
C	-3.30610900	0.22652200	2.54733300
H	-1.61375800	1.26701500	1.88548200
C	-3.92011200	-0.89009500	3.31547200
C	-5.03726300	-1.57759800	2.81353600
C	-3.42531800	-1.24599800	4.57867500
C	-5.62049700	-2.61458100	3.53860000
H	-5.43977100	-1.29414100	1.84592000
C	-4.01551500	-2.27593800	5.31092300
H	-2.56889700	-0.71127600	4.97930000
C	-5.11109800	-2.96738800	4.79150300
H	-6.47367700	-3.14764200	3.12707600
H	-3.61645900	-2.53953000	6.28688300
H	-5.56831700	-3.77309600	5.35978400
C	-4.21471100	1.31435000	2.10293300
C	-5.34812600	1.66872700	2.85827600
C	-3.96010200	2.02908000	0.91822700
C	-6.17884000	2.71295400	2.45433000
H	-5.56892700	1.12641200	3.77237600
C	-4.79104300	3.07207000	0.51390100

H	-3.11630500	1.74852200	0.29925100
C	-5.90391300	3.42210300	1.28200500
H	-7.04318100	2.97519800	3.05913500
H	-4.56987000	3.59811900	-0.40992200
H	-6.55565900	4.23222700	0.96592800
C	5.60675000	1.25018400	0.00495000
C	6.43849200	1.64857100	-1.05977900
C	6.11103900	1.14968500	1.31547200
C	7.77971700	1.93654900	-0.78952900
C	7.45790900	1.45160400	1.54086400
C	8.30730200	1.84766800	0.50292900
H	8.42835900	2.23730600	-1.61003500
H	7.85239600	1.37417000	2.55221700
C	-0.28279300	4.97459400	-0.49242400
C	-0.84423800	5.33803600	0.74659400
C	-0.07455000	5.93749700	-1.50020100
C	-1.19432900	6.67672300	0.95537000
C	-0.44295600	7.26208000	-1.24884300
C	-1.00701700	7.65100400	-0.02890000
H	-1.62322900	6.96341000	1.91355000
H	-0.28086500	8.00934800	-2.02328800
C	-3.47710500	-0.67107300	-3.11877100
C	-4.65156800	-1.04836300	-2.44037300
C	-3.47017200	-0.52843400	-4.52226300
C	-5.81359100	-1.27547400	-3.18601300
C	-4.65384400	-0.76928900	-5.22572200
C	-5.83503000	-1.14458200	-4.57724200
H	-6.72540300	-1.55886600	-2.66391500
H	-4.65247300	-0.66019500	-6.30857400
C	1.90112100	-4.58660500	-0.98711900
C	1.90280900	-5.26970700	0.24369700
C	2.21125000	-5.26060300	-2.18558100
C	2.18891200	-6.63849500	0.25192900
C	2.49691700	-6.62821700	-2.12936000
C	2.48203700	-7.33664500	-0.92321000
H	2.18608500	-7.16978100	1.20172000
H	2.74185900	-7.15212400	-3.05129400
C	0.53873900	5.54245100	-2.82420400
H	1.53632600	5.10883600	-2.68714200
H	-0.06409600	4.77982400	-3.33124800
H	0.62962400	6.40498300	-3.49129400
C	-1.08319700	4.30797600	1.82768400
H	-1.94447000	3.67627800	1.57976300
H	-0.22328000	3.64220600	1.95898800

H	-1.29451900	4.78812900	2.78827300
C	-1.42434200	9.08426500	0.20650800
H	-2.43410900	9.27065600	-0.18332400
H	-1.43679700	9.32905600	1.27396400
H	-0.74944000	9.78652500	-0.29541400
C	-4.66798500	-1.21377900	-0.93843500
H	-4.07983100	-2.08337700	-0.62214200
H	-4.24694400	-0.34249000	-0.42707100
H	-5.69000800	-1.35447300	-0.57315600
C	-2.21229100	-0.11060500	-5.24973200
H	-1.94680100	0.92809200	-5.01924200
H	-1.34823300	-0.71432200	-4.95139500
H	-2.33788700	-0.19645600	-6.33336800
C	-7.09273000	-1.42759700	-5.36559700
H	-7.09890200	-2.45945200	-5.74177800
H	-7.99005500	-1.29875100	-4.75093800
H	-7.17842200	-0.76627900	-6.23502200
C	1.62492500	-4.53079800	1.53047000
H	2.45346900	-3.85447800	1.77866600
H	0.72365000	-3.91720800	1.45512900
H	1.48945300	-5.22134000	2.36713600
C	2.24660000	-4.51916300	-3.50277800
H	1.24824000	-4.17008200	-3.79186600
H	2.88030600	-3.62682100	-3.44283400
H	2.62796100	-5.15849600	-4.30470000
C	2.75508500	-8.82264000	-0.89624400
H	3.16677800	-9.13832200	0.06851900
H	1.83314200	-9.39654100	-1.06083500
H	3.46276100	-9.11500000	-1.67985000
C	5.21388300	0.71355100	2.45038000
H	4.30811200	1.32693300	2.51278000
H	4.87445800	-0.31936600	2.30907000
H	5.73277100	0.77218900	3.41226700
C	5.88607300	1.76244500	-2.46219200
H	5.39873800	0.83394800	-2.78109100
H	5.12013200	2.54498400	-2.52255900
H	6.67583200	2.00202700	-3.18062900
C	9.75194200	2.19896800	0.77387500
H	9.86843000	3.27507800	0.96038100
H	10.13535600	1.67260100	1.65466100
H	10.39274600	1.94684200	-0.07825200
H	3.03621600	0.93863100	5.88205400
H	-2.21490000	-5.88118900	2.28245100

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C	-2.30379800	2.30573600	0.36149700
C	-2.36571500	3.74833700	0.31874500
C	-1.23290900	4.16978100	-0.31214900
C	-0.45385200	2.98907800	-0.59693500
N	-1.12305000	1.87071100	-0.17878000
H	-3.19215000	4.34012800	0.68577900
H	-0.93206000	5.17867600	-0.55620300
C	2.37982700	-0.19211600	-0.95821000
C	3.52349000	0.61949100	-1.30908400
C	3.05793100	1.88319400	-1.52625000
C	1.64812900	1.86179600	-1.22207000
N	1.26056900	0.58703300	-0.89108400
H	4.53846000	0.25853300	-1.38264300
H	3.61189400	2.76443900	-1.81738600
C	-2.95274400	-1.89751800	-0.21415100
C	-4.33073700	-1.93678800	0.22214100
C	-4.62028500	-0.69913300	0.71119000
C	-3.43463300	0.10812400	0.52248500
N	-2.43769500	-0.64589300	-0.02859100
H	-4.96526700	-2.81033000	0.17441300
H	-5.54729000	-0.34125400	1.13612200
C	-0.84637700	-3.01796300	-0.85179500
C	-0.05227200	-4.20921700	-1.06331200
C	1.25183300	-3.82217700	-1.00205400
C	1.24864800	-2.38768600	-0.81523800
N	-0.03411100	-1.92774900	-0.73026800
H	-0.45707800	-5.20048700	-1.20962500
H	2.14391900	-4.42454500	-1.10143200
C	-3.36875400	1.48771000	0.76964100
C	2.40484200	-1.59639500	-0.80862700
C	0.83546000	2.99920700	-1.15362100
C	-2.23728700	-3.01447100	-0.66937900
Fe	-0.57085000	-0.02920200	-0.39912500
Cl	-1.17787900	0.12292800	-2.68643800
O	-0.19149600	-0.25714700	1.27740500
H	0.31474600	0.67060900	1.83244300
C	4.49898100	0.60949400	2.16333200
C	4.65056900	-0.20992700	3.28423400
C	3.62649200	-0.35488200	4.22657400
C	2.42176600	0.29936000	4.01765200
C	2.21318200	1.09995900	2.87044700
C	3.28993600	1.25714800	1.96978500
H	5.30669100	0.69110200	1.44695200

H	3.77967300	-1.00027600	5.08281300
H	3.14934800	1.85871700	1.08100400
C	0.90185200	1.64656400	2.54878400
H	0.88111700	2.48069400	1.84905700
H	0.20021000	1.75358000	3.37714400
C	1.37222700	4.28719800	-1.69169500
C	1.97136100	5.23958500	-0.84532200
C	1.25582400	4.52488200	-3.07715300
C	2.44695900	6.43017500	-1.40493100
C	1.74087900	5.73132300	-3.59040900
C	2.34203400	6.69440000	-2.77366700
H	2.91046400	7.16872300	-0.75397300
H	1.64552500	5.92294900	-4.65737400
C	-4.53873000	2.14254700	1.43245200
C	-5.63335900	2.58786000	0.66656000
C	-4.51824700	2.31363200	2.82987800
C	-6.70509200	3.19899500	1.32522300
C	-5.61212900	2.92742300	3.44690500
C	-6.71591400	3.37364700	2.71287300
H	-7.55168900	3.54941500	0.73817600
H	-5.60081400	3.06187400	4.52674400
C	-2.98643900	-4.28610100	-0.90567400
C	-3.55057400	-4.51214600	-2.17686700
C	-3.12700700	-5.23194700	0.12690200
C	-4.25072200	-5.70237000	-2.39325400
C	-3.83663700	-6.40870000	-0.13488200
C	-4.40219500	-6.66352700	-1.38785200
H	-4.68978600	-5.88244800	-3.37261800
H	-3.95070800	-7.14203700	0.66084700
C	3.72733900	-2.25637600	-0.60045200
C	4.66477600	-2.40576100	-1.64033100
C	4.04167600	-2.66722400	0.71688600
C	5.95092000	-2.85940300	-1.32148500
C	5.33851100	-3.10544900	0.98674400
C	6.31781800	-3.17338200	-0.01023300
H	6.68426300	-2.96103600	-2.11895800
H	5.60186000	-3.37535100	2.00700000
C	0.62982100	3.49378500	-3.98860700
H	1.26341300	2.60227900	-4.06966500
H	-0.33534000	3.13840100	-3.61158100
H	0.48276900	3.89715300	-4.99508500
C	2.10857900	4.98751600	0.63919200
H	1.13178400	4.84245100	1.11499900
H	2.69713400	4.08474800	0.83944900

H	2.60464600	5.82548100	1.13785800
C	2.88939200	7.97360300	-3.36278000
H	2.93750500	8.77282200	-2.61552900
H	3.90650400	7.82535100	-3.74952400
H	2.27391400	8.32526200	-4.19814600
C	4.29043600	-2.11783500	-3.07916800
H	3.31366400	-2.54924000	-3.32587500
H	4.21816800	-1.04422200	-3.28623500
H	5.03163900	-2.53957900	-3.76497100
C	3.00289700	-2.65632000	1.81619100
H	2.44612700	-1.71539600	1.86027200
H	2.26120700	-3.44818000	1.65367000
H	3.47035200	-2.82649900	2.78909500
C	7.72711900	-3.57531600	0.35089000
H	8.39866900	-3.52433200	-0.51219400
H	8.11636800	-2.91213200	1.13289500
H	7.76226900	-4.59821100	0.74663800
C	-3.40639000	-3.48245500	-3.27400100
H	-3.88400700	-2.53502400	-2.99744900
H	-2.35474300	-3.24275300	-3.46834000
H	-3.85782700	-3.83332500	-4.20687800
C	-5.13753700	-7.95503800	-1.66132600
H	-5.99598100	-7.79469300	-2.32322400
H	-4.48180100	-8.68572300	-2.15339900
H	-5.50276000	-8.41407300	-0.73655300
C	-2.52918500	-4.97575300	1.49175900
H	-1.43980200	-4.86324100	1.43473200
H	-2.91826400	-4.04781900	1.92808000
H	-2.75075900	-5.79573900	2.18136500
C	-3.32809200	1.85149300	3.64040800
H	-3.11056100	0.79120800	3.46566300
H	-2.42265200	2.40483700	3.36097700
H	-3.49795800	1.99586600	4.71164100
C	-5.64118700	2.41960900	-0.83557100
H	-4.78080700	2.91958100	-1.29609800
H	-5.57574200	1.36272300	-1.11947100
H	-6.55280700	2.83493200	-1.27534600
C	-7.90187200	4.00464300	3.40481600
H	-8.41774000	4.71489500	2.74972200
H	-8.63552300	3.24338100	3.70211500
H	-7.60022400	4.53711800	4.31335500
H	1.61080700	0.17092800	4.72902900
N	5.86687300	-1.00176000	3.42029900
O	5.86848000	-1.91579100	4.25298300

O	6.81551500	-0.74598000	2.67430000
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C	-1.60267800	2.24298100	-0.77193200
C	-1.77983800	3.67408300	-0.89108200
C	-0.53790200	4.22566600	-0.83705900
C	0.39153900	3.13271200	-0.65452700
N	-0.27545100	1.94175400	-0.62330600
H	-2.73288200	4.16596200	-1.02238100
H	-0.25642100	5.26681200	-0.90364100
C	3.44424100	0.27978100	0.33008600
C	4.54009500	1.21478700	0.46784000
C	4.05023400	2.43976700	0.13582900
C	2.65055900	2.25441000	-0.17511100
N	2.31005400	0.93492200	-0.05792600
H	5.54495500	0.94578100	0.76028500
H	4.56544600	3.38928100	0.10877300
C	-1.51655400	-2.04949100	-1.11473500
C	-2.91148900	-2.23092600	-1.43540000
C	-3.50257300	-1.00953800	-1.30812800
C	-2.45664300	-0.07467900	-0.95994800
N	-1.26470700	-0.73156100	-0.82048200
H	-3.36353900	-3.17596300	-1.70127600
H	-4.53966500	-0.74532600	-1.45592200
C	0.72489800	-2.92716200	-0.57915200
C	1.63900400	-4.01605600	-0.33361700
C	2.77381100	-3.46407200	0.18026700
C	2.56809900	-2.03407100	0.20021100
N	1.30203700	-1.73400500	-0.23520100
H	1.42040500	-5.05708300	-0.52437700
H	3.68324100	-3.95923100	0.48910000
C	-2.64584900	1.31815200	-0.89095500
C	3.57506300	-1.10600000	0.50193900
C	1.77383700	3.29899400	-0.49059400
C	-0.58274500	-3.08975200	-1.06001700
Fe	0.50717200	0.10246500	-0.38029400
Cl	1.02732800	0.11002900	-2.69023800
O	0.18278500	0.22905600	1.31354200
C	4.90946800	-1.62631900	0.93867600
C	5.23045300	-1.65907300	2.30929300
C	5.84161600	-2.05229300	-0.02891800
C	6.48516400	-2.14125000	2.69449900
C	7.08530100	-2.52455500	0.40196400
C	7.42417300	-2.58322500	1.75744900

H	6.73580400	-2.16794800	3.75309000
H	7.80980100	-2.84945900	-0.34212100
C	-0.99162200	-4.43828100	-1.56360500
C	-1.53647500	-5.40797700	-0.70177600
C	-0.81714700	-4.71005600	-2.93677200
C	-1.90189300	-6.64968900	-1.23315900
C	-1.19599700	-5.96447200	-3.42296000
C	-1.73725600	-6.94822600	-2.58863900
H	-2.32669300	-7.40057200	-0.57008300
H	-1.06577200	-6.17757600	-4.48212100
C	-4.03880000	1.84350800	-1.04974000
C	-4.76850600	2.24484800	0.08496100
C	-4.60631200	1.93406800	-2.33974200
C	-6.08768600	2.68273800	-0.08540400
C	-5.91985400	2.39258100	-2.46204200
C	-6.68310800	2.75668200	-1.34606600
H	-6.65932300	2.97181500	0.79397700
H	-6.35914600	2.46886100	-3.45488800
C	2.34002400	4.67594700	-0.63159200
C	2.42384400	5.52413700	0.48847300
C	2.79052600	5.10048300	-1.89676700
C	2.96651200	6.80207800	0.32137200
C	3.32634700	6.38626000	-2.01722700
C	3.42031900	7.25200600	-0.92265800
H	3.03758100	7.46085500	1.18463900
H	3.67975100	6.71902600	-2.99118600
C	-1.73241900	-5.11968400	0.76901200
H	-0.78578900	-4.85295900	1.25350600
H	-2.41837800	-4.27838700	0.92512600
H	-2.14485700	-5.98816500	1.29107000
C	-0.23973300	-3.66258700	-3.86112000
H	-0.86974200	-2.76622700	-3.89577000
H	0.74468200	-3.32080500	-3.52181500
H	-0.13802600	-4.04922300	-4.87955800
C	-2.10787100	-8.30666300	-3.13673700
H	-2.50813800	-8.23244100	-4.15394300
H	-1.23099900	-8.96637400	-3.18118900
H	-2.85825400	-8.80199600	-2.51150500
C	-3.80834400	1.55981100	-3.56920200
H	-2.82013400	2.03372600	-3.56586800
H	-3.63400000	0.47867400	-3.62387700
H	-4.33037100	1.86289400	-4.48181400
C	-4.15011800	2.25780700	1.46436100
H	-3.40278500	1.47159100	1.59282900

H	-3.64294300	3.21432000	1.64863700
H	-4.91779200	2.12780700	2.23267600
C	-8.11834800	3.20041900	-1.50650200
H	-8.78926000	2.33596500	-1.59889100
H	-8.45697500	3.78618600	-0.64572700
H	-8.25080300	3.81004200	-2.40754900
C	2.69627200	4.18047800	-3.09242100
H	3.25799200	3.25297800	-2.93126200
H	1.66022100	3.87714300	-3.28352300
H	3.08363600	4.66358300	-3.99447900
C	1.93970000	5.05769200	1.84240500
H	0.87375500	4.80087800	1.81630000
H	2.47168400	4.15488000	2.16569400
H	2.08515700	5.83039800	2.60323500
C	3.97191700	8.64925900	-1.08732700
H	4.73407000	8.68978700	-1.87316400
H	3.17896600	9.35580200	-1.36707100
H	4.42149700	9.01614200	-0.15829900
C	5.51156000	-1.98768400	-1.50297800
H	4.69418400	-2.67154900	-1.76045200
H	5.18024500	-0.98454500	-1.79520200
H	6.38024700	-2.25280500	-2.11299700
C	4.24332300	-1.16870900	3.34367300
H	4.01384300	-0.10579300	3.20070300
H	3.29052000	-1.70436700	3.27373700
H	4.63440900	-1.29947100	4.35715200
C	8.76189800	-3.12998500	2.19870500
H	8.70976300	-4.21466900	2.36289100
H	9.53635400	-2.95251500	1.44465600
H	9.09174700	-2.67457300	3.13872300
C	-4.37384700	-0.25944500	4.02162600
C	-3.22528000	-0.24000900	4.81617300
C	-3.19434400	-1.38196000	2.26513800
C	-4.37255000	-0.83660000	2.74877900
H	-5.27876300	-0.82754700	2.15571700
C	-2.00223200	-1.35299900	3.02416000
C	-2.04876200	-0.77871800	4.31267800
C	0.39937500	-2.28478200	3.29426800
C	-0.75671700	-1.83982900	2.42185100
H	1.21330100	-2.65594500	2.66510800
H	-0.29790800	-0.78041800	1.80702300
H	-0.93150500	-2.49363700	1.56971900
H	0.09978000	-3.09202800	3.97780100
H	-3.26758900	0.21055600	5.80037100

H	0.79519000	-1.46203900	3.89976300
H	-1.14969500	-0.74277700	4.91883800
H	-3.17969200	-1.81762900	1.27166700
N	-5.59273900	0.37581200	4.51554800
O	-5.63375400	0.70993600	5.70123800
O	-6.51301700	0.55667900	3.71021200

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C	-0.56558700	-2.93668100	-0.55378000
C	-1.37581300	-4.09160400	-0.25665900
C	-2.50110600	-3.63091300	0.36046200
C	-2.39767000	-2.18992600	0.38988900
N	-1.19507300	-1.79522000	-0.13815700
H	-1.09841400	-5.11117400	-0.48443500
H	-3.34604800	-4.19500400	0.72885700
C	-2.89966800	2.03505900	-0.19969800
C	-4.27896200	2.12180200	0.22587000
C	-4.61899000	0.89168600	0.69969500
C	-3.45873500	0.04479300	0.52362800
N	-2.42762400	0.76677500	-0.00862000
H	-4.88215700	3.01709900	0.17536600
H	-5.56443800	0.56391700	1.10786000
C	2.36402400	0.14406000	-1.00634100
C	3.47562600	-0.71011300	-1.36159800
C	2.96743400	-1.96171800	-1.54605300
C	1.56570700	-1.89198300	-1.21330200
N	1.22500000	-0.59992300	-0.89026800
H	4.49898500	-0.38313400	-1.46699600
H	3.48695300	-2.86269300	-1.83969000
C	1.30385200	2.37737100	-0.90736500
C	1.34820200	3.80703000	-1.12406900
C	0.05663200	4.23646900	-1.15177900
C	-0.76959800	3.07598600	-0.89483800
N	0.00946200	1.96149000	-0.77887000
H	2.25648400	4.37664800	-1.26243900
H	-0.31979000	5.23784100	-1.30480300
C	0.71156800	-2.99765100	-1.13549200
C	-2.15399100	3.12207100	-0.67669900
C	-3.45125100	-1.33909300	0.75715600
C	2.43448900	1.55097200	-0.90201000
Fe	-0.57775200	0.08583600	-0.38526200
Cl	-1.21693000	-0.08156700	-2.66739100
O	-0.18007600	0.39781400	1.27771100
H	0.39794800	-0.40510500	1.99187000

C	4.20637500	0.48040400	3.98553200
C	4.98044800	0.11228900	2.88474300
C	4.46297700	-0.70712400	1.87997700
C	3.14476000	-1.12423500	1.96807000
C	2.30861300	-0.73601700	3.03748400
C	2.88338200	0.05799700	4.05391900
H	4.63782100	1.10986500	4.75436900
H	5.07890400	-0.96996600	1.03018000
H	2.73566100	-1.71576500	1.16046200
C	0.86649500	-1.09361500	3.02112600
C	-4.69819400	-1.96272700	1.30449900
C	-4.83681200	-2.14617900	2.69233700
C	-5.72482300	-2.35548900	0.42170600
C	-6.01290000	-2.72288800	3.18248900
C	-6.88303300	-2.92904700	0.95463600
C	-7.04610700	-3.12315600	2.33043300
H	-6.12384100	-2.86043700	4.25622700
H	-7.67920600	-3.23056500	0.27681000
C	1.16265600	-4.29218600	-1.73914900
C	0.76385500	-4.56356800	-3.06639700
C	1.95954300	-5.21029300	-1.02964700
C	1.19103500	-5.75296800	-3.66362900
C	2.36161100	-6.38836600	-1.66874700
C	1.99406200	-6.67551400	-2.98585100
H	0.88706700	-5.96305000	-4.68720100
H	2.97680200	-7.09905800	-1.12055600
C	3.78168200	2.17168000	-0.73538300
C	4.71823100	2.23837000	-1.78463100
C	4.12576200	2.61726400	0.56313500
C	6.03008400	2.62872900	-1.48736600
C	5.44455700	2.99777900	0.80980100
C	6.42371100	2.96299900	-0.18905900
H	6.76349600	2.65872800	-2.29066200
H	5.72909800	3.28725300	1.81867900
C	-2.86374800	4.41657000	-0.91290600
C	-3.43966800	4.65212500	-2.17652500
C	-2.94624900	5.37947900	0.11046700
C	-4.09269000	5.86899200	-2.39555300
C	-3.60969300	6.58193300	-0.15302800
C	-4.19008500	6.84457200	-1.39811600
H	-4.53473700	6.05934700	-3.37157100
H	-3.67330400	7.33130100	0.63351900
C	-5.57617800	-2.16021400	-1.06983700
H	-5.44223600	-1.10209900	-1.32333200

H	-4.69396900	-2.68578000	-1.45366200
H	-6.45485200	-2.53098800	-1.60590800
C	-3.73151600	-1.73012600	3.63464700
H	-2.82475300	-2.32311600	3.46353700
H	-3.45444100	-0.67988100	3.48625700
H	-4.02764700	-1.86188900	4.67971700
C	-8.29595000	-3.77401000	2.87595000
H	-8.48291700	-3.47846700	3.91383000
H	-9.17790700	-3.50856500	2.28267600
H	-8.21055800	-4.86879300	2.85803600
C	-3.35340700	3.60737700	-3.26546100
H	-2.31562200	3.32242200	-3.47279100
H	-3.86577800	2.68355800	-2.97149900
H	-3.80446200	3.96737000	-4.19504500
C	-2.32728400	5.11666200	1.46456800
H	-2.73305200	4.20305900	1.91556000
H	-1.24283000	4.97281100	1.38590600
H	-2.51136200	5.94753700	2.15223800
C	-4.92972400	8.13798700	-1.65044000
H	-4.86108200	8.44096800	-2.70089400
H	-5.99661900	8.03571800	-1.41046200
H	-4.53482200	8.95348400	-1.03488100
C	4.32259500	1.92128000	-3.21193900
H	4.28849800	0.84342400	-3.40769500
H	3.32618100	2.31330900	-3.44327600
H	5.03436700	2.36236200	-3.91677100
C	7.86166100	3.25487500	0.16199600
H	8.22964900	2.48900400	0.85626300
H	8.50550800	3.25653600	-0.72338400
H	7.96501700	4.22546400	0.66224800
C	3.09753200	2.69176300	1.66908500
H	2.38995400	3.50974100	1.48669400
H	2.50196400	1.77780800	1.74845500
H	3.57943800	2.87068200	2.63315700
C	2.35944700	-4.95685800	0.40526700
H	2.86587000	-3.99249200	0.52219700
H	1.48239500	-4.94082000	1.06270500
H	3.03571200	-5.73571100	0.77007300
C	-0.12429800	-3.60120200	-3.82108600
H	-1.13120600	-3.57137800	-3.38754300
H	0.24391500	-2.57094100	-3.77724400
H	-0.21609300	-3.89387100	-4.87142500
C	2.47053600	-7.93542600	-3.67011300
H	1.70737700	-8.33769300	-4.34562900

H	3.36709000	-7.74078200	-4.27370600
H	2.72756300	-8.71485100	-2.94493800
C	0.53768400	-2.53842700	2.67519400
H	-0.53992500	-2.66428200	2.53778100
H	1.02212400	-2.86335100	1.75483400
H	0.86330700	-3.21139500	3.48259200
C	0.00813100	-0.53210100	4.14151900
H	0.25251100	-0.99740500	5.10855400
H	0.12734600	0.55138300	4.23761600
H	-1.04622200	-0.72812300	3.93189900
H	2.28672600	0.36304700	4.90579000
N	6.33328200	0.64463000	2.74358600
O	7.02459800	0.23063400	1.80994300
O	6.70362800	1.50349300	3.54984000

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C	-1.55963400	-1.88788800	-1.34348400
C	-2.95461900	-1.94185800	-1.70587600
C	-3.45636500	-0.68875300	-1.51290900
C	-2.34683600	0.14997000	-1.11757400
N	-1.21268600	-0.60326400	-1.00397400
H	-3.47664000	-2.83664400	-2.01431900
H	-4.47631500	-0.35291900	-1.62422100
C	0.79771200	3.06243800	-0.90542300
C	-0.02179800	4.23228600	-1.13720800
C	-1.31577200	3.80854600	-1.12041900
C	-1.27823400	2.37389400	-0.93905200
N	0.01372300	1.94886400	-0.81577800
H	0.35958000	5.23524200	-1.26562100
H	-2.22070600	4.38635100	-1.24615700
C	2.38159500	-2.23036300	0.30743300
C	2.48160100	-3.67086600	0.26102400
C	1.35875400	-4.12203400	-0.36589300
C	0.55041700	-2.96184900	-0.65346800
N	1.18664400	-1.82596900	-0.23050100
H	3.32462000	-4.24083900	0.62475100
H	1.08516600	-5.13837200	-0.61106200
C	3.44816700	-0.00189400	0.49975400
C	4.60829000	0.83658000	0.71286300
C	4.28596700	2.07368600	0.24435600
C	2.91517300	1.99981100	-0.20958300
N	2.43239100	0.73159400	-0.04423900
H	5.54224200	0.49934800	1.13943500
H	4.89464400	2.96632300	0.21765200

C	-0.72625100	-3.00601600	-1.23687800
C	2.18139700	3.09818300	-0.67805000
C	-2.41280300	1.55263500	-0.97051700
C	3.42889600	-1.38951300	0.71106700
Fe	0.59073300	0.05692800	-0.47618000
Cl	1.26343500	-0.07727500	-2.73951100
O	0.15543700	0.29039700	1.20407000
H	-0.46068600	-0.70539400	1.70796000
C	-0.34877300	-1.38340200	3.80130100
C	-1.18172900	-0.23955900	4.43993100
C	-0.99975600	-1.59711000	2.43285000
C	-2.39208800	-1.15045300	2.58068400
C	-3.48535500	-1.34960000	1.73049300
C	-4.68252900	-0.69188500	1.99002700
C	-4.76766800	0.14901000	3.10329100
C	-3.70231100	0.32608200	3.99692300
C	-2.51248800	-0.32948400	3.72461800
H	-3.39277000	-1.97125500	0.84964100
H	-3.81617900	0.99661300	4.84044300
H	-5.53508300	-0.78258600	1.32899900
H	-0.71761700	0.73110200	4.21985100
H	0.71238700	-1.13613800	3.71980800
H	-0.79596200	-2.52317600	1.89444600
N	-5.97912600	0.94788900	3.27940300
O	-5.93982800	1.87862600	4.09168200
O	-6.96203600	0.68129600	2.58402800
C	-3.75792200	2.17868300	-0.79995100
C	-4.67265900	2.30373800	-1.86271100
C	-4.11640000	2.58367800	0.50812000
C	-5.97801300	2.72369900	-1.57634300
C	-5.43079000	2.98677400	0.74618700
C	-6.38615800	3.02924100	-0.27530000
H	-6.69318500	2.80694100	-2.39233000
H	-5.72480200	3.25454700	1.75870100
C	2.90012500	4.39206900	-0.88826300
C	3.48905900	4.64222600	-2.14341300
C	2.98813100	5.33515700	0.15261100
C	4.15899800	5.85399600	-2.33604500
C	3.66902200	6.53367400	-0.08478500
C	4.25697400	6.81302400	-1.32231500
H	4.61701600	6.05270900	-3.30304700
H	3.74262400	7.26489600	0.71772500
C	4.65074800	-2.02640500	1.29647600
C	5.72486700	-2.38465700	0.45745600

C	4.71381000	-2.25906000	2.68290900
C	6.85689700	-2.97014800	1.03273700
C	5.86625500	-2.84438000	3.21620600
C	6.94741600	-3.20868800	2.40798500
H	7.68968600	-3.24624200	0.38899100
H	5.92008200	-3.01877100	4.28902100
C	-1.22489000	-4.31309400	-1.76567500
C	-1.09878100	-4.56307600	-3.14804700
C	-1.79992200	-5.27259900	-0.91041500
C	-1.54974600	-5.78784700	-3.64910700
C	-2.24258400	-6.48139000	-1.45778900
C	-2.12719300	-6.75768600	-2.82332600
H	-1.44628800	-5.98866600	-4.71364100
H	-2.68817900	-7.22476300	-0.79981500
C	2.36435400	5.05283000	1.50057800
H	1.27940200	4.91611300	1.41644500
H	2.76425100	4.12992100	1.93777400
H	2.55043800	5.87126200	2.20246800
C	3.40544700	3.61408300	-3.24825500
H	3.90929900	2.68252300	-2.96427100
H	2.36761500	3.33898600	-3.46816100
H	3.86622500	3.98503000	-4.16872600
C	4.95868400	8.12826300	-1.56987500
H	5.81135700	8.00617300	-2.24699100
H	4.27929800	8.85676500	-2.03231600
H	5.32561500	8.57046700	-0.63747200
C	3.55140900	-1.88873500	3.57491800
H	3.27005300	-0.83628300	3.45051100
H	2.66325900	-2.48262800	3.32719900
H	3.78884100	-2.05816900	4.62954300
C	5.65293500	-2.14413000	-1.03321100
H	4.78433800	-2.64599900	-1.47563100
H	5.54517400	-1.07731900	-1.26148700
H	6.55258900	-2.51113400	-1.53610000
C	8.17019900	-3.87086100	2.99934700
H	8.32619700	-3.56982600	4.04088000
H	8.07120300	-4.96461300	2.98732300
H	9.07463800	-3.62096800	2.43406600
C	-1.94206300	-5.01108800	0.57214500
H	-0.96438400	-4.88752700	1.05292400
H	-2.50881700	-4.09342800	0.76581200
H	-2.46014600	-5.83575700	1.07065700
C	-0.49910800	-3.52607900	-4.07067100
H	-1.16883000	-2.66479200	-4.18327300

H	0.44291100	-3.12213600	-3.68432700
H	-0.31665500	-3.94442200	-5.06520700
C	-2.63891900	-8.05726600	-3.39972500
H	-3.65595500	-7.93857600	-3.79673800
H	-2.00823400	-8.40508700	-4.22534600
H	-2.67417900	-8.84754300	-2.64232800
C	-3.10388100	2.60594900	1.63119000
H	-2.52150100	1.68152200	1.68894300
H	-2.38225500	3.41866700	1.48260900
H	-3.59831700	2.76513500	2.59244900
C	-4.25687300	2.02515500	-3.29208600
H	-3.26813600	2.44679600	-3.50465500
H	-4.19175400	0.95280500	-3.50823900
H	-4.97196000	2.46241000	-3.99581700
C	-7.81278500	3.40296900	0.04721300
H	-8.46777600	3.29443700	-0.82328000
H	-8.19682700	2.76426500	0.85170400
H	-7.88486000	4.44119800	0.39559600
H	-1.26900700	-0.32175700	5.52875100
H	-0.43702500	-2.29930600	4.40294700

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C	-1.66626500	-1.86159900	-1.22804800
C	-3.06690000	-1.92683800	-1.56654500
C	-3.55999600	-0.66389600	-1.42973900
C	-2.44935700	0.17646900	-1.04882400
N	-1.31272400	-0.57267900	-0.91505400
H	-3.58956800	-2.82973900	-1.84791200
H	-4.57019200	-0.31384000	-1.58405100
C	0.62053600	3.14926500	-0.60181200
C	-0.22502800	4.31409800	-0.74306300
C	-1.50322500	3.85772200	-0.82739500
C	-1.43119000	2.41440900	-0.77045000
N	-0.13142900	2.00947600	-0.62872200
H	0.13220800	5.33370000	-0.76147700
H	-2.41805600	4.42164900	-0.93932700
C	2.43048300	-2.19080800	0.01401800
C	2.54278900	-3.62626600	-0.08957400
C	1.35298300	-4.07746100	-0.57519000
C	0.50546700	-2.92122600	-0.73206900
N	1.17593800	-1.78457600	-0.36017700
H	3.43174300	-4.19175600	0.15004300
H	1.05938600	-5.09060200	-0.80943600
C	3.46647300	0.04449000	0.25880900

C	4.61339100	0.89872300	0.47350800
C	4.20798600	2.16920100	0.20546900
C	2.80618300	2.09169300	-0.13850600
N	2.38077000	0.79306400	-0.10385000
H	5.59178800	0.55069200	0.77204000
H	4.78065300	3.08468900	0.24466900
C	-0.82047200	-2.97497700	-1.18295000
C	2.00771100	3.20947300	-0.41169300
C	-2.53807300	1.57475700	-0.93127400
C	3.50514900	-1.35310700	0.34621500
Fe	0.51522000	0.10852400	-0.43850800
Cl	1.02960400	0.13641400	-2.74643300
O	0.19376800	0.21319100	1.23186900
H	-0.16933200	-0.79737300	1.83295500
C	0.13000400	-1.67056100	3.81930100
C	-0.67040500	-1.09647500	4.76151000
C	-0.60262000	-1.82071600	2.55635100
C	-1.98374800	-1.41034700	2.86260500
C	-3.13269500	-1.37483400	2.07551800
C	-4.29931700	-0.81671800	2.59871200
C	-4.28972600	-0.30491800	3.90093200
C	-3.15968100	-0.35179400	4.72599300
C	-2.00138000	-0.90970900	4.19733100
H	-3.12617900	-1.74832500	1.05872900
H	-3.20893200	0.05145400	5.73034400
H	-5.20402400	-0.74637100	2.00834500
H	-0.38308000	-0.81319500	5.76780000
H	1.17580900	-1.92207500	3.94308100
H	-0.39666800	-2.64487600	1.87623700
N	-5.50069800	0.33948500	4.41005000
O	-5.55067800	0.61764300	5.60980800
O	-6.40731500	0.58550600	3.60603300
C	-3.88806600	2.20504900	-1.07340200
C	-4.41004500	2.44400000	-2.36268000
C	-4.62038400	2.55343600	0.07666300
C	-5.68095500	3.01272900	-2.47430800
C	-5.89467400	3.11020700	-0.08500100
C	-6.44407500	3.34251500	-1.34779900
H	-6.08603100	3.20311300	-3.46627900
H	-6.46883900	3.36513100	0.80335800
C	2.67045600	4.54845600	-0.47140700
C	3.19627700	4.99419000	-1.69949900
C	2.76866400	5.34003900	0.68853900
C	3.81844600	6.24553900	-1.74402700

C	3.40007000	6.58431600	0.59729200
C	3.92782700	7.05569800	-0.60915800
H	4.22870900	6.59484800	-2.68941700
H	3.48305400	7.19901900	1.49139200
C	4.79805900	-1.99799600	0.73691600
C	5.79977900	-2.19957000	-0.23420000
C	4.99758200	-2.40103900	2.07024200
C	6.99947600	-2.80049800	0.15826500
C	6.21523300	-2.99312500	2.41969100
C	7.22750400	-3.20319000	1.47857100
H	7.77603600	-2.95820700	-0.58758000
H	6.37506100	-3.29803000	3.45193500
C	-1.35394400	-4.28525100	-1.66956900
C	-1.34351600	-4.53707000	-3.05715700
C	-1.84913000	-5.24530800	-0.76633800
C	-1.83022700	-5.76434100	-3.51679600
C	-2.33120400	-6.45653800	-1.27320000
C	-2.33139900	-6.73479400	-2.64331800
H	-1.81637900	-5.96685000	-4.58587700
H	-2.71563600	-7.20071500	-0.57864700
C	2.20804000	4.84868400	2.00357900
H	1.12824000	4.67012100	1.93410700
H	2.66434600	3.89645300	2.29969000
H	2.38225100	5.57367200	2.80421100
C	3.09218300	4.13220100	-2.93689300
H	3.60946500	3.17476200	-2.80249400
H	2.04943800	3.88459100	-3.16745200
H	3.52511000	4.63520000	-3.80674100
C	4.57558800	8.41849100	-0.69101500
H	5.35671000	8.44607000	-1.45847800
H	3.83835900	9.19043800	-0.94940200
H	5.02698600	8.70687800	0.26443800
C	3.90771000	-2.21308900	3.10037200
H	3.52038400	-1.18768200	3.09851500
H	3.05696600	-2.87264400	2.88720200
H	4.26841900	-2.44284500	4.10752200
C	5.58035000	-1.77760900	-1.66905800
H	4.64776700	-2.19154200	-2.06970400
H	5.49902300	-0.68762300	-1.75661300
H	6.40451900	-2.10869900	-2.30783900
C	8.52258600	-3.87707400	1.86799600
H	8.74225200	-3.74121300	2.93226000
H	8.47635000	-4.95790200	1.67890600
H	9.36822200	-3.48370000	1.29326900

C	-1.85535000	-4.98539000	0.72294600
H	-0.83493300	-4.92316700	1.12043000
H	-2.34917000	-4.03898300	0.96889200
H	-2.37462700	-5.78385700	1.26102100
C	-0.82457400	-3.50014700	-4.02760200
H	-1.48833000	-2.62781400	-4.06623800
H	0.15906600	-3.11767000	-3.73358300
H	-0.74775200	-3.91154600	-5.03851600
C	-2.88522500	-8.03800300	-3.17054100
H	-3.94808700	-7.93844000	-3.42843800
H	-2.36030000	-8.35895800	-4.07684600
H	-2.80400000	-8.83916100	-2.42815100
C	-4.05103900	2.37808900	1.46611100
H	-3.34364200	1.54782000	1.52515900
H	-3.51263800	3.28276000	1.77902900
H	-4.84938900	2.19261300	2.19071800
C	-3.60877700	2.10069300	-3.59851700
H	-2.60298000	2.53480500	-3.55841000
H	-3.47493700	1.01724900	-3.70256600
H	-4.10381900	2.46788900	-4.50247900
C	-7.83586900	3.91125500	-1.49663400
H	-7.92788300	4.51478300	-2.40634900
H	-8.58317400	3.10910500	-1.56062900
H	-8.10663600	4.53950000	-0.64145900

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C	-1.31477200	2.35251600	-1.03093700
C	-1.37446900	3.78683200	-1.20746700
C	-0.08766600	4.23208700	-1.21163100
C	0.74919500	3.07541900	-0.97691100
N	-0.01587600	1.94876300	-0.89879900
H	-2.28787500	4.34982000	-1.33870100
H	0.27831800	5.24155300	-1.33350100
C	3.43633700	0.06078900	0.46562100
C	4.59374800	0.91026000	0.64749100
C	4.25325600	2.13977600	0.17253200
C	2.87802400	2.04907700	-0.26277500
N	2.40786100	0.77749900	-0.07498000
H	5.53727300	0.58503500	1.06154200
H	4.85403600	3.03695200	0.12695400
C	-1.51689500	-1.91426700	-1.41909000
C	-2.90747200	-1.99582500	-1.79542200
C	-3.43317100	-0.75005500	-1.61799100
C	-2.34215600	0.11107000	-1.21887600

N	-1.19659300	-0.61966000	-1.09009000
H	-3.41076800	-2.90216300	-2.10119100
H	-4.45756200	-0.43320100	-1.74329600
C	0.58951200	-2.94978400	-0.65944000
C	1.39371400	-4.09806700	-0.31540000
C	2.49636200	-3.62425200	0.33031600
C	2.39294200	-2.18301300	0.32748600
N	1.20715400	-1.80072200	-0.24954800
H	1.12962200	-5.12243900	-0.53641600
H	3.32940400	-4.17999000	0.73664300
C	-2.43452500	1.51297300	-1.06864900
C	3.43274200	-1.32356900	0.70843800
C	2.13111800	3.13321900	-0.74010500
C	-0.67007000	-3.01783800	-1.28069600
Fe	0.58588200	0.07621300	-0.52676700
Cl	1.31391800	-0.08053700	-2.77659800
O	0.09770200	0.29769400	1.12081000
H	-1.73267700	-1.00671500	5.63787000
C	4.68409700	-1.92732600	1.26937000
C	4.88192100	-1.98803000	2.66073800
C	5.67437200	-2.40110000	0.38187800
C	6.07377300	-2.53676000	3.14824600
C	6.84742300	-2.94274000	0.91340200
C	7.06505700	-3.02407500	2.29341300
H	6.23010900	-2.58009200	4.22434400
H	7.61532600	-3.30293000	0.23160400
C	-1.12981100	-4.33520800	-1.81959900
C	-1.74268100	-5.29232800	-0.98844100
C	-0.93653600	-4.59105400	-3.19317400
C	-2.15043000	-6.50687800	-1.54990900
C	-1.35618100	-5.82092700	-3.70887400
C	-1.96168700	-6.79223800	-2.90543100
H	-2.62965900	-7.24659900	-0.91178600
H	-1.20756200	-6.02330900	-4.76772700
C	-3.78846400	2.11687800	-0.89385700
C	-4.14842400	2.51617100	0.41599200
C	-4.70612700	2.23345500	-1.95512400
C	-5.46513100	2.91103500	0.65419400
C	-6.01498300	2.64060400	-1.66662200
C	-6.42299800	2.94429900	-0.36519100
H	-5.76028900	3.17789600	1.66648400
H	-6.73256600	2.71632400	-2.48120600
C	2.83016700	4.43793100	-0.95024200
C	2.91443200	5.37560300	0.09595100

C	3.40346900	4.70421700	-2.20909600
C	3.57699500	6.58452200	-0.13968000
C	4.05618600	5.92584500	-2.39952800
C	4.15050500	6.87947400	-1.38049000
H	3.64755600	7.31177000	0.66672900
H	4.50325200	6.13659800	-3.36907600
C	-1.97342100	-5.01665700	0.48009000
H	-1.03031200	-4.83119500	1.00721300
H	-2.60014400	-4.12936200	0.62750800
H	-2.47066100	-5.86080200	0.96710000
C	-0.31020500	-3.55068200	-4.09412900
H	-0.98778600	-2.70156700	-4.24574800
H	0.60496900	-3.12682100	-3.66695400
H	-0.07321800	-3.97306900	-5.07537200
C	-2.37697500	-8.12482800	-3.48411200
H	-2.72585300	-8.02173200	-4.51752300
H	-1.53463800	-8.82944500	-3.49518700
H	-3.17997800	-8.58506700	-2.89854800
C	-4.28923000	1.96248400	-3.38571900
H	-3.30824600	2.40097500	-3.60047800
H	-4.20663400	0.89167000	-3.60346100
H	-5.01310800	2.38827100	-4.08745500
C	-3.13900000	2.53605000	1.54236100
H	-2.56024900	1.60944200	1.60352000
H	-2.41386000	3.34624600	1.39777500
H	-3.63656200	2.69568900	2.50191200
C	-7.85236200	3.30228000	-0.03804900
H	-8.22647300	2.65384400	0.76327300
H	-7.93384400	4.33744200	0.31730100
H	-8.50801100	3.19266100	-0.90791600
C	3.32084300	3.68312800	-3.32045000
H	3.81875700	2.74726600	-3.04061800
H	2.28235100	3.41488600	-3.54615500
H	3.78635800	4.05809000	-4.23687900
C	2.30466300	5.07708400	1.44678300
H	1.22227800	4.91808300	1.36841100
H	2.72623800	4.16179100	1.87961400
H	2.47759300	5.89756900	2.14962700
C	4.83191800	8.20594600	-1.62472400
H	5.66573400	8.10479000	-2.32812000
H	4.13202000	8.93549200	-2.05373700
H	5.22121600	8.63540900	-0.69537300
C	5.47764700	-2.31316100	-1.11457400
H	4.62281200	-2.91657100	-1.44166300

H	5.27046900	-1.28436100	-1.43141700
H	6.36557500	-2.66328000	-1.64929700
C	3.82585500	-1.49565500	3.62406100
H	3.36340000	-0.56281200	3.28551600
H	3.01929000	-2.23184100	3.72867600
H	4.24822500	-1.32721200	4.61967600
C	8.33182400	-3.64055000	2.83957000
H	8.25631100	-4.73576300	2.86903600
H	9.19880500	-3.39349100	2.21671600
H	8.53787400	-3.29938200	3.85955400
C	-4.84405500	0.11436100	3.00328800
C	-3.84800900	0.25055900	3.97331900
C	-3.42421500	-1.27743300	1.68684900
C	-4.65534800	-0.66952000	1.86352600
H	-5.44416300	-0.74888500	1.12650300
C	-2.37805700	-1.11956600	2.61836000
C	-2.61273000	-0.36811900	3.79985200
C	-0.05398500	-1.73615200	3.45322000
C	-0.11638700	-0.46313600	4.30843600
C	-1.53453800	-0.25101700	4.86173900
C	-1.03987900	-1.63054100	2.30649300
H	0.95153600	-1.88285000	3.04791300
H	0.59994800	-0.51633000	5.13676400
H	-0.51617300	-0.66494400	1.59713500
H	-1.02265100	-2.45429100	1.59215300
H	-1.61181400	0.72297300	5.35992700
H	-0.28684500	-2.61879500	4.07139700
H	0.16790700	0.38702500	3.67733100
H	-4.04164500	0.86879600	4.84278500
H	-3.24169900	-1.85314800	0.78811800
N	-6.07790400	0.88188800	3.13190200
O	-7.01170100	0.61449500	2.37089300
O	-6.10892300	1.78752900	3.97269800

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C	-1.10812700	-2.08251500	-1.52279200
C	-2.44867200	-2.59127200	-1.68289000
C	-3.29416800	-1.58494300	-1.32273400
C	-2.47273300	-0.43100100	-1.03203300
N	-1.14640100	-0.77703800	-1.11638300
H	-2.69262800	-3.59683900	-1.99551700
H	-4.37192700	-1.60513000	-1.27356300
C	-0.36086900	3.31380500	-0.87523300
C	-1.50681300	4.16774900	-1.09173000

C	-2.60302200	3.36157000	-1.06286000
C	-2.12028400	2.01082400	-0.87324100
N	-0.76461900	2.00498300	-0.77652100
H	-1.45901700	5.23930600	-1.22332000
H	-3.64394700	3.62927700	-1.17684600
C	2.90519400	-1.24618100	-0.31116700
C	3.46574900	-2.54809400	-0.59244600
C	2.49353000	-3.26711300	-1.22471900
C	1.32081400	-2.42791700	-1.26680700
N	1.60350500	-1.20122400	-0.71659900
H	4.47319400	-2.85133100	-0.34690100
H	2.53762200	-4.28049600	-1.59756700
C	3.19374600	1.16040900	0.18182600
C	4.03085600	2.30637100	0.46291200
C	3.30596600	3.40893500	0.12567400
C	2.01194000	2.93442100	-0.31270200
N	1.96863000	1.57580700	-0.26997400
H	5.04601400	2.25083900	0.82976000
H	3.59515600	4.44923300	0.17201700
C	0.05651600	-2.85027800	-1.69001700
C	0.94310700	3.77254900	-0.68187000
C	-2.95727200	0.87683000	-0.85023100
C	3.63409400	-0.16413800	0.22680100
Fe	0.40263000	0.38710300	-0.64612800
Cl	0.83377300	0.68878000	-2.96913300
O	0.13536500	0.27743900	1.05554200
H	-0.12696000	-0.84345200	1.52069200
C	1.63224400	-2.79598000	5.10080800
C	2.73839900	-3.38757100	4.48617600
C	2.75181600	-3.52566300	3.09535300
C	1.67845800	-3.06692900	2.33950800
C	0.55857500	-2.45448300	2.93869700
C	0.55599400	-2.33576000	4.34133700
H	1.60042800	-2.69731100	6.18286900
H	3.60192700	-3.98190200	2.59535400
H	1.70345000	-3.17471300	1.26314700
H	-0.30157000	-1.91245700	4.85075400
C	-0.52957200	-1.98876800	2.04141700
H	-0.57025500	-2.58799900	1.13095300
C	-1.88528800	-1.65118100	2.53050000
C	-2.11095400	-0.69027300	3.53832400
C	-3.00843000	-2.22651700	1.90387200
C	-3.39848400	-0.32322100	3.90567000
H	-1.26645900	-0.18444500	3.99295600

C	-4.30201700	-1.85403100	2.24178100
C	-4.48420900	-0.89506200	3.23824500
H	-3.57511100	0.43566700	4.65740100
H	-5.16414500	-2.26722100	1.73320700
C	-4.41843400	1.08164900	-0.62717400
C	-5.37671900	0.79177900	-1.61906700
C	-4.83567100	1.52309700	0.65631300
C	-6.73502500	0.82536900	-1.27583900
C	-6.19776900	1.52775700	0.95261700
C	-7.16311000	1.14716900	0.01225700
H	-7.47288100	0.58629000	-2.03963300
H	-6.51613600	1.80817300	1.95399600
C	-0.06109400	-4.18610400	-2.35320500
C	-0.32816400	-5.35204800	-1.61159200
C	0.10309300	-4.24274000	-3.75294600
C	-0.42558700	-6.57163100	-2.29047000
C	-0.00140700	-5.48353500	-4.38807800
C	-0.26182200	-6.65888100	-3.67592200
H	-0.63447400	-7.47496400	-1.72091300
H	0.12198700	-5.53168900	-5.46820100
C	1.21853700	5.23315300	-0.83698800
C	1.73742400	5.69462500	-2.06312800
C	0.96386200	6.12494800	0.22207900
C	1.98203600	7.06325400	-2.21101500
C	1.22908200	7.48466500	0.03072700
C	1.73722000	7.97295900	-1.17718100
H	2.37328700	7.42707400	-3.15906900
H	1.03287900	8.17873400	0.84561400
C	4.97260200	-0.44369200	0.83011500
C	5.07049900	-0.52815900	2.23407200
C	6.11143800	-0.60603400	0.01559300
C	6.31161000	-0.84123300	2.79803900
C	7.33277200	-0.90746400	0.62578600
C	7.44999700	-1.04631800	2.01292200
H	6.39021000	-0.91808900	3.88078900
H	8.21598500	-1.03025200	0.00204800
C	3.88218900	-0.22922900	3.12042100
H	3.72248500	0.85467200	3.19027900
H	2.95501500	-0.66046300	2.73509600
H	4.03632800	-0.61656100	4.13115100
C	6.02550200	-0.42240200	-1.48326300
H	5.42055200	-1.20379700	-1.95708200
H	5.55220400	0.53344000	-1.73668500
H	7.01990000	-0.44256800	-1.93933200

C	8.77044500	-1.42103400	2.64467600
H	8.87058200	-2.51141500	2.73080600
H	9.61715800	-1.06348000	2.04867700
H	8.86561800	-1.00572600	3.65385900
C	0.41698500	5.62330400	1.53972800
H	-0.58832000	5.20162100	1.42051300
H	1.04528300	4.82529100	1.95319500
H	0.36128100	6.42995800	2.27686300
C	2.03008300	4.72714600	-3.18741200
H	2.86408400	4.06355800	-2.92749300
H	1.17848100	4.07059400	-3.39769600
H	2.29419800	5.25885000	-4.10656100
C	2.04368200	9.44242500	-1.35141600
H	3.08893900	9.66050500	-1.09425300
H	1.89100400	9.76390200	-2.38751700
H	1.41331200	10.06381300	-0.70623400
C	-3.85247000	2.00221800	1.70171900
H	-2.96060700	1.37335300	1.76105600
H	-3.50895800	3.01778200	1.46997700
H	-4.32523600	2.02512400	2.68661300
C	-4.99339800	0.48662700	-3.05374800
H	-3.94541100	0.71701900	-3.26072300
H	-5.15263300	-0.56863400	-3.30619200
H	-5.61117600	1.07800300	-3.73926600
C	-8.61799600	1.09522000	0.40935300
H	-8.74905300	0.42341600	1.26643300
H	-8.98432700	2.08350700	0.71449100
H	-9.25073900	0.73841500	-0.40964500
C	0.38234000	-2.98630100	-4.54562100
H	-0.41189000	-2.24226700	-4.41570300
H	1.30337800	-2.49445300	-4.21292400
H	0.47559500	-3.20699800	-5.61320100
C	-0.51774600	-5.29697500	-0.11299600
H	0.35730000	-4.87383700	0.39271800
H	-1.37440900	-4.66827800	0.15757900
H	-0.69286500	-6.29435500	0.30108000
C	-0.33621100	-7.99133500	-4.38462500
H	0.66359500	-8.42903600	-4.50686600
H	-0.94158400	-8.71187400	-3.82436900
H	-0.76911100	-7.88925100	-5.38587100
H	3.57468300	-3.74139000	5.08286800
H	-2.85771400	-2.95203800	1.11276800
N	-5.83367300	-0.41293000	3.52005500
O	-5.95163800	0.57484700	4.25372200

O	-6.78214600	-0.99163100	2.98587600
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C	2.52188600	0.24293100	-1.26802200
C	3.57593000	-0.63095000	-1.73321400
C	2.98413000	-1.80412100	-2.09678000
C	1.58153500	-1.67298100	-1.78743300
N	1.32583200	-0.41740100	-1.29208100
H	4.62172900	-0.36532900	-1.78303100
H	3.44410900	-2.69350600	-2.50322200
C	-2.46650700	-1.87512300	-0.38527600
C	-2.62898900	-3.30470000	-0.52175500
C	-1.51903300	-3.76756300	-1.16487100
C	-0.64900500	-2.63306900	-1.35530200
N	-1.23705500	-1.50022700	-0.86541500
H	-3.49607600	-3.86060100	-0.19539400
H	-1.28457300	-4.77909600	-1.46454600
C	-0.35381800	3.36417400	-0.67783500
C	0.57485700	4.47210600	-0.64599700
C	1.82411100	3.93200900	-0.65667900
C	1.65345000	2.49835700	-0.74156000
N	0.32271200	2.18119900	-0.74040000
H	0.28793200	5.51314900	-0.60528900
H	2.77998100	4.43602900	-0.64151000
C	-2.61929300	2.42248200	-0.41195000
C	-4.03015700	2.55465500	-0.12832100
C	-4.49519300	1.30050900	0.12354600
C	-3.37558100	0.40119700	-0.04958400
N	-2.25427500	1.10297700	-0.37783100
H	-4.56805600	3.49165900	-0.10803100
H	-5.49798300	0.99045200	0.38058000
C	2.70806400	1.59676700	-0.91856800
C	-3.47129000	-0.99677800	0.04973400
C	0.65213400	-2.71529000	-1.87864200
C	-1.74786200	3.50192300	-0.59129200
Fe	-0.44730900	0.32793500	-0.75635600
Cl	-0.92266200	0.63306200	-3.05789100
O	-0.13181000	0.18818800	0.92261700
H	0.26992400	-0.91126700	1.31785900
C	4.14783300	-0.73599800	3.87172000
C	4.31688600	-0.89543500	2.49193400
C	3.25517500	-1.36949100	1.72574800
C	2.04497100	-1.66993500	2.35158600
C	1.91291700	-1.56035100	3.76503700

C	2.96617100	-1.08630900	4.53594200
H	3.36743300	-1.48058700	0.65411400
H	2.89912800	-0.97021500	5.61110300
C	0.75085000	-2.06554800	1.77659300
C	-0.09486100	-2.40952200	2.93425800
C	-1.36375600	-2.98510000	2.98904500
C	-1.96318200	-3.18028700	4.23737300
C	-1.31082400	-2.79247200	5.41507600
C	-0.03370400	-2.22070400	5.36980500
C	0.57667600	-2.04093900	4.13069700
H	-1.87638100	-3.27442100	2.07651000
H	-1.79647100	-2.94597500	6.37495400
H	0.47672300	-1.93966400	6.28750200
C	1.06309000	-3.98267200	-2.55887400
C	0.76518200	-4.11958500	-3.93098600
C	1.73365700	-5.00505900	-1.86133600
C	1.15911000	-5.28948400	-4.58620800
C	2.10707100	-6.15898800	-2.55904900
C	1.82894800	-6.32063600	-3.91926300
H	0.93907800	-5.39619300	-5.64659700
H	2.62925100	-6.94986300	-2.02447600
C	-4.73452600	-1.56760200	0.60853500
C	-4.95753200	-1.48327200	1.99964900
C	-5.69678000	-2.15695700	-0.23911300
C	-6.11403900	-2.06658200	2.52779400
C	-6.84380500	-2.71298900	0.33482800
C	-7.06185300	-2.69661900	1.71650000
H	-6.28225100	-2.01538000	3.60182400
H	-7.59144800	-3.16203800	-0.31599300
C	-2.32634300	4.87937800	-0.64225100
C	-2.54191600	5.60219800	0.54649700
C	-2.65416800	5.43123900	-1.89586900
C	-3.09409600	6.88373200	0.45901900
C	-3.20571500	6.71562900	-1.93500300
C	-3.43038100	7.45806300	-0.77127200
H	-3.26621200	7.44623200	1.37454700
H	-3.46701400	7.14556000	-2.89987700
C	4.10766200	2.09924900	-0.76708700
C	4.61809600	2.29800900	0.53378400
C	4.91207600	2.34539900	-1.89989500
C	5.96617600	2.64344300	0.67773200
C	6.24628200	2.71473200	-1.70559900
C	6.79828100	2.84613500	-0.42681500
H	6.37208700	2.75285200	1.68118900

H	6.87052300	2.90425600	-2.57661900
C	2.03302300	-4.87710800	-0.38509900
H	2.57705400	-3.95361100	-0.15815300
H	1.10919600	-4.85574800	0.20612700
H	2.63508000	-5.71834000	-0.02929200
C	0.03134900	-3.02550400	-4.67235600
H	-0.98914500	-2.90283900	-4.28996300
H	0.51472300	-2.05022100	-4.54831800
H	-0.03076700	-3.24776100	-5.74185300
C	2.21591200	-7.58670600	-4.64750700
H	3.04751700	-8.09842800	-4.15161900
H	1.37446800	-8.29131100	-4.68707000
H	2.51250100	-7.37892400	-5.68155300
C	3.73933100	2.20609500	1.76195800
H	3.22210000	3.16096200	1.92523400
H	2.96681600	1.43838200	1.67788400
H	4.34073600	1.99191400	2.64953900
C	4.34425200	2.24799300	-3.29958800
H	4.14848000	1.21122500	-3.59585400
H	3.38913700	2.77985600	-3.37736200
H	5.03469900	2.67970700	-4.03052700
C	8.24426600	3.24261700	-0.24104200
H	8.34237700	4.32943400	-0.11720400
H	8.67415500	2.77484000	0.65122300
H	8.85414500	2.95616500	-1.10450500
C	-2.18391800	5.00224600	1.88714600
H	-2.75104700	4.08301900	2.07729900
H	-1.12242900	4.72999100	1.92982400
H	-2.38851900	5.70293600	2.70213200
C	-3.99423300	8.85825400	-0.84277600
H	-4.64806600	8.98410900	-1.71251700
H	-4.57098100	9.10568400	0.05507600
H	-3.19093100	9.60221600	-0.92888300
C	-2.41090700	4.64851500	-3.16594400
H	-1.34294400	4.44508300	-3.30949700
H	-2.90265300	3.66941000	-3.13970900
H	-2.77470000	5.19379400	-4.04199500
C	-4.01161000	-0.73101000	2.90997600
H	-4.10872900	-1.06906500	3.94565400
H	-2.96461500	-0.84521300	2.62035400
H	-4.23429900	0.34371700	2.88380000
C	-5.52697000	-2.15304700	-1.74317500
H	-5.19515100	-1.17321500	-2.10431200
H	-4.77536600	-2.87875900	-2.07401300

H	-6.47021400	-2.39838500	-2.24064200
C	-8.28560300	-3.34907400	2.31561200
H	-8.58182100	-2.86373500	3.25173200
H	-9.13781200	-3.31242800	1.62831400
H	-8.09600600	-4.40680800	2.54251400
H	0.71518300	-2.66456900	0.87163400
H	-2.95120600	-3.62976700	4.29109000
H	5.25654800	-0.60970200	2.03608400
N	5.23934500	-0.14365700	4.64538100
O	6.16103300	0.39563600	4.02217000
O	5.17540900	-0.19696500	5.87495500

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C	1.31187900	-2.13118200	-0.98482300
C	1.33632700	-3.57509700	-0.97717800
C	0.05655300	-3.98504200	-0.77697400
C	-0.74668600	-2.79220000	-0.64722500
N	0.04278900	-1.67250400	-0.72278600
H	2.22352200	-4.17384100	-1.12266100
H	-0.32993700	-4.99224300	-0.72156600
C	-3.54131700	0.42955700	-0.14289000
C	-4.73942800	-0.36932700	-0.06021000
C	-4.36051900	-1.66427800	-0.24583700
C	-2.92711300	-1.65668700	-0.40189300
N	-2.44908100	-0.37302100	-0.34266100
H	-5.73234000	0.02696500	0.09625200
H	-4.97779400	-2.55040200	-0.26725300
C	1.72135500	2.13930200	-1.35717600
C	3.10344500	2.15637500	-1.77629300
C	3.50753300	0.85945000	-1.84232100
C	2.37518300	0.05349700	-1.44844500
N	1.29885500	0.84794300	-1.16961500
H	3.66971400	3.05116400	-1.99064000
H	4.47461500	0.46734700	-2.12135400
C	-0.39681300	3.28960600	-0.80339700
C	-1.16758500	4.48552500	-0.54218400
C	-2.42441900	4.07493100	-0.22332900
C	-2.41718000	2.63046500	-0.29589400
N	-1.17403600	2.17859400	-0.65010500
H	-0.77937700	5.49230100	-0.60080300
H	-3.28690600	4.67353000	0.03255300
C	2.40470500	-1.34725000	-1.37256700
C	-3.54088800	1.83059100	-0.06888400
C	-2.14617000	-2.80877100	-0.56819100

C	0.95795500	3.29502300	-1.16431800
Fe	-0.55685000	0.24255300	-0.66743700
Cl	-1.03730900	0.12742400	-2.97547400
O	-0.25416400	0.54627900	0.99934100
H	0.08830100	-0.29135900	1.79917700
C	2.03336600	-4.76946100	2.78353700
C	0.66342900	-4.61873500	2.54472500
C	0.06188300	-3.35749800	2.58064200
C	0.83312700	-2.22970200	2.86568300
C	2.22555200	-2.39104000	3.07765500
C	2.82641000	-3.64845500	3.04426900
H	2.48533500	-5.75687700	2.75153100
H	-0.98687100	-3.26093600	2.34527900
H	3.89489500	-3.75475800	3.21346700
C	0.46119300	-0.78569700	2.98212200
C	1.77969800	-0.10050200	3.15560100
C	2.11414200	1.25834500	3.10187300
C	3.44867900	1.64607000	3.21052200
C	4.44092900	0.67109500	3.35498600
C	4.14705300	-0.69281800	3.37531500
C	2.81555500	-1.06620000	3.24913800
H	1.35581500	2.00961700	2.92936000
H	4.94882800	-1.41685200	3.44790600
C	-0.74778400	-0.39424300	3.89086100
C	-2.07075000	-0.95878400	3.33081000
C	-0.50052600	-0.97092400	5.30370800
C	-0.91148100	1.13516400	4.00622000
H	-2.21352800	-0.65640900	2.28917900
H	-2.11374500	-2.04789700	3.39459300
H	-2.91178800	-0.57417100	3.91954200
H	0.43474100	-0.58411100	5.72478000
H	-1.31985600	-0.68655100	5.97555000
H	-0.43800900	-2.06375200	5.28351100
H	-1.81965000	1.35927200	4.57799300
H	-0.07364600	1.59331700	4.53928000
H	-1.00338600	1.59294100	3.01739000
C	-2.84915700	-4.10766900	-0.82321900
C	-2.92745200	-4.54827100	-2.16657900
C	-3.44188400	-4.86148000	0.20724300
C	-3.59381400	-5.74410200	-2.44220000
C	-4.09703700	-6.05548600	-0.11963500
C	-4.18465900	-6.51445500	-1.43447800
H	-3.65941400	-6.08054100	-3.47509000
H	-4.55226100	-6.63789500	0.67917300

C	-4.83693800	2.51429100	0.23514400
C	-5.24882300	2.66132000	1.57328200
C	-5.63317700	2.99717300	-0.82190700
C	-6.46338100	3.30265000	1.83517800
C	-6.84261200	3.62771300	-0.51398100
C	-7.27292000	3.79447000	0.80642600
H	-6.78464100	3.41924900	2.86833500
H	-7.46472500	3.99636900	-1.32718900
C	1.63111300	4.61853100	-1.34557200
C	2.40046900	5.15716000	-0.29587500
C	1.48602800	5.31206600	-2.56278000
C	3.01852300	6.39692500	-0.48458700
C	2.12551300	6.54687900	-2.70914100
C	2.89707100	7.10474700	-1.68457200
H	3.60969600	6.81896800	0.32554900
H	2.01901400	7.08546100	-3.64873200
C	3.63422700	-2.04324600	-1.87189600
C	4.76635900	-2.19332200	-1.04885700
C	3.64136400	-2.52095800	-3.19950400
C	5.89623300	-2.83305900	-1.56727400
C	4.79476500	-3.15181000	-3.67608000
C	5.93125600	-3.31730600	-2.87841500
H	6.76977700	-2.95390100	-0.92975900
H	4.80559400	-3.51998200	-4.70010200
C	-3.36542500	-4.44488200	1.65941800
H	-2.47222900	-4.86258500	2.14125900
H	-3.32857400	-3.35931500	1.77872400
H	-4.23204900	-4.81424200	2.21753100
C	-2.30122900	-3.75585100	-3.29375000
H	-2.48052000	-2.67921200	-3.20281100
H	-1.21131900	-3.88144300	-3.30401000
H	-2.68526800	-4.09001700	-4.26243300
C	-4.92553800	-7.78717100	-1.77168200
H	-5.03750700	-8.43268400	-0.89429800
H	-5.93273500	-7.56806000	-2.15028700
H	-4.40593000	-8.35773800	-2.54975800
C	4.74750700	-1.69420000	0.37384500
H	4.46439800	-0.63775100	0.42978700
H	4.01072600	-2.24579100	0.96698500
H	5.72455600	-1.80313000	0.85433300
C	2.43031200	-2.36496700	-4.09220200
H	1.61084200	-3.01675000	-3.76507900
H	2.03441200	-1.34352500	-4.07320400
H	2.67198300	-2.62155600	-5.12806900

C	7.17645600	-3.97167500	-3.43008700
H	7.84119400	-3.22815000	-3.88987000
H	7.74783500	-4.47534700	-2.64286500
H	6.93346400	-4.71107400	-4.20097900
C	2.55039100	4.40987000	1.00959700
H	1.57274300	4.17339700	1.44733700
H	3.06661500	3.45423000	0.86419200
H	3.12024900	4.99530200	1.73761300
C	3.60679100	8.42407600	-1.88155800
H	3.04656100	9.08529500	-2.55162500
H	3.75339000	8.94777100	-0.93080600
H	4.59916600	8.27409800	-2.32742100
C	0.65462700	4.73371000	-3.68530200
H	0.95687100	3.70716200	-3.92221300
H	-0.40652200	4.68845200	-3.41146600
H	0.74451800	5.33640500	-4.59404900
C	-4.39469400	2.13066000	2.70148600
H	-4.29594100	1.04041600	2.64541800
H	-3.37694500	2.53522900	2.65972400
H	-4.82243000	2.38357300	3.67645800
C	-5.19011800	2.83030800	-2.25751100
H	-4.27128800	3.39459500	-2.45725000
H	-4.96617900	1.78246100	-2.48903700
H	-5.96071200	3.17839400	-2.95181500
C	-8.56615800	4.51291300	1.11402300
H	-9.00399600	4.16613000	2.05625100
H	-8.40308000	5.59485900	1.20894300
H	-9.30634600	4.36502800	0.32013800
H	0.05790100	-5.49029600	2.30953800
H	3.73573100	2.68875600	3.16664200
N	5.84357300	1.09028500	3.43216800
O	6.08614600	2.29879500	3.44746000
O	6.70607400	0.20886500	3.46980200

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C	3.01446600	-1.55067600	-0.60469800
C	3.44324600	-2.92824500	-0.57930400
C	2.32044500	-3.69070100	-0.68866900
C	1.20764400	-2.77736100	-0.76294500
N	1.64708800	-1.48292600	-0.70809100
H	4.47110800	-3.25043700	-0.49543000
H	2.23396400	-4.76717200	-0.70845700
C	-2.40149700	-0.48456600	-1.20828700
C	-3.31980900	-1.59689700	-1.27555100

C	-2.57744500	-2.72699500	-1.12689300
C	-1.20926100	-2.30309700	-0.95340100
N	-1.12936300	-0.92966200	-0.96455300
H	-4.38526900	-1.50417700	-1.42732500
H	-2.90468600	-3.75678900	-1.13753800
C	2.27604500	2.68918800	-0.65203900
C	3.64208800	3.12040900	-0.45677200
C	4.40341000	1.99430200	-0.42847500
C	3.49522900	0.87802200	-0.57668600
N	2.21293800	1.32499600	-0.72670100
H	3.95460200	4.15128100	-0.37146300
H	5.47390500	1.90487400	-0.31223100
C	-0.11946000	3.15148000	-1.04654000
C	-1.19556700	4.06636500	-1.34864600
C	-2.29563600	3.30519300	-1.59286100
C	-1.89918600	1.93022000	-1.39548300
N	-0.56534600	1.86057300	-1.09015300
H	-1.09535800	5.14154900	-1.38387400
H	-3.28965800	3.62487200	-1.86871000
C	3.89519900	-0.46377200	-0.53428600
C	-2.77994000	0.84590000	-1.46121800
C	-0.12861100	-3.18629000	-0.89286200
C	1.19286300	3.56449700	-0.77919800
Fe	0.53072500	0.19034600	-0.80958500
Cl	0.76855400	0.08238000	-3.15580700
O	0.48869300	0.40817900	0.88269100
H	-0.17012400	-0.22223300	1.70248200
C	-0.53081300	3.12777900	4.82462600
C	0.70670000	2.49088400	4.64984300
C	0.78476900	1.23075900	4.05048500
C	-0.39357200	0.61300900	3.63703700
C	-1.64404100	1.25044900	3.82069400
C	-1.71616000	2.51160200	4.41122500
H	-0.56909400	4.10947100	5.28892000
H	1.61538500	2.98640700	4.98106000
H	1.74127600	0.73823000	3.90182800
H	-2.67399800	3.00627700	4.55145500
C	-0.58379800	-0.66323000	2.89292400
C	-2.04878100	-0.79635500	2.76808100
C	-2.80495500	-1.81973400	2.19605700
C	-4.19059600	-1.69321300	2.13688800
C	-4.79585900	-0.54257200	2.65528200
C	-4.06409700	0.49482800	3.24492000
C	-2.68308400	0.36471000	3.29195900

H	-2.31645900	-2.69093600	1.77583500
H	-4.80868300	-2.45681800	1.68275600
H	-4.58043500	1.36628700	3.62816400
C	-0.39628600	-4.64396100	-1.11414700
C	-0.47234800	-5.10586200	-2.44777300
C	-0.54856300	-5.53439200	-0.03750800
C	-0.69896500	-6.46506400	-2.67273500
C	-0.77257200	-6.88951600	-0.31258900
C	-0.85405900	-7.37390600	-1.61897500
H	-0.74909300	-6.82637600	-3.69805600
H	-0.88367200	-7.58074300	0.52072000
C	-4.19388900	1.10270000	-1.87694400
C	-5.11734800	1.66850800	-0.97580300
C	-4.58766900	0.76177400	-3.19010700
C	-6.44084900	1.84651400	-1.39216900
C	-5.91583900	0.97779400	-3.56661200
C	-6.86004400	1.50894200	-2.68136700
H	-7.16005600	2.25574600	-0.68555400
H	-6.22235400	0.71925800	-4.57831900
C	1.44418700	5.03001000	-0.62312600
C	1.21966000	5.63009600	0.63000900
C	1.88951200	5.79157500	-1.72237300
C	1.45692700	7.00325900	0.76438800
C	2.10801200	7.15934100	-1.54255600
C	1.89957600	7.78349400	-0.30661000
H	1.28883300	7.47228700	1.73162500
H	2.44796400	7.75368100	-2.38862200
C	5.35843400	-0.75404900	-0.40897600
C	5.97547000	-0.72783400	0.85725100
C	6.10331700	-1.05114800	-1.56763700
C	7.34186600	-1.01293300	0.94293000
C	7.46755800	-1.32690400	-1.43408700
C	8.10532400	-1.31244900	-0.18964300
H	7.82099700	-1.00119500	1.91991700
H	8.04632400	-1.55806900	-2.32614100
C	-0.50647600	-5.05764200	1.39433300
H	0.14064800	-4.18894400	1.52922900
H	-1.50823100	-4.77298400	1.74172700
H	-0.14948400	-5.84496600	2.06485100
C	-0.31507800	-4.15030600	-3.60907600
H	-1.14454800	-3.43406200	-3.64868600
H	0.59883600	-3.55165400	-3.52598100
H	-0.28761800	-4.68982800	-4.56045500
C	-1.12326200	-8.83479200	-1.89542500

H	-0.87170400	-9.46078300	-1.03285600
H	-2.18369100	-9.00358900	-2.12547700
H	-0.54580400	-9.19274700	-2.75526700
C	5.18417700	-0.38955400	2.10079800
H	4.82102500	0.64501300	2.07100100
H	4.30016900	-1.02666600	2.20598800
H	5.79429100	-0.50792500	3.00128200
C	5.44011500	-1.07820800	-2.92602900
H	4.72911400	-1.90931300	-3.00512200
H	4.86636200	-0.16332200	-3.11273500
H	6.18056300	-1.18860400	-3.72390800
C	9.58779700	-1.58184800	-0.07626300
H	10.16635000	-0.65569800	-0.19325200
H	9.84582800	-2.00533600	0.90040100
H	9.92979100	-2.27783700	-0.84993300
C	0.72918600	4.81171400	1.80289300
H	-0.27790900	4.41587800	1.62458000
H	1.36761800	3.94138900	1.99094000
H	0.69558400	5.41014400	2.71796200
C	2.15142100	9.26506200	-0.14787500
H	1.53618400	9.84941100	-0.84333300
H	1.92523000	9.60625000	0.86739400
H	3.19880300	9.51457800	-0.35936900
C	2.11864700	5.13915400	-3.06673700
H	2.92223000	4.39456100	-3.01670500
H	1.22351000	4.60785400	-3.41104400
H	2.38930500	5.88002200	-3.82499000
C	-4.70836500	2.10629900	0.41102600
H	-3.86690700	1.52559800	0.79375700
H	-4.39354700	3.15811500	0.41070100
H	-5.53863600	2.00856300	1.11627200
C	-3.60562000	0.16895000	-4.17750600
H	-2.62672800	0.65803700	-4.13146200
H	-3.42938600	-0.89450300	-3.97298200
H	-3.98494800	0.25292500	-5.20064000
C	-8.28792800	1.74122700	-3.11681300
H	-8.98482400	1.62467200	-2.27992400
H	-8.41913900	2.75773100	-3.51155600
H	-8.58524500	1.04394500	-3.90745700
C	0.28057000	-1.84762000	3.20132400
C	1.55918000	-1.97827500	2.63841300
C	-0.16096700	-2.82875000	4.10457000
C	2.37288300	-3.06393000	2.96825700
H	1.89260900	-1.23413500	1.92424300

C	0.65795600	-3.90590000	4.44321300
H	-1.14924900	-2.73753200	4.54633800
C	1.92802000	-4.02891100	3.87408400
H	3.34690000	-3.16495200	2.49826200
H	0.30107200	-4.65202800	5.14853500
H	2.56134300	-4.87483700	4.12764300
N	-6.24724500	-0.40136700	2.53801300
O	-6.89165000	-1.35694300	2.10140300
O	-6.75249000	0.67629200	2.87339300

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C	2.47744100	0.14847600	-1.29793500
C	3.50359300	-0.76583400	-1.74603200
C	2.87143600	-1.91420700	-2.12409300
C	1.47249500	-1.73446400	-1.82292700
N	1.25884100	-0.46801400	-1.33927300
H	4.55980500	-0.54696400	-1.77439700
H	3.30302800	-2.82044000	-2.52529600
C	-2.51465300	-1.81619000	-0.26715400
C	-2.75107600	-3.23155600	-0.43542500
C	-1.68809200	-3.72839700	-1.13132700
C	-0.76812500	-2.63264800	-1.32004500
N	-1.29153200	-1.48541500	-0.78678600
H	-3.63122700	-3.75381000	-0.08918800
H	-1.51692600	-4.74079300	-1.46864200
C	-0.34539900	3.35488000	-0.94377500
C	0.60651400	4.44142200	-1.01546000
C	1.84518000	3.87700300	-0.96497400
C	1.64577100	2.44493600	-0.92352400
N	0.31260200	2.15765400	-0.91560500
H	0.34185400	5.48778500	-1.07094500
H	2.81189300	4.36023200	-0.98471100
C	-2.59928300	2.47050500	-0.46608200
C	-3.97767500	2.64559300	-0.06718700
C	-4.43456100	1.41771600	0.30593700
C	-3.34920900	0.48732600	0.08457600
N	-2.25036700	1.15221000	-0.37635500
H	-4.50013900	3.59164300	-0.06011200
H	-5.41496100	1.14289400	0.66844400
C	2.68770600	1.50556900	-0.96681500
C	-3.46410300	-0.90419800	0.22495600
C	0.51204600	-2.75142500	-1.88495400
C	-1.72964100	3.52045600	-0.79503800
Fe	-0.47969600	0.33122700	-0.79044800

Cl	-1.05631600	0.51583200	-3.08801800
O	-0.10625400	0.29850000	0.89054600
H	0.30592400	-0.81440900	1.31295000
C	4.57367100	-0.41015100	3.11046300
C	3.45626900	-0.27883300	3.94026100
C	3.28655900	-1.59526000	1.48332400
C	4.50841500	-1.07751700	1.88695000
H	3.55324000	0.25544500	4.87840600
H	5.39263700	-1.15107100	1.26676200
C	0.81624800	-1.90309500	1.81508400
C	2.13785400	-1.44593800	2.27664400
C	2.23235900	-0.79010900	3.52528100
C	0.96295500	-0.58730800	4.32570700
H	0.84230000	-2.55259400	0.94154100
H	1.19174300	-0.43390100	5.38627800
H	0.49356800	0.34424400	3.96840000
H	3.20822700	-2.09449900	0.52525700
C	-0.11521100	-2.33355900	2.87691500
C	-1.06859400	-3.34112000	2.66261100
C	-1.91886700	-3.74288900	3.69065700
C	-1.82240000	-3.14128600	4.94835800
C	-0.88114500	-2.13103900	5.16697200
C	-0.03178100	-1.71443500	4.14183200
H	-1.14151000	-3.80191900	1.68232500
H	-2.65578000	-4.52078700	3.51101000
H	-2.47830100	-3.45433600	5.75621000
H	-0.80814900	-1.66065100	6.14507800
C	0.87190400	-4.03072500	-2.57155000
C	0.70727700	-4.09721000	-3.97080300
C	1.36132200	-5.13686000	-1.85095300
C	1.02534200	-5.29121600	-4.62465600
C	1.66990000	-6.30950400	-2.54844700
C	1.50276900	-6.40893900	-3.93290900
H	0.89852000	-5.34758200	-5.70399300
H	2.05266200	-7.16491900	-1.99538500
C	4.06294500	1.95449000	-0.60177400
C	4.29418000	2.24485800	0.76941600
C	5.11908400	2.02559100	-1.52844500
C	5.59945500	2.49294500	1.18821300
C	6.41475200	2.28169900	-1.05707600
C	6.68059900	2.48224000	0.29709500
H	5.78812000	2.67201600	2.24431300
H	7.23372900	2.31775900	-1.77331500
C	-4.69724900	-1.43953900	0.87844600

C	-4.77363500	-1.41083300	2.28651600
C	-5.76642500	-1.93896100	0.10817500
C	-5.90564700	-1.94989700	2.90492900
C	-6.88318000	-2.45791600	0.77164800
C	-6.96462100	-2.48856100	2.16739500
H	-5.96350000	-1.94001200	3.99159700
H	-7.71337700	-2.84097700	0.18154500
C	-2.29760800	4.89737800	-0.92112700
C	-2.74589500	5.33073800	-2.18438300
C	-2.37739400	5.74002400	0.20343600
C	-3.27588000	6.61937300	-2.29774400
C	-2.91505500	7.02119700	0.04316700
C	-3.37176600	7.47764200	-1.19722900
H	-3.62087600	6.96143000	-3.27153100
H	-2.97722500	7.67790300	0.90865800
C	0.22085800	-2.89538100	-4.74843700
H	-0.67910900	-2.45212400	-4.30858800
H	0.97267100	-2.09676000	-4.74975700
H	0.00621700	-3.16039000	-5.78816000
C	1.56626500	-5.06475400	-0.35495900
H	2.24176400	-4.24527800	-0.08333700
H	0.62280700	-4.88690100	0.17424700
H	1.99590300	-5.99382900	0.03107000
C	1.80655300	-7.69726500	-4.66157600
H	0.90161100	-8.30944100	-4.77332000
H	2.19444600	-7.50647100	-5.66823400
H	2.54407400	-8.30068700	-4.12167300
C	3.16645000	2.28927600	1.77759600
H	2.55394600	3.18816900	1.63783600
H	2.48947100	1.43408800	1.68776200
H	3.56456900	2.30915800	2.79508400
C	4.89915100	1.88036200	-3.02078200
H	5.46831700	1.03890600	-3.43431100
H	3.84763000	1.72817600	-3.27505200
H	5.24187400	2.78336100	-3.54043000
C	8.08263600	2.67539300	0.82055100
H	8.20381400	3.66489200	1.27931100
H	8.29748600	1.93011600	1.59590200
H	8.83029600	2.57736700	0.02688600
C	-1.88715700	5.26899200	1.55378100
H	-2.41188700	4.36014900	1.87180200
H	-0.81906000	5.02149800	1.52469900
H	-2.03809900	6.03577900	2.31954500
C	-2.64937800	4.41834200	-3.38559700

H	-1.61489000	4.10799100	-3.57273600
H	-3.21653700	3.49264600	-3.23347600
H	-3.02919200	4.90958100	-4.28650900
C	-3.97964000	8.85354800	-1.34237400
H	-5.07297700	8.81378100	-1.24625800
H	-3.60934900	9.54015400	-0.57357000
H	-3.75653900	9.28865600	-2.32275300
C	-5.73042700	-1.88558200	-1.40335400
H	-5.44857000	-0.88755300	-1.75828900
H	-4.99459900	-2.58301300	-1.81981100
H	-6.70780600	-2.13534000	-1.82724500
C	-3.68247600	-0.76789700	3.11191100
H	-2.68408600	-1.07903600	2.79291400
H	-3.72091200	0.32459800	3.01416900
H	-3.78858000	-1.01951100	4.17004100
C	-8.16019100	-3.09825300	2.86148700
H	-9.06021300	-3.03772400	2.24017000
H	-7.98777900	-4.16011600	3.08302800
H	-8.37012700	-2.59865000	3.81364300
N	5.82355300	0.24036700	3.49014800
O	6.83969200	-0.02906800	2.84437500
O	5.79016800	1.05683200	4.41720500

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C	2.44895800	0.31443100	-1.33662800
C	3.52142900	-0.52402700	-1.82282100
C	2.95566300	-1.70311900	-2.21266800
C	1.55335000	-1.61713900	-1.88619800
N	1.27052500	-0.37333300	-1.37553500
H	4.56104800	-0.23807400	-1.86678800
H	3.43658700	-2.57204400	-2.63932900
C	-2.42140200	-1.94650900	-0.32348000
C	-2.56110300	-3.37667200	-0.47794800
C	-1.46878600	-3.80684900	-1.17377300
C	-0.62661900	-2.65294300	-1.37715900
N	-1.22377700	-1.54038100	-0.85071300
H	-3.40054800	-3.95671400	-0.12271300
H	-1.23008700	-4.80860800	-1.50185600
C	-0.54305400	3.34635000	-0.90843800
C	0.34835900	4.48569500	-0.92768300
C	1.61511900	3.98884200	-0.87396900
C	1.49444800	2.54713400	-0.88441500
N	0.17810700	2.18724300	-0.90472900
H	0.02720200	5.51726400	-0.95354600

H	2.55344900	4.52530100	-0.86236300
C	-2.75274700	2.33086800	-0.49780200
C	-4.14642800	2.42022700	-0.12333700
C	-4.53460800	1.16509900	0.23550500
C	-3.39180100	0.30268100	0.02590100
N	-2.32883800	1.03332300	-0.41489500
H	-4.72389000	3.33371600	-0.11901600
H	-5.50200800	0.82978200	0.58174900
C	2.58513400	1.67005100	-0.95692500
C	-3.42193200	-1.09306400	0.17228200
C	0.65776700	-2.69088600	-1.94600200
C	-1.93803000	3.43325700	-0.78747400
Fe	-0.51188300	0.31643200	-0.82077800
Cl	-1.07725700	0.51045400	-3.12229800
O	-0.15319300	0.26778700	0.86017200
H	0.33204100	-0.82992100	1.29309900
C	4.57948900	-0.26621600	3.08585900
C	3.50302600	-0.31238900	3.97185600
C	3.32361400	-1.39899800	1.39751800
C	4.51781800	-0.82427400	1.80757400
H	3.57419100	0.11957600	4.96149600
H	5.37532500	-0.75950500	1.15080800
C	0.87938400	-1.89471800	1.78865600
C	2.19858300	-1.43050400	2.23472000
C	2.32543100	-0.91020500	3.53962900
H	0.89127600	-2.54549700	0.91525600
H	3.24017900	-1.80334600	0.39701800
C	0.00800000	-2.33829300	2.89030900
C	-1.05796000	-3.23515700	2.72213100
C	-1.87796600	-3.58273500	3.79206100
C	-1.64658400	-3.02966600	5.05722400
C	-0.58611900	-2.14531800	5.25442700
C	0.23178900	-1.81523400	4.17614800
H	-1.24021800	-3.64534000	1.73406200
H	-2.70799600	-4.26568500	3.63794400
H	-2.28754700	-3.29175300	5.89423500
H	-0.37129900	-1.71589800	6.22752000
C	1.09601800	-3.94562400	-2.63285500
C	0.91004300	-4.03431700	-4.02812200
C	1.68073800	-5.00685900	-1.91604700
C	1.31275700	-5.20178400	-4.68309500
C	2.06994300	-6.15507700	-2.61401400
C	1.89070400	-6.27369100	-3.99537200
H	1.17203800	-5.27402400	-5.75973900

H	2.52660300	-6.97539200	-2.06387800
C	3.93106300	2.18190000	-0.56607300
C	4.13708200	2.43463900	0.81695600
C	4.98462700	2.35406200	-1.48220300
C	5.42055600	2.75725100	1.25214700
C	6.25818700	2.67921600	-0.99342000
C	6.50345700	2.85307500	0.36829600
H	5.59187100	2.91333300	2.31491300
H	7.07617500	2.79466300	-1.70233600
C	-4.60152500	-1.69551100	0.86313800
C	-4.66487400	-1.60321700	2.27004100
C	-5.63415000	-2.32133200	0.13514600
C	-5.73087900	-2.22135700	2.93164600
C	-6.68777500	-2.91081600	0.84064900
C	-6.74344900	-2.89091200	2.23827200
H	-5.77607700	-2.16531000	4.01756800
H	-7.49020400	-3.38988500	0.28306000
C	-2.57684000	4.78026400	-0.89532800
C	-2.98992400	5.23390100	-2.16323700
C	-2.75342600	5.57711500	0.25161500
C	-3.58559400	6.49523700	-2.25865400
C	-3.35265700	6.83258300	0.10848500
C	-3.77836300	7.30726500	-1.13620900
H	-3.90524600	6.85246700	-3.23562200
H	-3.48879500	7.45438200	0.99110600
C	0.30050000	-2.88469300	-4.79719300
H	-0.66129200	-2.57430400	-4.37424700
H	0.94015800	-1.99522800	-4.75830500
H	0.14819700	-3.15037700	-5.84761100
C	1.89560600	-4.91459700	-0.42249800
H	2.51636600	-4.05019100	-0.15955600
H	0.94600800	-4.80080400	0.11394200
H	2.39130800	-5.81074700	-0.03771800
C	2.28578800	-7.53686300	-4.72434700
H	1.43196500	-8.22131400	-4.81720900
H	2.63896000	-7.32054300	-5.73858100
H	3.07959600	-8.07525300	-4.19556400
C	3.00603500	2.36011400	1.81994500
H	2.33436200	3.22085100	1.71701100
H	2.38683900	1.46755200	1.68788500
H	3.39775300	2.36181900	2.84013100
C	4.78095700	2.25193100	-2.98029000
H	5.42971700	1.48792900	-3.42572100
H	3.74932400	2.01092400	-3.24644700

H	5.03554200	3.20515300	-3.45955400
C	7.88605000	3.12894200	0.90616500
H	7.93560600	4.11212500	1.39114600
H	8.14909400	2.38025000	1.66297600
H	8.64249300	3.10473900	0.11514500
C	-2.29898100	5.08571400	1.60726500
H	-2.80920600	4.15539700	1.88438800
H	-1.22429200	4.86739200	1.61174100
H	-2.49882500	5.82858300	2.38528700
C	-2.78472600	4.37331800	-3.38872200
H	-1.72232000	4.15963600	-3.55467200
H	-3.27298000	3.39771000	-3.28283900
H	-3.18031500	4.86093800	-4.28480800
C	-4.45527200	8.65244400	-1.26260900
H	-5.54662300	8.55312100	-1.18937500
H	-4.13691500	9.33882900	-0.47059800
H	-4.23681500	9.12228000	-2.22783000
C	-5.63601700	-2.31990400	-1.37829600
H	-5.39730700	-1.32613800	-1.77380300
H	-4.88942300	-3.00695400	-1.79231200
H	-6.61507400	-2.61613100	-1.76706000
C	-3.64849800	-0.80139100	3.05302900
H	-2.63135800	-0.92431300	2.67243300
H	-3.88216900	0.26941300	2.99027000
H	-3.64921900	-1.08793800	4.10768600
C	-7.86656200	-3.57991000	2.97766500
H	-8.79441100	-3.57308100	2.39529600
H	-7.61859700	-4.63042100	3.18107900
H	-8.06692800	-3.10055900	3.94198600
N	5.79077800	0.44744400	3.48336700
O	6.80363400	0.29563400	2.79637000
O	5.72322000	1.19052300	4.46688600
O	1.28440600	-0.95817900	4.43255100

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C	-0.82083500	-2.96401300	-0.81237900
C	-1.60827800	-4.08687400	-0.36313900
C	-2.64032700	-3.57390300	0.36541300
C	-2.51315600	-2.13534600	0.31135200
N	-1.37933000	-1.79284700	-0.38158900
H	-1.37844200	-5.12197300	-0.57292000
H	-3.44056400	-4.10184900	0.86433300
C	-2.94606300	2.09717100	-0.31286400
C	-4.28294700	2.22595700	0.22183700

C	-4.61122100	1.01360600	0.74710300
C	-3.48994000	0.13464500	0.49254900
N	-2.49258600	0.81750100	-0.14157200
H	-4.86698500	3.13503800	0.20321400
H	-5.52686900	0.71698600	1.23832200
C	2.13818900	0.00784800	-1.61376000
C	3.18029500	-0.88657800	-2.06749700
C	2.61387900	-2.12091900	-2.19089900
C	1.25130400	-1.99800500	-1.73194800
N	0.98568700	-0.69196200	-1.39887200
H	4.19923400	-0.59303400	-2.27254200
H	3.07150100	-3.04314900	-2.51988100
C	1.18971800	2.28052500	-1.37956000
C	1.27656500	3.71255200	-1.56259400
C	0.00600800	4.19410500	-1.47184900
C	-0.84415500	3.06128900	-1.17726100
N	-0.10672500	1.91404000	-1.14987800
H	2.19325500	4.25006800	-1.76048100
H	-0.33935300	5.21388700	-1.56478000
C	0.38424100	-3.07609000	-1.52679000
C	-2.20518100	3.15805600	-0.84945100
C	-3.49228700	-1.24259600	0.77031300
C	2.27683900	1.40744000	-1.50250300
Fe	-0.73025900	0.06259700	-0.72313100
Cl	-1.61463700	-0.08111000	-2.91460100
O	-0.12374100	0.27693900	0.88588500
C	2.83872700	0.93453900	5.93255600
C	3.95167300	0.84736800	5.12413000
C	3.88057000	0.17117800	3.87740700
C	2.62265000	-0.40878000	3.48169300
C	1.48545800	-0.29981600	4.34009500
C	1.61270900	0.35901300	5.54776800
C	4.96208600	0.07091900	2.93943000
C	2.50202300	-1.08793000	2.21926900
C	3.60200000	-1.15244800	1.36776300
C	4.81666200	-0.55830500	1.71531900
C	1.21844700	-1.65781800	1.82037800
C	0.29066900	-2.04681900	2.95280500
C	0.14359200	-0.85651300	3.90694400
H	-0.41015200	-0.06983700	3.37598600
H	-0.68224200	-2.34534600	2.55038000
H	2.91147700	1.45352800	6.88459800
H	4.88590200	1.28771600	5.43864400
H	0.75027900	0.43991500	6.20525600

H	5.65750200	-0.57976400	1.03341800
H	3.50892300	-1.65429800	0.41143200
H	0.58397200	-0.66155300	1.26166500
H	1.28056500	-2.36880800	0.99930800
N	6.28049200	0.65424600	3.19583600
O	6.67938200	0.75109800	4.35966300
O	6.94843500	1.00680400	2.21579600
C	-4.67817300	-1.80029400	1.49433700
C	-5.76801300	-2.31109900	0.76113800
C	-4.70604100	-1.78027700	2.90211600
C	-6.87083700	-2.81099600	1.46120500
C	-5.82857300	-2.29139500	3.56027800
C	-6.91866600	-2.81570200	2.85866500
H	-7.71666100	-3.20096600	0.89856300
H	-5.85305100	-2.27570300	4.64812200
C	-2.88003200	4.48092100	-1.02187400
C	-3.47378300	4.78141000	-2.26311300
C	-2.91940500	5.40288600	0.04142600
C	-4.10815600	6.01809800	-2.41704800
C	-3.56337200	6.62783800	-0.15826200
C	-4.16107400	6.95471400	-1.37990900
H	-4.57336800	6.25414300	-3.37205800
H	-3.59942000	7.34329400	0.66097600
C	3.65642000	1.97832000	-1.49645100
C	4.42012300	2.08464500	-2.67503600
C	4.19621500	2.36552500	-0.24860600
C	5.75322900	2.49831000	-2.57213300
C	5.53773600	2.74899700	-0.19282800
C	6.33736700	2.80451700	-1.33945700
H	6.35016800	2.57703900	-3.47864800
H	5.97631300	2.98578500	0.77252700
C	0.76405700	-4.41486500	-2.07590000
C	0.31046000	-4.75216200	-3.36832100
C	1.54393200	-5.31720200	-1.32864800
C	0.66082100	-5.99860300	-3.89505100
C	1.86908900	-6.55389100	-1.89624600
C	1.44184400	-6.91116500	-3.17826400
H	0.31196600	-6.26369900	-4.89115400
H	2.47019400	-7.25483100	-1.32055400
C	2.01854100	-4.96831400	0.06343900
H	2.66552900	-4.08310000	0.05676600
H	1.17567000	-4.74221000	0.72739400
H	2.58481200	-5.79273100	0.50685300
C	-0.54874800	-3.79080700	-4.15723700

H	-1.50386600	-3.60343500	-3.65259700
H	-0.07330800	-2.80952600	-4.26334800
H	-0.76125200	-4.18184100	-5.15673800
C	1.83295300	-8.23772000	-3.78684300
H	2.71819500	-8.13123300	-4.42797000
H	2.07434400	-8.97837500	-3.01704000
H	1.02938100	-8.64493600	-4.41048900
C	-3.54344900	-1.21838800	3.68763100
H	-2.63376800	-1.80664700	3.52366500
H	-3.31002100	-0.19202000	3.38196800
H	-3.75464000	-1.21601900	4.76130600
C	-5.75182600	-2.31050700	-0.75066700
H	-5.52154400	-1.31543800	-1.14837300
H	-4.98255800	-2.98708600	-1.14172100
H	-6.71811000	-2.62622800	-1.15514100
C	-8.10670900	-3.39267600	3.59257100
H	-7.95211900	-4.45654600	3.81718300
H	-8.27686900	-2.88131400	4.54636400
H	-9.02288600	-3.31570900	2.99731700
C	-2.27735900	5.07250100	1.36962100
H	-2.72309000	4.17527700	1.81576000
H	-1.20655700	4.86611100	1.25261600
H	-2.38901500	5.89735200	2.07974600
C	-3.42408000	3.78456100	-3.39818100
H	-2.39117200	3.57204900	-3.69820000
H	-3.85694100	2.82035900	-3.10809200
H	-3.96500500	4.15563400	-4.27389700
C	-4.82174900	8.29852900	-1.58285000
H	-4.09998100	9.04114400	-1.94861800
H	-5.63037800	8.24118700	-2.31947300
H	-5.24036700	8.68587000	-0.64754700
C	3.34410700	2.40545600	1.00048100
H	2.66077400	3.26361000	0.96972300
H	2.71886300	1.51601200	1.11452100
H	3.96568900	2.50286200	1.89366700
C	3.81102600	1.79340300	-4.02992800
H	3.62855200	0.72357900	-4.18349500
H	2.84247400	2.29402900	-4.14304700
H	4.46780700	2.13847000	-4.83435000
C	7.78716700	3.21480200	-1.23399200
H	8.27179000	2.71884900	-0.38539600
H	8.34502900	2.96508300	-2.14257100
H	7.88238000	4.29689700	-1.07379500
H	0.70528000	-2.91499400	3.48903600

H	-0.44679600	-1.12878300	4.78952300
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C	-0.46745300	-2.83132800	-1.23743400
C	-1.29853400	-4.00223800	-1.10532900
C	-2.50939900	-3.57233800	-0.65236000
C	-2.42481300	-2.13571800	-0.54028300
N	-1.16953800	-1.70918200	-0.89332200
H	-0.97450800	-5.01179400	-1.31273200
H	-3.39055200	-4.15485000	-0.42392200
C	-2.87241700	2.13086000	-0.69952700
C	-4.26598300	2.19010500	-0.31777500
C	-4.64259200	0.91630800	-0.02494800
C	-3.48438500	0.08080300	-0.25556100
N	-2.42152900	0.84213700	-0.65441300
H	-4.85502200	3.09531300	-0.28106500
H	-5.60828700	0.55370300	0.29640100
C	2.45109600	0.31715900	-1.41341300
C	3.60485500	-0.51953000	-1.65707300
C	3.14266200	-1.78877900	-1.82506300
C	1.71647600	-1.74193400	-1.61289800
N	1.31942600	-0.45047700	-1.36507200
H	4.62455200	-0.17035900	-1.70587700
H	3.70303700	-2.68523100	-2.04746900
C	1.34638200	2.52901400	-1.35802400
C	1.37709300	3.96251300	-1.54219400
C	0.08496500	4.38677800	-1.50857300
C	-0.72770600	3.21349600	-1.27687000
N	0.05880600	2.09549900	-1.22327500
H	2.27847700	4.54107200	-1.68640700
H	-0.30095000	5.39071600	-1.61255900
C	0.88519900	-2.86669500	-1.60851300
C	-2.10530600	3.25395800	-1.03269200
C	-3.49953200	-1.31689600	-0.16634000
C	2.49298000	1.72389100	-1.32954700
Fe	-0.53269800	0.18602200	-0.96227200
Cl	-1.01094500	0.15680800	-3.28452000
O	-0.28308600	0.35851400	0.73353200
H	0.32442300	-0.32349400	1.55512700
C	4.10044100	0.98788000	3.63427000
C	4.88105000	0.55217900	2.56354700
C	4.37204000	-0.32295900	1.60165600
C	3.05048400	-0.72876900	1.69935100
C	2.21555800	-0.27372800	2.74042100

C	2.77474900	0.57249700	3.71672000
H	4.52949600	1.65603400	4.37109500
H	4.99864600	-0.64106500	0.77951400
H	2.63637300	-1.38515900	0.94306000
H	2.15865000	0.91689100	4.53981700
C	0.78979200	-0.72410000	2.76416900
C	-0.17115600	0.06699600	3.60289100
C	-0.28399700	1.45956700	3.40300000
C	-1.02284900	-0.53682400	4.54314300
C	-1.21187500	2.21274300	4.11631200
C	-1.95328100	0.21989000	5.25723000
H	-0.95533200	-1.60520400	4.71732200
C	-2.05564600	1.59591900	5.04567300
H	-1.28525400	3.28230300	3.93732600
H	-2.59799800	-0.27009500	5.98239300
H	-2.78472700	2.18283200	5.59797100
C	-4.76871600	-1.97302100	0.28110600
C	-5.70624000	-2.39682500	-0.68416200
C	-5.02359800	-2.14447600	1.65527500
C	-6.88653500	-3.00625700	-0.25122000
C	-6.22213700	-2.75668800	2.04139800
C	-7.16348100	-3.19539100	1.10736900
H	-7.61104000	-3.33598700	-0.99330800
H	-6.42283600	-2.89159400	3.10253900
C	1.46720300	-4.18144900	-2.02121200
C	2.23027600	-4.94373600	-1.11590200
C	1.24067000	-4.63587000	-3.33699200
C	2.75797100	-6.16510600	-1.54792900
C	1.79330000	-5.85973900	-3.72523400
C	2.55074100	-6.64072500	-2.84592200
H	3.34633100	-6.75821400	-0.85038700
H	1.62852100	-6.21084700	-4.74200200
C	-2.78640600	4.58437000	-1.06270900
C	-3.39623300	5.02243300	-2.25292500
C	-2.81812600	5.37621100	0.10172900
C	-4.03150900	6.26837500	-2.25858100
C	-3.46710100	6.61333100	0.05139800
C	-4.07543600	7.07850300	-1.11955200
H	-4.50517100	6.61250800	-3.17579200
H	-3.49916500	7.22846100	0.94860400
C	3.82082800	2.38110700	-1.14484500
C	4.10413100	2.93052500	0.13222700
C	4.80558800	2.38603000	-2.15087000
C	5.40256900	3.35614600	0.40370200

C	6.09663700	2.82600700	-1.82876500
C	6.42693900	3.26666900	-0.54690600
H	5.63906900	3.72050000	1.40048200
H	6.86423700	2.80436700	-2.60013200
C	3.04238200	3.04860800	1.20265700
H	2.32794500	3.84521000	0.96414000
H	2.46514400	2.12599100	1.30961700
H	3.49470000	3.28019900	2.16956200
C	4.50876200	1.94424500	-3.56967700
H	4.94291600	0.96183400	-3.79182300
H	3.43515600	1.87722700	-3.76485600
H	4.93929300	2.65518500	-4.28391900
C	7.84321100	3.60507700	-0.15405100
H	8.19397100	2.88147400	0.59259700
H	8.52335200	3.57383800	-1.01122000
H	7.90879900	4.60103400	0.30036300
C	-2.16798300	4.89089800	1.37819300
H	-2.58421600	3.92876000	1.70014000
H	-1.09129000	4.73381400	1.23899800
H	-2.30520900	5.61187800	2.19010900
C	-3.37165900	4.15439800	-3.49015000
H	-2.34842000	3.87450300	-3.76585200
H	-3.91177100	3.21423700	-3.32514500
H	-3.82982600	4.66566000	-4.34212700
C	-4.73925800	8.43552500	-1.15896100
H	-4.01732100	9.22028100	-1.42203600
H	-5.54131600	8.46877800	-1.90415700
H	-5.16749100	8.70152700	-0.18632100
C	-4.02714600	-1.70817700	2.70638900
H	-3.23424500	-2.45459300	2.83666900
H	-3.53330100	-0.76603600	2.45106300
H	-4.51352200	-1.57858100	3.67829400
C	-5.44231300	-2.18938700	-2.15840500
H	-5.24771200	-1.13416000	-2.38312400
H	-4.55767400	-2.74530600	-2.49043600
H	-6.29496500	-2.51563900	-2.76138200
C	-8.46428900	-3.82471000	1.54931500
H	-8.37755200	-4.26914400	2.54647200
H	-9.26911200	-3.07868800	1.59198500
H	-8.78681300	-4.60836200	0.85471500
C	0.41484200	-3.82049700	-4.30629300
H	-0.64280300	-3.81275200	-4.01591600
H	0.72917400	-2.77135800	-4.33115600
H	0.48395600	-4.22672600	-5.31994300

C	2.49343600	-4.45245500	0.28836200
H	3.27663200	-3.68368500	0.29975100
H	1.60310900	-4.00592100	0.73780000
H	2.82193600	-5.26793900	0.93870900
C	3.10485000	-7.97788200	-3.27977300
H	4.01908800	-8.23116000	-2.73210800
H	2.38110000	-8.78331700	-3.09586200
H	3.33616500	-7.98805700	-4.35046800
C	0.61954300	-2.21749200	2.81891100
C	-0.51213800	-2.81567300	2.24458200
C	1.52993800	-3.03652200	3.50765400
C	-0.73907800	-4.18577800	2.36562900
H	-1.20766000	-2.18991300	1.69976500
C	1.30280500	-4.40806500	3.63293900
H	2.41167500	-2.59284400	3.95992500
C	0.16663800	-4.98821800	3.06503500
H	-1.61575700	-4.62358200	1.89885400
H	2.01525800	-5.02245900	4.17732100
H	-0.00718700	-6.05677800	3.15827500
H	0.33982300	1.93715500	2.65577000
N	6.24082600	1.06647900	2.40720200
O	6.93821400	0.59655000	1.50562400
O	6.60970100	1.96542100	3.16887300

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C	-2.82591600	2.24603100	-0.01355100
C	-4.11744200	2.50838200	-0.60745700
C	-4.84650300	1.36703900	-0.47471700
C	-3.98664800	0.39868000	0.16875500
N	-2.76639200	0.94994900	0.42912000
H	-4.41420900	3.45311900	-1.03993600
H	-5.86408400	1.17592700	-0.78406400
C	-1.62498600	-2.96598700	1.33714900
C	-2.66093000	-3.97234900	1.25604600
C	-3.82664600	-3.31244800	1.01696800
C	-3.49062300	-1.90838400	0.90875700
N	-2.15741100	-1.72494100	1.15685300
H	-2.49327000	-5.03295900	1.38056700
H	-4.82099300	-3.71752700	0.89459300
C	0.96778700	2.00425800	2.00334800
C	1.21587800	3.42286500	2.07457200
C	0.22561200	4.02948700	1.36046200
C	-0.64195600	2.97982600	0.88179900
N	-0.17107300	1.75658000	1.27760700

H	2.05507500	3.87434600	2.58388500
H	0.07312600	5.08351500	1.17817100
C	1.58747500	-0.34478200	2.42787600
C	2.54937500	-1.36241100	2.77308400
C	2.00589900	-2.55535800	2.40351000
C	0.67884400	-2.27294100	1.90500400
N	0.45776900	-0.92268800	1.90904700
H	3.51748400	-1.17187800	3.21326400
H	2.44830000	-3.53740600	2.46935100
C	-1.84278200	3.21968300	0.19247900
C	-0.26788400	-3.25342500	1.54991200
C	-4.36929500	-0.92343500	0.44887100
C	1.81442900	1.03096200	2.54891600
Fe	-1.13444400	0.00431900	1.13159400
Cl	-1.94414300	0.38983600	3.32324800
O	-0.72631300	-0.41080400	-0.47881300
H	0.22829400	-0.05966500	-1.20122300
C	1.01612400	0.04691500	-2.25648000
C	1.76792500	-1.24502000	-2.14830800
C	1.79319300	-2.21025100	-3.17088600
C	2.43475200	-1.53768300	-0.94237700
C	2.43069600	-3.43275700	-2.99212000
H	1.30494800	-1.99795800	-4.11505800
C	3.07540200	-2.75044600	-0.74754600
H	2.41592600	-0.81054300	-0.13901800
C	3.04865800	-3.70043100	-1.77049600
H	2.43986800	-4.18429700	-3.77194700
H	3.55896100	-2.98485800	0.19043900
C	-0.05528400	0.15214400	-3.30444100
C	-1.07679400	-0.81731600	-3.37590300
C	-0.10975100	1.23912200	-4.19238200
C	-2.10381400	-0.70340200	-4.30847700
H	-1.07057600	-1.64212800	-2.67276600
C	-1.14374400	1.35519700	-5.12396800
H	0.66674800	1.99701600	-4.15198200
C	-2.14463600	0.38519900	-5.18674800
H	-2.88174700	-1.46161500	-4.34391000
H	-1.16288200	2.20498500	-5.80146600
C	1.75639900	1.30890500	-1.99690500
C	3.05739700	1.60119500	-2.25339800
H	1.12899300	2.09857800	-1.59277300
C	3.94337200	0.66029700	-2.99972500
C	5.11130800	0.14784700	-2.41522600
C	3.62584100	0.28486200	-4.31273600

C	5.92079400	-0.74718000	-3.11284200
H	5.36949300	0.44110300	-1.40232200
C	4.44341000	-0.59905500	-5.01789400
H	2.72267700	0.67705800	-4.77111100
C	5.58925700	-1.12358500	-4.41764800
H	6.80986500	-1.15349300	-2.63798600
H	4.18055000	-0.88297900	-6.03352000
H	6.22144000	-1.82012400	-4.96162400
C	3.63113000	2.91686800	-1.87304000
C	4.73411400	3.45136300	-2.56426900
C	3.08488000	3.67453300	-0.82036900
C	5.25708100	4.69900300	-2.22320200
H	5.17712200	2.88724800	-3.37849300
C	3.60457400	4.91992900	-0.48126900
H	2.26442400	3.27275200	-0.24099700
C	4.69566100	5.44153100	-1.18210600
H	6.10662700	5.09210200	-2.77563700
H	3.16349300	5.47358200	0.34357500
H	5.10854000	6.41037500	-0.91435800
C	-5.78233700	-1.31720300	0.16050200
C	-6.76193800	-1.13919400	1.15603800
C	-6.11635500	-1.85619400	-1.09638700
C	-8.07788900	-1.51657500	0.87268900
C	-7.44607700	-2.21617400	-1.33758800
C	-8.44013700	-2.05372900	-0.36725900
H	-8.83868800	-1.38784400	1.64009200
H	-7.71081400	-2.63472700	-2.30658900
C	-2.13478300	4.62545600	-0.23080700
C	-1.57682600	5.13245100	-1.41992100
C	-2.95879000	5.43552100	0.57904000
C	-1.87257800	6.44763200	-1.79391100
C	-3.21927900	6.74640200	0.17004800
C	-2.68816800	7.27095600	-1.01318700
H	-1.45189100	6.83684200	-2.71896500
H	-3.85363700	7.37408900	0.79286000
C	3.03147400	1.48902400	3.28791100
C	4.28273300	1.54210300	2.64620700
C	2.89522300	1.87832000	4.63732200
C	5.39013500	1.99650400	3.37136300
C	4.02999400	2.31892000	5.32307700
C	5.28594300	2.38528200	4.70909000
H	6.35654900	2.04945700	2.87376500
H	3.92988500	2.62128500	6.36366600
C	0.22162600	-4.63961100	1.29365800

C	0.29010700	-5.05039000	-0.06314400
C	0.71583800	-5.47417400	2.31238900
C	0.95608400	-6.23479700	-0.36885900
C	1.37778600	-6.65641700	1.95377300
C	1.55254500	-7.02726000	0.62030600
H	1.06753600	-6.52158500	-1.41146200
H	1.78671100	-7.28692900	2.74118700
C	-3.54685000	4.90414800	1.86729000
H	-4.31173000	4.14300400	1.67285700
H	-2.78380000	4.42468800	2.49079300
H	-4.00939700	5.70766900	2.44832700
C	-0.66067000	4.28749900	-2.27424700
H	0.33888500	4.22101200	-1.82588500
H	-1.03236500	3.26471600	-2.39206000
H	-0.54225800	4.71970200	-3.27288800
C	-2.96437800	8.70043400	-1.41745100
H	-2.25262800	9.38888200	-0.94244800
H	-2.87565400	8.83603600	-2.50060000
H	-3.96953500	9.01580500	-1.11654200
C	4.45142200	1.09857300	1.21114200
H	4.59866100	0.01233700	1.14679100
H	3.57819900	1.33642700	0.59994800
H	5.31861400	1.58256300	0.75152300
C	1.54737000	1.83399700	5.32078400
H	0.86229800	2.57879400	4.89834500
H	1.05464700	0.86427500	5.18929500
H	1.64349200	2.03060600	6.39287300
C	6.50066700	2.84063600	5.48389800
H	6.95339100	2.00457400	6.03359800
H	7.27035000	3.25028400	4.82111500
H	6.24149900	3.60936400	6.22029300
C	-0.31125400	-4.22046700	-1.17541700
H	-1.40696700	-4.26371000	-1.15418300
H	-0.03475200	-3.16554100	-1.09223700
H	0.02230600	-4.58322600	-2.15027200
C	0.55002400	-5.13756400	3.78026000
H	1.51056400	-4.89861300	4.25294100
H	-0.11425000	-4.28369100	3.93683700
H	0.13141000	-5.99506100	4.31998400
C	2.39652100	-8.21163100	0.22109200
H	1.85860900	-8.87812600	-0.46368800
H	3.29070500	-7.85479000	-0.30523000
H	2.71661200	-8.79622700	1.08953000
C	-5.05582200	-2.04437300	-2.15816500

H	-4.52755600	-1.10710500	-2.36906300
H	-4.29506200	-2.76556100	-1.83445600
H	-5.49337800	-2.40858100	-3.09296500
C	-6.39005000	-0.54750600	2.49620200
H	-5.58118500	-1.11041200	2.97609200
H	-6.02242100	0.47990100	2.38570400
H	-7.24825600	-0.53134500	3.17473400
C	-9.87668900	-2.42107600	-0.65906600
H	-10.44224200	-1.54940600	-1.01481200
H	-9.94525500	-3.19254400	-1.43349000
H	-10.38535100	-2.79301400	0.23715900
H	-2.95034400	0.47480900	-5.91048700
N	3.62878500	-5.01898300	-1.52963800
O	4.20786300	-5.21304000	-0.45822100
O	3.48607700	-5.88369500	-2.40064100

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C	-1.91927600	2.62308900	0.07039200
C	-1.73377700	4.05137700	-0.03983800
C	-0.47218400	4.24803200	-0.50654300
C	0.12727400	2.94315900	-0.64193300
N	-0.77488300	1.96964500	-0.28843300
H	-2.48586400	4.79761100	0.17040500
H	0.00801600	5.18630800	-0.74181700
C	2.40749600	-0.68834800	-0.62951900
C	3.69565500	-0.09262000	-0.90877000
C	3.46674900	1.21402600	-1.19765400
C	2.05399800	1.43903100	-1.01687200
N	1.42515300	0.26854600	-0.68993500
H	4.64953000	-0.59437300	-0.87749700
H	4.19516500	1.97130600	-1.44741300
C	-3.19114000	-1.46147900	-0.26943100
C	-4.58532900	-1.26090700	0.06144400
C	-4.72047400	0.04478200	0.40740300
C	-3.41942800	0.65396900	0.24059400
N	-2.50751000	-0.29015300	-0.15930100
H	-5.34489200	-2.02887800	0.05994400
H	-5.61615400	0.55293500	0.73165900
C	-1.24934700	-2.95645800	-0.61307700
C	-0.63861100	-4.26483500	-0.71395100
C	0.69795300	-4.08189100	-0.57125000
C	0.91022300	-2.65455600	-0.44552300
N	-0.27867700	-1.99510200	-0.48001700
H	-1.16757500	-5.19433500	-0.86189600

H	1.47918200	-4.82771300	-0.59291600
C	-3.14437700	2.01373200	0.39711100
C	2.18210200	-2.05492800	-0.41121800
C	1.44966900	2.70303300	-1.02331800
C	-2.62235900	-2.71638100	-0.55404200
Fe	-0.52551400	-0.00402800	-0.35130400
Cl	-0.86621800	0.02513500	-2.67154700
O	-0.38655500	-0.16290400	1.36087300
H	0.16509500	0.74458700	1.91516300
C	4.47235400	0.93022300	2.00231800
C	4.60450300	-0.36972000	2.49527400
C	3.56719800	-1.00231200	3.18845300
C	2.35274900	-0.34751200	3.31119600
C	2.16238900	0.94663600	2.77130900
C	3.25862000	1.58402700	2.15222000
H	5.30364600	1.39055300	1.48384700
H	3.70842500	-2.00656200	3.56505600
H	3.13315300	2.58721200	1.76015000
C	0.83230900	1.54353200	2.74974200
H	0.75553700	2.54921000	2.33642100
H	0.20665400	1.37887200	3.62831900
C	2.30773100	3.87273200	-1.36058600
C	2.69347200	4.79460400	-0.38383500
C	2.77901200	4.07600400	-2.66127700
C	3.50996600	5.88251100	-0.67684100
C	3.59665000	5.15892400	-2.98029000
C	3.95987300	6.06456300	-1.98441700
C	-4.22973200	2.90635200	0.89079500
C	-5.38390000	3.16444300	0.14489000
C	-4.10668100	3.54330400	2.13061200
C	-6.38546700	4.01066800	0.61580600
C	-5.09365200	4.39444200	2.62013800
C	-6.23759300	4.62706000	1.85750800
C	-3.55577200	-3.86434900	-0.72309700
C	-4.42179600	-3.91951200	-1.82122600
C	-3.62723500	-4.90502600	0.20845200
C	-5.31518700	-4.97385900	-1.99638000
C	-4.51118800	-5.96965900	0.05178800
C	-5.35736800	-6.00204600	-1.05575100
C	3.34434400	-2.93836500	-0.12742700
C	4.40547900	-3.14529600	-1.01576200
C	3.42150300	-3.58376100	1.11425900
C	5.52086000	-3.90106000	-0.66350200
C	4.52747200	-4.33578400	1.49018700

C	5.58741200	-4.48876500	0.59895200
H	1.51555100	-0.85234100	3.78298800
N	5.82388100	-1.11711700	2.20703100
O	6.00411500	-2.18678000	2.79729500
O	6.59430000	-0.65820000	1.35722100
F	2.42260300	-3.45175000	2.00076000
F	4.58615200	-4.88088500	2.70581100
F	6.65566900	-5.20021700	0.94800200
F	6.52238600	-4.06946900	-1.53037200
F	4.37314100	-2.60262800	-2.24079800
F	-2.83460200	-4.89212300	1.28816200
F	-4.55884200	-6.95155200	0.95708200
F	-6.20823000	-7.01643500	-1.21418900
F	-6.12792900	-5.00651200	-3.05567100
F	-4.40499400	-2.94190100	-2.73172600
F	-3.01437500	3.33809900	2.87827900
F	-4.95366000	4.98504800	3.81030800
F	-7.19025700	5.43924700	2.31609000
F	-7.47937000	4.23945300	-0.11573700
F	-5.54781700	2.59282800	-1.05364600
F	2.28496000	4.63113700	0.88855300
F	3.86633200	6.74416800	0.27988200
F	4.74178000	7.10280800	-2.27985600
F	4.03087000	5.33553800	-4.22996900
F	2.45108900	3.21696900	-3.62939100

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C	-1.70169000	2.17576800	-0.59754500
C	-1.91087200	3.60369800	-0.68166000
C	-0.68402800	4.17647700	-0.77008000
C	0.28712000	3.10839500	-0.68188500
N	-0.35848000	1.90421300	-0.59786700
H	-2.87567900	4.08844900	-0.71242000
H	-0.44938800	5.22522800	-0.87430700
C	3.42290500	0.31963300	0.21503400
C	4.47679600	1.29458400	0.38289600
C	3.96221000	2.49648300	0.01893300
C	2.57534600	2.27417800	-0.32395500
N	2.27943900	0.94297900	-0.20763500
H	5.47896100	1.07940100	0.72259900
H	4.45635900	3.45703100	0.01561700
C	-1.52795500	-2.08284500	-1.11588500
C	-2.93281300	-2.28119500	-1.37355800
C	-3.54631400	-1.08824500	-1.15653800

C	-2.51183100	-0.13698200	-0.82515100
N	-1.29464900	-0.76588600	-0.79982100
H	-3.38572200	-3.21896700	-1.66119900
H	-4.59916200	-0.86409000	-1.23300100
C	0.74231500	-2.91831100	-0.68182600
C	1.68400700	-3.98702500	-0.46442800
C	2.82240800	-3.41884600	0.01676100
C	2.59481800	-1.99537400	0.06306100
N	1.31588500	-1.71740000	-0.35104200
H	1.48790700	-5.03381600	-0.64625400
H	3.74706200	-3.90931100	0.28391600
C	-2.72931600	1.23358300	-0.64048300
C	3.57530600	-1.05661500	0.39517200
C	1.66911700	3.29778800	-0.60860600
C	-0.58081600	-3.10386300	-1.08543000
Fe	0.47960800	0.08478100	-0.44590500
Cl	0.85221600	0.15215900	-2.71727900
O	0.26115500	0.20218600	1.20187800
C	4.87789900	-1.57165800	0.90228900
C	4.96983500	-2.17079700	2.16250100
C	6.04819000	-1.50021500	0.13968400
C	6.17172300	-2.67418000	2.65332300
C	7.26388500	-1.99040400	0.61175200
C	7.32328400	-2.58102700	1.87309400
C	-1.02285700	-4.49056500	-1.40338900
C	-1.78282000	-5.23316000	-0.49698100
C	-0.67534600	-5.10510400	-2.60936400
C	-2.20051100	-6.53175500	-0.77305800
C	-1.07689300	-6.40630200	-2.90834100
C	-1.84302900	-7.11863700	-1.98679400
C	-4.13059800	1.73179800	-0.54440900
C	-4.61047000	2.26302600	0.65658400
C	-5.01259300	1.71124600	-1.62926900
C	-5.91260600	2.73545700	0.79153400
C	-6.32172300	2.17338900	-1.51944400
C	-6.77253800	2.68619200	-0.30344500
C	2.21086000	4.67774800	-0.75725400
C	1.98318800	5.66897300	0.20227600
C	2.99540200	5.02083300	-1.86365500
C	2.49789200	6.95585000	0.06618500
C	3.52579500	6.30008500	-2.01778800
C	3.27329800	7.26997000	-1.04895200
C	-4.39147000	-0.11802300	3.27991800
C	-3.29784300	0.28744100	4.04703200

C	-3.05687700	-1.74509500	2.14097600
C	-4.28924300	-1.13591300	2.33267000
H	-5.15929500	-1.42306000	1.75573200
C	-1.91956400	-1.33638500	2.86540300
C	-2.06788700	-0.31736200	3.82952300
C	0.47654000	-2.06959000	3.56233500
C	-0.59094700	-1.87718400	2.49678300
H	1.42125000	-2.36786200	3.10003100
H	-0.16214000	-1.00178400	1.79036300
H	-0.67088400	-2.73313200	1.81964400
H	0.17672300	-2.85184100	4.27255700
H	-3.41965400	1.08763800	4.76640500
H	0.66167200	-1.15221400	4.12951900
H	-1.20452500	0.02789400	4.38780100
H	-2.96022100	-2.53263800	1.40306800
N	-5.66796200	0.58749500	3.43056300
O	-5.79180800	1.36288400	4.37580900
O	-6.54018100	0.36995000	2.58359900
F	-3.80637600	2.32187900	1.72947300
F	-6.33546100	3.22197400	1.95786300
F	-8.02416000	3.13035900	-0.19184200
F	-7.14447800	2.13496300	-2.57250300
F	-4.60615400	1.22687200	-2.81140800
F	1.24891000	5.39089100	1.28820800
F	2.26171700	7.88478700	0.99817700
F	3.77427800	8.49861200	-1.18759400
F	4.27029000	6.60271600	-3.08520700
F	3.25685000	4.10751000	-2.80410500
F	3.87852400	-2.27508000	2.93690600
F	6.22906300	-3.23916700	3.86320600
F	8.48086900	-3.05685700	2.33385400
F	8.36698800	-1.90581200	-0.13724900
F	6.01801000	-0.94481700	-1.07728500
F	-2.12505300	-4.69393600	0.68822800
F	-2.92817600	-7.21795300	0.11334300
F	-2.23342700	-8.36329200	-2.26408200
F	-0.73593100	-6.97263300	-4.06867100
F	0.06195900	-4.44296500	-3.50506500

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C	-0.13251900	-2.88480600	-0.84433500
C	-0.84436600	-4.13234800	-0.73800000
C	-2.05689800	-3.84945300	-0.18565500
C	-2.11455700	-2.41955300	-0.00939300

N	-0.93021600	-1.85869700	-0.40569600
H	-0.45063500	-5.09838000	-1.01954000
H	-2.85885900	-4.53571900	0.04573800
C	-3.04253300	1.72978500	-0.37153900
C	-4.43240500	1.65087400	0.02002900
C	-4.65517900	0.37648800	0.43481200
C	-3.42045000	-0.34807700	0.23781000
N	-2.45879900	0.50303400	-0.24236100
H	-5.12736900	2.47800400	0.01173900
H	-5.57467500	-0.04460800	0.81349900
C	2.46764800	0.50668400	-0.56833600
C	3.70780400	-0.21220600	-0.75770200
C	3.37894300	-1.48572300	-1.09846100
C	1.94278300	-1.58334800	-1.02893600
N	1.41204100	-0.36171100	-0.69811800
H	4.69978900	0.19765600	-0.64887800
H	4.04943900	-2.29865600	-1.33552400
C	1.14298000	2.58484500	-0.53425900
C	1.03481600	4.01411400	-0.72760500
C	-0.28212300	4.29048300	-0.90578900
C	-0.99738800	3.04225400	-0.76264000
N	-0.10029400	2.02177500	-0.56957400
H	1.86842500	4.70020900	-0.76299000
H	-0.73642900	5.25070400	-1.09986300
C	1.21732200	-2.76636800	-1.18182500
C	-2.38621600	2.91974900	-0.70763700
C	-3.25477200	-1.72262500	0.40990900
C	2.35763900	1.89657800	-0.42662400
Fe	-0.50932600	0.07066100	-0.42589600
Cl	-0.79872000	0.08429100	-2.71823000
O	-0.40042600	0.23546300	1.23069900
H	0.15914000	-0.81637500	1.97064600
C	3.54941100	0.99290900	3.14441900
C	4.58239100	0.22278500	2.60967700
C	4.39070800	-1.11253500	2.25931800
C	3.12906800	-1.67261300	2.41316100
C	2.04055500	-0.90989600	2.88114800
C	2.28478500	0.43172100	3.24927000
H	3.73069500	2.02336000	3.41599000
H	5.21337600	-1.68412900	1.84831100
H	2.98719800	-2.70431300	2.12456100
C	0.64503700	-1.45056200	2.88163400
C	-4.35858700	-2.52003300	1.00970000
C	-4.18494300	-3.13040300	2.25645800

C	-5.58417200	-2.71683300	0.36630600
C	-5.18323600	-3.89805800	2.84914800
C	-6.60119500	-3.47658600	0.94097500
C	-6.39760900	-4.07008400	2.18583700
C	1.92406600	-3.99129400	-1.65174100
C	1.70840700	-4.48243200	-2.94363000
C	2.79819100	-4.70788700	-0.83205200
C	2.34323500	-5.63483400	-3.40433500
C	3.44817000	-5.85843800	-1.26922700
C	3.21744900	-6.32204000	-2.56370200
C	3.58385900	2.70325100	-0.18472000
C	4.66854300	2.74924500	-1.06830800
C	3.69673400	3.45954500	0.98925800
C	5.83552800	3.44713100	-0.76633100
C	4.85112200	4.16150900	1.31390400
C	5.93123800	4.14841400	0.43426100
C	-3.22544800	4.13172900	-0.91713800
C	-4.08428100	4.22006500	-2.01865300
C	-3.21791000	5.20487900	-0.02039900
C	-4.89333700	5.33442500	-2.23037900
C	-4.01387600	6.33097600	-0.21481700
C	-4.85492600	6.39340700	-1.32479300
C	0.48225400	-2.92434600	2.53353600
H	-0.57819100	-3.17631200	2.45832000
H	0.96085700	-3.19135900	1.58973000
H	0.92265500	-3.55044200	3.32295900
C	-0.24397600	-1.04117000	4.05767500
H	0.10630300	-1.52412500	4.98029500
H	-0.25875700	0.03868900	4.22196700
H	-1.27207400	-1.36500600	3.87123200
H	1.46690400	1.05836400	3.58380900
N	5.86973000	0.85863300	2.32841800
O	6.64739600	0.26854300	1.57358200
O	6.09240000	1.96306500	2.83031900
F	-3.02580800	-2.98112700	2.92119600
F	-4.98779600	-4.46468300	4.04357600
F	-7.36363500	-4.80190100	2.74233300
F	-7.76308800	-3.64705600	0.30417700
F	-5.80447800	-2.16713400	-0.83380900
F	-2.43016200	5.16590800	1.06311500
F	-3.98482500	7.34296700	0.65845900
F	-5.62409800	7.46605200	-1.51877200
F	-5.70180300	5.39544800	-3.29242200
F	-4.14411000	3.21630200	-2.89922300

F	2.67783000	3.49469400	1.86507200
F	4.93433300	4.81899700	2.47183200
F	7.04665700	4.80967200	0.73490300
F	6.85733100	3.45624300	-1.62656800
F	4.60955000	2.10411700	-2.24171400
F	3.02944900	-4.29316000	0.42738500
F	4.27923500	-6.52083900	-0.45841800
F	3.83101200	-7.42463400	-2.99531800
F	2.12148400	-6.08303100	-4.64254700
F	0.87225800	-3.84475500	-3.76658900

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C	-1.66861100	-1.95184300	-1.28825100
C	-3.08613800	-2.05016400	-1.53748300
C	-3.61758600	-0.82553200	-1.28029800
C	-2.51845400	0.04578800	-0.93522900
N	-1.34668200	-0.66133000	-0.94651500
H	-3.60245300	-2.94867800	-1.84347100
H	-4.65351000	-0.52927400	-1.34043700
C	0.49957100	3.08445500	-0.79702600
C	-0.39682800	4.21840500	-0.85427900
C	-1.65836200	3.73172700	-0.73518400
C	-1.54801000	2.29160500	-0.67021000
N	-0.22705000	1.92861000	-0.70740800
H	-0.09263800	5.24934900	-0.95702300
H	-2.58732800	4.28315100	-0.73678000
C	2.42412100	-2.16390600	-0.03364300
C	2.54906800	-3.59980900	-0.08043100
C	1.39084200	-4.08218600	-0.60756800
C	0.53460100	-2.94776500	-0.84545200
N	1.18495400	-1.79348600	-0.49191400
H	3.42658800	-4.15652900	0.21471600
H	1.12688700	-5.11096800	-0.80606000
C	3.41494500	0.08487000	0.13305100
C	4.53457000	0.98271400	0.30843700
C	4.11791600	2.21248600	-0.08798700
C	2.72340100	2.08817900	-0.45032200
N	2.33035100	0.78375400	-0.32309100
H	5.51248700	0.70066100	0.66906200
H	4.68222400	3.13360200	-0.09833800
C	-0.79273600	-3.03514000	-1.26800000
C	1.89320000	3.17329300	-0.74075700
C	-2.63842800	1.42213700	-0.70274100
C	3.45647000	-1.29677100	0.33598200

Fe	0.48074700	0.05725600	-0.57682700
Cl	0.86074200	0.11879700	-2.84909200
O	0.24824400	0.16606900	1.06876900
H	-0.15829800	-1.07279300	1.63121600
C	0.21832800	-1.59558600	3.68804800
C	-0.46724800	-0.33093000	4.27053600
C	-0.58552500	-1.88034900	2.41595800
C	-1.93667700	-1.36078100	2.67900400
C	-3.12941800	-1.60410200	1.98959600
C	-4.25860700	-0.86413800	2.31909100
C	-4.17256400	0.09005400	3.33881100
C	-3.00144700	0.32205400	4.06777300
C	-1.87604800	-0.41178000	3.72472800
H	-3.16678400	-2.34405800	1.19985100
H	-2.99469000	1.07470700	4.84696300
H	-5.19770800	-0.99994700	1.79803600
H	0.02169900	0.57140600	3.87989500
H	1.28442700	-1.45973200	3.49021300
H	-0.48593400	-2.84980300	1.92154700
N	-5.35352800	0.91565800	3.62283900
O	-5.31915400	1.65497400	4.60401300
O	-6.31041700	0.82760900	2.84744300
C	-3.99590600	2.01063300	-0.52657700
C	-4.92697500	2.09399700	-1.56606200
C	-4.37782600	2.53148100	0.71424000
C	-6.19009500	2.64923200	-1.37681200
C	-5.63066800	3.09915200	0.92762200
C	-6.54205500	3.15319600	-0.12499400
C	2.53421000	4.50895400	-0.89783000
C	3.32749700	4.79140900	-2.01491700
C	2.39706000	5.51353800	0.06493800
C	3.95222200	6.02646400	-2.17672200
C	3.00669800	6.75733300	-0.07866700
C	3.78814100	7.01202100	-1.20472000
C	4.67941900	-1.90162900	0.93192200
C	5.90462000	-1.93212400	0.25878800
C	4.63068900	-2.48853400	2.20088100
C	7.03979400	-2.50767900	0.82576300
C	5.74966800	-3.07470200	2.78610600
C	6.95966500	-3.08187900	2.09350900
C	-1.33209000	-4.38635400	-1.58916000
C	-1.06946100	-5.00580600	-2.81332600
C	-2.10345200	-5.08934400	-0.66103000
C	-1.56506200	-6.27506700	-3.10945600

C	-2.61344600	-6.35520000	-0.93361300
C	-2.33982800	-6.94840100	-2.16610800
H	-0.43090300	-0.27908500	5.36385100
H	0.11172000	-2.44054400	4.38289500
F	-2.36590700	-4.54143000	0.54021300
F	-3.35023500	-7.00490600	-0.02733500
F	-2.81916800	-8.16236000	-2.44074700
F	-1.30445800	-6.84821800	-4.28723600
F	-0.32623600	-4.38027800	-3.73006900
F	-3.52340200	2.48866800	1.74813600
F	-5.95691400	3.58282600	2.12555300
F	-7.74819400	3.68935000	0.06086200
F	-7.06167100	2.71019800	-2.38873900
F	-4.61496500	1.62355100	-2.78234900
F	1.66067300	5.29049500	1.16235800
F	2.85675600	7.70064200	0.85684300
F	4.38006700	8.19875900	-1.35031400
F	4.70321100	6.27185200	-3.25425600
F	3.50473300	3.86157700	-2.95858200
F	3.47766600	-2.50283200	2.88874800
F	5.67242900	-3.62533400	4.00156200
F	8.03987300	-3.63841200	2.64346300
F	8.19858000	-2.52081100	0.16102000
F	6.00866100	-1.39527000	-0.96277900

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C	-1.71469200	-1.92900200	-1.27376400
C	-3.13340000	-2.01648300	-1.53103800
C	-3.66347900	-0.80171000	-1.23165200
C	-2.55936400	0.05794300	-0.86611300
N	-1.39302800	-0.64446400	-0.89717500
H	-3.65445900	-2.90104000	-1.86605400
H	-4.69883700	-0.50158700	-1.28340400
C	0.45541200	3.09010500	-0.79811700
C	-0.43825500	4.22975400	-0.82702700
C	-1.69674000	3.74788000	-0.66599000
C	-1.58812800	2.30662000	-0.60679300
N	-0.26674400	1.94017200	-0.68633100
H	-0.13434400	5.25960300	-0.94013500
H	-2.62381800	4.30174700	-0.63675900
C	2.36121400	-2.14920300	0.04907700
C	2.47242400	-3.58728600	0.03632900
C	1.32092700	-4.06785700	-0.50749500
C	0.48037900	-2.92887600	-0.78412300

N	1.12871300	-1.77847600	-0.43352700
H	3.33892900	-4.14771500	0.35585000
H	1.05296600	-5.09823100	-0.69086200
C	3.37333500	0.09907400	0.13395600
C	4.50468300	0.99221400	0.26288500
C	4.09153200	2.21257400	-0.16458900
C	2.68855800	2.08872700	-0.49599800
N	2.28973100	0.78902500	-0.32522200
H	5.48661400	0.71453100	0.61523600
H	4.66300200	3.12808500	-0.21156600
C	-0.83962500	-3.01149300	-1.25391100
C	1.85597100	3.17058000	-0.78466400
C	-2.67555800	1.43740200	-0.61469400
C	3.39981000	-1.27978600	0.38886900
Fe	0.43568000	0.07302900	-0.53391000
Cl	0.79233200	0.08966300	-2.82889800
O	0.21693500	0.19959300	1.11172000
H	0.12327400	-0.91448000	1.84356000
C	0.45504700	-1.28085400	3.89381100
C	-0.41804800	-0.49961300	4.61029700
C	-0.20610500	-1.79204300	2.69756600
C	-1.63088600	-1.40130300	2.84566000
C	-2.73064300	-1.63708100	2.03570300
C	-3.92730800	-0.96278800	2.30825700
C	-3.98919100	-0.08274800	3.39009500
C	-2.90766800	0.13765300	4.25087700
C	-1.72069500	-0.53411400	3.97029900
H	-2.67008300	-2.31049200	1.19020900
H	-3.00971600	0.82737200	5.07991000
H	-4.80005100	-1.09872400	1.68309000
H	-0.18407000	0.06636600	5.50482300
H	1.50406000	-1.43182000	4.11371800
H	0.08786300	-2.73549500	2.23725500
N	-5.22398100	0.67700500	3.60379200
O	-5.31398600	1.36381100	4.61964000
O	-6.10353500	0.59522400	2.73948400
C	-4.03158600	2.02096600	-0.41155900
C	-4.96699100	2.13379600	-1.44418900
C	-4.40686700	2.50046100	0.84690000
C	-6.22968400	2.68053200	-1.23179600
C	-5.66166800	3.05401400	1.08494900
C	-6.57671200	3.14147900	0.03811200
C	2.49890400	4.49842900	-0.99082300
C	3.26053700	4.74767200	-2.13769500

C	2.39577700	5.52690400	-0.04925600
C	3.88623000	5.97474900	-2.34861400
C	3.00802300	6.76274200	-0.24161300
C	3.75656400	6.98475500	-1.39669700
C	4.61111300	-1.87591700	1.01556000
C	5.84980700	-1.92321100	0.36835400
C	4.53542600	-2.44280300	2.29276700
C	6.97148100	-2.49062000	0.96941600
C	5.64014300	-3.01963200	2.91243600
C	6.86451500	-3.04118900	2.24567000
C	-1.33932200	-4.35146900	-1.66897200
C	-0.84405200	-4.96978700	-2.82262700
C	-2.28876500	-5.05464500	-0.92210900
C	-1.28330600	-6.22929300	-3.22538500
C	-2.74733900	-6.31156200	-1.30689800
C	-2.23973000	-6.89994600	-2.46439900
F	-2.78539300	-4.52156200	0.20735400
F	-3.65691600	-6.95801700	-0.57173300
F	-2.66775300	-8.10514800	-2.84145600
F	-0.79690000	-6.79600200	-4.33249000
F	0.07807400	-4.35066700	-3.56492400
F	-3.54796300	2.42167700	1.87367000
F	-5.98711700	3.48908900	2.30084100
F	-7.78430900	3.66596200	0.24711900
F	-7.10611900	2.77285200	-2.23713700
F	-4.65781700	1.70056300	-2.67525700
F	1.69146100	5.33468500	1.07450000
F	2.89178400	7.72941200	0.67424100
F	4.35001100	8.16371400	-1.58936200
F	4.60587400	6.18900800	-3.45353000
F	3.40419500	3.79387400	-3.06242900
F	3.36629700	-2.44732100	2.95513400
F	5.53510500	-3.54852800	4.13506100
F	7.93173000	-3.58911400	2.82764400
F	8.14285500	-2.51895900	0.32840900
F	5.98080900	-1.41232500	-0.86175800

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C	-1.53600400	-1.99410100	-1.39748300
C	-2.93717200	-2.14551900	-1.70552300
C	-3.52942700	-0.94862800	-1.44859900
C	-2.48250100	-0.04001000	-1.04358600
N	-1.28162200	-0.69519300	-1.02779700
H	-3.40400600	-3.05728500	-2.04901900

H	-4.57330400	-0.69498200	-1.54986600
C	0.38151300	3.12611200	-0.77326100
C	-0.56298800	4.22144900	-0.74027800
C	-1.80151400	3.67269900	-0.64903900
C	-1.62624100	2.23801900	-0.67984200
N	-0.28952700	1.93772200	-0.74793400
H	-0.29954100	5.26894900	-0.75679200
H	-2.75367700	4.18101700	-0.60398600
C	2.54158600	-2.03257800	-0.06297800
C	2.72080700	-3.46395400	-0.08160700
C	1.58490600	-3.99813800	-0.60640300
C	0.68998500	-2.89994000	-0.87482300
N	1.28900300	-1.71745500	-0.52851100
H	3.61644000	-3.98175000	0.22963100
H	1.36106000	-5.03965900	-0.78647300
C	3.44368800	0.25745800	0.06081300
C	4.54639800	1.18802500	0.15847800
C	4.07090200	2.40160700	-0.21866700
C	2.65878600	2.23685500	-0.48484200
N	2.31377900	0.91838600	-0.33198100
H	5.55384300	0.93443800	0.45342300
H	4.61464500	3.33179000	-0.28831400
C	-0.62002500	-3.04255200	-1.33937300
C	1.77169900	3.28471800	-0.73440300
C	-2.67219600	1.32007500	-0.75898100
C	3.54654600	-1.12071700	0.26746400
Fe	0.50197200	0.10271700	-0.61432200
O	0.22698800	0.19171700	1.02375600
C	-1.09300000	-4.41525200	-1.67083200
C	-0.69474200	-5.06065000	-2.84446600
C	-1.93279000	-5.11606200	-0.80149300
C	-1.12479600	-6.35111800	-3.14993200
C	-2.37975100	-6.40310600	-1.08557400
C	-1.97138800	-7.02085600	-2.26761800
C	-4.05601800	1.83068500	-0.55047100
C	-5.00283600	1.91130200	-1.57524700
C	-4.44840300	2.27594300	0.71672400
C	-6.29094600	2.39013700	-1.34829500
C	-5.72533800	2.76959700	0.96640600
C	-6.65268200	2.82067300	-0.07220700
C	2.30942100	4.66605900	-0.88020400
C	2.89898800	5.35122900	0.18675600
C	2.20895800	5.34186600	-2.10153400
C	3.38733300	6.64808700	0.04810800

C	2.68493100	6.64133900	-2.26182500
C	3.27754100	7.29435700	-1.18216000
C	4.82956000	-1.66842200	0.79267400
C	5.98436300	-1.72122800	0.00641200
C	4.91467200	-2.17137300	2.09382000
C	7.18087900	-2.24319200	0.49338000
C	6.09709900	-2.70405100	2.60129500
C	7.23424300	-2.73805400	1.79563700
F	-2.32267500	-4.54715100	0.35400500
F	-3.18330400	-7.05001200	-0.23597200
F	-2.38934100	-8.25509600	-2.55155300
F	-0.73445300	-6.94764200	-4.27928500
F	0.12101300	-4.43985100	-3.70118000
F	-3.58090800	2.23096400	1.73895200
F	-6.05962700	3.18409200	2.18863000
F	-7.88203400	3.28430800	0.14990800
F	-7.17724500	2.44832700	-2.34736700
F	-4.68235800	1.51165900	-2.81475700
F	3.00687000	4.75881300	1.38422800
F	3.94835600	7.27741700	1.08573600
F	3.73808000	8.53808000	-1.32585400
F	2.57937000	7.26339100	-3.43945100
F	1.63892400	4.74040200	-3.15040000
F	3.83732400	-2.14868300	2.89428800
F	6.14952900	-3.17617300	3.85058800
F	8.37318400	-3.24341500	2.27147300
F	8.27077100	-2.27964400	-0.27852000
F	5.95703700	-1.25601100	-1.24786800
C1	0.93121900	0.19197800	-2.88112200
C	-4.27773000	-0.99818100	2.14634100
C	-3.06001600	-1.59877500	1.87579600
C	-3.30230600	-0.00844300	4.15388700
C	-4.37542000	-0.19465200	3.28385000
H	-5.13468700	-1.12530500	1.49757800
H	-2.95342100	-2.22577900	0.99884400
C	-2.07325700	-0.60673300	3.88013600
C	-1.94319200	-1.39901300	2.71149600
C	0.45938600	-0.70137100	4.19288300
C	0.44286300	-2.00104100	3.37710400
C	-0.62449800	-1.91466900	2.29680000
C	-0.91001700	-0.44594600	4.84083500
H	1.23295400	-0.74315100	4.96771100
H	1.41919100	-2.18423900	2.91909900
H	-1.05476400	-1.15978000	5.66677500

H	-0.94243400	0.55178700	5.29421800
H	-0.68404800	-2.77754800	1.62585100
H	0.71211900	0.12740600	3.52075600
H	0.22753500	-2.85870100	4.03431400
H	-0.22961900	-1.02975200	1.57862900
H	-3.43527000	0.61947900	5.02744100
N	-5.63941000	0.50215800	3.54965600
O	-6.52702500	0.41435500	2.69577300
O	-5.74200800	1.13714300	4.59720600

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C	-2.05985700	-1.28371700	-1.28105500
C	-3.48508100	-1.08117500	-1.36871400
C	-3.71864000	0.21991900	-1.06232500
C	-2.43178000	0.83794500	-0.84294100
N	-1.43938800	-0.10037700	-0.96684900
H	-4.21115100	-1.84978300	-1.58849000
H	-4.67355800	0.71675400	-0.99662600
C	1.18062400	3.15981800	-0.73488700
C	0.54793600	4.46039700	-0.75104700
C	-0.78775800	4.25026000	-0.63944900
C	-0.98433300	2.81856400	-0.61038400
N	0.22367200	2.18111200	-0.67568100
H	1.06571300	5.40481300	-0.82750700
H	-1.57955600	4.98489100	-0.61809600
C	1.98749800	-2.43548900	-0.44926400
C	1.80404500	-3.85849900	-0.59979000
C	0.52810100	-4.04936900	-1.02838800
C	-0.09143900	-2.74918800	-1.09190100
N	0.81401700	-1.78229100	-0.73717900
H	2.56151400	-4.60848400	-0.42716200
H	0.04505100	-4.98401500	-1.27256800
C	3.42831800	-0.45319000	-0.17565700
C	4.72633500	0.16423800	-0.02494500
C	4.55617100	1.49207900	-0.24978500
C	3.14785600	1.69762000	-0.50469100
N	2.48837600	0.49972500	-0.45854500
H	5.64369700	-0.36168300	0.19666800
H	5.30336300	2.27171500	-0.22502900
C	-1.44121500	-2.52954200	-1.37891400
C	2.56022200	2.95124100	-0.69295400
C	-2.23803600	2.20397900	-0.60660400
C	3.20373200	-1.82949900	-0.12583300
Fe	0.51149600	0.19376100	-0.65704500

C1	0.82625600	0.30818100	-2.94689300
O	0.37166700	0.22996100	1.00211600
H	-0.34126900	-0.82512400	1.55915600
C	0.15202500	-1.69689700	5.81015000
C	1.42040500	-2.27000200	5.67507400
C	1.88724600	-2.63797300	4.40737200
C	1.08915100	-2.43794700	3.28786200
C	-0.19583700	-1.86414500	3.40890100
C	-0.64649100	-1.48776300	4.68894900
H	-0.21601700	-1.41536800	6.79285500
H	2.87995500	-3.06039500	4.29343900
H	1.45513800	-2.70549800	2.30059600
H	-1.63291600	-1.05103000	4.80354500
C	-0.99096100	-1.65320600	2.17242200
H	-0.94776200	-2.51760200	1.50272000
C	-2.35958300	-1.06777600	2.25992900
C	-2.53032800	0.27635700	2.64218700
C	-3.49303600	-1.82681400	1.92209200
C	-3.79545300	0.84775900	2.69083600
H	-1.65690700	0.88021000	2.86616200
C	-4.76511500	-1.26491800	1.95599000
C	-4.89624000	0.07281400	2.32775100
H	-3.93582700	1.87850400	2.98202600
H	-5.64528900	-1.83334400	1.68172100
C	-3.42840400	3.05187800	-0.32462100
C	-4.45317200	3.27297800	-1.25019200
C	-3.58316200	3.62829800	0.94070900
C	-5.60281400	3.98591900	-0.91685100
C	-4.72796800	4.32796400	1.30334400
C	-5.74477800	4.50747500	0.36827500
C	-2.29399400	-3.70095700	-1.72518800
C	-2.63150500	-4.66772800	-0.77479800
C	-2.81327200	-3.86180400	-3.01386500
C	-3.44517300	-5.75477000	-1.07875800
C	-3.63156600	-4.94090700	-3.34444300
C	-3.94507700	-5.89070500	-2.37340700
C	3.46412000	4.13228000	-0.78133000
C	4.30148800	4.31052300	-1.88797300
C	3.53080000	5.08884200	0.23649500
C	5.16502600	5.39950400	-1.98621700
C	4.38207000	6.18826200	0.15713400
C	5.20255700	6.34143500	-0.95935400
C	4.35038800	-2.70644000	0.24646300
C	4.79816900	-2.76383100	1.56832500

C	5.02032500	-3.49559400	-0.69276800
C	5.85506000	-3.58209400	1.95630100
C	6.08355700	-4.32082500	-0.33083100
C	6.50203800	-4.36169800	0.99876100
H	2.04370500	-2.42679700	6.55097700
H	-3.36745900	-2.86076300	1.62006700
N	-6.22114300	0.70393400	2.28239000
O	-6.28547400	1.91806400	2.49459900
O	-7.18910200	-0.00794900	2.01563700
F	-2.62359600	3.47288300	1.86988400
F	-4.86079000	4.80136500	2.54378700
F	-6.84741100	5.17693500	0.69884600
F	-6.56897100	4.17142500	-1.82120400
F	-4.35585400	2.77246500	-2.48963900
F	2.75973800	4.96149900	1.32476700
F	4.42339400	7.08887300	1.14429100
F	6.02456600	7.38882800	-1.04397800
F	5.95295100	5.54770100	-3.05524100
F	4.28956500	3.41808200	-2.88331500
F	4.19056500	-2.02350200	2.50835300
F	6.24406500	-3.62721200	3.23490200
F	7.51721400	-5.15032400	1.35455000
F	6.70509200	-5.06893900	-1.24677900
F	4.63385100	-3.48007500	-1.97330900
F	-2.17497600	-4.55530800	0.48866800
F	-3.75235600	-6.65888900	-0.14351900
F	-4.72605200	-6.92699900	-2.68012200
F	-4.11326900	-5.07237900	-4.58264600
F	-2.53442900	-2.96226200	-3.96085500

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C	2.48885800	0.51760500	-1.25677200
C	3.69425900	-0.14726600	-1.69729000
C	3.34390000	-1.41975400	-2.02755100
C	1.94038900	-1.56059000	-1.72062100
N	1.43921600	-0.34983600	-1.29928800
H	4.66696900	0.31068800	-1.78364700
H	3.97927600	-2.20315800	-2.41458600
C	-2.01957300	-2.41415600	-0.30039500
C	-1.87530200	-3.84960500	-0.24653900
C	-0.67760900	-4.14781600	-0.82049900
C	-0.05646800	-2.89387600	-1.17203200
N	-0.88201500	-1.85849400	-0.83896700
H	-2.60861900	-4.53990000	0.14244800

H	-0.23876500	-5.12346500	-0.97191400
C	-0.93036000	3.05921300	-1.05480500
C	-0.22115100	4.31615100	-0.93393500
C	1.09110300	4.01290400	-0.75617600
C	1.19989400	2.57302500	-0.83746000
N	-0.04742800	2.02623300	-1.01128300
H	-0.68152000	5.29335500	-0.95066700
H	1.92227000	4.69165500	-0.62987400
C	-2.99822900	1.73767200	-0.84402400
C	-4.42241300	1.60538700	-0.62310200
C	-4.63943300	0.33146200	-0.20669400
C	-3.35909900	-0.34234600	-0.23697100
N	-2.38966600	0.52331000	-0.63784200
H	-5.14960800	2.39385000	-0.74724300
H	-5.57843400	-0.13102600	0.06151700
C	2.40150500	1.87078300	-0.87265600
C	-3.17640200	-1.70717300	0.03441400
C	1.25030400	-2.76846100	-1.66732400
C	-2.33056800	2.93833400	-1.08140300
Fe	-0.46333300	0.08041200	-0.90109700
Cl	-0.87557400	0.09700300	-3.18655800
O	-0.21396300	0.18719400	0.73995300
H	0.37937400	-0.87341400	1.30220600
C	4.26204200	0.44913000	3.34840900
C	4.41111500	-0.18636400	2.11279200
C	3.36842100	-0.97012400	1.61962100
C	2.20217600	-1.09278900	2.37181400
C	2.08021900	-0.46698900	3.64194100
C	3.11378100	0.31490500	4.13967000
H	3.46710700	-1.47463100	0.66699600
H	3.05990100	0.81944400	5.09670200
C	0.92046900	-1.73956600	2.02853800
C	0.09712300	-1.63841600	3.24750400
C	-1.19341900	-2.10659400	3.49526900
C	-1.81021700	-1.77325500	4.70451600
C	-1.14622200	-0.97407100	5.64369400
C	0.14642100	-0.48802900	5.39576700
C	0.76510600	-0.81754400	4.19469200
H	-1.70871200	-2.70690100	2.75117900
H	-1.64221600	-0.71926200	6.57599100
H	0.64859400	0.13579100	6.13031800
C	1.97766200	-4.01875000	-2.01779300
C	1.65188500	-4.75278700	-3.16187100
C	2.99021700	-4.51928100	-1.19435000

C	2.31973100	-5.93240200	-3.48626400
C	3.67415600	-5.69249500	-1.49917700
C	3.33444800	-6.40007500	-2.65222900
C	-4.29749600	-2.43378100	0.69077600
C	-4.64451900	-2.12584300	2.01133900
C	-5.03566300	-3.43563200	0.05281600
C	-5.65143700	-2.80710200	2.68844700
C	-6.05684200	-4.12287300	0.70621500
C	-6.36391600	-3.80769100	2.02958900
C	-3.12135200	4.18593900	-1.26321400
C	-3.89796200	4.73396100	-0.23688900
C	-3.07929400	4.87906700	-2.47866100
C	-4.62196900	5.91066300	-0.41231900
C	-3.79186400	6.05986300	-2.67480800
C	-4.56687100	6.57488200	-1.63673600
C	3.63365600	2.58890100	-0.44654500
C	3.76142400	2.96147800	0.89827900
C	4.68807100	2.91681300	-1.30145700
C	4.88939600	3.61889800	1.37839100
C	5.83323900	3.56289100	-0.84089100
C	5.93408600	3.91435300	0.50484700
H	0.90713800	-2.63641200	1.40713000
H	-2.82146800	-2.11462200	4.90451200
H	5.33071600	-0.05564700	1.55693000
N	5.35598500	1.30033100	3.83168300
O	6.31372800	1.48836500	3.07555000
O	5.25651200	1.78324500	4.95848800
F	-3.98227200	-1.16475500	2.66815200
F	-5.92686700	-2.51162300	3.96326200
F	-7.33467000	-4.46561100	2.66411800
F	-6.74388200	-5.07804000	0.07332000
F	-4.76202900	-3.76408600	-1.21561500
F	-3.95667700	4.12721300	0.95610700
F	-5.35800500	6.40999500	0.58552100
F	-5.25466500	7.70365300	-1.81429300
F	-3.73963900	6.69814800	-3.84709900
F	-2.33823300	4.40922300	-3.48679500
F	2.78314300	2.67430500	1.76695000
F	4.97184200	3.95743900	2.66589700
F	7.02271000	4.53814400	0.95020700
F	6.82874700	3.85656800	-1.68337100
F	4.61886900	2.59821700	-2.60358000
F	3.31631800	-3.86670400	-0.06534100
F	4.63898900	-6.14831100	-0.69501500

F	3.97911400	-7.52747900	-2.95482300
F	1.99688500	-6.61481100	-4.58778300
F	0.67812000	-4.32616000	-3.97085800

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C	1.55996200	-1.83965800	-1.13518500
C	1.72281200	-3.26624200	-1.26352800
C	0.53657100	-3.83507200	-0.93483700
C	-0.39278200	-2.76068700	-0.68454200
N	0.26184600	-1.55328200	-0.77004200
H	2.63784400	-3.76936900	-1.53208000
H	0.30622100	-4.88703700	-0.88200900
C	-3.58719900	0.10992500	-0.68141300
C	-4.67574200	-0.83896200	-0.73304600
C	-4.12717300	-2.07538900	-0.62183300
C	-2.69544900	-1.89169300	-0.54666000
N	-2.39305600	-0.56198100	-0.59451500
H	-5.72048800	-0.58472100	-0.83290600
H	-4.63443500	-3.02902000	-0.62524300
C	1.58738700	2.37131400	-0.36588700
C	3.00265900	2.58352100	-0.55391800
C	3.52691300	1.39882500	-0.96211100
C	2.43951800	0.44957500	-0.99568300
N	1.27345300	1.06250300	-0.62478000
H	3.52162900	3.51774400	-0.39723100
H	4.56058900	1.17327300	-1.17964900
C	-0.70264600	3.24444700	-0.10368900
C	-1.64773500	4.32186000	0.07055900
C	-2.88182700	3.80351600	-0.15977300
C	-2.70131400	2.39713900	-0.43804900
N	-1.37115100	2.08404100	-0.40330800
H	-1.39183200	5.34062300	0.32248800
H	-3.83374200	4.31270400	-0.12076000
C	2.58505500	-0.90756700	-1.30657600
C	-3.75074800	1.49378000	-0.63386800
C	-1.76759400	-2.93921300	-0.51668400
C	0.68316100	3.38939600	-0.05235000
Fe	-0.55136500	0.24088000	-0.54707100
Cl	-0.68721600	0.47192100	-2.83685000
O	-0.61892000	0.26383200	1.12417100
H	0.00502600	-0.66290300	1.88366200
C	2.07604100	-5.09921100	2.12430500
C	0.69373200	-4.97323500	2.28955600
C	0.11007500	-3.72309100	2.51944600

C	0.92050200	-2.58569000	2.59331400
C	2.31648300	-2.72245300	2.38783900
C	2.89745300	-3.96758000	2.16753800
H	2.51571000	-6.07784600	1.95315500
H	-0.96193900	-3.65169700	2.61738400
H	3.96899600	-4.06013600	2.02472300
C	0.58212300	-1.15097800	2.86995400
C	1.90802800	-0.45070400	2.75800800
C	2.20671000	0.91565000	2.74985500
C	3.50015600	1.33631400	2.45193600
C	4.47187000	0.38710800	2.13163000
C	4.21416300	-0.98363100	2.14172400
C	2.92097400	-1.39078600	2.44471900
H	1.44204900	1.66168700	2.90306000
H	4.98944700	-1.67979600	1.85631300
C	-0.42008700	-0.82042700	4.02676000
C	-1.84453700	-1.31215300	3.68267700
C	0.07805100	-1.51625900	5.31431400
C	-0.51052700	0.69558100	4.29243800
H	-2.16368200	-0.93906100	2.70429800
H	-1.92909900	-2.39970700	3.68603700
H	-2.54832200	-0.93930700	4.43545500
H	1.09049400	-1.18376100	5.57131300
H	-0.58524300	-1.26705700	6.15119900
H	0.09392400	-2.60464700	5.20193300
H	-1.29165400	0.88288100	5.03770800
H	0.42348400	1.09409100	4.69777300
H	-0.77195800	1.24346300	3.38204900
C	-2.30352200	-4.32280700	-0.37703900
C	-2.23919000	-5.25907800	-1.41476000
C	-2.93263700	-4.73037700	0.80423400
C	-2.73487300	-6.55363500	-1.27189600
C	-3.43597900	-6.01703100	0.97289500
C	-3.33550100	-6.93328600	-0.07303000
C	-5.13036600	2.05013000	-0.71621400
C	-6.06246800	1.85668400	0.30788100
C	-5.53250500	2.81190000	-1.81837800
C	-7.34953100	2.38396000	0.23921800
C	-6.81327100	3.35365900	-1.90637400
C	-7.72359100	3.13631300	-0.87319800
C	1.24052500	4.73552700	0.26540200
C	1.87073300	4.99099700	1.48529500
C	1.17077300	5.78888500	-0.65199500
C	2.41873000	6.23392400	1.78998800

C	1.70531700	7.04426900	-0.36949900
C	2.33307000	7.26494100	0.85578100
C	3.90165300	-1.33412900	-1.86193700
C	4.76253000	-2.23613400	-1.23064000
C	4.35366900	-0.78227500	-3.07074700
C	6.01191600	-2.56604900	-1.74661100
C	5.59942500	-1.09528100	-3.60853600
C	6.43430200	-1.99041800	-2.94196600
H	0.05948700	-5.85410800	2.23615000
H	3.74126900	2.38828300	2.40283400
N	5.76948800	0.85229600	1.63283400
O	6.01380400	2.05826300	1.69017100
O	6.52966700	0.01191600	1.14264600
F	-5.72494100	1.14582500	1.39269700
F	-8.22140500	2.18174800	1.23259800
F	-8.95288500	3.64933700	-0.94783300
F	-7.17480700	4.07519200	-2.97123700
F	-4.67611500	3.03838100	-2.81954300
F	1.96218300	4.02059600	2.41225700
F	3.01383900	6.44450800	2.96723900
F	2.84830500	8.46266400	1.13530400
F	1.62472600	8.03359300	-1.26324900
F	0.57633700	5.60215700	-1.83534500
F	4.39492700	-2.83716500	-0.08533000
F	6.79988300	-3.43117400	-1.10127900
F	7.62741700	-2.29926100	-3.45006000
F	5.99642300	-0.54649400	-4.75970400
F	3.58508900	0.08458700	-3.73775800
F	-3.06587700	-3.86592900	1.82540300
F	-4.01749000	-6.37432400	2.12201200
F	-3.81441000	-8.16938000	0.07318700
F	-2.64859900	-7.42699800	-2.27911800
F	-1.68277500	-4.92508800	-2.58507200

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C	2.63784200	1.07318800	-0.62136400
C	3.95415100	0.47801700	-0.66943700
C	3.78484900	-0.81403100	-1.04948200
C	2.36369700	-1.02651700	-1.18858000
N	1.68580200	0.13209400	-0.91043800
H	4.87864800	0.97819000	-0.42247100
H	4.54842800	-1.56095800	-1.20734400
C	-1.74421300	-2.25252700	-1.08232700
C	-1.52381900	-3.63792100	-1.41808200

C	-0.20834000	-3.76411600	-1.72965300
C	0.39679400	-2.47345100	-1.52053400
N	-0.56102100	-1.56144700	-1.15491300
H	-2.27625800	-4.40970900	-1.42710900
H	0.31903300	-4.65965300	-2.02338700
C	-1.00866400	3.34376900	-0.80227800
C	-0.41513600	4.65119900	-0.63399900
C	0.91101700	4.45675100	-0.41957700
C	1.13959000	3.03123300	-0.48292300
N	-0.04249600	2.37923500	-0.71457100
H	-0.95360500	5.58721600	-0.65812400
H	1.67501700	5.20290900	-0.25751700
C	-2.96918900	1.85179100	-0.93551500
C	-4.39337000	1.60788700	-0.87112300
C	-4.55616400	0.26832900	-0.72421300
C	-3.23511600	-0.31694500	-0.76059700
N	-2.29252400	0.66158400	-0.89278900
H	-5.15960200	2.36707000	-0.91953900
H	-5.47954500	-0.28712400	-0.64383100
C	2.39695000	2.43081300	-0.38433100
C	-2.98978000	-1.69267600	-0.77392700
C	1.77437400	-2.24314000	-1.53653800
C	-2.38162800	3.11835200	-0.94689100
Fe	-0.30314500	0.38782900	-0.85042000
Cl	-0.28784500	0.68575200	-3.15793100
O	-0.39173100	0.34789600	0.81316500
H	-0.11482800	-0.70430100	1.63550900
C	-2.93959900	-0.04748300	5.21781000
C	-1.84117300	0.81028600	5.08835200
C	-0.74925900	0.45938600	4.28749300
C	-0.76328900	-0.76970200	3.62895300
C	-1.86568600	-1.64334100	3.77848200
C	-2.95814400	-1.28401400	4.56280400
H	-3.78424300	0.24800800	5.83389900
H	-1.83689300	1.76265700	5.61080000
H	0.09316700	1.13550400	4.19304500
H	-3.81394500	-1.94676400	4.65578600
C	0.20531500	-1.36728500	2.64812200
C	-0.33159500	-2.73552200	2.39254100
C	0.17792700	-3.78339600	1.62439300
C	-0.57201900	-4.95712400	1.49628700
C	-1.82785500	-5.07520800	2.10165800
C	-2.35228800	-4.02460200	2.86489200
C	-1.59819000	-2.86434800	3.01738400

H	1.13468000	-3.69159900	1.12425900
H	-0.17963100	-5.77923100	0.90487600
H	-2.40153100	-5.99019000	1.98036100
H	-3.33241000	-4.11242600	3.32598200
C	2.66509100	-3.38629100	-1.88557900
C	2.74434500	-3.86507000	-3.19697500
C	3.44318700	-4.02991500	-0.92011700
C	3.56630600	-4.93865000	-3.53568600
C	4.27374800	-5.10190500	-1.23265600
C	4.33493500	-5.55566400	-2.54976500
C	-4.10928300	-2.60200500	-0.40547500
C	-4.57500600	-2.59690700	0.91447600
C	-4.69957000	-3.51483500	-1.28353800
C	-5.53194100	-3.49970800	1.36444200
C	-5.67591500	-4.41503400	-0.86090300
C	-6.08763000	-4.41308400	0.47164200
C	-3.26940100	4.31163600	-1.04336800
C	-4.12067900	4.68294500	0.00166300
C	-3.26155900	5.11775200	-2.18648800
C	-4.94443900	5.80256900	-0.08532400
C	-4.07275600	6.24550400	-2.29323000
C	-4.91740500	6.58627200	-1.23789000
C	3.55578500	3.30137900	-0.04150400
C	3.66491400	3.87374900	1.22864800
C	4.57598100	3.57853500	-0.95662300
C	4.74801900	4.66576800	1.59478100
C	5.66985800	4.37124400	-0.61660500
C	5.75429500	4.91682500	0.66341400
C	1.66937400	-1.07535000	2.73306700
C	2.11109100	0.25558900	2.59039000
C	2.63333800	-2.08565400	2.90014700
C	3.46222400	0.56120600	2.57804100
H	1.39096500	1.04553300	2.41565000
C	3.99411300	-1.79465800	2.86567800
H	2.31678500	-3.11197600	3.04154200
C	4.39110600	-0.47201700	2.68190800
H	3.80463200	1.57686100	2.45738700
H	4.74092700	-2.57413400	2.95332800
N	5.81186700	-0.15684000	2.51996500
O	6.63230800	-1.04298800	2.75507900
O	6.10439100	0.97992200	2.13161700
F	-4.07732200	-1.72176500	1.79441800
F	-5.89438000	-3.50736000	2.65453800
F	-7.00864200	-5.28379200	0.88789900

F	-6.21704000	-5.28175500	-1.72249200
F	-4.31407800	-3.55767100	-2.56594300
F	-4.16118300	3.95061500	1.12292800
F	-5.75182400	6.13316300	0.92776000
F	-5.69991500	7.66279100	-1.33031700
F	-4.04830900	6.99836300	-3.39678700
F	-2.45523700	4.81505200	-3.20879700
F	2.71517400	3.63163800	2.15083600
F	4.82847300	5.18146600	2.82430300
F	6.79603200	5.67841800	0.99666300
F	6.63074000	4.61929000	-1.51034900
F	4.52068100	3.06917400	-2.19272500
F	3.39331600	-3.61834500	0.36016100
F	5.00230800	-5.69784400	-0.28400400
F	5.12432600	-6.58336200	-2.86431300
F	3.62418800	-5.37760600	-4.79554600
F	2.01196600	-3.29597000	-4.15859200

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C	2.60981100	-0.75331200	-0.85716700
C	3.38047800	-1.95490000	-1.08084700
C	2.51086700	-2.90666300	-1.51320100
C	1.19522500	-2.31272400	-1.48965900
N	1.28633400	-1.00067000	-1.10515800
H	4.44801200	-2.04697400	-0.95287500
H	2.73011200	-3.92496500	-1.80027800
C	-2.84310500	-1.13288800	-0.71249200
C	-3.43940200	-2.44009100	-0.85688600
C	-2.47142000	-3.26449400	-1.34310000
C	-1.26167700	-2.48359700	-1.43435800
N	-1.51878200	-1.18964500	-1.06104100
H	-4.47051000	-2.68457400	-0.65337300
H	-2.55486500	-4.31306600	-1.59053900
C	0.82299100	3.13881600	-0.97476200
C	2.04090000	3.90058100	-0.80727600
C	3.03067400	3.00850900	-0.54173800
C	2.43397200	1.69254300	-0.59902500
N	1.09481200	1.80486100	-0.85704000
H	2.11231700	4.97739000	-0.85750400
H	4.07656200	3.20904100	-0.36005600
C	-1.63536200	2.97476400	-0.98244200
C	-2.95268300	3.55074200	-0.81843900
C	-3.78801800	2.53283300	-0.48341000
C	-3.00148300	1.31977000	-0.51829400

N	-1.70894100	1.61574000	-0.83482500
H	-3.19294800	4.59851900	-0.92068600
H	-4.84769400	2.57930400	-0.27650500
C	3.15137500	0.49481700	-0.52001100
C	-3.52507500	0.03349200	-0.34480800
C	0.00374800	-3.01430500	-1.69082200
C	-0.45066900	3.70468600	-1.11210600
Fe	-0.21441700	0.30254500	-0.91834300
Cl	-0.24192900	0.53278200	-3.23028400
O	-0.19500600	0.26261700	0.73988600
H	-0.41646100	-1.04978400	1.23747700
C	3.42895600	-1.29766900	3.59377100
C	2.31498100	-0.65353300	4.13252600
C	2.05912000	-2.52735900	2.06817800
C	3.32104300	-2.23827100	2.56876600
H	2.45510400	0.07661400	4.92105800
H	4.21195700	-2.71253000	2.17750600
C	-0.40541100	-2.04064000	1.94381800
C	0.92591700	-1.87011300	2.56964100
C	1.05483200	-0.92615700	3.61096400
C	-0.17429500	-0.16447200	4.05809800
H	-0.47490700	-2.88620800	1.25571400
H	-0.05710300	0.19541300	5.08630900
H	-0.24770100	0.73042900	3.41787700
H	1.94598000	-3.24784700	1.26606500
C	-1.57334100	-1.85439100	2.82795200
C	-2.78694200	-2.52568600	2.60518300
C	-3.87551300	-2.30883200	3.44471000
C	-3.76319000	-1.41026000	4.51215700
C	-2.55958100	-0.73552800	4.73573800
C	-1.46318700	-0.94050500	3.89977500
H	-2.86264400	-3.21571700	1.76984700
H	-4.80971400	-2.83590300	3.27143800
H	-4.61515200	-1.22563800	5.15928100
H	-2.47888400	-0.03406900	5.56249400
C	0.08837400	-4.45801200	-2.04948200
C	-0.18688000	-4.90599700	-3.34361300
C	0.42622900	-5.41635200	-1.09135800
C	-0.11609400	-6.25833300	-3.67674900
C	0.50757400	-6.77095400	-1.39882200
C	0.23396500	-7.19026500	-2.70086700
C	4.57697100	0.57426400	-0.09550900
C	4.89578800	0.94260800	1.21590200
C	5.64346200	0.31403000	-0.96135100

C	6.21066200	1.03410600	1.66249900
C	6.96773100	0.39141000	-0.53724300
C	7.25117000	0.75255900	0.77957100
C	-4.86177000	-0.07997000	0.29794000
C	-4.98491000	0.27778600	1.64660800
C	-6.00609800	-0.55256700	-0.34847000
C	-6.18380000	0.13403000	2.33747700
C	-7.21982900	-0.69577100	0.32093000
C	-7.30564400	-0.35439600	1.67021700
C	-0.53173700	5.18164200	-1.28881300
C	-0.12177000	5.77802400	-2.48615100
C	-0.98342200	6.02594700	-0.26991800
C	-0.17076000	7.15829900	-2.67085000
C	-1.04541900	7.40748500	-0.43394900
C	-0.63590500	7.97356300	-1.64027400
N	4.76261600	-0.93233500	4.08111700
O	5.73568700	-1.36532700	3.45529900
O	4.83996300	-0.20695800	5.07067000
F	0.67623600	-5.03362000	0.17535800
F	0.83420100	-7.66649000	-0.46220300
F	0.30502200	-8.48560900	-3.01026400
F	-0.37913900	-6.66564300	-4.92095700
F	-0.52761100	-4.03123700	-4.29320400
F	-3.92445000	0.75196300	2.30742800
F	-6.26046900	0.44408900	3.63692900
F	-8.46094800	-0.49789500	2.32233100
F	-8.29923900	-1.15542500	-0.31987200
F	-5.94995400	-0.89787000	-1.64238500
F	-1.37139900	5.50874700	0.90418800
F	-1.48413900	8.19099500	0.55661000
F	-0.68825400	9.29595600	-1.80760200
F	0.22234900	7.70395100	-3.82522800
F	0.33433100	5.01860100	-3.48654400
F	3.91490700	1.21445900	2.09033900
F	6.47231200	1.38321300	2.92121800
F	8.51681100	0.83156300	1.18992600
F	7.96653700	0.13138500	-1.38692600
F	5.40336100	-0.02679800	-2.23566300

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C	2.44964400	-1.23708200	-0.89418700
C	2.98316200	-2.55917000	-1.12865400
C	1.94517400	-3.33595400	-1.53962200
C	0.76203400	-2.50879600	-1.49696800

N	1.09967400	-1.23567500	-1.12166200
H	4.01909300	-2.84421700	-1.02656700
H	1.96916900	-4.37647100	-1.82956300
C	-2.99948000	-0.58629800	-0.76050800
C	-3.82938600	-1.75855900	-0.91250100
C	-3.02364000	-2.75747200	-1.36600600
C	-1.68727700	-2.21812100	-1.43868200
N	-1.70345300	-0.89439900	-1.08111100
H	-4.89310300	-1.80206100	-0.73572100
H	-3.29862200	-3.77401900	-1.60804100
C	1.41466300	2.92044700	-0.94635200
C	2.75489500	3.44063700	-0.78551200
C	3.56405600	2.37687500	-0.54639000
C	2.73121500	1.19564800	-0.61124000
N	1.43303900	1.55772900	-0.84736000
H	3.02481700	4.48597400	-0.82271100
H	4.63107200	2.37728100	-0.37788100
C	-1.02996200	3.22107700	-0.95435500
C	-2.21689900	4.03535100	-0.80251600
C	-3.23631000	3.19069600	-0.50059000
C	-2.69256900	1.85081400	-0.54104500
N	-1.36031000	1.89908900	-0.82816600
H	-2.25236600	5.11074700	-0.89276600
H	-4.27212500	3.43475100	-0.31276700
C	3.21657900	-0.11387500	-0.55675800
C	-3.45676100	0.68807800	-0.40043800
C	-0.54154200	-2.97922700	-1.67925900
C	0.27073100	3.71774600	-1.07058900
Fe	-0.13759800	0.32565800	-0.91563300
Cl	-0.11362800	0.57074600	-3.23398800
O	-0.13626300	0.24682900	0.73574000
H	-0.65744300	-1.02379100	1.25182100
C	3.03652900	-1.76748800	3.68440400
C	1.98405200	-1.09738800	4.29647400
C	1.57932800	-2.73925900	2.05170300
C	2.85456200	-2.60298100	2.57754400
H	2.14746300	-0.46204500	5.15694600
H	3.70626700	-3.10702900	2.14031800
C	-0.82803100	-1.98070300	1.95807900
C	0.49330000	-2.05152300	2.60985400
C	0.71353100	-1.25240100	3.74792200
H	-1.04673600	-2.80380500	1.27329400
H	1.41305700	-3.36139900	1.18001500
C	-1.92726700	-1.59247900	2.85909400

C	-3.27973800	-1.85580600	2.59216400
C	-4.27594700	-1.37377200	3.43226300
C	-3.93759000	-0.59259000	4.54945700
C	-2.60425400	-0.33031600	4.84647600
C	-1.61152000	-0.84073800	4.00892300
H	-3.52934000	-2.43747700	1.71010400
H	-5.31854100	-1.58856900	3.21787800
H	-4.71961900	-0.18729600	5.18349400
H	-2.31314500	0.25603000	5.71137000
C	-0.72810800	-4.42153400	-2.00320800
C	-1.12862600	-4.84261500	-3.27354500
C	-0.53123000	-5.40367100	-1.02961600
C	-1.31650800	-6.19270600	-3.56834600
C	-0.70803000	-6.75716300	-1.29896000
C	-1.10295900	-7.15011700	-2.57781100
C	4.64049800	-0.29788000	-0.15908300
C	5.04944500	0.00850200	1.14394300
C	5.62667400	-0.73212800	-1.05019500
C	6.37434800	-0.10963600	1.55399200
C	6.95587100	-0.87591000	-0.66028900
C	7.32988500	-0.56144800	0.64570200
C	-4.81023200	0.82787900	0.20034400
C	-4.91231200	1.20389700	1.54614400
C	-6.00052000	0.57480300	-0.48608400
C	-6.13988000	1.27848800	2.19674800
C	-7.24181700	0.65616400	0.14181100
C	-7.30958100	1.00515300	1.49021700
C	0.46838100	5.18508800	-1.23462100
C	0.99176900	5.70206000	-2.42490100
C	0.17440200	6.09290300	-0.21260800
C	1.20381000	7.06805500	-2.59974100
C	0.37342100	7.46263300	-0.36709600
C	0.89132200	7.94951500	-1.56615500
N	4.39592100	-1.57205800	4.20526300
O	5.31923700	-2.11919500	3.59703000
O	4.53530800	-0.87701600	5.20839600
O	-0.31062900	-0.57696000	4.35911200
F	-0.16787400	-5.04396400	0.21682200
F	-0.51244400	-7.67509300	-0.34736400
F	-1.27870500	-8.44380500	-2.85061700
F	-1.69643300	-6.57396400	-4.79046700
F	-1.34373500	-3.94307000	-4.23669200
F	-3.80760400	1.47527400	2.24819600
F	-6.19955300	1.58794400	3.49788900

F	-8.49267200	1.07230100	2.10370400
F	-8.36493600	0.40352500	-0.53761000
F	-5.96626300	0.22582200	-1.77940500
F	-0.31380900	5.65116500	0.95455100
F	0.08104300	8.30882500	0.62603000
F	1.08844600	9.25954300	-1.72373900
F	1.70126000	7.53771100	-3.74746400
F	1.30555600	4.87684600	-3.42807500
F	4.14973900	0.44030200	2.04133000
F	6.72935900	0.20766800	2.79799800
F	8.60287300	-0.68761300	1.02150800
F	7.87579400	-1.29879200	-1.53326400
F	5.30242300	-1.02425300	-2.31765200

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C	0.53984100	3.02189000	-0.88380800
C	1.25581500	4.20427400	-0.47169100
C	2.37435200	3.78226900	0.17820100
C	2.36931000	2.33960400	0.12908600
N	1.23442900	1.90503500	-0.50620300
H	0.93108900	5.21993800	-0.64638900
H	3.15506800	4.38682000	0.61658000
C	3.08080500	-1.83942400	-0.50066700
C	4.43609700	-1.87365200	0.00374800
C	4.69636700	-0.64590700	0.52227700
C	3.52421400	0.16700700	0.28375900
N	2.56002100	-0.58555500	-0.32835100
H	5.08001800	-2.74102500	-0.00549400
H	5.60243400	-0.31041600	1.00463200
C	-2.21864900	-0.18242300	-1.45025800
C	-3.33069800	0.60744100	-1.92582900
C	-2.86512700	1.87258800	-2.11143300
C	-1.48963900	1.88248300	-1.67786100
N	-1.11292100	0.60915700	-1.31872200
H	-4.32094900	0.23271100	-2.13329800
H	-3.40677400	2.73063200	-2.48275000
C	-1.10452300	-2.35401800	-1.14152300
C	-1.09916100	-3.79551300	-1.25768300
C	0.20249000	-4.17843900	-1.31805100
C	1.00105700	-2.98170900	-1.15337700
N	0.18122500	-1.89101400	-1.08394900
H	-1.98237500	-4.41294500	-1.33877100
H	0.59331900	-5.17790000	-1.43745100
C	-0.71948200	3.02852700	-1.49322200

C	2.38571000	-2.96337800	-0.95513900
C	3.42318400	1.53233700	0.56768100
C	-2.25257300	-1.56679900	-1.21923100
Fe	0.70269100	0.01029700	-0.76663900
Cl	1.36604700	0.13652200	-2.97760000
O	0.29345400	-0.20431500	0.83431100
C	-3.01200500	-2.07172700	5.17790600
C	-4.07871900	-1.73884300	4.36950900
C	-3.93649200	-0.72244500	3.39144600
C	-2.65965100	-0.07429500	3.24152600
C	-1.57872600	-0.42922800	4.09945100
C	-1.77487800	-1.41288000	5.05418000
C	-4.96593500	-0.33642800	2.47738900
C	-2.46884300	0.91563400	2.21692900
C	-3.51659600	1.22001500	1.34726800
C	-4.75605000	0.59038000	1.47050000
C	-1.16346100	1.55698500	2.05073600
C	-0.30731300	1.61918000	3.30705100
C	-0.22020100	0.22139100	3.93263600
H	0.38950700	-0.41181600	3.27356600
H	0.69344600	1.98755200	3.06405200
H	-3.13083300	-2.85231900	5.92398000
H	-5.02330700	-2.25171500	4.47591600
H	-0.95320100	-1.68728200	5.71119300
H	-5.56805400	0.82726500	0.79398700
H	-3.36990600	1.96566700	0.57596300
H	-0.54573700	0.78654300	1.33773200
H	-1.20041800	2.47766800	1.46099100
N	-6.32155000	-0.90018100	2.54695200
O	-6.78683500	-1.18484100	3.64924000
O	-6.93390000	-1.02434100	1.48154900
C	4.52619300	2.19393400	1.31864200
C	5.79827700	2.37673700	0.76723100
C	4.31169300	2.68530800	2.61012400
C	6.82091400	3.00821000	1.47214400
C	5.31511000	3.32635300	3.33176700
C	6.57575000	3.48603700	2.75852500
C	3.15687000	-4.22598500	-1.12959300
C	4.08684900	-4.35069000	-2.16768800
C	3.01480700	-5.31179800	-0.26024000
C	4.83741200	-5.51131300	-2.34441000
C	3.74923000	-6.48401700	-0.42149300
C	4.66479600	-6.58142100	-1.46810700
C	-3.56474500	-2.22902500	-0.99020300

C	-4.55381800	-2.39176900	-1.96144800
C	-3.85896400	-2.68005900	0.30285800
C	-5.79428500	-2.95112600	-1.65976400
C	-5.09173200	-3.23143500	0.62798500
C	-6.06709000	-3.36571300	-0.35713600
C	-1.31421500	4.34784000	-1.84392800
C	-0.85898600	5.08199700	-2.94270700
C	-2.33204500	4.91104200	-1.07024500
C	-1.40376300	6.32332100	-3.26832700
C	-2.89637000	6.14559300	-1.37704300
C	-2.42647900	6.85341700	-2.48305600
H	-0.75856600	2.32878300	4.01690500
H	0.29109200	0.26230000	4.90107100
F	-2.78825000	4.25670000	0.01427300
F	-3.87074300	6.65819300	-0.61909100
F	-2.95507900	8.03960500	-2.78745600
F	-0.95545400	7.00560700	-4.32532700
F	0.12356600	4.59645100	-3.70622000
F	3.10913300	2.54626300	3.19048500
F	5.07950700	3.78291900	4.56590900
F	7.54648100	4.09515200	3.44121600
F	8.02801400	3.16665000	0.92156700
F	6.05899800	1.93619600	-0.46922300
F	2.15146300	-5.24099500	0.76300500
F	3.59043100	-7.50772200	0.42405700
F	5.37647900	-7.69842300	-1.62974200
F	5.71731000	-5.60551700	-3.34554400
F	4.27642300	-3.33720600	-3.01786000
F	-2.94646600	-2.55166600	1.27583000
F	-5.35784300	-3.58341500	1.89235800
F	-7.25700100	-3.87885000	-0.05509900
F	-6.72393200	-3.08611100	-2.61080300
F	-4.32907700	-1.98551700	-3.22031500

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C	-0.69092700	-2.92695600	-1.03024500
C	-1.61034900	-4.02638600	-0.85979800
C	-2.82957800	-3.48097000	-0.61915800
C	-2.65648600	-2.04697600	-0.63446200
N	-1.34740500	-1.73597400	-0.89638400
H	-1.34927400	-5.07275900	-0.91303200
H	-3.76627200	-3.99327200	-0.45518300
C	-2.70794700	2.25407400	-0.73995500
C	-4.10466400	2.42590400	-0.40818900

C	-4.62458400	1.18472500	-0.24397200
C	-3.55048600	0.24678600	-0.48249700
N	-2.39737200	0.91974900	-0.78355100
H	-4.60863000	3.37504000	-0.30175400
H	-5.63795900	0.91928700	0.01880900
C	2.46040400	-0.00875500	-1.41670900
C	3.52776100	-0.94717800	-1.66841500
C	2.96903900	-2.18386700	-1.69939200
C	1.56356000	-2.01757900	-1.43041500
N	1.27007700	-0.67926100	-1.28207700
H	4.56678500	-0.69626200	-1.80661800
H	3.46011000	-3.12862800	-1.88168900
C	1.56063800	2.28035100	-1.29763300
C	1.71426200	3.71228900	-1.41932200
C	0.46980300	4.24603600	-1.35807100
C	-0.44861900	3.14583500	-1.17044900
N	0.23499500	1.95955100	-1.17521100
H	2.65278800	4.22633300	-1.56565800
H	0.18913800	5.28582200	-1.43735600
C	0.67440000	-3.07844800	-1.28200300
C	-1.81773700	3.30702300	-0.94408500
C	-3.69009000	-1.13874500	-0.40455000
C	2.62775100	1.38115500	-1.32927800
Fe	-0.54072800	0.11073200	-0.97767800
Cl	-0.90675000	0.10497000	-3.26525200
O	-0.47658900	0.22636100	0.67713300
H	0.46621400	-0.24105700	1.59641400
C	4.46096400	0.96719600	2.90984100
C	5.10006900	0.14885400	1.97947700
C	4.43713700	-0.91008900	1.35855400
C	3.09493600	-1.11063000	1.63339200
C	2.39864800	-0.27636000	2.53184800
C	3.11365300	0.74825900	3.18077600
H	5.00546000	1.78361000	3.36784400
H	4.96201600	-1.53123900	0.64637200
H	2.56474500	-1.90640800	1.12636400
H	2.60498200	1.39369700	3.88698400
C	0.92340400	-0.48576300	2.71020400
C	0.18336300	0.56266000	3.50010300
C	0.11760000	1.88126300	3.00279800
C	-0.47934700	0.26062000	4.69985100
C	-0.58888000	2.86507000	3.68690900
C	-1.17465500	1.25164900	5.39290100
H	-0.44141600	-0.75158000	5.08979700

C	-1.23718000	2.55259500	4.88707100
H	-0.65431800	3.86590200	3.27118000
H	-1.67197900	1.00563500	6.32721300
H	-1.79261300	3.31857300	5.42152900
C	-5.02187800	-1.68931500	-0.02578400
C	-6.11867200	-1.63233100	-0.89033500
C	-5.21763600	-2.28760700	1.22211600
C	-7.36188600	-2.15009400	-0.53128000
C	-6.44684900	-2.81921400	1.60112400
C	-7.52349700	-2.74726800	0.71805200
C	1.21695900	-4.46493800	-1.35173500
C	2.00919300	-4.98178800	-0.32255700
C	0.93661300	-5.30778500	-2.43138100
C	2.50692400	-6.28131200	-0.35691800
C	1.42148700	-6.61310100	-2.48784700
C	2.21029900	-7.09916900	-1.44611900
C	-2.34508100	4.69652100	-0.84009200
C	-3.23368400	5.21785000	-1.78546200
C	-1.97635900	5.52957300	0.22159300
C	-3.73620000	6.51371600	-1.68382500
C	-2.46110200	6.82873200	0.34208900
C	-3.34608600	7.32086200	-0.61638000
C	3.99600000	1.94572800	-1.16886700
C	4.30680400	2.65180200	0.00310700
C	5.02590300	1.80420600	-2.10432900
C	5.57795000	3.15539500	0.25635200
C	6.31196900	2.28390700	-1.86569700
C	6.59265800	2.95720400	-0.67765600
C	0.47304700	-1.90839700	2.92257300
C	-0.84223600	-2.26638900	2.56471600
C	1.31465200	-2.89713500	3.45991300
C	-1.29053500	-3.57388100	2.72271500
H	-1.49729500	-1.51554300	2.13566200
C	0.86360200	-4.20710400	3.61865900
H	2.32643500	-2.63902400	3.75530000
C	-0.43702500	-4.55154500	3.24563700
H	-2.30306400	-3.82664300	2.42862600
H	1.53052600	-4.95752500	4.03408200
H	-0.78571500	-5.57404300	3.36389300
H	0.60186300	2.11623100	2.05997200
N	6.47475400	0.45337500	1.57461100
O	6.91941800	-0.12815600	0.58052000
O	7.09337700	1.30165800	2.21801300
F	2.30999800	-4.22109900	0.74189400

F	3.25898200	-6.74820800	0.64524000
F	2.68005800	-8.34695800	-1.49017600
F	1.13858400	-7.39863000	-3.53083600
F	0.17581700	-4.86777200	-3.43908300
F	-4.19830800	-2.36188000	2.09468900
F	-6.60295700	-3.38792000	2.80088800
F	-8.70849600	-3.24891600	1.06998400
F	-8.39532200	-2.08279100	-1.37532600
F	-5.98938300	-1.06413700	-2.09390100
F	-1.12302300	5.08311200	1.15756900
F	-2.08900100	7.60178900	1.36754200
F	-3.81889000	8.56385900	-0.51124900
F	-4.58298900	6.98762700	-2.60225500
F	-3.62770500	4.46311800	-2.81661500
F	3.36373900	2.85204300	0.93719000
F	5.82941400	3.79664000	1.40114200
F	7.81777700	3.41960900	-0.44447800
F	7.27341000	2.11403200	-2.77635200
F	4.79595600	1.17923500	-3.26830400

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C	1.03901200	3.29178500	-0.70852300
C	1.98162600	4.28151500	-0.24010900
C	3.20187600	3.68988700	-0.24485300
C	3.00231700	2.32195700	-0.66898800
N	1.68099000	2.10794200	-0.95462800
H	1.73922100	5.29506000	0.04109600
H	4.15230100	4.12962600	0.01910700
C	2.83821500	-1.92877800	-1.27019100
C	4.25165600	-2.18979800	-1.10726500
C	4.85664300	-0.98759500	-0.94515100
C	3.81405800	0.01418200	-0.99496000
N	2.60404400	-0.58051100	-1.23043200
H	4.70819700	-3.16843400	-1.12682800
H	5.90634100	-0.78771700	-0.78788100
C	-2.10306800	0.69876500	-2.12501400
C	-3.09022500	1.73192900	-2.32663100
C	-2.53061300	2.90067700	-1.91671800
C	-1.19194800	2.59279900	-1.48296800
N	-0.93899300	1.25496800	-1.65470400
H	-4.08140900	1.58449600	-2.72593600
H	-2.97192500	3.88676900	-1.92286800
C	-1.37795900	-1.66054800	-2.08440000
C	-1.64278100	-3.08128100	-2.13547100

C	-0.47024100	-3.70914500	-1.86917500
C	0.52406000	-2.67576400	-1.68092000
N	-0.05099600	-1.44144900	-1.82239700
H	-2.60010300	-3.53054000	-2.35522500
H	-0.28629600	-4.77155800	-1.81662900
C	-0.31588400	3.53528100	-0.93910300
C	1.87244000	-2.92651200	-1.40915500
C	4.01834200	1.36627000	-0.71863200
C	-2.35303100	-0.67514500	-2.24564500
Fe	0.80938000	0.33225200	-1.37581900
Cl	1.28403700	0.64709500	-3.62769100
O	0.61116600	0.02300800	0.23174800
H	-0.51308800	0.39846100	1.10378200
C	-1.02212800	0.37580400	2.20124100
C	-0.54175400	-1.00963800	2.56520500
C	0.30383100	-1.27367200	3.65006300
C	-0.85706700	-2.05883800	1.68016100
C	0.81534300	-2.55273300	3.85927900
H	0.56675900	-0.47325200	4.33328200
C	-0.35486100	-3.33355400	1.87034800
H	-1.48230700	-1.85603300	0.81918800
C	0.48443300	-3.56575400	2.96184600
H	1.47144100	-2.77075400	4.69288200
H	-0.57897400	-4.13445000	1.17800300
C	-0.32742100	1.56388500	2.82955300
C	1.05837300	1.74821300	2.65113700
C	-1.04882700	2.54200500	3.53298700
C	1.69590000	2.87903300	3.15249900
H	1.62020100	1.01571800	2.08247300
C	-0.40905100	3.67542100	4.03679800
H	-2.11746700	2.41510800	3.68006700
C	0.96291700	3.85000900	3.84432000
H	2.76043300	3.00757400	2.98319200
H	-0.98498100	4.42132400	4.57810800
C	-2.45460500	0.60194900	1.91062700
C	-3.57020100	-0.14427700	2.20283900
H	-2.61251300	1.52226600	1.35608700
C	-3.54241200	-1.27050100	3.17094800
C	-4.10725700	-2.52039300	2.85781400
C	-2.94696900	-1.09654800	4.43071400
C	-4.03709000	-3.57417300	3.76607700
H	-4.58162500	-2.66541700	1.89441400
C	-2.88633300	-2.14889100	5.34171500
H	-2.52344700	-0.12955500	4.68628900

C	-3.42279400	-3.39456100	5.00859300
H	-4.45864800	-4.54005800	3.50177800
H	-2.41607400	-1.99789100	6.30929000
H	-3.36681900	-4.21892100	5.71401400
C	-4.87242400	0.21010400	1.59438200
C	-6.09039000	-0.18029400	2.18994100
C	-4.93902200	0.93036300	0.38359200
C	-7.31158500	0.11825100	1.59009200
H	-6.07642400	-0.72102900	3.12952600
C	-6.15848100	1.23765800	-0.20903900
H	-4.02612900	1.22083200	-0.11877600
C	-7.35481400	0.82476400	0.38515000
H	-8.23405900	-0.20060200	2.06700800
H	-6.17324900	1.78264700	-1.14935600
H	-8.30805600	1.04996300	-0.08472800
C	5.39541700	1.79812600	-0.34463300
C	6.41464300	1.90813800	-1.29372100
C	5.71611000	2.09519100	0.98304100
C	7.70374700	2.30364100	-0.94024700
C	6.99343600	2.50000800	1.35970500
C	7.99104900	2.60210000	0.39071500
C	-0.87754200	4.86310500	-0.57074900
C	-1.82885100	4.97117200	0.45046700
C	-0.48956500	6.04617700	-1.20822300
C	-2.35848700	6.19742500	0.84048100
C	-1.00574900	7.28567600	-0.83584000
C	-1.94391800	7.35989000	0.19251600
C	-3.77541000	-1.10903900	-2.35456300
C	-4.38104300	-1.75322400	-1.26997600
C	-4.59307400	-0.82983400	-3.45296500
C	-5.72978600	-2.08386900	-1.25045900
C	-5.95073300	-1.14595300	-3.45876400
C	-6.52283500	-1.77099600	-2.35067800
C	2.30206900	-4.33626600	-1.18998800
C	2.73510700	-4.75242100	0.07397000
C	2.28595100	-5.29524500	-2.20733900
C	3.12838400	-6.06244600	0.33011000
C	2.66866800	-6.61406300	-1.97608400
C	3.09067200	-6.99690800	-0.70316000
H	1.45937900	4.73621100	4.23080400
N	1.05668700	-4.90211000	3.14120600
O	0.79865800	-5.75462200	2.28503100
O	1.76075400	-5.10465000	4.12916200
F	-2.25904900	3.87262300	1.09075000

F	-3.25751300	6.26612100	1.82794000
F	-2.44557300	8.54171100	0.55520600
F	-0.61415100	8.39976900	-1.46122700
F	0.40620300	6.00690400	-2.20141900
F	4.77423900	1.99468500	1.93647800
F	7.27012300	2.78235800	2.63703500
F	9.22110100	2.98507800	0.73831800
F	8.66212500	2.40168600	-1.86596100
F	6.16466900	1.62199200	-2.57558700
F	2.78135500	-3.87213800	1.08495500
F	3.53623900	-6.42262700	1.54600100
F	3.46195900	-8.25833300	-0.47820700
F	2.64070000	-7.51247400	-2.96640500
F	1.88381000	-4.95517900	-3.43969900
F	-3.65488400	-2.04507400	-0.17740800
F	-6.26820100	-2.66158500	-0.16964900
F	-7.82458300	-2.06220300	-2.34438100
F	-6.70934900	-0.85071900	-4.51896900
F	-4.08459000	-0.20457000	-4.52251900

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C	-2.27262000	2.33027300	0.35805600
C	-2.29771400	3.77705000	0.32823700
C	-1.15421500	4.17824700	-0.29464600
C	-0.39660300	2.98270200	-0.59047200
N	-1.09873200	1.87838000	-0.18374800
H	-3.11028300	4.38631400	0.69986700
H	-0.83052100	5.18371400	-0.52644200
C	2.36824400	-0.25591100	-0.97458700
C	3.52675500	0.54128700	-1.31792500
C	3.08517100	1.81465100	-1.52544300
C	1.67151100	1.81997600	-1.22264100
N	1.26319000	0.55123000	-0.90819100
H	4.53579400	0.16240000	-1.39439800
H	3.65789800	2.68811400	-1.80629700
C	-2.98415700	-1.86143300	-0.20337500
C	-4.36350400	-1.87382100	0.23830500
C	-4.63431600	-0.62781200	0.71622500
C	-3.43710200	0.16431100	0.51919100
N	-2.45625000	-0.61347700	-0.02875900
H	-5.01225200	-2.73834700	0.20138300
H	-5.55643700	-0.25438000	1.14045300
C	-0.90952500	-3.01538600	-0.84331500
C	-0.13236500	-4.22226200	-1.04576500

C	1.17809700	-3.85574900	-0.99805300
C	1.20299100	-2.41716500	-0.83101400
N	-0.07258100	-1.94006200	-0.74425800
H	-0.55258900	-5.21034600	-1.17482000
H	2.05962500	-4.47544800	-1.09314300
C	-3.35472700	1.53981300	0.76009000
C	2.37336200	-1.65231500	-0.84091200
C	0.88970900	2.97630600	-1.13883800
C	-2.29350800	-2.99295800	-0.64828200
Fe	-0.57974700	-0.03284400	-0.41114700
Cl	-1.20222400	0.13755800	-2.72285400
O	-0.18652600	-0.25134300	1.24859200
H	0.33734400	0.64223500	1.79352500
C	4.52504500	0.56350700	2.15199100
C	4.68287400	-0.24111900	3.28766800
C	3.65275500	-0.36235900	4.23201700
C	2.45626900	0.29984000	4.01972800
C	2.24285500	1.09054900	2.86042800
C	3.32423900	1.21844000	1.95295900
H	5.32570600	0.62330600	1.42549800
H	3.80235100	-0.99699700	5.09712600
H	3.18220200	1.79763100	1.04968000
C	0.94652900	1.64472000	2.53927900
H	0.92229600	2.46150800	1.82060700
H	0.23715000	1.75304400	3.36063500
C	1.45272800	4.25696400	-1.67374200
C	2.06097400	5.20717600	-0.83079100
C	1.35561800	4.49858100	-3.06078600
C	2.55672900	6.39210500	-1.38734600
C	1.86160800	5.69653400	-3.57591500
C	2.46716700	6.65440100	-2.75700600
H	3.02455900	7.12662700	-0.73357600
H	1.77917200	5.88568700	-4.64522700
C	-4.52204900	2.21991500	1.40697000
C	-5.60174800	2.68284300	0.62950600
C	-4.52397500	2.40432500	2.80330500
C	-6.67300200	3.31838600	1.26704800
C	-5.61352800	3.04371100	3.40388800
C	-6.69921000	3.50415400	2.65265600
H	-7.50575400	3.67981100	0.66552400
H	-5.61316800	3.18713200	4.48342300
C	-3.06467900	-4.25816200	-0.86288000
C	-3.65651600	-4.49167000	-2.12056200
C	-3.20477500	-5.19986100	0.17401000

C	-4.37562200	-5.67456900	-2.32023200
C	-3.93213100	-6.37143000	-0.06580400
C	-4.52124400	-6.62787700	-1.30710900
H	-4.83401400	-5.85509700	-3.29150400
H	-4.04176700	-7.09862800	0.73728800
C	3.69107400	-2.32995800	-0.62758100
C	4.61983400	-2.51907800	-1.66690800
C	4.02048700	-2.70897900	0.69532400
C	5.90679500	-2.97774000	-1.35103400
C	5.31405100	-3.15663900	0.96756000
C	6.28218300	-3.26346500	-0.03673100
H	6.63441000	-3.09841300	-2.15238800
H	5.58527100	-3.39603600	1.99394300
C	0.73274600	3.46928400	-3.97597500
H	1.38632300	2.59465700	-4.07991400
H	-0.21124600	3.07954800	-3.58112200
H	0.55703300	3.88457800	-4.97426100
C	2.18418600	4.95685200	0.65495300
H	1.20126700	4.83222300	1.12268500
H	2.74590500	4.03838700	0.85789600
H	2.69813400	5.78467800	1.15482700
C	3.03762700	7.92522200	-3.34503300
H	3.08195100	8.72866300	-2.60095100
H	4.05977200	7.76910900	-3.71713500
H	2.43761100	8.28010100	-4.19116300
C	4.23987800	-2.23715800	-3.10482800
H	3.24704900	-2.64039200	-3.33291300
H	4.19122800	-1.16271700	-3.31534800
H	4.96330000	-2.68397100	-3.79568000
C	2.99078000	-2.65011800	1.80025400
H	2.46296700	-1.69235200	1.82466900
H	2.22183100	-3.41815000	1.65034800
H	3.45768300	-2.81683500	2.77464700
C	7.69235800	-3.66827300	0.32322700
H	8.36083300	-3.62588100	-0.54391000
H	8.08803200	-3.00024000	1.09826100
H	7.72939900	-4.68915900	0.72632600
C	-3.52259000	-3.46772100	-3.22387700
H	-4.00298800	-2.52248200	-2.94569500
H	-2.47355100	-3.21736600	-3.41563800
H	-3.97500800	-3.82613200	-4.15476400
C	-5.27411100	-7.91460900	-1.56007300
H	-6.13166800	-7.75410600	-2.22420900
H	-4.63145000	-8.66611200	-2.03951100

H	-5.64659600	-8.35285700	-0.62719200
C	-2.58257800	-4.94053300	1.52692600
H	-1.49340500	-4.84442200	1.44845500
H	-2.94639900	-3.99786900	1.95213100
H	-2.80876700	-5.74889300	2.23041900
C	-3.35347900	1.92596000	3.63199500
H	-3.15992200	0.85998700	3.46697100
H	-2.43280000	2.45018100	3.34840000
H	-3.52905500	2.08873700	4.70076200
C	-5.59086900	2.50303900	-0.87079300
H	-4.70897800	2.97678700	-1.31709200
H	-5.53830700	1.44235400	-1.14139000
H	-6.48705700	2.93444500	-1.32928400
C	-7.88393000	4.16099000	3.32457000
H	-8.37719600	4.87776200	2.65800900
H	-8.63894500	3.41840200	3.61820100
H	-7.58508500	4.69506300	4.23397200
H	1.64654100	0.18824400	4.73606400
N	5.88764700	-1.02549800	3.43850000
O	5.90542400	-1.91109700	4.30858400
O	6.83883700	-0.80159100	2.67782000

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C	-1.56563400	2.28563400	-0.76606100
C	-1.71480100	3.72385400	-0.86554600
C	-0.46434600	4.25327000	-0.79346300
C	0.44858200	3.14204200	-0.61892200
N	-0.24567000	1.96459800	-0.61172400
H	-2.65833900	4.23567100	-0.99527800
H	-0.16662500	5.29169500	-0.84150400
C	3.44715600	0.21913300	0.32130400
C	4.55708400	1.13848800	0.47601800
C	4.08540300	2.37708200	0.16977200
C	2.68050000	2.22139800	-0.14559000
N	2.32578000	0.90431200	-0.05307300
H	5.55914600	0.85024700	0.76259600
H	4.61669800	3.31893200	0.16242300
C	-1.55800900	-2.00079400	-1.11721600
C	-2.95976800	-2.15282400	-1.43903500
C	-3.52574400	-0.91916000	-1.32025900
C	-2.46218500	-0.00052200	-0.97264300
N	-1.28418800	-0.68851700	-0.83084300
H	-3.43279400	-3.08988200	-1.69941600
H	-4.55793400	-0.63563900	-1.47178400

C	0.65827400	-2.92259500	-0.59309500
C	1.55478200	-4.03134300	-0.35260000
C	2.70645800	-3.50401400	0.14775600
C	2.53483300	-2.06655900	0.16935300
N	1.27100900	-1.74428500	-0.25588600
H	1.31155800	-5.06893300	-0.53628600
H	3.60664400	-4.02084600	0.45079900
C	-2.62725800	1.38684800	-0.90217500
C	3.56045400	-1.16651800	0.47350100
C	1.82670300	3.28583900	-0.44299300
C	-0.65213900	-3.06345200	-1.05792000
Fe	0.50761500	0.11174000	-0.38731700
Cl	1.02887900	0.11983800	-2.72672000
O	0.17828800	0.21106000	1.29956900
C	4.89185400	-1.71726600	0.88902800
C	5.23586700	-1.77542300	2.25363800
C	5.80787800	-2.15430600	-0.08971600
C	6.48529900	-2.28757100	2.62047100
C	7.04710100	-2.65991200	0.31769800
C	7.40220800	-2.74026000	1.66759700
H	6.74861100	-2.33063300	3.67625200
H	7.75472200	-2.99399700	-0.43966100
C	-1.09042400	-4.40399600	-1.56488900
C	-1.65947700	-5.36860900	-0.71271400
C	-0.92160800	-4.68251600	-2.93817000
C	-2.05107800	-6.60250400	-1.24617300
C	-1.32606000	-5.92693300	-3.43149200
C	-1.88997400	-6.90117300	-2.60149800
H	-2.49380000	-7.34611000	-0.58529000
H	-1.19847600	-6.13961400	-4.49185100
C	-4.00906400	1.94302400	-1.07936400
C	-4.76745900	2.33020000	0.04218900
C	-4.54576100	2.07975500	-2.37834100
C	-6.06963300	2.80993900	-0.15105400
C	-5.84530400	2.57200800	-2.52761300
C	-6.62813600	2.93142100	-1.42462700
H	-6.65793800	3.09247500	0.72033100
H	-6.25697200	2.67833700	-3.53035500
C	2.41833700	4.65696900	-0.56013700
C	2.50497200	5.49622000	0.56678500
C	2.89423000	5.09526200	-1.81182200
C	3.06908300	6.76874200	0.42409800
C	3.45206900	6.37415100	-1.91332500
C	3.54513300	7.22610300	-0.80835100

H	3.13939800	7.41665800	1.29660800
H	3.82332000	6.71249600	-2.87957000
C	-1.85054900	-5.07986000	0.75823300
H	-0.89627000	-4.84338700	1.24234000
H	-2.50363700	-4.21329300	0.91287900
H	-2.29436100	-5.93607000	1.27703800
C	-0.32046800	-3.64404300	-3.85689900
H	-0.92839500	-2.73270200	-3.88144200
H	0.66758200	-3.32250700	-3.50985800
H	-0.22605100	-4.02736400	-4.87852000
C	-2.28733200	-8.25154600	-3.15357700
H	-2.67882000	-8.16831900	-4.17424700
H	-1.42823600	-8.93574200	-3.19249300
H	-3.05554700	-8.72887500	-2.53469400
C	-3.72567000	1.70435600	-3.59199500
H	-2.72725900	2.15343600	-3.55164300
H	-3.57027700	0.62058400	-3.64849700
H	-4.21789000	2.02797900	-4.51542500
C	-4.19105900	2.27949500	1.43858400
H	-3.45192000	1.48351900	1.54660100
H	-3.67898800	3.22153700	1.67692000
H	-4.97847900	2.12234700	2.18319400
C	-8.04883200	3.41430500	-1.60975500
H	-8.75090200	2.57139000	-1.67372200
H	-8.37215600	4.04239600	-0.77213900
H	-8.15829000	3.99628600	-2.53262600
C	2.80342600	4.18868200	-3.01742100
H	3.35647200	3.25633300	-2.85681800
H	1.76784000	3.88776300	-3.21171300
H	3.19889200	4.67894700	-3.91346500
C	1.99736300	5.02026300	1.90831500
H	0.92865100	4.78041300	1.86179300
H	2.50664500	4.10017200	2.21755800
H	2.14884800	5.77887800	2.68361800
C	4.11832100	8.61821200	-0.95037300
H	4.88939100	8.65764200	-1.72854700
H	3.34121200	9.34402700	-1.22802000
H	4.56616500	8.96643500	-0.01247500
C	5.45792300	-2.06859400	-1.55757000
H	4.62661700	-2.73829400	-1.80645200
H	5.12711100	-1.05961300	-1.82740400
H	6.31507700	-2.33547400	-2.18495600
C	4.27284700	-1.27377800	3.30470900
H	4.07114100	-0.20408100	3.17414600

H	3.30411700	-1.77835700	3.22952500
H	4.66849600	-1.43074000	4.31388200
C	8.73304200	-3.32382300	2.08526500
H	8.66835800	-4.41305600	2.21621900
H	9.50804500	-3.13449700	1.33348000
H	9.07579200	-2.90308600	3.03757200
C	-4.36629500	-0.29286700	4.07778200
C	-3.21643500	-0.34307500	4.87501900
C	-3.19320400	-1.33888000	2.26312300
C	-4.36020300	-0.79868100	2.77038500
H	-5.25997100	-0.73789100	2.17061600
C	-2.00038900	-1.38308100	3.02880400
C	-2.05054600	-0.87873800	4.35100000
C	0.40544700	-2.29991400	3.25831100
C	-0.77168500	-1.86039300	2.41224300
H	1.20410300	-2.66516300	2.60660500
H	-0.31013800	-0.76988300	1.78488100
H	-0.94546700	-2.48788200	1.54166500
H	0.13430400	-3.10764200	3.95530800
H	-3.25502500	0.05288900	5.88271900
H	0.81457100	-1.47161500	3.84905100
H	-1.15524400	-0.89851300	4.96391000
H	-3.17777700	-1.70926400	1.24356400
N	-5.56975500	0.32062100	4.60125700
O	-5.59610700	0.64130800	5.79711200
O	-6.51859900	0.50473500	3.82442800

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C	-0.54783700	-2.93514500	-0.55341000
C	-1.35587000	-4.09488500	-0.25430600
C	-2.48696700	-3.64033500	0.35532700
C	-2.39741700	-2.19526100	0.37967000
N	-1.19461800	-1.79878500	-0.14455800
H	-1.06919800	-5.11479200	-0.47261200
H	-3.32777400	-4.21148300	0.72463400
C	-2.90821900	2.02733700	-0.19782200
C	-4.28961900	2.10529200	0.23168200
C	-4.62603200	0.87128300	0.69760600
C	-3.46347800	0.02454600	0.51529300
N	-2.43873900	0.75747800	-0.01496800
H	-4.89680600	2.99926800	0.18957100
H	-5.57123400	0.54033200	1.10595200
C	2.36276100	0.16748200	-0.99763100
C	3.48186500	-0.68720400	-1.33747200

C	2.98239600	-1.94305500	-1.51394600
C	1.57393800	-1.88137900	-1.19272900
N	1.22751400	-0.59090800	-0.88461200
H	4.50445200	-0.35512300	-1.44327900
H	3.51129400	-2.84297900	-1.79646300
C	1.29025200	2.38225100	-0.91833700
C	1.32503700	3.81496200	-1.13063900
C	0.03186000	4.23995500	-1.14894300
C	-0.79230700	3.07552900	-0.88977000
N	-0.00217200	1.96638600	-0.78380300
H	2.23055800	4.38980900	-1.27143700
H	-0.34748300	5.24192700	-1.29602100
C	0.73170000	-2.99586700	-1.11404300
C	-2.17103300	3.11990500	-0.66496600
C	-3.45477300	-1.35547600	0.74807400
C	2.42650400	1.56729400	-0.92267800
Fe	-0.58540700	0.09049800	-0.39197900
Cl	-1.21875100	-0.09319400	-2.70867300
O	-0.19225400	0.38424800	1.26910800
H	0.39825600	-0.38385500	1.96414100
C	4.18646600	0.50658900	4.01299100
C	4.98481700	0.14153500	2.92510100
C	4.48071100	-0.68448800	1.91418000
C	3.16796900	-1.11546600	1.98624000
C	2.30883000	-0.73382000	3.04494100
C	2.86909500	0.07325900	4.06512000
H	4.60165100	1.14216800	4.78592400
H	5.10316700	-0.93619900	1.06560400
H	2.77288300	-1.70287300	1.16870100
C	0.88008000	-1.09979000	3.01419700
C	-4.70159500	-1.98772100	1.29089200
C	-4.84655900	-2.18444400	2.67688400
C	-5.73018000	-2.38245500	0.41065400
C	-6.01973800	-2.77052800	3.16535000
C	-6.88782600	-2.96518600	0.93678800
C	-7.05073900	-3.16966800	2.31072400
H	-6.13004700	-2.91660900	4.23884500
H	-7.68263800	-3.26618000	0.25585000
C	1.19387600	-4.28763700	-1.72077800
C	0.79279900	-4.56798500	-3.04633700
C	2.00582400	-5.20262000	-1.02359400
C	1.22988200	-5.75098700	-3.65109400
C	2.42115700	-6.37517300	-1.66643100
C	2.04973200	-6.66411600	-2.98153200

H	0.92069800	-5.96321400	-4.67349400
H	3.04954200	-7.07931100	-1.12314000
C	3.77756600	2.19369100	-0.76856400
C	4.69905400	2.27548200	-1.82825800
C	4.15083500	2.62251700	0.52694100
C	6.01938200	2.65844300	-1.55100400
C	5.47407200	2.99819200	0.75955900
C	6.43532500	2.97634000	-0.25675900
H	6.74149200	2.68715000	-2.36576700
H	5.77751600	3.26639900	1.76954100
C	-2.88792100	4.41511200	-0.89029400
C	-3.50098400	4.64853100	-2.13751500
C	-2.94821300	5.38932800	0.12428500
C	-4.16060600	5.86387000	-2.34995200
C	-3.61798000	6.59191400	-0.12730300
C	-4.23112700	6.84656400	-1.35765400
H	-4.62914700	6.04754900	-3.31574600
H	-3.66095900	7.34683500	0.65644800
C	-5.57921800	-2.17611400	-1.07865600
H	-5.44996400	-1.11507400	-1.32025500
H	-4.68663000	-2.68644300	-1.45780300
H	-6.45261800	-2.55241800	-1.62179100
C	-3.74297700	-1.76942800	3.62129200
H	-2.83289200	-2.35332100	3.43969300
H	-3.47074800	-0.71840900	3.47351500
H	-4.03634300	-1.91027800	4.66707400
C	-8.29746800	-3.83241100	2.85179900
H	-8.48920100	-3.54058400	3.89066000
H	-9.18128700	-3.57060400	2.25834800
H	-8.20848200	-4.92760100	2.83264700
C	-3.44904800	3.59337700	-3.21811600
H	-2.42180800	3.27039400	-3.41884000
H	-3.98583500	2.68867700	-2.90940700
H	-3.89305200	3.95831600	-4.15052300
C	-2.29410000	5.13483400	1.46301800
H	-2.66725100	4.20683500	1.91137900
H	-1.20986300	5.01206000	1.35599400
H	-2.48160500	5.95829300	2.16043900
C	-4.97890500	8.13855900	-1.59901700
H	-4.92752400	8.44152500	-2.65126700
H	-6.04296300	8.03886600	-1.34260200
H	-4.57477900	8.95655900	-0.99154700
C	4.28065300	1.95288200	-3.24698400
H	4.22431400	0.87287900	-3.42557000

H	3.28430100	2.35351200	-3.46228800
H	4.98908200	2.37577500	-3.96796000
C	7.88147800	3.25696900	0.07535100
H	8.24909400	2.50047900	0.78038300
H	8.51583300	3.23395400	-0.81773100
H	8.00537400	4.23662900	0.55488600
C	3.13640000	2.68365400	1.64497400
H	2.41309600	3.48867800	1.46645300
H	2.55335800	1.76179800	1.72233100
H	3.62531200	2.86781100	2.60521700
C	2.41284600	-4.94708500	0.40882500
H	2.92596100	-3.98577400	0.51709900
H	1.53674700	-4.91404100	1.06610300
H	3.08250600	-5.73184000	0.77631500
C	-0.11909800	-3.61948700	-3.78948100
H	-1.13048300	-3.63995500	-3.36608400
H	0.20251300	-2.57645600	-3.70610600
H	-0.18648800	-3.88800200	-4.84931700
C	2.54115300	-7.91567300	-3.67274000
H	1.78151700	-8.32573100	-4.34872000
H	3.43538100	-7.71218100	-4.27812200
H	2.80783300	-8.69582000	-2.95062900
C	0.54971000	-2.53417900	2.63046400
H	-0.52585400	-2.64797700	2.46933000
H	1.04087400	-2.83677400	1.70674900
H	0.85636600	-3.23377200	3.42482200
C	0.00422100	-0.55889400	4.13095500
H	0.23181500	-1.03156700	5.10038600
H	0.11377800	0.52489400	4.24109500
H	-1.04573800	-0.75518900	3.89904900
H	2.25805600	0.37602700	4.90794100
N	6.32847800	0.67612800	2.80960400
O	7.04764200	0.26580400	1.89102500
O	6.68882600	1.53684600	3.62563600

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C	-1.57583500	-1.87587000	-1.32127500
C	-2.97808300	-1.92412300	-1.67009300
C	-3.46889200	-0.66430300	-1.49715600
C	-2.34998500	0.17658900	-1.12649400
N	-1.21959500	-0.58970600	-1.01401900
H	-3.51089900	-2.82107900	-1.95546800
H	-4.48769200	-0.32249300	-1.60904400
C	0.81392100	3.06569400	-0.89428100

C	-0.00335100	4.23975200	-1.12729900
C	-1.29819600	3.81967800	-1.13070200
C	-1.27052400	2.38140000	-0.96130700
N	0.01945500	1.95571400	-0.82625600
H	0.38101900	5.24398100	-1.24226600
H	-2.20013700	4.40244700	-1.26118000
C	2.38303000	-2.23630200	0.28111300
C	2.46401000	-3.68115700	0.24937300
C	1.32702500	-4.12656600	-0.35423400
C	0.52359900	-2.96004400	-0.64595900
N	1.18614800	-1.82907100	-0.24650200
H	3.30458000	-4.25842100	0.60946800
H	1.03871500	-5.14391900	-0.58071700
C	3.45560700	-0.02395600	0.47403400
C	4.61654000	0.81532500	0.69519100
C	4.29173000	2.05965900	0.24916900
C	2.91722100	1.99525800	-0.20330400
N	2.44048500	0.72334500	-0.05524200
H	5.55314900	0.47311000	1.11393000
H	4.90150600	2.95276700	0.23632400
C	-0.75774900	-3.00339800	-1.20448000
C	2.19017100	3.10084900	-0.65437600
C	-2.41028900	1.57295500	-1.00697800
C	3.43889900	-1.40781800	0.67694600
Fe	0.59457700	0.06702300	-0.48499700
Cl	1.27206300	-0.08099600	-2.78343500
O	0.15575800	0.26046900	1.17307100
H	-0.44749800	-0.66032600	1.64994600
C	-0.31722200	-1.38734800	3.76148800
C	-1.13147600	-0.23327400	4.40936800
C	-1.01031300	-1.61044100	2.41781800
C	-2.38046400	-1.15463700	2.58219500
C	-3.49656600	-1.34312600	1.75147400
C	-4.68152800	-0.67763100	2.03268600
C	-4.75118200	0.16430900	3.15031000
C	-3.65887000	0.33710100	4.02026100
C	-2.48177000	-0.32341500	3.72816300
H	-3.42026300	-1.95549600	0.86243800
H	-3.75205300	1.01097900	4.86383800
H	-5.54272300	-0.75943300	1.38157300
H	-0.66846000	0.73099400	4.16074600
H	0.74030600	-1.13617300	3.64342900
H	-0.79957900	-2.51240700	1.84573300
N	-5.94805400	0.95512000	3.35277000

O	-5.90864300	1.87059800	4.19007100
O	-6.94777400	0.70812200	2.66516300
C	-3.75826600	2.20490700	-0.84385400
C	-4.66079100	2.34778400	-1.91325500
C	-4.14190600	2.59174700	0.46223300
C	-5.97128500	2.76754100	-1.64313700
C	-5.45830700	2.99606600	0.69013000
C	-6.39706000	3.05906100	-0.34545800
H	-6.67672300	2.85498300	-2.46835500
H	-5.76749000	3.24229000	1.70418900
C	2.91405500	4.39800100	-0.84267900
C	3.54641400	4.65401000	-2.07590000
C	2.97204400	5.34686300	0.19571400
C	4.21993200	5.86749600	-2.25138100
C	3.65646600	6.54848400	-0.01906200
C	4.28226800	6.82846500	-1.23736100
H	4.70914900	6.06591000	-3.20393800
H	3.70346300	7.28097100	0.78544100
C	4.66521100	-2.05544100	1.24585300
C	5.73904900	-2.40149400	0.40069900
C	4.74085000	-2.31902000	2.62674900
C	6.87452500	-3.00052400	0.95673200
C	5.89369500	-2.91852200	3.14551600
C	6.97056800	-3.26815300	2.32585500
H	7.70447400	-3.26501100	0.30313900
H	5.95131600	-3.11585100	4.21495800
C	-1.27223700	-4.31106100	-1.72286900
C	-1.17414400	-4.56606600	-3.10747300
C	-1.83619500	-5.27483900	-0.86458000
C	-1.63507600	-5.78957100	-3.60458000
C	-2.28827800	-6.48523300	-1.40324500
C	-2.19707600	-6.76063100	-2.77019200
H	-1.55151900	-5.98865000	-4.67202400
H	-2.72247100	-7.22952800	-0.73740800
C	2.30842600	5.06271400	1.52373100
H	1.22491300	4.94376300	1.40604800
H	2.67761800	4.12454900	1.95405900
H	2.49138400	5.87001100	2.24094000
C	3.50885700	3.62014800	-3.17750100
H	4.04675600	2.71169700	-2.88187300
H	2.48497900	3.29703300	-3.39420600
H	3.96008100	4.00527100	-4.09824800
C	4.98565200	8.14764000	-1.46435400
H	5.84507300	8.03392400	-2.13543500

H	4.31285700	8.88553700	-1.92324100
H	5.34607800	8.57854900	-0.52320100
C	3.58345700	-1.96240600	3.53029200
H	3.30762600	-0.90719400	3.42248300
H	2.69092800	-2.54228800	3.26761600
H	3.82200700	-2.15558400	4.58166500
C	5.66116800	-2.12579400	-1.08313500
H	4.76331700	-2.57579900	-1.52138900
H	5.59172700	-1.05017400	-1.28213400
H	6.53967700	-2.51853200	-1.60606900
C	8.19430800	-3.94747800	2.89801400
H	8.35254100	-3.67345100	3.94740100
H	8.09923100	-5.04164800	2.85892000
H	9.09915200	-3.68203900	2.33904600
C	-1.95408100	-5.01428000	0.61994700
H	-0.96777100	-4.90082000	1.08438600
H	-2.50136800	-4.08674400	0.81918700
H	-2.47705500	-5.83290300	1.12562200
C	-0.59820100	-3.52485100	-4.04000300
H	-1.29779500	-2.69004000	-4.17008900
H	0.31935300	-3.07630000	-3.64528900
H	-0.39042000	-3.95203000	-5.02707800
C	-2.72021300	-8.06010100	-3.33927200
H	-3.74408800	-7.94504100	-3.72141800
H	-2.10231800	-8.40965100	-4.17477000
H	-2.74312000	-8.85127600	-2.58125600
C	-3.14386300	2.59010400	1.59696300
H	-2.57943600	1.65469100	1.64857100
H	-2.40279900	3.38679200	1.45704700
H	-3.64486400	2.75131300	2.55508400
C	-4.22911600	2.05963900	-3.33525100
H	-3.23294700	2.47043600	-3.53234300
H	-4.16392800	0.98429500	-3.53685100
H	-4.93296800	2.49480400	-4.05332000
C	-7.82820100	3.43548600	-0.04016900
H	-8.47502400	3.31217200	-0.91596400
H	-8.22085200	2.80850700	0.76972400
H	-7.90948500	4.47955600	0.29109500
H	-1.18979500	-0.29894700	5.50208800
H	-0.37997100	-2.29416500	4.38285800

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C	-1.67772300	-1.83813200	-1.22391700
C	-3.08467200	-1.89298800	-1.55088500

C	-3.56925800	-0.62746300	-1.41685600
C	-2.45179800	0.21311100	-1.05000000
N	-1.31853900	-0.54980800	-0.92477100
H	-3.61679300	-2.79489000	-1.81981600
H	-4.58006500	-0.27336600	-1.56179200
C	0.64583500	3.14751100	-0.59530700
C	-0.19547700	4.31802000	-0.73056600
C	-1.47670100	3.87131800	-0.82145500
C	-1.41906500	2.42582900	-0.77618100
N	-0.12122600	2.01603300	-0.63586900
H	0.16709700	5.33662200	-0.73756900
H	-2.38748800	4.44401900	-0.92780300
C	2.42104400	-2.19399200	-0.00174700
C	2.51183000	-3.63357600	-0.09831800
C	1.31689500	-4.07321600	-0.57949900
C	0.47729900	-2.90900700	-0.74353800
N	1.16888100	-1.78049600	-0.38021500
H	3.39329100	-4.20996700	0.14610800
H	1.01089600	-5.08569800	-0.80347200
C	3.46380300	0.01886900	0.25407000
C	4.61263700	0.87059600	0.47976700
C	4.21387400	2.14481000	0.22051600
C	2.81120300	2.08031300	-0.13068400
N	2.38635500	0.78016900	-0.10767400
H	5.58907700	0.51702800	0.78080200
H	4.79173400	3.05728600	0.27133500
C	-0.84724600	-2.95968800	-1.17978600
C	2.02666500	3.20339900	-0.39676900
C	-2.53469500	1.60289800	-0.93865700
C	3.50121300	-1.37492600	0.33443200
Fe	0.51675700	0.11582900	-0.44878200
Cl	1.03407500	0.14279800	-2.77862100
O	0.18647900	0.18117100	1.20165800
H	-0.18781800	-0.79545600	1.79459900
C	0.12283600	-1.73083700	3.78894800
C	-0.65402300	-1.14715200	4.75165300
C	-0.62898600	-1.86993300	2.54293600
C	-1.98604200	-1.45040800	2.86427600
C	-3.15286600	-1.39352600	2.09282700
C	-4.30278700	-0.82860400	2.63097400
C	-4.27591000	-0.31883400	3.94158600
C	-3.13220300	-0.37699900	4.74703400
C	-1.98346300	-0.94807600	4.20827500
H	-3.15938200	-1.75459700	1.07098900

H	-3.16253200	0.03005900	5.75087000
H	-5.21311800	-0.74569800	2.05106900
H	-0.34208800	-0.85570100	5.74869200
H	1.16970700	-1.99059300	3.89314400
H	-0.41981400	-2.65649000	1.82259700
N	-5.46794000	0.32317600	4.46786400
O	-5.49096500	0.64059900	5.66430700
O	-6.41333600	0.53642800	3.69375500
C	-3.88106100	2.24631800	-1.08412900
C	-4.39102200	2.51483700	-2.37197300
C	-4.63126600	2.57914500	0.06017400
C	-5.65595000	3.09750100	-2.49249600
C	-5.89750200	3.15447300	-0.10544100
C	-6.42839700	3.41650600	-1.37022500
H	-6.04829600	3.30623100	-3.48676800
H	-6.48072000	3.39852400	0.78076600
C	2.69799200	4.54155700	-0.44139000
C	3.23672900	5.00077900	-1.65931800
C	2.79668300	5.32871400	0.72194600
C	3.86684600	6.24938000	-1.69256200
C	3.43470000	6.57168300	0.64737900
C	3.97284400	7.05012900	-0.55116000
H	4.28577400	6.60392000	-2.63307400
H	3.51457400	7.17920500	1.54757600
C	4.79351200	-2.03137700	0.71608300
C	5.79614800	-2.22989500	-0.25534600
C	5.00189100	-2.45325400	2.04287900
C	6.99627900	-2.84012100	0.12408800
C	6.21687200	-3.05795800	2.38351900
C	7.22570900	-3.26121100	1.43787500
H	7.77082400	-2.99125900	-0.62633300
H	6.37733900	-3.37758500	3.41200300
C	-1.39262100	-4.26634000	-1.67101600
C	-1.38700800	-4.51690100	-3.05965900
C	-1.89780300	-5.23192200	-0.77892800
C	-1.88533400	-5.73615800	-3.52980500
C	-2.38933600	-6.43833700	-1.29145600
C	-2.39363600	-6.70807000	-2.66252500
H	-1.87476900	-5.93144700	-4.60107600
H	-2.77852000	-7.18434600	-0.60038000
C	2.22460300	4.82932300	2.02852700
H	1.14548300	4.65541600	1.94543400
H	2.67029900	3.86888700	2.31221200
H	2.39841100	5.54524100	2.83876100

C	3.13768700	4.14779800	-2.90289600
H	3.65159100	3.18902300	-2.76825500
H	2.09591000	3.89729300	-3.13231900
H	3.57331200	4.65677800	-3.76930000
C	4.62690400	8.41180300	-0.61809200
H	5.41262300	8.44282800	-1.38174000
H	3.89723500	9.19326400	-0.87216000
H	5.07697100	8.68912300	0.34208000
C	3.91645900	-2.27157800	3.07803600
H	3.53168100	-1.24591300	3.08066900
H	3.06124800	-2.92192800	2.85715700
H	4.27802100	-2.51295700	4.08318400
C	5.57454700	-1.78795200	-1.68340200
H	4.63284000	-2.18450700	-2.07891700
H	5.49893100	-0.69653400	-1.75285400
H	6.39286000	-2.11858100	-2.33178600
C	8.51807400	-3.94897300	1.81578100
H	8.74766100	-3.81647300	2.87914200
H	8.46465600	-5.03017900	1.62675000
H	9.36400300	-3.56151700	1.23617000
C	-1.90081000	-4.98206800	0.71148400
H	-0.87931700	-4.92399700	1.10537000
H	-2.38400400	-4.03206500	0.96145300
H	-2.42434000	-5.78130900	1.24625100
C	-0.86149100	-3.47710100	-4.02287100
H	-1.52060600	-2.60118600	-4.05265800
H	0.11947200	-3.09721900	-3.71838300
H	-0.78398300	-3.88226000	-5.03745200
C	-2.96068300	-8.00313900	-3.19857900
H	-4.01977200	-7.89266800	-3.46999800
H	-2.42920700	-8.33113900	-4.09948500
H	-2.89811900	-8.80733600	-2.45666400
C	-4.08233100	2.36199600	1.45144800
H	-3.41811300	1.49687100	1.49954100
H	-3.49507600	3.23255000	1.77391900
H	-4.89127100	2.20920400	2.17289200
C	-3.57985400	2.17692500	-3.60227600
H	-2.57279200	2.60502500	-3.54503000
H	-3.44536800	1.09358300	-3.70407900
H	-4.06559700	2.54923900	-4.51054200
C	-7.81389500	4.00178000	-1.52436500
H	-7.89951000	4.59622000	-2.44150700
H	-8.57587500	3.21181000	-1.57639800
H	-8.07445300	4.64576000	-0.67676300

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C	-1.29422300	2.35941100	-1.06188500
C	-1.34375600	3.79683200	-1.23250500
C	-0.05584300	4.23816500	-1.21642900
C	0.77769200	3.07788400	-0.97332000
N	0.00120100	1.95510000	-0.91511500
H	-2.25384400	4.36475400	-1.37143500
H	0.31328500	5.24861400	-1.32677400
C	3.43998300	0.04338600	0.47798700
C	4.59342900	0.89684700	0.68381900
C	4.25585500	2.13141100	0.22078600
C	2.88354400	2.04610200	-0.23369500
N	2.41815700	0.77173400	-0.06434100
H	5.53401700	0.57010300	1.10547700
H	4.85704900	3.02998900	0.19437700
C	-1.52141500	-1.90306100	-1.40361100
C	-2.91800400	-1.97861300	-1.77129800
C	-3.43356200	-0.72635600	-1.61254700
C	-2.33483300	0.13684500	-1.23273900
N	-1.19260700	-0.60882800	-1.10265100
H	-3.43113000	-2.88636000	-2.05860100
H	-4.45667100	-0.40372300	-1.74099000
C	0.57275500	-2.94773900	-0.65166100
C	1.38004100	-4.09978000	-0.31504500
C	2.49313000	-3.63104200	0.31472400
C	2.39731300	-2.18641300	0.31661400
N	1.20807100	-1.80279000	-0.24769000
H	1.10905800	-5.12436500	-0.53018700
H	3.32751400	-4.19280600	0.71193200
C	-2.42023500	1.53182300	-1.11309500
C	3.44013700	-1.33800200	0.70492400
C	2.14911700	3.13552900	-0.71086000
C	-0.68801300	-3.01591900	-1.25382200
Fe	0.59565300	0.08128600	-0.53493200
Cl	1.34581100	-0.09671400	-2.80819300
O	0.08990300	0.29263500	1.10004500
H	-1.72559500	-1.00333000	5.61872300
C	4.69698100	-1.95654600	1.24261100
C	4.88507500	-2.11168100	2.62837400
C	5.70540700	-2.36552900	0.34352300
C	6.07768400	-2.67678800	3.09670000
C	6.88065200	-2.92820100	0.85029700
C	7.08482900	-3.09492900	2.22415000

H	6.22172100	-2.78997300	4.17021600
H	7.65868700	-3.23944300	0.15476000
C	-1.16070200	-4.33397500	-1.78563400
C	-1.76453400	-5.29503200	-0.95192200
C	-0.99081600	-4.59581100	-3.16186700
C	-2.17990600	-6.51175800	-1.50528000
C	-1.41825500	-5.82526100	-3.67446000
C	-2.01069200	-6.79731100	-2.86284200
H	-2.64968900	-7.25211200	-0.85952200
H	-1.28594100	-6.02682400	-4.73644200
C	-3.77703900	2.14195900	-0.94398900
C	-4.15807300	2.52201400	0.36530900
C	-4.68648500	2.27551600	-2.00857900
C	-5.47660000	2.91592600	0.59791500
C	-6.00090400	2.67830800	-1.73143400
C	-6.42250000	2.96630400	-0.43175000
H	-5.78336200	3.16272500	1.61243300
H	-6.71211100	2.75609000	-2.55264600
C	2.85606400	4.44217700	-0.89866500
C	2.91112500	5.38543500	0.14496600
C	3.47478000	4.71291100	-2.13542500
C	3.58127000	6.59540300	-0.06741900
C	4.13488900	5.93417900	-2.30823400
C	4.19536200	6.88917500	-1.28850000
H	3.62612100	7.32366600	0.74104200
H	4.61485400	6.14350100	-3.26313400
C	-1.97577600	-5.01809600	0.51903100
H	-1.02514500	-4.82782800	1.02951700
H	-2.59657300	-4.12777300	0.67036100
H	-2.46747700	-5.86178000	1.01478800
C	-0.38409800	-3.55216000	-4.07192100
H	-1.08306600	-2.72223600	-4.23255300
H	0.51297000	-3.09533200	-3.64114100
H	-0.13247800	-3.97974500	-5.04855900
C	-2.43189200	-8.13207100	-3.43487900
H	-2.78815900	-8.03210700	-4.46681200
H	-1.59373100	-8.84269500	-3.45010600
H	-3.23374200	-8.58814600	-2.84305100
C	-4.25776300	1.99750800	-3.43362600
H	-3.26801800	2.42220600	-3.63387100
H	-4.17955000	0.92400200	-3.64026500
H	-4.97045200	2.42617600	-4.14685000
C	-3.15824500	2.52130300	1.49908500
H	-2.59167700	1.58705800	1.55056400

H	-2.41864700	3.31953200	1.36098700
H	-3.65911200	2.67956800	2.45781700
C	-7.85671400	3.31980300	-0.11480700
H	-8.23259200	2.67842600	0.69173300
H	-7.95065200	4.35933900	0.22716800
H	-8.50717600	3.19535900	-0.98776100
C	3.43301600	3.68765800	-3.24474800
H	3.93877200	2.76214400	-2.94621400
H	2.40458300	3.39551000	-3.48355800
H	3.91100800	4.06740600	-4.15412200
C	2.25882200	5.08628600	1.47518900
H	1.17901500	4.93581300	1.35963300
H	2.65575700	4.16050300	1.90779100
H	2.41986300	5.90052800	2.18977600
C	4.88343500	8.21703500	-1.51176900
H	5.73025400	8.11941100	-2.20106400
H	4.19554700	8.95527800	-1.94711300
H	5.25888200	8.63852600	-0.57218700
C	5.51716200	-2.18754600	-1.14533700
H	4.62878100	-2.72283100	-1.49869500
H	5.35831100	-1.13367800	-1.40048500
H	6.38739400	-2.55267600	-1.70100100
C	3.80897900	-1.69181400	3.60279400
H	3.39803900	-0.70891800	3.35069000
H	2.96904900	-2.39656100	3.58178000
H	4.19231700	-1.65833600	4.62841800
C	8.35243800	-3.73359500	2.74518300
H	8.28672000	-4.83028200	2.72051200
H	9.22262100	-3.44996300	2.14147600
H	8.55178800	-3.44302500	3.78287700
C	-4.87763100	0.13588100	3.01653000
C	-3.86697000	0.26896800	3.97713800
C	-3.46432500	-1.25956300	1.68693000
C	-4.69003300	-0.64831500	1.87286200
H	-5.47957000	-0.72100800	1.13581600
C	-2.40595700	-1.10806300	2.61124700
C	-2.63781000	-0.35226200	3.79565600
C	-0.06788200	-1.70234000	3.41894300
C	-0.13606000	-0.42770700	4.27190300
C	-1.54859300	-0.23635300	4.84736300
C	-1.07853400	-1.61518800	2.29186900
H	0.93040600	-1.82165200	2.98815100
H	0.59562300	-0.46494100	5.08900000
H	-0.54557800	-0.63051200	1.56160800

H	-1.05449400	-2.42797900	1.56683300
H	-1.63012200	0.73206800	5.35725300
H	-0.26096400	-2.58772800	4.04868100
H	0.12326800	0.42253200	3.63054200
H	-4.05194000	0.88701800	4.84884900
H	-3.28634000	-1.82518700	0.78075600
N	-6.10460200	0.89068000	3.16072400
O	-7.04477200	0.64129200	2.39429600
O	-6.15047100	1.77537800	4.02952100

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C	-1.13922700	-2.05919100	-1.46539600
C	-2.49565500	-2.49164400	-1.71646800
C	-3.30131400	-1.42259400	-1.46702000
C	-2.43690900	-0.31045500	-1.13173900
N	-1.13180600	-0.73657100	-1.10500200
H	-2.77699800	-3.49319100	-2.01208700
H	-4.37968800	-1.37257100	-1.51102600
C	-0.18245300	3.32410700	-0.74686000
C	-1.28808200	4.23716800	-0.94697700
C	-2.41365200	3.47737200	-1.01981000
C	-1.99469500	2.09646800	-0.89990500
N	-0.63978000	2.03360400	-0.74363700
H	-1.19394600	5.31271900	-1.00556600
H	-3.43781500	3.79533700	-1.15928400
C	2.92506600	-1.36976800	-0.26649400
C	3.40433300	-2.71871300	-0.47625400
C	2.37594100	-3.42421900	-1.02544500
C	1.24765700	-2.52444100	-1.10486200
N	1.60702600	-1.28677500	-0.63832000
H	4.40497600	-3.05870300	-0.24818900
H	2.35714700	-4.46145400	-1.32981100
C	3.32013900	1.02055800	0.16758500
C	4.20980000	2.13490900	0.42569200
C	3.50035000	3.26787600	0.17415300
C	2.16769000	2.84844600	-0.20679700
N	2.08686800	1.48466100	-0.19543700
H	5.24294400	2.03881000	0.72997600
H	3.82496500	4.29728700	0.23957500
C	-0.02947400	-2.90476800	-1.52692100
C	1.13170500	3.73250200	-0.51678800
C	-2.87450700	1.01285000	-0.98811700
C	3.72911900	-0.31547300	0.17860900
Fe	0.46359800	0.35994200	-0.59325000

Cl	0.96926500	0.63527700	-2.92656400
O	0.15113600	0.24742500	1.08568700
H	-0.29335500	-0.76625400	1.55817200
C	1.02325600	-3.07878500	5.27343900
C	2.24138300	-3.49195800	4.73096700
C	2.43705600	-3.38528200	3.35023200
C	1.43745600	-2.86016100	2.53790400
C	0.20406400	-2.42704500	3.06688500
C	0.01769100	-2.55820600	4.45638700
H	0.84492800	-3.17030200	6.34284800
H	3.37643700	-3.69656700	2.89950300
H	1.60636700	-2.77252600	1.47386300
H	-0.93167100	-2.28337600	4.90302200
C	-0.81525500	-1.91487600	2.11596300
H	-0.82887900	-2.50079900	1.19665500
C	-2.16341000	-1.52380200	2.54150100
C	-2.40482200	-0.65186900	3.63147900
C	-3.28356900	-1.95815800	1.79706400
C	-3.68860900	-0.24897300	3.96364400
H	-1.56258300	-0.25435300	4.18773400
C	-4.57148200	-1.55358900	2.10714800
C	-4.76914200	-0.69729100	3.19406100
H	-3.86881400	0.44508400	4.77530000
H	-5.42098700	-1.86408400	1.51160300
C	-4.34778900	1.27525600	-0.91423500
C	-5.18142100	1.13360200	-2.04096500
C	-4.90951200	1.62886100	0.33614200
C	-6.56986100	1.23542100	-1.87613700
C	-6.29813000	1.70447900	0.46024100
C	-7.14723700	1.48512400	-0.62984500
H	-7.21289700	1.10892200	-2.74601900
H	-6.72935800	1.92280000	1.43537600
C	-0.20630000	-4.27402500	-2.10940800
C	-0.46112300	-5.39277300	-1.29349600
C	-0.10960200	-4.42301600	-3.50894500
C	-0.60664200	-6.65027300	-1.89123300
C	-0.26084000	-5.69693900	-4.06622400
C	-0.50507500	-6.82324100	-3.27423100
H	-0.80578200	-7.51431400	-1.25917600
H	-0.18644900	-5.81132300	-5.14661600
C	1.44807600	5.19392800	-0.59932700
C	1.94751000	5.71815600	-1.80850900
C	1.24535200	6.03572700	0.51061800
C	2.23017100	7.08596500	-1.88652600

C	1.54194300	7.39816000	0.39264000
C	2.03600000	7.94111500	-0.79717600
H	2.60941100	7.49327000	-2.82259500
H	1.38224900	8.04989800	1.25033500
C	5.13050300	-0.61969200	0.61374000
C	5.43165300	-0.68793200	1.98915800
C	6.14750600	-0.81281900	-0.34410700
C	6.73982400	-0.99255600	2.38282300
C	7.44261100	-1.11263400	0.09204100
C	7.75627500	-1.21805800	1.45058700
H	6.96911800	-1.04946500	3.44586200
H	8.22713500	-1.26023200	-0.64873500
C	4.37227600	-0.39119500	3.02544500
H	4.14085400	0.68128700	3.04401200
H	3.43308800	-0.90663400	2.80926700
H	4.70243500	-0.68700800	4.02685400
C	5.84911600	-0.67735300	-1.82016900
H	5.18367300	-1.47446400	-2.17032100
H	5.33315400	0.26567500	-2.03254900
H	6.76929900	-0.71305900	-2.41309100
C	9.15349600	-1.58401700	1.89755700
H	9.27735900	-2.67360800	1.96990900
H	9.90935000	-1.21916900	1.19234600
H	9.38191100	-1.16611000	2.88473800
C	0.70995400	5.47067100	1.80629700
H	-0.30401000	5.07463700	1.67516300
H	1.32586000	4.63332200	2.15389900
H	0.68342600	6.23301300	2.59215900
C	2.17785500	4.80869700	-2.99327900
H	2.96824900	4.07958800	-2.77943800
H	1.28677000	4.21646100	-3.22798400
H	2.46612400	5.38027700	-3.88197000
C	2.38139700	9.41006600	-0.89547100
H	3.43682600	9.59004100	-0.64760500
H	2.21804200	9.79360000	-1.90929400
H	1.77923700	10.01184100	-0.20512800
C	-4.03265400	1.95918200	1.52134100
H	-3.22677400	1.23270700	1.65137800
H	-3.55035500	2.93423900	1.38072400
H	-4.61893400	2.00342900	2.44295900
C	-4.60238300	0.89020900	-3.41869100
H	-3.66684500	1.44185800	-3.55681700
H	-4.36574400	-0.16704400	-3.58637300
H	-5.30892800	1.20204000	-4.19601600

C	-8.64612200	1.54110600	-0.44591700
H	-8.95711900	0.90701200	0.39323300
H	-8.98637800	2.56109400	-0.22149400
H	-9.17609300	1.20425400	-1.34376100
C	0.13379400	-3.21831900	-4.38860200
H	-0.71953500	-2.53053500	-4.35767400
H	0.99363700	-2.63111000	-4.04872200
H	0.29866100	-3.51589400	-5.42968200
C	-0.59805700	-5.24106000	0.20383700
H	0.27777200	-4.75392000	0.64522800
H	-1.46303800	-4.61695600	0.45819000
H	-0.72961200	-6.21255700	0.69147800
C	-0.62668900	-8.19586200	-3.89651800
H	0.35854100	-8.66670000	-4.02013900
H	-1.23140000	-8.86675900	-3.27570400
H	-1.08751100	-8.14710200	-4.89002400
H	3.02278100	-3.89466600	5.37067000
H	-3.12388100	-2.60223200	0.94035600
N	-6.09928500	-0.18402600	3.45848900
O	-6.21930500	0.73000300	4.28776400
O	-7.05152100	-0.65988200	2.82805200

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C	2.54669700	0.09807100	-1.23443200
C	3.54680600	-0.84056400	-1.69431000
C	2.89968600	-2.00727200	-1.96952600
C	1.51049100	-1.80568500	-1.62584200
N	1.32248900	-0.52031600	-1.18713900
H	4.59805600	-0.61326800	-1.80226700
H	3.31104700	-2.93474400	-2.34315300
C	-2.58802000	-1.75304400	-0.34033600
C	-2.82149100	-3.17654200	-0.45571200
C	-1.70115100	-3.71841500	-1.00956600
C	-0.75590200	-2.63957500	-1.18164800
N	-1.31010100	-1.46256000	-0.75064900
H	-3.74142100	-3.67267000	-0.17897700
H	-1.50595900	-4.75069600	-1.26553700
C	-0.15996300	3.35281500	-0.56342700
C	0.82685400	4.41152800	-0.55999600
C	2.04459500	3.81224000	-0.64807100
C	1.80287600	2.38751400	-0.73825600
N	0.45947800	2.13869700	-0.67184900
H	0.59547300	5.46522400	-0.48690400
H	3.02342300	4.27053000	-0.67459700

C	-2.46397100	2.54108300	-0.29927200
C	-3.87440400	2.75734200	-0.05810100
C	-4.43482000	1.53056400	0.11539300
C	-3.37338000	0.55875600	-0.04574200
N	-2.19330000	1.19924400	-0.30056500
H	-4.34928500	3.72785300	-0.01839400
H	-5.46796800	1.28367700	0.31667300
C	2.80818300	1.44544900	-0.96753700
C	-3.57416500	-0.82391500	0.00490000
C	0.54188400	-2.81166900	-1.66946300
C	-1.53349200	3.57087300	-0.44210100
Fe	-0.41770900	0.32778000	-0.66253700
Cl	-0.87697800	0.61905100	-2.99097400
O	-0.10737900	0.17733600	0.99280600
H	0.24000100	-0.89108000	1.41487500
C	4.18504000	-0.98826200	3.92065300
C	4.30288800	-1.20472100	2.53670700
C	3.19327400	-1.60791200	1.80686100
C	1.96956600	-1.79661000	2.46326000
C	1.88174200	-1.62257500	3.88120400
C	2.98668800	-1.20999300	4.61251500
H	3.27067000	-1.75080400	0.73524600
H	2.94928700	-1.04923700	5.68354100
C	0.65069900	-2.10876000	1.93523300
C	-0.20146100	-2.31945600	3.11083600
C	-1.52534300	-2.75518400	3.20983900
C	-2.12163400	-2.82596900	4.47118300
C	-1.41542400	-2.45616400	5.62668500
C	-0.08972400	-2.02325400	5.53950200
C	0.52023200	-1.96511400	4.28572300
H	-2.07749000	-3.03080800	2.31479400
H	-1.90279400	-2.51173300	6.59712600
H	0.46111300	-1.74760700	6.43628200
C	0.89563300	-4.11922100	-2.31071300
C	0.60331900	-4.28517300	-3.68175800
C	1.51443800	-5.15598600	-1.58730400
C	0.94358500	-5.48939000	-4.30520500
C	1.83881600	-6.34615500	-2.25015700
C	1.56081200	-6.53213500	-3.60653100
H	0.72398500	-5.61460700	-5.36443800
H	2.32219800	-7.14549100	-1.69077000
C	-4.94365600	-1.32376700	0.35276100
C	-5.38129800	-1.30581600	1.69332500
C	-5.80684000	-1.78375200	-0.66538400

C	-6.65510000	-1.79906400	1.99873600
C	-7.07402100	-2.26242800	-0.31659300
C	-7.51173300	-2.29140100	1.01094100
H	-6.98625700	-1.79216400	3.03609200
H	-7.73891400	-2.61462200	-1.10389800
C	-2.03156200	4.98335000	-0.44948200
C	-2.23399100	5.67651000	0.75880400
C	-2.30416500	5.60772000	-1.68325200
C	-2.71238900	6.99092600	0.71486500
C	-2.78289200	6.92183400	-1.68442100
C	-2.99064900	7.63048500	-0.49660000
H	-2.87123400	7.52659400	1.64949500
H	-3.00007000	7.40311700	-2.63684300
C	4.22986300	1.92005800	-1.00917900
C	4.93865100	2.12402500	0.19182700
C	4.85450900	2.16589500	-2.25114100
C	6.28045300	2.52056800	0.12749400
C	6.19258600	2.57019200	-2.26948300
C	6.92542500	2.74483300	-1.09050000
H	6.83114100	2.65463500	1.05698200
H	6.67472900	2.75362400	-3.22864100
C	1.81653300	-4.99954400	-0.11494100
H	2.40196600	-4.09602400	0.08453900
H	0.89398400	-4.90854000	0.47051300
H	2.37477300	-5.85956400	0.26919700
C	-0.07222100	-3.17721200	-4.45686300
H	-1.08195500	-2.98675400	-4.07471300
H	0.46059400	-2.22553700	-4.35619500
H	-0.14725100	-3.42801600	-5.52030400
C	1.89234300	-7.83489700	-4.29850600
H	2.67736700	-8.38427200	-3.76690500
H	1.01364200	-8.49238500	-4.35405700
H	2.23394400	-7.66719800	-5.32677500
C	4.27003300	1.96981700	1.53890700
H	3.79808300	2.91516200	1.83931100
H	3.48135800	1.21545400	1.52330100
H	4.99485500	1.69237400	2.31134000
C	4.08954700	2.00179900	-3.54550800
H	3.88079800	0.94710700	-3.75922300
H	3.11614900	2.50224300	-3.49633300
H	4.65198600	2.41546800	-4.38940100
C	8.36617800	3.20138300	-1.13467000
H	8.43681700	4.29781500	-1.15918300
H	8.92149800	2.85993100	-0.25398800

H	8.88016800	2.82457400	-2.02666300
C	-1.94318000	5.00352400	2.08048600
H	-2.59079600	4.13157600	2.22977200
H	-0.91263000	4.63195700	2.11544400
H	-2.09253600	5.69172900	2.91907300
C	-3.47422300	9.06287100	-0.52612000
H	-4.16981100	9.23500200	-1.35583800
H	-3.98446200	9.33459800	0.40491400
H	-2.63771100	9.76364600	-0.65550400
C	-2.07588300	4.86289800	-2.97828400
H	-1.01342000	4.62997100	-3.11573000
H	-2.59393800	3.89766800	-2.98453000
H	-2.41491200	5.44972600	-3.83860100
C	-4.51637700	-0.71951700	2.78515800
H	-4.86265500	-1.03090400	3.77634300
H	-3.46821700	-1.00943900	2.68345700
H	-4.53900600	0.37711900	2.74768500
C	-5.38537300	-1.74507400	-2.11767100
H	-4.90189000	-0.79446000	-2.36665900
H	-4.65440200	-2.52989600	-2.34508300
H	-6.24765100	-1.88267100	-2.77897400
C	-8.86793700	-2.85613900	1.36749100
H	-9.26035100	-2.40960100	2.28825300
H	-9.59832300	-2.68204600	0.56872600
H	-8.81771000	-3.94198400	1.52893600
H	0.53135500	-2.70563100	1.03744800
H	-3.15116400	-3.16531100	4.55719900
H	5.25546700	-1.02308100	2.05534500
N	5.33802000	-0.49583100	4.65223200
O	6.34059900	-0.15244400	4.00796400
O	5.27061200	-0.43013100	5.88665300

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C	1.27784200	-2.14204300	-1.02759400
C	1.28712700	-3.58800100	-1.01619300
C	0.00880700	-3.98759700	-0.79008600
C	-0.78758800	-2.78928300	-0.64607000
N	0.01425000	-1.67781800	-0.74550400
H	2.16768600	-4.19542300	-1.17037400
H	-0.38200200	-4.99294300	-0.71898300
C	-3.54362400	0.45428000	-0.10036800
C	-4.73932100	-0.34457500	0.04035200
C	-4.37019100	-1.64272600	-0.13729500
C	-2.94090100	-1.64564600	-0.34763300

N	-2.46271400	-0.36188100	-0.32453100
H	-5.72608800	0.05525900	0.22840700
H	-4.99044700	-2.52768900	-0.11850500
C	1.71385400	2.11861500	-1.38364400
C	3.10243400	2.12361300	-1.78966300
C	3.49606300	0.82430300	-1.86140000
C	2.35397900	0.02077100	-1.48308700
N	1.28420300	0.82833200	-1.21061300
H	3.68015200	3.01483900	-1.99114100
H	4.46404700	0.42705800	-2.13240700
C	-0.38900000	3.27934100	-0.84824000
C	-1.15765700	4.48176600	-0.60159600
C	-2.41522100	4.08109600	-0.27332900
C	-2.41684900	2.63353700	-0.32208500
N	-1.17866300	2.17668600	-0.67928000
H	-0.76584400	5.48704300	-0.67325200
H	-3.27352000	4.68839100	-0.02090900
C	2.37766500	-1.37459900	-1.41132400
C	-3.54149900	1.84935300	-0.05692700
C	-2.17742700	-2.80459200	-0.51938400
C	0.96235700	3.27956900	-1.19961300
Fe	-0.56972300	0.23951900	-0.68985400
Cl	-1.08988500	0.11302600	-3.01243400
O	-0.23053400	0.51484700	0.95999600
H	0.15019800	-0.27652600	1.72855600
C	2.11865300	-4.76298700	2.77564100
C	0.74646200	-4.61609200	2.53741100
C	0.13741000	-3.36035500	2.58070400
C	0.89968100	-2.22596500	2.87522600
C	2.29639600	-2.38331300	3.07889600
C	2.90419200	-3.63880900	3.03672700
H	2.57673800	-5.74779800	2.73163000
H	-0.90780000	-3.26687700	2.32800100
H	3.97620900	-3.73647700	3.19188400
C	0.52372900	-0.78833500	2.97914700
C	1.82414500	-0.09924900	3.15653200
C	2.15790000	1.26536800	3.10951100
C	3.48538400	1.66129600	3.22972800
C	4.49045300	0.69394600	3.37981100
C	4.20323200	-0.67326900	3.37789100
C	2.87642800	-1.05772800	3.24486600
H	1.39800300	2.01331100	2.92932800
H	5.00923000	-1.39303800	3.45005700
C	-0.71225400	-0.38767300	3.84619000

C	-2.02168200	-0.95893600	3.26161200
C	-0.50839300	-0.94462300	5.27410100
C	-0.88479600	1.14264100	3.94033100
H	-2.14083400	-0.66840700	2.21478500
H	-2.06203200	-2.04766600	3.33534600
H	-2.87759600	-0.57085500	3.82812500
H	0.41079900	-0.54541900	5.71964700
H	-1.35155200	-0.66297700	5.91900600
H	-0.43374500	-2.03741800	5.26585400
H	-1.80844500	1.37032000	4.48674100
H	-0.06104500	1.61027800	4.48784800
H	-0.95486300	1.58621100	2.94338000
C	-2.89831500	-4.09934200	-0.76343500
C	-3.03388300	-4.52742500	-2.10655800
C	-3.45627400	-4.86974400	0.27441900
C	-3.71297500	-5.71889800	-2.37483300
C	-4.13183900	-6.05659500	-0.04062800
C	-4.27051200	-6.49887700	-1.35641500
H	-3.81496000	-6.04349900	-3.40933300
H	-4.56115100	-6.64676600	0.76784000
C	-4.83007200	2.54785500	0.25616900
C	-5.21856400	2.73748800	1.59650600
C	-5.65225500	3.00675800	-0.79196600
C	-6.42614600	3.38931700	1.86882200
C	-6.85324400	3.65244700	-0.47868300
C	-7.25543300	3.85656200	0.84483800
H	-6.72567500	3.53427500	2.90571300
H	-7.49076800	4.00256500	-1.28917700
C	1.64867500	4.59978300	-1.37510500
C	2.40618700	5.14081700	-0.31745800
C	1.53332300	5.29639800	-2.59384600
C	3.03934500	6.37519000	-0.49757200
C	2.18194000	6.52800400	-2.73471800
C	2.94191000	7.08186700	-1.69994900
H	3.62268800	6.79361700	0.32101700
H	2.09262100	7.06633000	-3.67715200
C	3.60236600	-2.08075900	-1.91510900
C	4.73101700	-2.25852400	-1.09259700
C	3.61526600	-2.54771100	-3.24659000
C	5.85628200	-2.90860900	-1.61089500
C	4.76026500	-3.19302300	-3.72635600
C	5.89063100	-3.38149500	-2.92570300
H	6.72557800	-3.04760500	-0.97010100
H	4.76902300	-3.55472700	-4.75353400

C	-3.32601800	-4.46579200	1.72590500
H	-2.39189700	-4.84642600	2.15829600
H	-3.32506400	-3.38035600	1.84804900
H	-4.14831900	-4.87614700	2.32266600
C	-2.44114100	-3.72420200	-3.24318100
H	-2.61321200	-2.64869200	-3.13030500
H	-1.35160900	-3.84637300	-3.28055800
H	-2.85137600	-4.04895100	-4.20550700
C	-5.03156500	-7.76410000	-1.68150800
H	-5.11165000	-8.42121200	-0.80827100
H	-6.05326500	-7.54002300	-2.01803700
H	-4.54523200	-8.32850800	-2.48609000
C	4.71486500	-1.76397000	0.33156700
H	4.52129300	-0.68720400	0.38205700
H	3.91392300	-2.24701700	0.89889100
H	5.66511600	-1.96030600	0.83909400
C	2.40810000	-2.36762500	-4.13909000
H	1.57544900	-2.99937000	-3.80690900
H	2.03238500	-1.33912900	-4.11253000
H	2.64302400	-2.62926900	-5.17639000
C	7.12990900	-4.04849600	-3.47839700
H	7.80615700	-3.31493600	-3.93905600
H	7.69559800	-4.56020000	-2.69128400
H	6.87905400	-4.78607400	-4.24961100
C	2.52950000	4.39408900	0.99067400
H	1.54181900	4.15741800	1.40370100
H	3.04195600	3.43555500	0.85314800
H	3.08722900	4.97746300	1.73094000
C	3.66650000	8.39546300	-1.88864900
H	3.12378200	9.05946000	-2.57145100
H	3.79784800	8.92261400	-0.93676000
H	4.66763000	8.24073600	-2.31446300
C	0.71389100	4.72137500	-3.72635200
H	1.00769800	3.68899000	-3.94582900
H	-0.35042900	4.68542200	-3.46483500
H	0.82387400	5.31801100	-4.63820300
C	-4.34221800	2.23454500	2.71990300
H	-4.24532300	1.14352800	2.68669200
H	-3.32451200	2.63174400	2.63850900
H	-4.74689500	2.51525100	3.69820800
C	-5.23790900	2.79951700	-2.23036900
H	-4.31832600	3.35129100	-2.45817400
H	-5.01728000	1.74530300	-2.43190800
H	-6.02039700	3.13187100	-2.92079700

C	-8.53928600	4.59014200	1.16075300
H	-8.96944100	4.25571100	2.11181800
H	-8.37054500	5.67287100	1.24397900
H	-9.29133700	4.43958700	0.37766500
H	0.14633900	-5.48790200	2.28741700
H	3.76305900	2.70679200	3.18991400
N	5.87647100	1.12256800	3.50332300
O	6.11574300	2.33579100	3.52346200
O	6.75274100	0.25233400	3.58466900

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C	3.02180000	-1.52529600	-0.60219300
C	3.45395800	-2.90434500	-0.57746900
C	2.33796100	-3.67138800	-0.70964500
C	1.21581500	-2.76638200	-0.79239800
N	1.65578200	-1.46956900	-0.72603600
H	4.48196100	-3.22323200	-0.47606500
H	2.25869800	-4.74900700	-0.73334000
C	-2.40162000	-0.48567200	-1.22699800
C	-3.31005300	-1.60782400	-1.27856400
C	-2.55905700	-2.73230300	-1.13276300
C	-1.18770200	-2.30402100	-0.97950300
N	-1.12172800	-0.93152300	-0.99793900
H	-4.37909100	-1.52247800	-1.41249200
H	-2.88240300	-3.76408700	-1.12902000
C	2.24636500	2.70182500	-0.66829000
C	3.61072700	3.13883000	-0.46664100
C	4.37887300	2.01770800	-0.42428100
C	3.48230500	0.89120500	-0.57369300
N	2.19907100	1.33610300	-0.73947300
H	3.91738100	4.17222500	-0.38260500
H	5.44941900	1.93721800	-0.29641700
C	-0.13876900	3.15254100	-1.04606000
C	-1.23149800	4.06007800	-1.31764100
C	-2.32783300	3.29332500	-1.55862400
C	-1.91918100	1.91584200	-1.39314000
N	-0.58190100	1.85837200	-1.10691800
H	-1.14339600	5.13743200	-1.33294700
H	-3.33031800	3.60925700	-1.80968200
C	3.89669000	-0.44051100	-0.51798800
C	-2.79551300	0.83209600	-1.46627100
C	-0.10929700	-3.18626700	-0.92228000
C	1.16619500	3.57495900	-0.79462800
Fe	0.52595300	0.19662800	-0.83236400

C1	0.77246800	0.08918400	-3.19510600
O	0.43180300	0.36734400	0.84255900
H	-0.19749200	-0.22948100	1.64999800
C	-0.47588900	3.11179500	4.78993100
C	0.75306900	2.45834400	4.59849300
C	0.80950000	1.19134800	4.01606100
C	-0.38098700	0.57163100	3.63083600
C	-1.62348600	1.22608400	3.83540000
C	-1.67081600	2.49914100	4.40840900
H	-0.49504400	4.10332200	5.23557500
H	1.67383300	2.95228900	4.89991600
H	1.76077300	0.69310900	3.85157100
H	-2.62299300	3.00448000	4.55451200
C	-0.60013600	-0.70592700	2.90978200
C	-2.05230400	-0.83122700	2.81786800
C	-2.83978800	-1.85137000	2.26611600
C	-4.22111800	-1.71865700	2.24624400
C	-4.81496600	-0.56085800	2.77807100
C	-4.05620800	0.47968000	3.32924300
C	-2.67583500	0.34438000	3.34269700
H	-2.36842200	-2.72299300	1.82691900
H	-4.85408900	-2.48055200	1.80968500
H	-4.55606400	1.35966900	3.71557400
C	-0.37011200	-4.64383800	-1.16679900
C	-0.46025800	-5.09027900	-2.50392200
C	-0.50379700	-5.55883700	-0.10653400
C	-0.68216900	-6.44811700	-2.75166300
C	-0.72302900	-6.91094800	-0.39873500
C	-0.81850700	-7.37443700	-1.71249200
H	-0.74426200	-6.79216100	-3.78300800
H	-0.81966600	-7.61715500	0.42453400
C	-4.21421300	1.08548700	-1.87877400
C	-5.15216300	1.60699100	-0.96614400
C	-4.60264300	0.79130600	-3.20410600
C	-6.47360600	1.80048100	-1.38505500
C	-5.93012000	1.01135300	-3.58445600
C	-6.88154600	1.51017000	-2.68897000
H	-7.19965600	2.18106500	-0.66867300
H	-6.22952800	0.78258000	-4.60626700
C	1.41587900	5.04409400	-0.64434900
C	1.23377600	5.64895600	0.61579500
C	1.82818600	5.81167500	-1.75012100
C	1.47223100	7.02142700	0.74600400
C	2.05464300	7.18170600	-1.57796600

C	1.87955900	7.80462000	-0.33862500
H	1.33613500	7.48945300	1.71977800
H	2.37488200	7.77522200	-2.43296400
C	5.36189700	-0.72100500	-0.36932100
C	5.96934700	-0.67300300	0.90183600
C	6.12966400	-1.03451500	-1.50919400
C	7.33642500	-0.95037000	1.01191900
C	7.49361900	-1.30545000	-1.35592600
C	8.11550800	-1.26753900	-0.10453000
H	7.80302700	-0.91917000	1.99531900
H	8.08444800	-1.55080200	-2.23712300
C	-0.43051800	-5.09675300	1.32764300
H	0.36879800	-4.37003200	1.48550600
H	-1.36308900	-4.60652600	1.63186700
H	-0.26673100	-5.93642100	2.01049100
C	-0.32560000	-4.11405600	-3.65027800
H	-1.16772100	-3.41220900	-3.67002700
H	0.57389200	-3.49649900	-3.55547700
H	-0.29246400	-4.63718700	-4.61181600
C	-1.08746600	-8.83289500	-2.00681500
H	-0.75583600	-9.47695600	-1.18447700
H	-2.16045400	-9.01895700	-2.15373500
H	-0.57587100	-9.15926800	-2.91991000
C	5.16287300	-0.31473300	2.12950400
H	4.80152900	0.71909500	2.07556400
H	4.27406900	-0.94533400	2.22666100
H	5.76015600	-0.42193700	3.04102800
C	5.48473700	-1.08707500	-2.87523000
H	4.78807400	-1.93023800	-2.95103800
H	4.89285000	-0.18651800	-3.07165700
H	6.23715300	-1.19146300	-3.66416100
C	9.59827100	-1.52900800	0.03354300
H	10.17851200	-0.60199900	-0.07414900
H	9.84206900	-1.95111600	1.01525900
H	9.95671700	-2.22577800	-0.73285600
C	0.78854900	4.82548100	1.80225300
H	-0.21093700	4.40369000	1.64590100
H	1.44918300	3.96845200	1.97153300
H	0.76310700	5.42495000	2.71786600
C	2.09463100	9.29296400	-0.18095200
H	1.15856900	9.84940500	-0.32850900
H	2.46316200	9.54162700	0.82106300
H	2.81712600	9.67441500	-0.91153600
C	2.02444000	5.15882500	-3.09901000

H	2.81954400	4.40496700	-3.06126900
H	1.11818700	4.63199000	-3.41886300
H	2.28569000	5.89764100	-3.86410900
C	-4.74815700	1.97838300	0.44008200
H	-3.94744100	1.33547300	0.80962100
H	-4.36470000	3.00671700	0.47741200
H	-5.59344200	1.90851500	1.13153200
C	-3.60977500	0.23006100	-4.19800500
H	-2.64119400	0.73742100	-4.13912600
H	-3.40864500	-0.82984100	-3.99848500
H	-3.98992400	0.31479200	-5.22186000
C	-8.30698100	1.75720300	-3.12825800
H	-9.00985300	1.62445700	-2.29802300
H	-8.43736200	2.78178700	-3.50394800
H	-8.60261700	1.07631500	-3.93475300
C	0.28569000	-1.88112400	3.17863200
C	1.56622300	-1.97235600	2.60897100
C	-0.12475400	-2.89784100	4.05857900
C	2.40961700	-3.04236700	2.91599400
H	1.87840500	-1.21164400	1.90254300
C	0.72029300	-3.96276900	4.37086100
H	-1.11433500	-2.84047800	4.50397900
C	1.99412900	-4.03889600	3.80159400
H	3.38180000	-3.10895200	2.43596000
H	0.38161200	-4.73559400	5.05745500
H	2.64994500	-4.87450500	4.03402000
N	-6.25776900	-0.42265200	2.71911400
O	-6.92840600	-1.38680700	2.32949000
O	-6.75994900	0.66041000	3.05875100

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C	2.47423900	0.24402200	-1.26822500
C	3.53190300	-0.65214300	-1.68576800
C	2.93785500	-1.81960600	-2.06520100
C	1.52499100	-1.67589800	-1.79437400
N	1.27267300	-0.41271100	-1.32948800
H	4.58399000	-0.40629200	-1.68901400
H	3.40257600	-2.71924600	-2.44556100
C	-2.48306100	-1.86604300	-0.30532300
C	-2.66968200	-3.29112300	-0.47417500
C	-1.58148500	-3.75647000	-1.15126900
C	-0.68856300	-2.63318100	-1.33091200
N	-1.26131300	-1.50330300	-0.80993800
H	-3.53740800	-3.84175500	-0.13836500

H	-1.37394800	-4.76565000	-1.47991900
C	-0.43968700	3.36123900	-0.89427600
C	0.48649900	4.47441400	-0.93050100
C	1.73970500	3.94228500	-0.89085100
C	1.58218900	2.50296600	-0.89183700
N	0.25560200	2.18419500	-0.89530000
H	0.19543300	5.51569400	-0.95361100
H	2.69325600	4.45308600	-0.88838000
C	-2.66530400	2.41566200	-0.45694100
C	-4.05431300	2.54853700	-0.07007400
C	-4.48619300	1.30441800	0.27662900
C	-3.37753200	0.39963000	0.05135300
N	-2.29234000	1.10240600	-0.38593300
H	-4.60031800	3.48184400	-0.05130600
H	-5.46446400	1.00177300	0.62450100
C	2.64986900	1.60131900	-0.96042900
C	-3.46583700	-0.99152700	0.17297100
C	0.60046900	-2.72294900	-1.86760100
C	-1.82386200	3.49245700	-0.75170100
Fe	-0.49429300	0.33621500	-0.79232700
Cl	-1.06105100	0.52094800	-3.12175500
O	-0.12942400	0.27715100	0.87546000
H	0.31985900	-0.77557300	1.29050300
C	4.59435600	-0.38039000	3.17663100
C	3.45818400	-0.27131500	3.99055800
C	3.33271100	-1.55097300	1.51202200
C	4.54203700	-1.02762000	1.93842300
H	3.53582700	0.25239600	4.93657800
H	5.43148300	-1.07921500	1.32343600
C	0.86516300	-1.89732500	1.81686000
C	2.16659600	-1.42751900	2.29080200
C	2.24604400	-0.78150000	3.55103100
C	0.95719200	-0.58431600	4.32260900
H	0.89959800	-2.52845700	0.93127100
H	1.15926200	-0.40397200	5.38510600
H	0.47862100	0.32866200	3.93110400
H	3.27025000	-2.02867000	0.54203200
C	-0.07094500	-2.34519500	2.86463000
C	-1.00833800	-3.36639500	2.64129600
C	-1.85838600	-3.78853100	3.66227800
C	-1.77981700	-3.19889600	4.92653000
C	-0.85616200	-2.17391600	5.15458500
C	-0.01072900	-1.73463400	4.13614700
H	-1.07403500	-3.81617600	1.65536000

H	-2.58643600	-4.57215600	3.46806000
H	-2.43774400	-3.52663500	5.72767400
H	-0.79695200	-1.70452200	6.13499600
C	1.00717700	-3.99106800	-2.55344000
C	0.87515500	-4.05731200	-3.95688800
C	1.51085600	-5.09407200	-1.83723200
C	1.23546200	-5.23747700	-4.61556800
C	1.86115500	-6.25584900	-2.53505300
C	1.72439800	-6.34908900	-3.92274500
H	1.13264700	-5.28788200	-5.69849200
H	2.25305200	-7.10664400	-1.97974700
C	4.02674900	2.08082500	-0.62177300
C	4.32168900	2.29895400	0.74553300
C	5.03016200	2.25179100	-1.59328600
C	5.64079000	2.55965400	1.12003000
C	6.34143700	2.51919000	-1.17422800
C	6.67164800	2.63877100	0.17732400
H	5.87605800	2.67986600	2.17570600
H	7.12245500	2.62676300	-1.92565100
C	-4.69674400	-1.56648800	0.80238300
C	-4.80321600	-1.56098400	2.20931500
C	-5.74327100	-2.08536500	0.01401700
C	-5.93348000	-2.13147200	2.80401700
C	-6.85954400	-2.64145000	0.64961100
C	-6.96589900	-2.68757700	2.04267300
H	-6.01007500	-2.13525400	3.89024600
H	-7.66834800	-3.04166300	0.03994600
C	-2.42515000	4.85994000	-0.85141400
C	-2.85061900	5.32783200	-2.11068000
C	-2.56122000	5.67017500	0.29176900
C	-3.41299500	6.60538400	-2.20213100
C	-3.12813600	6.94259200	0.15827900
C	-3.56300900	7.42569600	-1.07943000
H	-3.74009900	6.96891500	-3.17515800
H	-3.23112800	7.57048900	1.04203200
C	0.37761600	-2.86030400	-4.73417900
H	-0.53678100	-2.43869000	-4.30375000
H	1.11003200	-2.04458400	-4.70768500
H	0.19058500	-3.11988100	-5.78172800
C	1.68586600	-5.02786800	-0.33756100
H	2.33399500	-4.19231700	-0.05093800
H	0.72877000	-4.87000000	0.17195300
H	2.12930500	-5.95013300	0.05195400
C	2.07087900	-7.62654700	-4.65351700

H	1.18880900	-8.27172900	-4.76914400
H	2.45505200	-7.42201400	-5.65960400
H	2.82832200	-8.20611600	-4.11347600
C	3.23105400	2.27770900	1.79194000
H	2.57993700	3.15403200	1.68509400
H	2.58287500	1.40174200	1.69670400
H	3.65811800	2.29089400	2.79805500
C	4.70481100	2.16798400	-3.06964100
H	4.59577800	1.13328000	-3.41409300
H	3.75452200	2.66676300	-3.28899100
H	5.49112400	2.63994800	-3.66909700
C	8.09479500	2.85159300	0.63756000
H	8.23256600	3.84998400	1.07424300
H	8.35494100	2.12097800	1.41303600
H	8.80741600	2.74752200	-0.18822400
C	-2.09616200	5.16826600	1.63945700
H	-2.62629500	4.25104600	1.92137400
H	-1.02961500	4.91572500	1.61844200
H	-2.25984300	5.91741200	2.42143000
C	-2.69037700	4.45805300	-3.33601800
H	-1.63749300	4.21112700	-3.51326300
H	-3.19900800	3.49537200	-3.21320500
H	-3.08751100	4.95309700	-4.22869400
C	-4.20623600	8.78903700	-1.19822300
H	-5.30024400	8.72304600	-1.11729000
H	-3.86271800	9.46607600	-0.40772500
H	-3.98198500	9.25587400	-2.16439700
C	-5.67692200	-2.02060700	-1.49557000
H	-5.39467500	-1.01731500	-1.83339700
H	-4.91945900	-2.70345900	-1.89695700
H	-6.64214200	-2.28064800	-1.94341100
C	-3.73959100	-0.90544200	3.05968400
H	-2.73227300	-1.19594500	2.75089400
H	-3.79360700	0.18643800	2.96428300
H	-3.85847100	-1.16686600	4.11496900
C	-8.15832200	-3.33485000	2.70986500
H	-9.04816500	-3.29393300	2.07115000
H	-7.96573100	-4.39396900	2.93117000
H	-8.40148000	-2.84600700	3.66049900
N	5.82491300	0.26983500	3.57930900
O	6.85300500	0.04546600	2.92705900
O	5.78757000	1.04715900	4.54517700

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C	2.43892900	0.34887300	-1.32599700
C	3.51857100	-0.49699500	-1.78903300
C	2.96127500	-1.68372800	-2.16584300
C	1.55198900	-1.60025100	-1.85355500
N	1.26288500	-0.35279600	-1.36664200
H	4.55926000	-0.20901300	-1.81858400
H	3.45087500	-2.55857700	-2.57174400
C	-2.43728300	-1.94317800	-0.32697300
C	-2.56468300	-3.37693400	-0.48274300
C	-1.45961500	-3.80268300	-1.15932500
C	-0.61702600	-2.64400300	-1.35558300
N	-1.23312400	-1.53545600	-0.83904700
H	-3.40633500	-3.96200100	-0.13876500
H	-1.21058000	-4.80544800	-1.47869900
C	-0.57091100	3.35669200	-0.86144200
C	0.31821000	4.50055400	-0.87282800
C	1.58780800	4.00918300	-0.84461500
C	1.47679000	2.56550500	-0.87905900
N	0.16156000	2.20321700	-0.88692500
H	-0.00690100	5.53194900	-0.87357800
H	2.52388400	4.55097400	-0.83191000
C	-2.76539000	2.33290800	-0.44865000
C	-4.16193600	2.41411700	-0.07381600
C	-4.55262800	1.15299300	0.25834000
C	-3.41030100	0.28974500	0.03575000
N	-2.34692800	1.03288800	-0.38656200
H	-4.74008500	3.32774700	-0.05241600
H	-5.52260300	0.81302900	0.59480900
C	2.57282800	1.70271100	-0.98139000
C	-3.44999900	-1.10379500	0.15417500
C	0.66838900	-2.68343800	-1.90785100
C	-1.95903400	3.44101400	-0.72317000
Fe	-0.52498700	0.32894300	-0.80506000
Cl	-1.10827400	0.52148200	-3.13275600
O	-0.14957600	0.25683000	0.86157200
H	0.36185700	-0.77981200	1.28416400
C	4.64832400	-0.30142500	3.11631500
C	3.56453300	-0.36081700	4.00113600
C	3.37663800	-1.39485000	1.40804100
C	4.57373900	-0.83409400	1.82673400
H	3.63921400	0.04893600	4.99975700
H	5.42634100	-0.75701600	1.16488200
C	0.93264500	-1.88302200	1.79244800
C	2.24641700	-1.43305300	2.24209700

C	2.38358800	-0.93515600	3.55870500
H	0.93290900	-2.50839700	0.90185500
H	3.28830100	-1.77391700	0.39822300
C	0.05605800	-2.33644300	2.88423100
C	-1.01559600	-3.22292500	2.70288400
C	-1.83733900	-3.58756300	3.76855600
C	-1.60120700	-3.06615700	5.04396700
C	-0.53161600	-2.19236600	5.25386400
C	0.28271200	-1.84175200	4.18097600
H	-1.20781000	-3.60572600	1.70557500
H	-2.67677200	-4.25566800	3.59682500
H	-2.24389900	-3.33842700	5.87712300
H	-0.31133300	-1.78142500	6.23428400
C	1.11792500	-3.93878900	-2.59050000
C	0.95261400	-4.02972900	-3.98894400
C	1.69450800	-5.00563800	-1.87500700
C	1.35976200	-5.19641300	-4.64407700
C	2.08894300	-6.15567800	-2.56887300
C	1.92511500	-6.27177000	-3.95185300
H	1.23258100	-5.26555800	-5.72336800
H	2.53747000	-6.97852100	-2.01433800
C	3.93267800	2.22174900	-0.63276900
C	4.21730600	2.41850200	0.74141800
C	4.92814500	2.45954100	-1.59757000
C	5.52131200	2.73620200	1.12234200
C	6.22515600	2.78111900	-1.17014600
C	6.54779700	2.88976700	0.18325700
H	5.75051900	2.84585800	2.18039600
H	7.00038700	2.94274700	-1.91802900
C	-4.65103400	-1.72065900	0.80050200
C	-4.76286400	-1.67220500	2.20676700
C	-5.66653300	-2.32345600	0.02988200
C	-5.85503100	-2.29644800	2.81991500
C	-6.74638500	-2.92737400	0.68357200
C	-6.84899100	-2.94064500	2.07790600
H	-5.93377100	-2.26907100	3.90571000
H	-7.53072600	-3.39162600	0.08743300
C	-2.60328900	4.78981300	-0.80556100
C	-3.01847400	5.27180200	-2.06280300
C	-2.78751700	5.56976900	0.35203300
C	-3.62044800	6.53244900	-2.13794900
C	-3.39269300	6.82590200	0.23445300
C	-3.81923800	7.32206500	-1.00110400
H	-3.94022300	6.90678700	-3.10929700

H	-3.53268300	7.43065600	1.12919000
C	0.36257700	-2.87324000	-4.76240500
H	-0.58575300	-2.53474100	-4.33181300
H	1.02170900	-1.99804000	-4.72743300
H	0.19983300	-3.14156500	-5.81175000
C	1.89613800	-4.91382600	-0.37994700
H	2.51181800	-4.04689200	-0.11522600
H	0.94188000	-4.79431700	0.14575400
H	2.38831900	-5.81062200	0.01057900
C	2.32250900	-7.53695200	-4.67809200
H	1.47081500	-8.22431900	-4.77692900
H	2.68273900	-7.32220700	-5.69091800
H	3.11416000	-8.07537200	-4.14460900
C	3.13255500	2.30999700	1.78945000
H	2.44341800	3.16056400	1.72058000
H	2.52066200	1.41237600	1.66193400
H	3.56248600	2.30136200	2.79454200
C	4.61890300	2.38542200	-3.07835900
H	4.72997800	1.36941200	-3.47587700
H	3.58699300	2.68871200	-3.28122200
H	5.29167400	3.03750700	-3.64689700
C	7.95709900	3.16749500	0.65107000
H	8.03915900	4.15958900	1.11521100
H	8.25693800	2.43141100	1.40674600
H	8.67432700	3.12579600	-0.17620200
C	-2.33080000	5.05435500	1.69747900
H	-2.83966000	4.11778600	1.95372800
H	-1.25762000	4.83101900	1.68973900
H	-2.52742100	5.78345600	2.49069800
C	-2.80339800	4.43674700	-3.30380500
H	-1.73730800	4.24965900	-3.47608300
H	-3.26122800	3.44623600	-3.20579800
H	-3.21780300	4.92923400	-4.19003200
C	-4.50500700	8.66595100	-1.10205100
H	-5.59617000	8.56491000	-1.01860400
H	-4.18055100	9.34386500	-0.30419800
H	-4.29844500	9.15122400	-2.06302900
C	-5.61262300	-2.29168500	-1.48162400
H	-5.35287800	-1.29097500	-1.84382300
H	-4.84666700	-2.96872200	-1.87630100
H	-6.57664900	-2.58012100	-1.91449700
C	-3.76107000	-0.90558100	3.04080500
H	-2.73748600	-1.03691100	2.68270700
H	-3.97387800	0.17028800	2.99238300

H	-3.79695000	-1.21642400	4.08899500
C	-7.99914900	-3.64217500	2.76416000
H	-8.90426000	-3.62954100	2.14582300
H	-7.76057100	-4.69554200	2.96751300
H	-8.23968000	-3.17381900	3.72552400
N	5.85709700	0.38839700	3.52520600
O	6.86378400	0.28406400	2.81266900
O	5.81780800	1.07120200	4.55838700
O	1.33621400	-0.98466300	4.45087000

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C	-0.79135000	-2.97373600	-0.80743700
C	-1.56109900	-4.10285500	-0.33436300
C	-2.59149200	-3.59732600	0.40071500
C	-2.48681500	-2.15479900	0.33385500
N	-1.36902600	-1.80797100	-0.38031000
H	-1.31826000	-5.13799700	-0.53276600
H	-3.37608600	-4.13346700	0.91714200
C	-2.97208000	2.06353700	-0.29989500
C	-4.29095300	2.18397400	0.28619500
C	-4.59223700	0.97171300	0.82744500
C	-3.47587200	0.09460800	0.53513600
N	-2.50852900	0.78786800	-0.13621900
H	-4.88217300	3.08951500	0.28760200
H	-5.48817300	0.67312800	1.35430100
C	2.10693200	0.03743400	-1.68106700
C	3.16400800	-0.85521900	-2.10879800
C	2.61549200	-2.09939900	-2.21129900
C	1.24552000	-1.98955000	-1.76131600
N	0.96224500	-0.68321100	-1.46334900
H	4.18146100	-0.55343500	-2.31266500
H	3.09064600	-3.02150000	-2.51720200
C	1.12322500	2.28353600	-1.48026700
C	1.18367300	3.71634400	-1.68055700
C	-0.09205700	4.18098500	-1.57436400
C	-0.92373500	3.04109800	-1.24452800
N	-0.16295000	1.90612700	-1.22556100
H	2.08970700	4.26562100	-1.89848800
H	-0.45167500	5.19605000	-1.67321200
C	0.40412300	-3.08188900	-1.52552600
C	-2.26748300	3.12824100	-0.87003100
C	-3.46366700	-1.27679500	0.81582700
C	2.22560600	1.43171800	-1.60059400
Fe	-0.75127700	0.05432600	-0.75879000

C1	-1.69508300	-0.13768900	-2.95402700
O	-0.09976800	0.27651200	0.82141800
C	2.84910900	0.95561800	5.92073600
C	3.97191300	0.91065900	5.12057800
C	3.93281200	0.26172200	3.85777400
C	2.69187500	-0.34221800	3.44266200
C	1.54283100	-0.27170700	4.28917300
C	1.64007000	0.36487700	5.51262100
C	5.02914900	0.20887000	2.92517900
C	2.58776000	-1.00723600	2.16630800
C	3.70041600	-1.02252100	1.32002200
C	4.89124800	-0.40566100	1.68485700
C	1.33326100	-1.60301000	1.75296000
C	0.38959100	-2.01624000	2.86348300
C	0.21506600	-0.83615000	3.82464900
H	-0.33083800	-0.05012600	3.28449800
H	-0.57322000	-2.31224800	2.43633100
H	2.90296000	1.45801400	6.88387500
H	4.89136100	1.36922700	5.44960700
H	0.76606200	0.41702400	6.15832100
H	5.73432500	-0.39665000	1.00607600
H	3.62233200	-1.50428300	0.35189600
H	0.65161900	-0.59869300	1.17888800
H	1.41150200	-2.29302300	0.91661500
N	6.32612800	0.80602600	3.18889800
O	6.67519100	1.02988400	4.35804500
O	7.06110900	1.05845400	2.21929100
C	-4.62824500	-1.84925200	1.56704500
C	-5.75457800	-2.32329100	0.86404500
C	-4.60543400	-1.89246400	2.97450200
C	-6.83554000	-2.84347900	1.58400700
C	-5.70729200	-2.41758900	3.65848700
C	-6.82936800	-2.90295300	2.98087000
H	-7.70593500	-3.20626300	1.03940400
H	-5.68857100	-2.44564600	4.74699000
C	-2.96681500	4.44342500	-1.02279200
C	-3.69147500	4.69861600	-2.20380300
C	-2.91053900	5.40938100	0.00034300
C	-4.34617200	5.92710000	-2.34308700
C	-3.57939000	6.62550600	-0.17728400
C	-4.29882500	6.90367100	-1.34346900
H	-4.90852000	6.12464100	-3.25449500
H	-3.53897900	7.37172000	0.61486600
C	3.60178400	2.01765200	-1.55567300

C	4.40977400	2.13109600	-2.70206800
C	4.10605700	2.39623200	-0.28951100
C	5.74340000	2.53465100	-2.55325400
C	5.44673500	2.77312200	-0.18255000
C	6.28666400	2.82849700	-1.30002800
H	6.37366900	2.60890200	-3.43845000
H	5.85542800	2.99754600	0.79950300
C	0.80185800	-4.42394800	-2.05962200
C	0.32134900	-4.80336700	-3.33117300
C	1.62683000	-5.29736700	-1.32576300
C	0.68836500	-6.04958400	-3.84927800
C	1.97010900	-6.53615900	-1.87991700
C	1.51549900	-6.92762700	-3.14190400
H	0.31647800	-6.34186600	-4.83016600
H	2.60691400	-7.21083500	-1.30978300
C	2.13268900	-4.91080700	0.04488400
H	2.77240900	-4.02198600	-0.00307500
H	1.30331700	-4.66504600	0.71767000
H	2.71288800	-5.72156800	0.49791300
C	-0.59293500	-3.88245000	-4.10557800
H	-1.54866700	-3.74857400	-3.58576500
H	-0.17423600	-2.87512900	-4.20132500
H	-0.79608200	-4.27748500	-5.10669300
C	1.92800500	-8.25350800	-3.74012200
H	2.80915300	-8.14224800	-4.38725100
H	2.18558600	-8.98262500	-2.96343900
H	1.12851200	-8.68259200	-4.35541800
C	-3.40279800	-1.38272000	3.73397700
H	-2.52363700	-2.00687400	3.53936000
H	-3.13334500	-0.36786200	3.42237800
H	-3.58539200	-1.37935300	4.81392900
C	-5.79338600	-2.25907200	-0.64526100
H	-5.64571800	-1.23275200	-0.99993900
H	-4.98616100	-2.85402000	-1.08726400
H	-6.74854600	-2.62810300	-1.03365600
C	-7.99394300	-3.50066000	3.73753700
H	-7.85495700	-4.57904700	3.89707400
H	-8.11025900	-3.04021600	4.72546800
H	-8.93587900	-3.37314100	3.19178000
C	-2.14098700	5.12774900	1.27030100
H	-2.50884600	4.21839200	1.75938700
H	-1.07940400	4.95644800	1.05723600
H	-2.22154200	5.95971100	1.97800600
C	-3.76589200	3.64999900	-3.28945000

H	-2.76784600	3.33403200	-3.61209100
H	-4.25850700	2.74027500	-2.92715700
H	-4.31646100	4.01977200	-4.16111900
C	-4.98492400	8.23801700	-1.53173300
H	-4.32267300	8.96150200	-2.02745500
H	-5.88278300	8.14360500	-2.15346600
H	-5.28244200	8.67610300	-0.57202400
C	3.20997200	2.43181100	0.92812800
H	2.55116100	3.30887000	0.88759700
H	2.55220700	1.56158500	0.99051700
H	3.79836600	2.48974600	1.84761900
C	3.85126700	1.83000200	-4.07617600
H	3.74385700	0.75298000	-4.25031800
H	2.85205300	2.26245400	-4.19709200
H	4.50150700	2.23405500	-4.85992900
C	7.73765600	3.21935800	-1.13750700
H	8.18216300	2.70960600	-0.27476300
H	8.32590600	2.96676500	-2.02696400
H	7.84605900	4.29922800	-0.96591600
H	0.79548900	-2.88812400	3.40288600
H	-0.39289500	-1.11545400	4.69380700

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C	-0.44805400	-2.82770500	-1.22495600
C	-1.27609000	-4.00407100	-1.09367300
C	-2.49353000	-3.58224200	-0.65266400
C	-2.42526400	-2.14182400	-0.54559200
N	-1.16910200	-1.71186600	-0.89246800
H	-0.94244000	-5.01345500	-1.28982600
H	-3.37062200	-4.17290700	-0.42614600
C	-2.88369600	2.12047500	-0.69833300
C	-4.28128400	2.16866800	-0.32131900
C	-4.65500400	0.89150300	-0.04087900
C	-3.49334300	0.05752000	-0.27247100
N	-2.43504000	0.83029000	-0.66242200
H	-4.87444700	3.07166200	-0.27649400
H	-5.62143100	0.52465300	0.27582200
C	2.44635200	0.34369900	-1.38840700
C	3.60761600	-0.49462800	-1.60305900
C	3.15476700	-1.76764100	-1.76259100
C	1.72165100	-1.72952900	-1.57422600
N	1.31912100	-0.43782600	-1.34673100
H	4.62712300	-0.13978100	-1.64153600
H	3.72491300	-2.66356700	-1.96427300

C	1.33478200	2.53638800	-1.34442700
C	1.35563800	3.97471100	-1.50361600
C	0.06219900	4.39357100	-1.45826000
C	-0.74963500	3.21348200	-1.24572500
N	0.04735700	2.10096200	-1.21180700
H	2.25486300	4.56035600	-1.63812400
H	-0.32619100	5.39918500	-1.54215500
C	0.90363600	-2.86102700	-1.57630200
C	-2.12462500	3.24979400	-1.01128900
C	-3.50850800	-1.33643300	-0.18420600
C	2.48513100	1.74309500	-1.33556200
Fe	-0.54130400	0.18990800	-0.96209900
Cl	-1.00336900	0.14787100	-3.30648600
O	-0.29587400	0.33282300	0.72183900
H	0.31987700	-0.29700000	1.51377400
C	4.09765500	1.01352600	3.66362600
C	4.89984700	0.56556300	2.61047800
C	4.39972700	-0.32504800	1.65387000
C	3.08084200	-0.73695900	1.74147900
C	2.22505300	-0.27227400	2.76600800
C	2.77492200	0.59628700	3.73399000
H	4.51408100	1.69389700	4.39664800
H	5.03061200	-0.64415100	0.83520900
H	2.67635400	-1.39411000	0.98059800
H	2.14647900	0.95326800	4.54260100
C	0.80842100	-0.72031100	2.77749800
C	-0.16463100	0.07348400	3.59518900
C	-0.27905700	1.46478600	3.38218900
C	-1.03678000	-0.51932000	4.52479200
C	-1.21942000	2.22373600	4.07262400
C	-1.98433300	0.24185200	5.21189500
H	-0.97556400	-1.58729800	4.70582000
C	-2.08279500	1.61639300	4.99042800
H	-1.29176000	3.29087600	3.87788100
H	-2.64765900	-0.24543100	5.92311600
H	-2.82622000	2.20747900	5.51975800
C	-4.78258800	-2.00066600	0.24368200
C	-5.70689500	-2.43335500	-0.72976800
C	-5.06240000	-2.17700700	1.61345800
C	-6.89084200	-3.05227700	-0.31634000
C	-6.26203500	-2.79664100	1.98474600
C	-7.18693400	-3.24204400	1.03711200
H	-7.60119800	-3.38942600	-1.06981000
H	-6.47707200	-2.93366300	3.04347100

C	1.49854700	-4.17338600	-1.98732000
C	2.26013800	-4.94132100	-1.08494700
C	1.28888300	-4.62831900	-3.30652300
C	2.80119800	-6.15758400	-1.51835300
C	1.84899000	-5.84821000	-3.69902900
C	2.60553600	-6.62874700	-2.81907900
H	3.38991800	-6.74982700	-0.81926000
H	1.69208400	-6.19585000	-4.71908700
C	-2.81150400	4.58018500	-1.02620900
C	-3.41771600	5.03930800	-2.21096600
C	-2.85751900	5.36072100	0.14574100
C	-4.05892300	6.28299100	-2.20560800
C	-3.50983800	6.59758800	0.11114700
C	-4.11264700	7.07723000	-1.05620800
H	-4.52897600	6.63814800	-3.12140700
H	-3.54922800	7.20009600	1.01746500
C	3.82141700	2.40199400	-1.18262700
C	4.16560600	2.92160800	0.08847100
C	4.76313000	2.43207700	-2.22850100
C	5.47850100	3.33257500	0.31925800
C	6.07182200	2.85417100	-1.95325700
C	6.45943300	3.25997500	-0.67545100
H	5.75934300	3.66660300	1.31590900
H	6.80811600	2.84192500	-2.75563700
C	3.13902600	3.03621600	1.19136600
H	2.41081900	3.82474300	0.96721000
H	2.56927200	2.11093300	1.31137900
H	3.61717600	3.27333200	2.14494400
C	4.38588000	2.00897300	-3.63257700
H	4.44456600	0.92215700	-3.76532900
H	3.35586600	2.29473700	-3.86891700
H	5.05349500	2.47096600	-4.36855600
C	7.89553400	3.57794500	-0.33467900
H	8.26241600	2.85919800	0.40926600
H	8.54469700	3.52403800	-1.21561700
H	7.99748400	4.57953700	0.10255900
C	-2.21461700	4.85807400	1.41842700
H	-2.62902500	3.88827500	1.71674000
H	-1.13832600	4.70181800	1.27887800
H	-2.35805700	5.56550100	2.24245400
C	-3.38151700	4.18862900	-3.45947600
H	-2.35429800	3.91925800	-3.72906400
H	-3.90908000	3.24016200	-3.30450500
H	-3.84190000	4.70674100	-4.30752700

C	-4.78000900	8.43389200	-1.08147100
H	-4.06374500	9.22681000	-1.33833500
H	-5.58489100	8.47192500	-1.82449300
H	-5.20838400	8.68928600	-0.10529800
C	-4.08407100	-1.72305700	2.67315700
H	-3.20726000	-2.37941100	2.71278200
H	-3.70538700	-0.71517100	2.47877400
H	-4.54627300	-1.72903500	3.66603300
C	-5.41920700	-2.22826400	-2.19945200
H	-5.20807300	-1.17511200	-2.41644000
H	-4.53060800	-2.78814100	-2.51294500
H	-6.26490600	-2.54873900	-2.81717300
C	-8.49080100	-3.87886300	1.46230600
H	-8.40340800	-4.35517000	2.44545800
H	-9.29555300	-3.13374700	1.53207600
H	-8.81832700	-4.64072900	0.74522400
C	0.46364900	-3.81345400	-4.27627100
H	-0.59561200	-3.81955900	-3.99267000
H	0.76211600	-2.75981500	-4.28000600
H	0.54759000	-4.20834200	-5.29448100
C	2.51106900	-4.45634000	0.32308000
H	3.28800000	-3.68166200	0.34181000
H	1.61491600	-4.01265200	0.76207900
H	2.83857900	-5.27293300	0.97387500
C	3.16970800	-7.96193700	-3.25560100
H	4.07985500	-8.21503600	-2.69972600
H	2.44986200	-8.77518000	-3.08719300
H	3.41461300	-7.96380000	-4.32410700
C	0.62859100	-2.21082200	2.82916700
C	-0.49487600	-2.80645600	2.23371900
C	1.52059500	-3.03781400	3.53421000
C	-0.73234500	-4.17504900	2.35540900
H	-1.17171500	-2.18073600	1.66530700
C	1.28647800	-4.40861600	3.65478100
H	2.39754300	-2.59742100	3.99993800
C	0.15570200	-4.98328100	3.07058500
H	-1.60055800	-4.60655700	1.86746800
H	1.98938600	-5.02700400	4.20858000
H	-0.02470200	-6.05179100	3.15900300
H	0.35245900	1.93552400	2.63669400
N	6.25098600	1.08070300	2.46992200
O	6.97119700	0.60792500	1.58362200
O	6.61346500	1.98711300	3.23318700

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C	-2.83987100	2.21854600	0.00983900
C	-4.13554400	2.47719100	-0.58165800
C	-4.85561500	1.32856700	-0.46821300
C	-3.99090000	0.35263500	0.16142700
N	-2.77514900	0.91768600	0.43157900
H	-4.43968100	3.42562100	-1.00242800
H	-5.87117300	1.13531500	-0.78512500
C	-1.60931700	-3.00403000	1.31247800
C	-2.63978900	-4.01414800	1.19937300
C	-3.80675600	-3.35875600	0.95262500
C	-3.48149300	-1.94875300	0.86874500
N	-2.15418800	-1.76496800	1.13829400
H	-2.46607800	-5.07639100	1.30700700
H	-4.79605100	-3.77069400	0.80830300
C	0.95708700	1.96664100	2.00599600
C	1.19669700	3.38863300	2.08954100
C	0.20043600	3.99940100	1.38852400
C	-0.67205800	2.95407300	0.90370600
N	-0.18835200	1.72855500	1.28647300
H	2.03966900	3.83913500	2.59481700
H	0.04655100	5.05566200	1.21677700
C	1.59049800	-0.37203700	2.39719700
C	2.56762300	-1.39158500	2.70615600
C	2.02474700	-2.58310700	2.33367800
C	0.68083900	-2.30776400	1.87038400
N	0.45591900	-0.95595100	1.89905600
H	3.54615800	-1.20050400	3.12402200
H	2.47656000	-3.56357800	2.37414500
C	-1.86918300	3.20002600	0.22470100
C	-0.26091500	-3.29117200	1.54093300
C	-4.36743000	-0.96827900	0.41768900
C	1.81578800	0.99943300	2.53223400
Fe	-1.14382000	-0.02823100	1.12770300
Cl	-1.95890500	0.34074700	3.34236800
O	-0.69101000	-0.40906500	-0.46255900
H	0.20764300	-0.05267600	-1.16213100
C	1.03248900	0.08625600	-2.27377800
C	1.79272100	-1.19023800	-2.18099300
C	1.81201900	-2.15695900	-3.20794800
C	2.48350400	-1.48980300	-0.98608500
C	2.46505400	-3.37085400	-3.04903900
H	1.30420000	-1.94530100	-4.14231300
C	3.13716800	-2.69730400	-0.81028000

H	2.46004500	-0.77539800	-0.17125300
C	3.11023300	-3.64411000	-1.83983500
H	2.47015600	-4.11619400	-3.83498000
H	3.62520900	-2.93489300	0.12470100
C	-0.05505100	0.19070600	-3.29884100
C	-1.06900900	-0.78872700	-3.36587100
C	-0.14387300	1.28797400	-4.17313100
C	-2.11457300	-0.67551200	-4.27713400
H	-1.04238000	-1.61944500	-2.66967400
C	-1.20074900	1.40684800	-5.07921000
H	0.62443700	2.05498700	-4.13815600
C	-2.18986900	0.42531700	-5.13860900
H	-2.88523500	-1.44185200	-4.30384000
H	-1.24616100	2.26993200	-5.73960000
C	1.74675000	1.35451300	-2.00271700
C	3.04658900	1.67234900	-2.24365700
H	1.10528700	2.13350300	-1.59712600
C	3.95367200	0.75711700	-2.99619600
C	5.14691600	0.28507600	-2.42824800
C	3.63391100	0.36460300	-4.30433300
C	5.98121000	-0.57872600	-3.13647600
H	5.40515900	0.58654100	-1.41792600
C	4.47229200	-0.49163400	-5.01862500
H	2.70795600	0.71956400	-4.74767500
C	5.64687700	-0.97062000	-4.43564500
H	6.88977400	-0.95292900	-2.67121600
H	4.20206100	-0.79194900	-6.02805300
H	6.29552700	-1.64706100	-4.98649700
C	3.59368100	2.99269900	-1.84509600
C	4.68093200	3.56806400	-2.53038900
C	3.03120700	3.72351700	-0.78166700
C	5.17046300	4.82512200	-2.17506300
H	5.13805200	3.02602800	-3.35227000
C	3.51574000	4.98005400	-0.43052100
H	2.22513800	3.29287400	-0.20309400
C	4.59051000	5.54156900	-1.12523100
H	6.00899400	5.24713200	-2.72456200
H	3.05795000	5.50846300	0.40194700
H	4.97737700	6.51852700	-0.84615000
C	-5.77840000	-1.36991800	0.11788600
C	-6.76881800	-1.21046000	1.10659100
C	-6.11011900	-1.90141400	-1.14322600
C	-8.08229500	-1.59416000	0.81651500
C	-7.43603100	-2.27065900	-1.39551300

C	-8.43551000	-2.12362000	-0.42889900
H	-8.84778800	-1.47704200	1.58218500
H	-7.69320500	-2.68356900	-2.36977000
C	-2.17897500	4.61218100	-0.17145000
C	-1.64086000	5.15248500	-1.35596300
C	-3.00497400	5.40334900	0.65506900
C	-1.95234000	6.47175100	-1.70458100
C	-3.28750800	6.71879800	0.27307600
C	-2.77148400	7.27117100	-0.90342800
H	-1.54246400	6.88314000	-2.62572900
H	-3.92621600	7.32712800	0.91174100
C	3.03283800	1.45650900	3.27640600
C	4.28835800	1.53038500	2.64402300
C	2.89797000	1.82623500	4.63215500
C	5.39354100	1.97828400	3.37828000
C	4.02711200	2.26549900	5.32943000
C	5.28425000	2.34704200	4.72070700
H	6.36148200	2.04341300	2.88371000
H	3.92172600	2.55351700	6.37434900
C	0.24616700	-4.67722100	1.29101800
C	0.39006800	-5.07953500	-0.05837800
C	0.68940200	-5.51984700	2.32628300
C	1.08864100	-6.25282800	-0.34226400
C	1.39031100	-6.68868300	1.99659200
C	1.64454100	-7.04233800	0.67008200
H	1.26199500	-6.52580900	-1.38068000
H	1.77053500	-7.31897100	2.79919700
C	-3.57806300	4.83897800	1.93539100
H	-4.32834700	4.06736100	1.72675800
H	-2.80304400	4.35496400	2.53949800
H	-4.05049800	5.62386200	2.53560300
C	-0.72405500	4.33251100	-2.23300800
H	0.27481600	4.25499300	-1.78545400
H	-1.09356400	3.31167400	-2.36930400
H	-0.60724000	4.78940900	-3.22167800
C	-3.06524400	8.70565800	-1.28043900
H	-2.33259900	9.39334900	-0.83552300
H	-3.02812700	8.85105400	-2.36610900
H	-4.05591200	9.01864100	-0.93082400
C	4.46257300	1.11429900	1.20214700
H	4.58585900	0.02685800	1.11553300
H	3.59614600	1.37988800	0.59362500
H	5.34379700	1.59089800	0.76017500
C	1.54812900	1.76647700	5.30986500

H	0.86476200	2.51763500	4.89653100
H	1.05529000	0.80168900	5.14912800
H	1.63958000	1.94072100	6.38731600
C	6.49581700	2.79640400	5.50568100
H	6.95681700	1.95622900	6.04341900
H	7.26359300	3.22329700	4.85050400
H	6.23140700	3.55226900	6.25443600
C	-0.18356500	-4.25033500	-1.18416900
H	-1.27980600	-4.28632300	-1.17836600
H	0.09285500	-3.19631800	-1.09045400
H	0.16630200	-4.61403300	-2.15329200
C	0.43497700	-5.16768600	3.77644400
H	1.14088100	-4.41500800	4.14672500
H	-0.56637000	-4.74445500	3.90921300
H	0.52546300	-6.05390100	4.41434200
C	2.53382400	-8.20642100	0.30493300
H	2.03000500	-8.90635800	-0.37391200
H	3.42478100	-7.83195200	-0.21513200
H	2.85909300	-8.76429200	1.19002800
C	-5.04334500	-2.07133900	-2.20095200
H	-4.52278000	-1.12690800	-2.39532100
H	-4.27640100	-2.78397600	-1.87419700
H	-5.47139300	-2.43274900	-3.14234700
C	-6.40694900	-0.62656400	2.45248700
H	-5.58698900	-1.18068100	2.92261200
H	-6.04941000	0.40464900	2.34840700
H	-7.26636400	-0.62817700	3.13141300
C	-9.86909200	-2.49765300	-0.73133900
H	-10.43933300	-1.63180600	-1.09577900
H	-9.92798500	-3.27327800	-1.50340300
H	-10.38389500	-2.86990700	0.16206000
H	-3.01428300	0.51664600	-5.84157000
N	3.70866800	-4.94945300	-1.62488600
O	4.31251700	-5.15393300	-0.56576100
O	3.57009500	-5.81110900	-2.50550300

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C	-2.05169100	1.69084300	-0.91749800
C	-2.49098000	3.04514900	-1.16486400
C	-1.37839700	3.83427200	-1.12518400
C	-0.25889800	2.96643700	-0.84497800
N	-0.69287700	1.66964200	-0.70963400
H	-3.51365900	3.33145000	-1.36780000
H	-1.30400900	4.90116700	-1.28434600

C	3.34503600	0.78961800	0.04092100
C	4.21482600	1.93846900	0.18430400
C	3.46614800	3.03654300	-0.10250500
C	2.12832900	2.56596500	-0.39776700
N	2.08787700	1.19929500	-0.30912300
H	5.26071200	1.88556600	0.45240800
H	3.76756300	4.07469700	-0.11374400
C	-1.17484200	-2.52341300	-0.77068000
C	-2.53725200	-2.98834300	-0.89741200
C	-3.33369800	-1.88433000	-0.87736300
C	-2.45928500	-0.73600900	-0.77531600
N	-1.15338000	-1.15575200	-0.66590600
H	-2.82356800	-4.02657000	-0.99103700
H	-4.41021200	-1.83000900	-0.95946100
C	1.23267700	-2.91809700	-0.53416700
C	2.37869500	-3.78884700	-0.39999300
C	3.43525000	-3.00086300	-0.06456000
C	2.95059400	-1.63784100	-0.03498800
N	1.60715600	-1.61597600	-0.31275700
H	2.35149700	-4.86091700	-0.53587900
H	4.45930000	-3.29024300	0.12507300
C	-2.90752000	0.58217800	-0.90366400
C	3.77255500	-0.53223900	0.19074100
C	1.05727700	3.41310500	-0.68789400
C	-0.06399900	-3.37140000	-0.77803100
Fe	0.47259100	0.01184900	-0.45917300
Cl	0.74641800	-0.01816800	-2.77776800
O	0.30476600	0.14299700	1.26246300
C	1.33035900	4.87844900	-0.83487200
C	1.12128100	5.75620000	0.24529400
C	1.79687100	5.37394000	-2.06953800
C	1.37861000	7.12062400	0.07885700
C	2.03978800	6.74516000	-2.19762600
C	1.84047000	7.63443700	-1.13648900
H	1.21683700	7.79714400	0.91615000
H	2.39353900	7.12916400	-3.15250900
C	-4.36512400	0.81731900	-1.17135500
C	-4.85556600	0.64995100	-2.48558300
C	-5.23805600	1.21503300	-0.14176900
C	-6.21299100	0.87208300	-2.73326200
C	-6.59204400	1.42074200	-0.42944900
C	-7.10001800	1.25047300	-1.71912500
H	-6.58878200	0.74698900	-3.74701300
H	-7.26263900	1.71854500	0.37431300

C	-0.26902900	-4.81181700	-1.13976300
C	-0.29507400	-5.15517700	-2.50871500
C	-0.43398900	-5.80458300	-0.15620000
C	-0.47929700	-6.49441000	-2.86454000
C	-0.61802400	-7.13310100	-0.55598600
C	-0.63930700	-7.49889400	-1.90442500
H	-0.49982200	-6.75948400	-3.91999900
H	-0.74852100	-7.89936800	0.20577400
C	5.19664600	-0.78045400	0.58287800
C	6.21107800	-0.79162700	-0.39419200
C	5.50774400	-1.01753000	1.93575900
C	7.52958100	-1.03348800	0.00569100
C	6.83838600	-1.25363500	2.29457500
C	7.86433600	-1.26191900	1.34417100
H	8.31426600	-1.04776700	-0.74837200
H	7.07935700	-1.43776000	3.33998700
C	2.03260100	4.43565700	-3.23061600
H	2.85150100	3.73962100	-3.01366300
H	1.15256300	3.81518100	-3.43297800
H	2.28574600	4.98816600	-4.14066300
C	0.61098400	5.23721300	1.57232400
H	-0.44576800	4.94263600	1.48985600
H	1.18426700	4.36016600	1.89796700
H	0.68083500	6.00126400	2.35300800
C	2.14630100	9.10619000	-1.29168000
H	1.55505700	9.71552500	-0.59954200
H	3.20516100	9.31335500	-1.08637500
H	1.94037800	9.45304500	-2.31025700
C	5.87608300	-0.55525000	-1.84897000
H	5.10224400	-1.24957200	-2.19628000
H	5.47767400	0.45409500	-2.00649200
H	6.75918100	-0.67681900	-2.48380600
C	4.41396500	-1.03101200	2.98027200
H	3.81527300	-0.11315400	2.94162800
H	3.71910100	-1.86310400	2.81044800
H	4.82881500	-1.13280000	3.98816100
C	9.30102900	-1.48596300	1.75627100
H	9.87920800	-1.95992900	0.95551700
H	9.79667800	-0.53553000	1.99622600
H	9.36966100	-2.12134300	2.64614600
C	-0.14169800	-4.09118700	-3.57161600
H	-0.98744200	-3.39338900	-3.55786300
H	0.75248800	-3.47932100	-3.41041100
H	-0.08329000	-4.53677400	-4.56951900

C	-0.80460900	-8.94300000	-2.31792900
H	-1.28631400	-9.53442400	-1.53189800
H	-1.40813800	-9.03259200	-3.22824200
H	0.16807400	-9.40766000	-2.52824500
C	-0.41479700	-5.45078900	1.31284800
H	0.55704400	-5.03927700	1.61043400
H	-1.16883800	-4.69163500	1.55137000
H	-0.61315500	-6.32861700	1.93562100
C	-4.73379000	1.45258700	1.26349800
H	-3.95897900	0.72525100	1.52541400
H	-4.31076800	2.46551400	1.35510700
H	-5.53239700	1.36008500	2.00465600
C	-3.93132200	0.23836900	-3.60901300
H	-3.02679500	0.85571300	-3.63507800
H	-3.59207700	-0.79679000	-3.48399700
H	-4.43274600	0.31627400	-4.57859400
C	-8.57029700	1.44192500	-2.00998900
H	-8.72868800	1.87905700	-3.00221300
H	-9.10420000	0.48242700	-1.98974300
H	-9.04539300	2.09542800	-1.27064300
K	-1.32138500	1.90212000	2.18668000
C	-3.41520000	-0.45417500	4.27167500
C	-2.22435500	-0.20351500	4.97018800
C	-2.24171800	-1.83926100	2.69222300
C	-3.43133000	-1.29959300	3.15216100
H	-4.36766400	-1.48854300	2.64109600
C	-1.00655300	-1.56962800	3.33866600
C	-1.04113000	-0.76619800	4.51104800
C	0.24739900	-1.93892700	2.71922900
H	0.40005600	-0.87513900	1.87515900
H	0.22557100	-2.76478700	2.01397300
H	-2.25047700	0.42336400	5.85428200
H	-0.11371500	-0.57614400	5.04602100
H	-2.24666400	-2.43951100	1.78841700
N	-4.63752100	0.21445800	4.68571900
O	-4.55163700	1.08129100	5.56461900
O	-5.69079800	-0.09549600	4.11896500
H	1.13938300	-1.90791500	3.34546700

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C	-2.18690400	1.48561300	-1.02469500
C	-2.74318300	2.79120000	-1.29755200
C	-1.71297900	3.68316200	-1.22385600
C	-0.52703300	2.92638400	-0.89916900

N	-0.84047800	1.59427800	-0.77109600
H	-3.78026500	2.97906900	-1.53836200
H	-1.73415600	4.75163900	-1.38849200
C	3.24203800	1.10134500	0.08708200
C	4.00901300	2.32516900	0.19982300
C	3.16225700	3.34802800	-0.09099700
C	1.87127200	2.75475500	-0.37268400
N	1.95001000	1.39159400	-0.25425900
H	5.05873000	2.36948200	0.45359700
H	3.37067500	4.40835200	-0.12260400
C	-0.92833500	-2.62953200	-0.81241700
C	-2.23643500	-3.22081200	-0.98457000
C	-3.13233800	-2.19603200	-1.00327500
C	-2.37237000	-0.96955800	-0.88172700
N	-1.03833300	-1.26508800	-0.72061300
H	-2.42158700	-4.28186300	-1.07767300
H	-4.20570300	-2.24352600	-1.12235500
C	1.49245800	-2.79759500	-0.45562600
C	2.70486200	-3.55969800	-0.25558300
C	3.67617100	-2.67137900	0.08798100
C	3.07328500	-1.35547500	0.05895100
N	1.74043100	-1.46356000	-0.25231500
H	2.77626800	-4.63341400	-0.35843900
H	4.71466200	-2.86403700	0.31792900
C	-2.93584300	0.30144100	-1.03195900
C	3.79167100	-0.17355000	0.25206900
C	0.73530700	3.49584500	-0.70375200
C	0.25529500	-3.37091500	-0.75685200
Fe	0.46135000	0.05433800	-0.46061000
Cl	0.84911700	0.03888600	-2.76632800
O	0.20861300	0.16438900	1.25465900
C	0.87776500	4.97696300	-0.87607100
C	0.58215400	5.85311500	0.18425500
C	1.30878500	5.48801300	-2.11767200
C	0.71981700	7.23179200	-0.00673700
C	1.43113500	6.87245000	-2.27074700
C	1.14531900	7.76090800	-1.22851900
H	0.49101700	7.90703100	0.81578100
H	1.75842900	7.26804800	-3.23036900
C	-4.40211400	0.40452700	-1.33442800
C	-4.85517500	0.14273800	-2.64737200
C	-5.32261600	0.78204600	-0.33839500
C	-6.22126300	0.24456900	-2.92361300
C	-6.68351100	0.86542600	-0.65410500

C	-7.15378300	0.59506200	-1.94064800
H	-6.56798100	0.04830900	-3.93649500
H	-7.38928600	1.14819100	0.12463500
C	0.20359300	-4.82594000	-1.11718900
C	0.29372900	-5.17165600	-2.48342600
C	0.06519500	-5.82928700	-0.14041300
C	0.24864600	-6.52177600	-2.84191700
C	0.02385500	-7.16930500	-0.54293900
C	0.11768900	-7.53615000	-1.88766100
H	0.31735200	-6.78848000	-3.89496000
H	-0.08565600	-7.94354800	0.21400300
C	5.25447400	-0.27169500	0.56735100
C	6.18390900	-0.43141700	-0.48103500
C	5.69567700	-0.19346500	1.90159600
C	7.54405500	-0.52145700	-0.16888800
C	7.06534800	-0.28669400	2.17098500
C	8.00529900	-0.45060300	1.14969600
H	8.26209100	-0.64839000	-0.97702200
H	7.40515900	-0.23105300	3.20354000
C	1.63514400	4.55159700	-3.25795500
H	2.50232300	3.92538100	-3.01724800
H	0.80966600	3.86030300	-3.46087700
H	1.85751700	5.10675800	-4.17441100
C	0.10502000	5.31571200	1.51608300
H	-0.91762400	4.91977400	1.42644200
H	0.75491800	4.50486900	1.86849400
H	0.08918900	6.09870300	2.28077200
C	1.32146600	9.25036800	-1.41263800
H	0.70451100	9.81920500	-0.70872900
H	2.36567800	9.54799700	-1.24749700
H	1.05349400	9.56274700	-2.42807600
C	5.71751600	-0.50804000	-1.91681500
H	5.10596600	-1.40148600	-2.08984300
H	5.08744700	0.34971400	-2.17799100
H	6.56630000	-0.53656400	-2.60700300
C	4.70386700	-0.00808700	3.02706700
H	4.15680800	0.93666900	2.92018300
H	3.95221500	-0.80445900	3.02774200
H	5.20393900	-0.00631600	4.00082400
C	9.48383600	-0.51930200	1.45515700
H	10.00027500	-1.21311700	0.78227900
H	9.95960500	0.46318900	1.33350500
H	9.66729000	-0.84550200	2.48458300
C	0.42759600	-4.09935700	-3.54054300

H	-0.45143600	-3.44451000	-3.55799000
H	1.28326900	-3.44327500	-3.34669600
H	0.54648600	-4.53984400	-4.53534500
C	0.10457600	-8.98895400	-2.30355400
H	-0.33884900	-9.62552900	-1.53047000
H	-0.46256700	-9.13508500	-3.22992400
H	1.12299500	-9.35666700	-2.48732800
C	-0.04943800	-5.47608000	1.32439700
H	0.82170100	-4.90653200	1.66824500
H	-0.93303500	-4.85490400	1.51474300
H	-0.13209700	-6.37435400	1.94418500
C	-4.86602200	1.13678600	1.05872100
H	-4.00488400	0.52780200	1.34857300
H	-4.57830800	2.19843600	1.11208900
H	-5.65144000	0.96975100	1.80175700
C	-3.88338900	-0.23353000	-3.74310500
H	-3.01530300	0.43421700	-3.75941700
H	-3.48922600	-1.24612600	-3.59583500
H	-4.36686100	-0.19836400	-4.72431900
C	-8.62881800	0.65593800	-2.26239200
H	-8.80296200	1.05680400	-3.26732200
H	-9.08117100	-0.34428200	-2.23047400
H	-9.17191600	1.28303100	-1.54744600
K	-1.52217600	1.85351800	2.10745600
C	-3.61270900	-0.53779500	4.25963600
C	-2.41893800	-0.29047900	4.95055400
C	-2.43862300	-1.86271500	2.63304600
C	-3.63155200	-1.35406900	3.11969200
H	-4.57211000	-1.54820500	2.61905500
C	-1.20118400	-1.59693000	3.27435600
C	-1.23112800	-0.82705100	4.46601600
C	1.34314600	-2.08823300	3.37847000
C	0.04275700	-1.97105600	2.61126900
H	2.14697800	-2.36205400	2.68891200
H	0.19879000	-0.91530100	1.83586200
H	-0.09349700	-2.74272700	1.85762800
H	1.28977000	-2.85780200	4.16223200
H	-2.44293300	0.31337600	5.85056200
H	1.62842100	-1.14358900	3.85622900
H	-0.30761700	-0.63825800	5.00458700
H	-2.44466100	-2.44767200	1.71821300
N	-4.84345100	0.09733900	4.70920200
O	-4.76922400	0.90225200	5.64436600
O	-5.89047300	-0.18118100	4.11529900

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C	-1.95034500	1.87175400	-0.94999500
C	-2.29433300	3.24982200	-1.22121800
C	-1.14108500	3.97197300	-1.11358800
C	-0.09174600	3.03683500	-0.77780100
N	-0.60778400	1.76889900	-0.67494000
H	-3.28574300	3.59589600	-1.47928900
H	-0.99413700	5.03251500	-1.26472100
C	3.38735200	0.63400200	0.06219100
C	4.32991700	1.72602400	0.18757300
C	3.63127400	2.87388800	-0.01889600
C	2.25830200	2.48909600	-0.27404000
N	2.13994800	1.12467200	-0.20949200
H	5.38394000	1.60519000	0.39461000
H	3.99297600	3.89263500	-0.01600700
C	-1.35768900	-2.38111500	-0.66213200
C	-2.74434600	-2.76206500	-0.81128800
C	-3.46760800	-1.60952300	-0.84753300
C	-2.52175800	-0.51797500	-0.75121100
N	-1.25056900	-1.01666000	-0.58329800
H	-3.09445300	-3.78212700	-0.88638300
H	-4.53545600	-1.48781200	-0.96437100
C	1.02121500	-2.92883300	-0.40895900
C	2.11554700	-3.87152700	-0.34204500
C	3.23668100	-3.15511900	-0.06383400
C	2.83972800	-1.76433000	0.00508100
N	1.48261800	-1.65613900	-0.17535200
H	2.01460500	-4.93749600	-0.49019300
H	4.25055700	-3.50947400	0.05811200
C	-2.87588900	0.81993100	-0.94797100
C	3.74783200	-0.71405600	0.15062700
C	1.24208800	3.40184000	-0.56312300
C	-0.30168200	-3.29791700	-0.65958900
Fe	0.44862700	0.04903000	-0.35516900
Cl	0.75996600	-0.05341000	-2.67932400
O	0.21990600	0.29001300	1.35638800
C	1.60210800	4.85133500	-0.68145800
C	1.40396700	5.72564600	0.40318900
C	2.13571100	5.33758100	-1.89311500
C	1.74106300	7.07622900	0.26616700
C	2.45728100	6.69468600	-1.99222100
C	2.27128300	7.57978200	-0.92489600
H	1.58796000	7.74947500	1.10774800

H	2.86295300	7.07155500	-2.92919600
C	-4.29713700	1.13107300	-1.31525600
C	-4.69571400	0.98016700	-2.66189100
C	-5.22706100	1.56072700	-0.35090400
C	-6.01951000	1.26264700	-3.00974600
C	-6.54521900	1.82608700	-0.73813500
C	-6.96017800	1.68612800	-2.06440600
H	-6.32654100	1.14420000	-4.04717700
H	-7.26332800	2.14255400	0.01580900
C	-0.58818200	-4.69849400	-1.11939400
C	-0.66519200	-4.92180100	-2.51283800
C	-0.78112500	-5.76551800	-0.22220100
C	-0.92169500	-6.21590700	-2.97587000
C	-1.04083000	-7.04396600	-0.72909800
C	-1.10933000	-7.29127800	-2.10233200
H	-0.97923200	-6.38697400	-4.04922900
H	-1.19500200	-7.86545900	-0.03190200
C	5.20543300	-1.04549400	0.27962500
C	5.98495000	-1.17264600	-0.88897000
C	5.79186600	-1.22754900	1.54514100
C	7.34261000	-1.48366400	-0.76390500
C	7.15366800	-1.53631000	1.62777800
C	7.94667300	-1.66697400	0.48416800
H	7.94377800	-1.58604000	-1.66542500
H	7.60445400	-1.67870700	2.60822400
C	2.35883600	4.40483600	-3.06121300
H	3.14127900	3.67093800	-2.83431500
H	1.45756400	3.82696800	-3.29365500
H	2.65857200	4.95763900	-3.95683500
C	0.81607000	5.22073700	1.70329900
H	-0.25787800	5.01284800	1.58355800
H	1.30738900	4.29431000	2.02514000
H	0.92093700	5.96122100	2.50267300
C	2.66172200	9.03433900	-1.05024900
H	2.11430900	9.66138700	-0.33828700
H	3.73309500	9.17431400	-0.85340200
H	2.46620800	9.41574500	-2.05861600
C	5.36071400	-0.98092000	-2.25187100
H	4.54438700	-1.69266900	-2.42046400
H	4.91933400	0.01749600	-2.35073500
H	6.10073600	-1.11093600	-3.04752900
C	4.95970500	-1.09367300	2.79859900
H	4.47427500	-0.11154200	2.84521800
H	4.16033400	-1.84387100	2.82275000

H	5.56910900	-1.21830100	3.69925600
C	9.42363000	-1.96859200	0.59226800
H	9.77321300	-2.56908200	-0.25487400
H	10.01663600	-1.04404900	0.60108000
H	9.65667000	-2.51355900	1.51354200
C	-0.50357300	-3.78214100	-3.49351800
H	-1.38212200	-3.12504900	-3.47622600
H	0.35102800	-3.14073200	-3.25472400
H	-0.38492200	-4.15819000	-4.51458300
C	-1.35421100	-8.68533100	-2.63168800
H	-1.88235100	-9.30662800	-1.90024400
H	-1.94779900	-8.66603000	-3.55255000
H	-0.40784100	-9.19058900	-2.86734500
C	-0.71092300	-5.55098500	1.27129200
H	0.30392700	-5.28233900	1.58610400
H	-1.37220200	-4.73760300	1.59178300
H	-1.00241600	-6.45473200	1.81550400
C	-4.82323600	1.75654800	1.09242300
H	-4.14836900	0.95847600	1.41908100
H	-4.31249800	2.72381400	1.22260500
H	-5.68923800	1.75228000	1.75956500
C	-3.71293800	0.50534100	-3.70801800
H	-2.77661400	1.07270100	-3.67307900
H	-3.43911400	-0.54392100	-3.54404400
H	-4.13580500	0.59281100	-4.71360000
C	-8.37888100	2.00576500	-2.47484500
H	-8.45883000	3.03419000	-2.85204600
H	-8.72382800	1.34071700	-3.27435500
H	-9.07209100	1.91166000	-1.63218300
K	-1.44003700	2.09602500	2.13246400
C	-3.79175400	-0.50224100	3.79541300
C	-2.90152800	0.03276800	4.73091400
C	-2.00453800	-1.69734900	2.72535500
C	-3.35315700	-1.39149400	2.80610400
H	-4.05602500	-1.78496200	2.08224800
C	-1.05357700	-1.13071400	3.61046200
C	-1.54862100	-0.28686800	4.63689200
C	0.39195700	-1.27651300	3.33223100
H	0.41875300	-0.57648200	2.18907900
H	-3.27675100	0.68644800	5.51024500
H	-0.86581800	0.12303000	5.37386000
H	-1.66666000	-2.32105000	1.90765900
N	-5.18576000	-0.07583200	3.81006700
O	-5.48890900	0.87158800	4.54484300

O	-5.97536900	-0.65372400	3.06101500
C	1.35050300	-0.50721400	4.22549900
H	1.09129200	0.55593300	4.29831800
H	1.38086200	-0.91641700	5.24735700
H	2.36182300	-0.56431300	3.81629300
C	0.89232000	-2.66564500	2.97256500
H	1.90241200	-2.61504200	2.55714400
H	0.92086500	-3.31115300	3.86394900
H	0.26510400	-3.14956700	2.22673500

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C	-3.31140200	0.91911900	0.03417500
C	-4.14177300	2.09402700	0.20461500
C	-3.34854700	3.17302200	-0.02695200
C	-2.02738800	2.66283900	-0.33292600
N	-2.03461500	1.29334500	-0.28206300
H	-5.19287200	2.07063400	0.45585200
H	-3.61186600	4.22132000	-0.00435000
C	2.08766300	1.64856900	-1.07954300
C	2.56338100	2.99122800	-1.32445600
C	1.48665300	3.82045000	-1.19806000
C	0.35286900	2.98728600	-0.87267400
N	0.74260400	1.67198900	-0.79512000
H	3.58242400	3.24477300	-1.58196100
H	1.44384900	4.89295100	-1.32878400
C	-1.31679700	-2.86164600	-0.51456500
C	-2.48930800	-3.69665700	-0.37518200
C	-3.52758500	-2.87048500	-0.07910800
C	-3.00031400	-1.52230600	-0.05978400
N	-1.65133800	-1.54609100	-0.31030000
H	-2.49282100	-4.77127700	-0.49274100
H	-4.56371800	-3.12482800	0.09428900
C	1.09195300	-2.54053900	-0.85637600
C	2.42874400	-3.04691100	-1.07249000
C	3.25514400	-1.96651800	-1.12415200
C	2.42292800	-0.79259700	-0.96991500
N	1.11585400	-1.17160800	-0.76732300
H	2.67806700	-4.09378400	-1.17505200
H	4.32424300	-1.94386600	-1.28263900
C	-3.79340400	-0.38930300	0.13342100
C	2.90405500	0.51121100	-1.12381900
C	-0.93552800	3.47826300	-0.63567400
C	-0.04140000	-3.35586900	-0.79112000
Fe	-0.46603800	0.05163300	-0.49757100

Cl	-0.84439200	0.02417000	-2.80518300
O	-0.22432700	0.17651500	1.22422800
C	-1.15816500	4.95655400	-0.73355200
C	-0.87082400	5.79613500	0.35874700
C	-1.66726800	5.50208300	-1.93019700
C	-1.09302000	7.17206300	0.24317200
C	-1.87291700	6.88296000	-2.00808400
C	-1.59068800	7.73536300	-0.93539600
H	-0.87692900	7.81786200	1.09239900
H	-2.26651900	7.30426100	-2.93115600
C	-5.25936200	-0.58457000	0.38017300
C	-6.16027100	-0.51020800	-0.70221900
C	-5.73213100	-0.83981200	1.68072600
C	-7.52489100	-0.69109800	-0.45734800
C	-7.10533700	-1.01298800	1.88396500
C	-8.01752900	-0.94465900	0.82712200
H	-8.22139600	-0.63275600	-1.29174000
H	-7.47046900	-1.20502700	2.89123900
C	0.10773400	-4.80597400	-1.14398800
C	0.05935500	-5.16462800	-2.50902900
C	0.28653500	-5.79355100	-0.15829700
C	0.18801100	-6.51210800	-2.85694100
C	0.41404400	-7.13131700	-0.55017900
C	0.36885700	-7.51055600	-1.89392900
H	0.14485300	-6.78973600	-3.90853400
H	0.55075900	-7.89381800	0.21426000
C	4.35386700	0.70241200	-1.46124900
C	4.77244000	0.54364000	-2.80121700
C	5.29204700	1.04065600	-0.46825100
C	6.12311800	0.72078000	-3.11223800
C	6.63724900	1.20294100	-0.81964400
C	7.07223600	1.04984600	-2.13755900
H	6.44491000	0.59632600	-4.14452400
H	7.35907400	1.45095700	-0.04373600
C	-1.99674000	4.60521100	-3.10121500
H	-1.15814200	3.94667600	-3.35280000
H	-2.84132800	3.94644700	-2.86646700
H	-2.25723700	5.19178800	-3.98757200
C	-0.32090300	5.22300700	1.64700000
H	-0.90228700	4.35001600	1.96912000
H	0.72402800	4.90643200	1.51089300
H	-0.33837400	5.96317800	2.45321200
C	-1.79544000	9.22749600	-1.05869500
H	-1.95011400	9.69481000	-0.08016000

H	-0.92177000	9.70991400	-1.51718700
H	-2.66122100	9.46229800	-1.68770000
C	3.77994300	0.17885200	-3.88159300
H	3.40749600	-0.84379600	-3.74823100
H	2.89939700	0.82991900	-3.85768900
H	4.23608700	0.24762700	-4.87401500
C	4.87028500	1.25143600	0.96820800
H	4.51663800	2.28374700	1.11968400
H	4.06597400	0.56173300	1.24128400
H	5.69482800	1.08493300	1.66779700
C	8.52170800	1.25637800	-2.51125200
H	8.84613800	0.53496500	-3.26969900
H	8.68271100	2.25897200	-2.92951800
H	9.18005600	1.15417900	-1.64212200
C	-0.12298200	-4.10909000	-3.57582500
H	-1.00178100	-3.48385200	-3.38420100
H	0.73107900	-3.42212500	-3.60408700
H	-0.22862200	-4.56388400	-4.56568300
C	0.53607200	-8.95545300	-2.30399000
H	0.33404300	-9.63686000	-1.47071700
H	-0.13746300	-9.21809400	-3.12777200
H	1.55982200	-9.15310900	-2.64906900
C	0.33207700	-5.42661900	1.30689200
H	1.10014000	-4.67048800	1.50646400
H	-0.62472100	-5.00623000	1.64002900
H	0.54937800	-6.30040700	1.92914200
C	-4.76682500	-0.93553100	2.83978800
H	-4.11641500	-1.81270200	2.73479600
H	-4.10956400	-0.05891400	2.88288000
H	-5.29628300	-1.01816400	3.79430600
C	-5.65906600	-0.23525500	-2.10155100
H	-5.22790200	0.77000300	-2.17824300
H	-4.86263600	-0.93230800	-2.38569400
H	-6.46806300	-0.31646000	-2.83410600
C	-9.49445700	-1.16749000	1.05741000
H	-10.10264900	-0.53473500	0.40124700
H	-9.77432000	-2.20953100	0.85177500
H	-9.77741600	-0.95225100	2.09349600
K	1.54088800	1.86840500	2.03612200
C	-0.98654600	-1.63877100	3.82998500
C	-0.18805600	-0.64558200	4.72155500
C	-0.06273400	-1.91044900	2.64421600
C	1.29227000	-1.63344600	3.10026300
C	2.52031700	-1.91263400	2.47718500

C	3.68850500	-1.36480500	2.99685400
C	3.62052400	-0.52435300	4.11708800
C	2.40641700	-0.25918500	4.77894300
C	1.24979400	-0.82741300	4.26947800
H	2.55755800	-2.51237300	1.57404200
H	2.40584900	0.37901900	5.65604000
H	4.64941300	-1.54490800	2.53095700
H	-0.52185400	0.38572900	4.53625500
H	-1.95427700	-1.23558600	3.52118200
H	-0.23377300	-0.89534500	1.81969400
H	-0.25302700	-2.76893600	2.00662700
N	4.83229900	0.14600600	4.57344500
O	4.72112900	0.98363000	5.47642800
O	5.89891000	-0.13342700	4.01660800
H	-0.31910800	-0.82793000	5.79382500
H	-1.17960000	-2.57037300	4.38074900

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C	-3.36127800	0.79772900	-0.07235400
C	-4.23229200	1.94120500	0.08956400
C	-3.47037700	3.04836200	-0.11266800
C	-2.12633300	2.58823500	-0.39013300
N	-2.09061200	1.21773800	-0.36166000
H	-5.28673600	1.87897200	0.31868100
H	-3.76778900	4.08713400	-0.08264300
C	2.04341000	1.73312000	-1.03747800
C	2.47619400	3.09754900	-1.22055700
C	1.36833200	3.88436500	-1.09701300
C	0.25482400	3.00444700	-0.83835900
N	0.68958800	1.70059800	-0.79350200
H	3.49359600	3.39341100	-1.43528400
H	1.29170200	4.95901300	-1.18773200
C	-1.20373900	-2.89465900	-0.56281000
C	-2.34252000	-3.77337700	-0.43284000
C	-3.42028800	-2.98864800	-0.16497200
C	-2.95399100	-1.62122500	-0.15567600
N	-1.60084300	-1.59084800	-0.38948100
H	-2.29838900	-4.84843000	-0.53495800
H	-4.44715800	-3.28435700	-0.00342900
C	1.19197200	-2.48398900	-0.87328200
C	2.55092800	-2.94052800	-1.05554900
C	3.33736100	-1.83144200	-1.10047600
C	2.46152800	-0.68850600	-0.97104600
N	1.16426900	-1.11408900	-0.80244600

H	2.84044500	-3.97877100	-1.13630600
H	4.40851600	-1.76909400	-1.23058100
C	-3.79634100	-0.52460300	0.02509100
C	2.90169400	0.63047400	-1.09566200
C	-1.05477600	3.44699800	-0.63437400
C	0.09389900	-3.34312500	-0.80671600
Fe	-0.46552700	0.04206300	-0.53845300
Cl	-0.78962700	0.01288600	-2.84490800
O	-0.25096100	0.12490400	1.14174900
C	-1.32251100	4.92003600	-0.68998000
C	-1.11801100	5.72322300	0.44749900
C	-1.79138200	5.49539700	-1.88861100
C	-1.38357600	7.09426300	0.37380200
C	-2.04288700	6.87040000	-1.92323400
C	-1.84379800	7.68758400	-0.80540400
H	-1.23217100	7.71215000	1.25699900
H	-2.40634200	7.31515000	-2.84761500
C	-5.24811300	-0.77967000	0.29449500
C	-6.17166500	-0.75439600	-0.76903000
C	-5.68133500	-1.04369600	1.60822000
C	-7.52248200	-0.99296300	-0.49442100
C	-7.04038900	-1.27446100	1.84071100
C	-7.97654100	-1.25606000	0.80160900
H	-8.23746400	-0.97323900	-1.31466700
H	-7.37631000	-1.47300400	2.85683800
C	0.31031600	-4.79776700	-1.09918400
C	0.37974900	-5.20585500	-2.44839500
C	0.43288000	-5.74440700	-0.06397600
C	0.57195600	-6.56099400	-2.73439400
C	0.62683900	-7.08985900	-0.39499700
C	0.70189500	-7.51804400	-1.72337900
H	0.61856100	-6.87711400	-3.77478200
H	0.72060500	-7.82104000	0.40568800
C	4.34824800	0.87602900	-1.40708800
C	4.79140100	0.74882800	-2.74169000
C	5.25767300	1.22931800	-0.39270300
C	6.14088600	0.97249600	-3.02842100
C	6.60171400	1.43913100	-0.72073800
C	7.06256000	1.31786500	-2.03378900
H	6.48296600	0.87161300	-4.05668500
H	7.30297800	1.69792500	0.07011100
C	-2.02761700	4.63573500	-3.10888600
H	-1.14125400	4.04209800	-3.35906900
H	-2.83763000	3.91750100	-2.93500200

H	-2.29264700	5.24598800	-3.97762700
C	-0.60944600	5.11710800	1.73752600
H	-1.18075700	4.21988000	2.00605000
H	0.44751400	4.82933300	1.63523400
H	-0.67825800	5.82778800	2.56700700
C	-2.09565400	9.17559900	-0.88046500
H	-2.31961100	9.59624300	0.10574600
H	-1.21622300	9.70565300	-1.27007100
H	-2.93399300	9.40693400	-1.54671600
C	3.82849300	0.36622700	-3.84267900
H	3.48712100	-0.66960400	-3.72851600
H	2.92738900	0.98906100	-3.82639200
H	4.29798800	0.46197700	-4.82651900
C	4.80287900	1.40112700	1.03856300
H	4.34218400	2.39158800	1.17949300
H	4.07089600	0.63427200	1.31122800
H	5.63520400	1.32062500	1.74294300
C	8.51068700	1.57698900	-2.37868300
H	8.85650900	0.91405000	-3.17959100
H	8.65487300	2.60844700	-2.72728900
H	9.16300800	1.43085500	-1.51123300
C	0.25363200	-4.19763300	-3.56828700
H	-0.62163000	-3.55173200	-3.43887300
H	1.12205600	-3.52840400	-3.59811800
H	0.17683100	-4.69614900	-4.53949200
C	0.94485200	-8.97143100	-2.05863600
H	0.55407900	-9.63494900	-1.27948600
H	0.47370800	-9.24790900	-3.00824500
H	2.01880800	-9.18024500	-2.15572300
C	0.33967700	-5.32826600	1.38591200
H	1.01950100	-4.50091400	1.61437600
H	-0.67188700	-4.98503200	1.63562900
H	0.58417600	-6.16005700	2.05358700
C	-4.68717400	-1.08695600	2.74612900
H	-4.00164300	-1.93631300	2.63327700
H	-4.06583800	-0.18402600	2.76814100
H	-5.19211800	-1.18404500	3.71241500
C	-5.71020800	-0.47100800	-2.18024800
H	-5.31931200	0.54931400	-2.27293200
H	-4.89471100	-1.14096700	-2.47592500
H	-6.52991300	-0.58815000	-2.89571600
C	-9.43555200	-1.54389900	1.07049300
H	-10.08252100	-1.07606800	0.32065000
H	-9.63607900	-2.62351900	1.04658400

H	-9.74139100	-1.17977800	2.05764200
K	1.39616200	1.81234700	2.17136600
C	-0.99610900	-1.22586000	3.91998200
C	-0.16748700	-0.53940600	4.76882400
C	-0.22989700	-1.82568600	2.82950300
C	1.16783200	-1.59197300	3.16714900
C	2.35693800	-1.91897500	2.50219600
C	3.56291000	-1.38614400	2.94670200
C	3.56763300	-0.50091700	4.04124600
C	2.40481100	-0.17086200	4.74847800
C	1.19744800	-0.72745400	4.31839200
H	2.34366100	-2.54960400	1.62004900
H	2.46463400	0.50300200	5.59628600
H	4.49565800	-1.60825500	2.44392700
H	-0.46375900	0.05008300	5.62969000
H	-2.07664300	-1.26747500	3.99131900
H	-0.33859700	-0.87682200	1.85969700
H	-0.56372700	-2.71265900	2.29782400
N	4.81851200	0.15519400	4.40967100
O	4.77145000	1.06333100	5.24823500
O	5.85570200	-0.20452900	3.84407700

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C	-2.33251600	1.29971500	-1.13468400
C	-2.98361800	2.55530300	-1.43104100
C	-2.02308200	3.52274600	-1.37142500
C	-0.78549300	2.86283400	-1.02906400
N	-0.99866700	1.51257800	-0.88211900
H	-4.03142700	2.66145100	-1.67530900
H	-2.12357400	4.58379200	-1.55373800
C	3.10908300	1.33320500	-0.02854900
C	3.77615800	2.61248100	0.10155300
C	2.85194700	3.56851700	-0.18201700
C	1.61312500	2.87827000	-0.47649000
N	1.79732700	1.52458500	-0.36647700
H	4.81856500	2.73736300	0.35846000
H	2.97693200	4.64216000	-0.20401400
C	-0.76990600	-2.70647700	-0.89267300
C	-2.03448900	-3.39628600	-1.01762700
C	-3.00460600	-2.44106400	-1.02850600
C	-2.33496200	-1.15966900	-0.94803400
N	-0.97913400	-1.35348100	-0.81727400
H	-2.14174600	-4.46970700	-1.08984400
H	-4.07426500	-2.56910600	-1.11790900

C	1.66558600	-2.68687400	-0.60329100
C	2.94322400	-3.34849600	-0.45758000
C	3.84773500	-2.38982100	-0.12226300
C	3.13724600	-1.12872800	-0.10259500
N	1.80978500	-1.34036100	-0.38175100
H	3.10159100	-4.40968400	-0.58825600
H	4.90544300	-2.49968900	0.07183100
C	-2.99234000	0.06365600	-1.11301200
C	3.76121400	0.10344100	0.10347100
C	0.42739600	3.52914600	-0.82438000
C	0.46847700	-3.35494300	-0.87073000
Fe	0.41661300	0.07614000	-0.57564000
Cl	0.79576500	0.09429600	-2.88497800
O	0.16164700	0.15696900	1.14079400
H	0.39479400	-1.35829600	5.84146700
C	5.23690400	0.11846900	0.37394500
C	5.71949600	0.13183900	1.69562500
C	6.13725000	0.14062000	-0.71131400
C	7.10096000	0.16049600	1.91548000
C	7.51048700	0.16559300	-0.44887300
C	8.01293400	0.17237900	0.85653300
H	7.47220500	0.17491200	2.93860500
H	8.20584700	0.18523800	-1.28602400
C	0.51948200	-4.80899700	-1.23428600
C	0.58510100	-5.81947600	-0.25566600
C	0.50620900	-5.14868700	-2.60491200
C	0.64563400	-7.15705400	-0.66208100
C	0.56893800	-6.49779600	-2.96677900
C	0.64351800	-7.51680600	-2.01237300
H	0.69420900	-7.93621600	0.09626000
H	0.56152800	-6.75899600	-4.02339200
C	-4.46608300	0.05353900	-1.39583900
C	-5.39658600	0.39489900	-0.39550200
C	-4.91849800	-0.27699200	-2.69319500
C	-6.76409600	0.37284900	-0.69074400
C	-6.29254100	-0.28043000	-2.94932200
C	-7.23293800	0.03202300	-1.96135100
H	-7.47667300	0.62910000	0.09100400
H	-6.63907900	-0.53014200	-3.95040400
C	0.45897800	5.01527100	-1.00960800
C	0.05426800	5.87630500	0.02738900
C	0.90372500	5.54732600	-2.23770500
C	0.09386600	7.25958900	-0.17439500
C	0.92556600	6.93582900	-2.40220900

C	0.52254900	7.80886200	-1.38623900
H	-0.21376100	7.92268300	0.63213400
H	1.26860400	7.34700500	-3.34971300
C	0.57089700	-5.48034600	1.21729600
H	1.36919700	-4.77584400	1.47567300
H	-0.37754700	-5.01059500	1.50617700
H	0.69785500	-6.37743400	1.83137300
C	0.40803200	-4.07700700	-3.66727100
H	-0.58751300	-3.61612000	-3.67099100
H	1.11580400	-3.25925400	-3.49515200
H	0.59098000	-4.49335400	-4.66282700
C	0.74842600	-8.96461200	-2.43255200
H	0.17552200	-9.15949200	-3.34604000
H	1.79103900	-9.24153300	-2.63913800
H	0.38091800	-9.63840400	-1.65098100
C	-3.93827400	-0.61198000	-3.79486300
H	-3.12336100	0.11829600	-3.84471300
H	-3.46680300	-1.58750900	-3.62608800
H	-4.43787100	-0.64146800	-4.76812500
C	-4.94376200	0.82087600	0.98269800
H	-4.05479200	0.26034500	1.28600500
H	-4.70036100	1.89473100	0.99218000
H	-5.71435200	0.65042400	1.74039600
C	-8.71340500	-0.02112500	-2.25875200
H	-9.28539500	0.61155300	-1.57170400
H	-8.92809100	0.30701900	-3.28192900
H	-9.09912900	-1.04453900	-2.15907400
C	1.36294300	4.63085800	-3.34839300
H	2.29326900	4.11855400	-3.07512000
H	0.63083500	3.84162400	-3.55086100
H	1.53966000	5.18875600	-4.27313300
C	-0.42465800	5.31742400	1.34959800
H	-1.40123500	4.82636800	1.22668700
H	0.28435100	4.57744400	1.74286200
H	-0.54379900	6.10703600	2.09808600
C	0.52723100	9.30416500	-1.60430900
H	1.36934200	9.61500400	-2.23252900
H	-0.39143300	9.63245800	-2.10875100
H	0.59175500	9.84912100	-0.65635700
C	5.62425500	0.14586400	-2.13282000
H	5.02210300	-0.74565000	-2.34273500
H	4.97083300	1.00676500	-2.31599500
H	6.44925300	0.18058200	-2.85094200
C	4.76082200	0.10800400	2.86328900

H	3.98669600	0.87668800	2.76310100
H	4.23965200	-0.85439200	2.92332600
H	5.28472300	0.26655700	3.81143600
C	9.50242100	0.16740900	1.11206700
H	9.90192900	-0.85568000	1.10155300
H	10.04297200	0.73331200	0.34515200
H	9.74489300	0.60155500	2.08814700
C	-3.47134800	-0.61961800	4.23717400
C	-2.25204900	-0.32006400	4.86273500
C	-2.34801400	-1.98889200	2.62283100
C	-3.53257900	-1.49133800	3.14269000
H	-4.49101000	-1.72527400	2.69653100
C	-1.09668800	-1.66242600	3.19532000
C	-1.06343600	-0.85253600	4.36927500
C	1.43993800	-1.91114700	3.26702800
C	1.46729700	-0.63140900	4.11429900
C	0.26016600	-0.58830300	5.06659200
C	0.13900500	-1.98850100	2.49291700
H	2.27713700	-1.92765500	2.56194600
H	2.39501400	-0.56364900	4.69310300
H	0.19406000	-0.94892400	1.69810700
H	0.05798000	-2.80604700	1.78114800
H	0.21746800	0.36986000	5.60049900
H	1.55154500	-2.79364800	3.91808500
H	1.44452400	0.22800200	3.43221600
H	-2.25403400	0.32823300	5.73299300
H	-2.37224400	-2.60588100	1.72892400
N	-4.68822600	0.03396700	4.69864600
O	-5.76118000	-0.31058000	4.19225600
O	-4.57814100	0.92223900	5.55248700
K	-1.64541200	1.77189600	1.99469200

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C	-0.95249400	-2.56001300	-0.99013100
C	-2.21779000	-3.24352600	-1.13874900
C	-3.18482700	-2.28573600	-1.14265900
C	-2.51437900	-1.01017400	-1.01621900
N	-1.15872600	-1.20749000	-0.88359300
H	-2.32748600	-4.31470100	-1.23416600
H	-4.25375000	-2.40829200	-1.24676000
C	-1.01004000	3.02013600	-0.76142700
C	-2.26981600	3.69588300	-0.96595100
C	-3.21493900	2.72588600	-1.13778600
C	-2.53537500	1.45552000	-1.02645500

N	-1.19657200	1.65939000	-0.79064300
H	-2.39316300	4.76966000	-0.99816200
H	-4.27135800	2.84192800	-1.33628800
C	3.01745100	-0.97750700	-0.57144400
C	3.72214600	-2.23584700	-0.68074000
C	2.78166200	-3.20303500	-0.84199500
C	1.49464100	-2.54404600	-0.82362200
N	1.66203400	-1.19324300	-0.63554600
H	4.79749400	-2.33834800	-0.64862000
H	2.92241400	-4.26676800	-0.97246500
C	2.99117900	1.47596500	-0.40896700
C	3.66017700	2.74951100	-0.24710400
C	2.69323800	3.70451500	-0.25129300
C	1.42959500	3.02003500	-0.43416100
N	1.64184100	1.66742100	-0.51443900
H	4.72956000	2.87011900	-0.14649200
H	2.80341900	4.77594900	-0.15894900
C	0.28294900	-3.21328500	-0.99982900
C	0.20615300	3.67991900	-0.55503900
C	-3.17993500	0.21498600	-1.10901600
C	3.66459300	0.25355200	-0.46873200
Fe	0.25088900	0.22149300	-0.65769400
Cl	0.44089300	0.33959600	-2.98366900
O	0.10342900	0.25659900	1.06492200
C	-4.65075400	0.20635200	-1.40460400
C	-5.60112300	0.37255100	-0.37992100
C	-5.07566800	0.03391300	-2.74034500
C	-6.96360500	0.35606800	-0.69834100
C	-6.44554600	0.03131900	-3.01787800
C	-7.40600400	0.19062500	-2.01290500
H	-7.69354100	0.47126500	0.10066000
H	-6.77249300	-0.10124600	-4.04749700
C	0.31285100	-4.67027800	-1.35901000
C	0.23240000	-5.02134500	-2.72479600
C	0.42612100	-5.67366600	-0.37806800
C	0.26501600	-6.37376600	-3.07768900
C	0.45362700	-7.01525400	-0.77480900
C	0.37670300	-7.38612500	-2.11969900
H	0.20363200	-6.64327200	-4.13043800
H	0.53711600	-7.78827400	-0.01328100
C	5.16296100	0.27329400	-0.51567700
C	5.80267700	0.43170400	-1.76221600
C	5.91943300	0.12720700	0.66103500
C	7.20023000	0.43757000	-1.80539900

C	7.31593300	0.14081500	0.57410200
C	7.97460300	0.29619600	-0.64895600
H	7.69655500	0.55451300	-2.76703700
H	7.90150100	0.02605000	1.48446900
C	0.19793100	5.17759700	-0.50897200
C	0.48580600	5.91249800	-1.67810100
C	-0.08859700	5.84953300	0.69323800
C	0.47950400	7.30903600	-1.61581300
C	-0.08316700	7.24828700	0.71622900
C	0.19664200	7.99653200	-0.43020400
H	0.70335400	7.87631400	-2.51730600
H	-0.29804000	7.76430100	1.65019800
C	-4.06874400	-0.15888800	-3.85173600
H	-3.26703200	0.58599000	-3.80767800
H	-3.57976000	-1.13765200	-3.77540700
H	-4.54923700	-0.09584500	-4.83300400
C	-5.17688700	0.58757900	1.05508300
H	-4.30465800	-0.02663600	1.30069500
H	-4.92181900	1.64511300	1.22727900
H	-5.97057400	0.32016600	1.75781000
C	-8.87962000	0.20884200	-2.34673200
H	-9.49069700	-0.07677300	-1.48389700
H	-9.20139900	1.21158200	-2.65858300
H	-9.11275000	-0.47580600	-3.16974800
C	0.80509200	5.19812900	-2.97095300
H	1.74173100	4.63413700	-2.88904300
H	0.02982000	4.46723400	-3.22629800
H	0.90248600	5.90529800	-3.80029100
C	-0.41050900	5.07349300	1.95178200
H	-1.40869900	4.61667000	1.87304600
H	0.31849100	4.27135900	2.12024500
H	-0.41620900	5.72379600	2.83218700
C	0.17375500	9.50726400	-0.40168600
H	0.99028500	9.93091700	-0.99734700
H	-0.76488800	9.89641600	-0.81809600
H	0.26440200	9.89223500	0.61952100
C	4.99067900	0.59349800	-3.02690200
H	4.27999300	-0.23036600	-3.15877300
H	4.38944600	1.51003500	-2.99718000
H	5.63726900	0.63712600	-3.90885000
C	9.48374400	0.34072400	-0.71965800
H	9.94191800	-0.19296300	0.12015500
H	9.85518600	-0.10594800	-1.64875500
H	9.85103000	1.37545800	-0.68846600

C	5.23039500	-0.04321800	1.99210400
H	4.54488600	0.78678200	2.19563600
H	4.62122900	-0.95340300	2.02168900
H	5.95142500	-0.09661500	2.81315100
C	0.52328500	-5.32028800	1.08785400
H	1.41271200	-4.71094800	1.28698500
H	-0.34465900	-4.73977900	1.42165500
H	0.58367700	-6.21871700	1.70999000
C	0.10282900	-3.95815600	-3.79217800
H	-0.87802400	-3.46949100	-3.74797600
H	0.84337800	-3.16104600	-3.66643600
H	0.22145800	-4.38892800	-4.79127900
C	0.44338400	-8.83814400	-2.53298400
H	-0.19244600	-9.03676000	-3.40303700
H	1.46742700	-9.12383000	-2.80875500
H	0.12628100	-9.50252300	-1.72195200
K	-1.88545600	1.56042200	2.08368400
C	3.09957800	-0.06138300	4.65115500
C	1.99105900	-0.27319900	3.83254600
C	1.69073500	-1.55416600	3.33645000
C	2.57127000	-2.60573300	3.64071700
C	3.68600600	-2.39444900	4.45269300
C	3.94687400	-1.12461600	4.97298400
H	3.31450600	0.93755400	5.02196000
H	1.36186500	0.56269600	3.53937700
H	2.36467700	-3.59899800	3.25062800
H	4.35046000	-3.22352300	4.68165000
C	0.47570400	-1.79973700	2.51337500
H	0.37812300	-0.76559800	1.66595300
C	-0.86295600	-1.72684500	3.11005300
C	-1.96981600	-2.22319700	2.37429800
C	-1.13904300	-1.05489400	4.32891800
C	-3.27484100	-2.00584600	2.78437100
C	-2.44488400	-0.81792200	4.74483300
H	-0.31471000	-0.71542300	4.94724800
C	-3.51002700	-1.26935400	3.95411900
H	-2.65615400	-0.29389300	5.67015600
H	0.57915900	-2.62642400	1.81290500
H	4.81374500	-0.96067600	5.60710700
H	-1.79327600	-2.74714200	1.44226800
H	-4.11221300	-2.36696000	2.19961200
N	-4.87477700	-0.93528700	4.33371800
O	-5.03533000	-0.15364200	5.27841900
O	-5.79680200	-1.42670500	3.67512000

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C	3.02658000	0.45098000	-0.60139700
C	4.30161400	-0.21888800	-0.69982000
C	4.04300000	-1.53003700	-0.97513000
C	2.60829500	-1.67257500	-1.02489800
N	2.00977700	-0.45944300	-0.76660800
H	5.26005900	0.27102800	-0.60198700
H	4.74540600	-2.33481400	-1.14319100
C	-1.57838800	-2.59483600	-0.91211800
C	-1.44830400	-4.03093600	-1.02376300
C	-0.12728800	-4.29409700	-1.22265300
C	0.56172700	-3.02284900	-1.18931600
N	-0.34519700	-2.00985300	-1.00689900
H	-2.27602600	-4.72501400	-0.98328300
H	0.35631400	-5.24970800	-1.37059600
C	-0.46341600	2.94634100	-0.92439900
C	0.21868600	4.21282300	-0.78611800
C	1.52068400	3.93258600	-0.50812400
C	1.65348600	2.49188100	-0.51360100
N	0.42298400	1.91655900	-0.73043400
H	-0.25775400	5.17759100	-0.88967500
H	2.33875800	4.62093200	-0.34829600
C	-2.49052800	1.59525300	-1.18573900
C	-3.92697800	1.45394300	-1.25787500
C	-4.20441400	0.13690500	-1.05274200
C	-2.93700000	-0.54720000	-0.92157200
N	-1.91493800	0.36555600	-1.00056700
H	-4.61454400	2.27410200	-1.41017000
H	-5.16877800	-0.34862400	-1.00663800
C	2.88482800	1.83564200	-0.44956800
C	-2.80524100	-1.93324800	-0.81069900
C	1.95073400	-2.88561700	-1.25371400
C	-1.82645800	2.82334200	-1.20410000
Fe	0.02361000	-0.04079400	-0.83663200
Cl	0.22874900	0.07177900	-3.16071800
O	-0.13064400	-0.19631900	0.85189700
C	2.77232400	-4.09064500	-1.59533700
C	3.28631700	-4.93075000	-0.59116900
C	3.02480900	-4.37432500	-2.95389300
C	4.04805200	-6.04665800	-0.95338900
C	3.79285300	-5.49724000	-3.27570100
C	4.31077900	-6.34756200	-2.29272400
H	4.44444000	-6.69426300	-0.17365600

H	3.99193900	-5.71452700	-4.32336100
C	4.13873600	2.66263300	-0.44406200
C	4.61984200	3.15477500	-1.67915300
C	4.85528600	2.91428600	0.73946500
C	5.80546600	3.89395400	-1.69665400
C	6.04105800	3.65647500	0.67742900
C	6.53071300	4.15890800	-0.52958000
H	6.17816900	4.26636800	-2.64897800
H	6.59408200	3.84335200	1.59606300
C	-2.60004600	4.05134100	-1.57865200
C	-2.72992400	4.36052700	-2.94937200
C	-3.17860800	4.88564900	-0.60383300
C	-3.44005000	5.50697100	-3.31763900
C	-3.88134400	6.02347200	-1.01632500
C	-4.02548600	6.34995400	-2.36751200
H	-3.53619700	5.74900900	-4.37440900
H	-4.32573300	6.66987800	-0.26192500
C	-4.03437100	-2.75758100	-0.58463500
C	-4.89325400	-3.08903200	-1.65132800
C	-4.31413500	-3.20309700	0.72339800
C	-6.04568600	-3.83441300	-1.38102200
C	-5.47981100	-3.94167600	0.94970600
C	-6.36014600	-4.26394800	-0.08765000
H	-6.71313400	-4.08848600	-2.20242700
H	-5.70354000	-4.27497800	1.96147100
C	2.47155300	-3.47722700	-4.03681200
H	1.37570600	-3.46071400	-4.01813000
H	2.78816300	-2.43734800	-3.89906100
H	2.79390700	-3.80966300	-5.02825000
C	3.03075800	-4.63108500	0.86964600
H	3.54046800	-3.70268900	1.16722200
H	1.95585500	-4.51651100	1.06307900
H	3.40527200	-5.43143100	1.51499700
C	5.10869700	-7.57259300	-2.67469700
H	5.73409900	-7.92104100	-1.84595400
H	4.44683000	-8.40183700	-2.95791100
H	5.76128000	-7.37332900	-3.53205000
C	-4.57282000	-2.65789700	-3.06491800
H	-4.66756900	-1.57266600	-3.18844700
H	-3.54007100	-2.91019900	-3.33115200
H	-5.24184600	-3.13952300	-3.78480500
C	-3.35421600	-2.92176100	1.85761400
H	-2.45027100	-3.53724600	1.75382600
H	-3.03059700	-1.87717400	1.87104800

H	-3.80880800	-3.14400300	2.82666400
C	-7.59885300	-5.08957800	0.17360100
H	-8.41327700	-4.81854700	-0.50730300
H	-7.39872500	-6.15999700	0.03002500
H	-7.95795200	-4.96097500	1.20048900
C	-2.11184700	3.46659600	-4.00021300
H	-1.04151000	3.31291100	-3.82317500
H	-2.56203200	2.46699100	-3.98902600
H	-2.24063200	3.88833000	-5.00184800
C	-4.81554500	7.56547600	-2.79419100
H	-4.84673700	8.32292600	-2.00362700
H	-4.38726400	8.02776000	-3.69061400
H	-5.85393800	7.29833900	-3.03239600
C	-3.04008800	4.57231800	0.86788100
H	-3.40784300	3.56704700	1.10121500
H	-1.99106700	4.60919300	1.18601900
H	-3.60025600	5.28562900	1.48008500
C	4.35482100	2.42393900	2.07758500
H	3.58857900	3.09910700	2.47901000
H	3.89778300	1.43286300	2.00042600
H	5.16444900	2.37199000	2.81286700
C	3.86957300	2.88700500	-2.96438800
H	3.65763900	1.82026500	-3.09635200
H	2.89719200	3.39354700	-2.96877500
H	4.43878100	3.23631200	-3.83121400
C	7.79635600	4.98299800	-0.57646900
H	8.37958800	4.77070400	-1.47957900
H	7.56776200	6.05713100	-0.58441000
H	8.43412300	4.79086700	0.29285200
K	1.69298600	-1.44000600	2.13713800
H	-0.80206300	0.63733400	1.44971000
C	1.43789500	0.41602600	5.29801300
C	1.90859400	1.33087800	4.33587300
C	1.03916400	1.80288600	3.35570200
C	-0.29435000	1.36552400	3.34808800
C	-0.76490800	0.46888300	4.36294500
C	0.10319100	-0.01206700	5.33800700
H	1.39362800	2.47423600	2.57933300
H	-0.21296300	-0.70647000	6.10820700
C	-1.32797200	1.51950100	2.33428500
C	-2.52311000	0.86757000	2.89062800
C	-3.83291400	0.78946900	2.40732800
C	-4.77680800	0.05442300	3.12616800
C	-4.42718600	-0.61329300	4.31111000

C	-3.12051800	-0.55506800	4.79774300
C	-2.17259600	0.19034300	4.09239400
H	-4.10744600	1.27688400	1.47805100
H	-5.17992600	-1.18078600	4.85136700
H	-2.85060400	-1.06737000	5.71833800
H	-5.79662400	-0.01142400	2.75658500
H	2.94553600	1.64021700	4.37122000
N	2.38475500	-0.13618400	6.26290600
O	1.94552300	-0.86663100	7.15568400
O	3.58252000	0.13603500	6.11767100
H	-1.39144500	2.40975600	1.71502600

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C	2.83563900	-1.72984600	-0.33491300
C	3.19023100	-3.11371200	-0.55887200
C	2.11594200	-3.71164400	-1.14279200
C	1.07843500	-2.71197000	-1.23738000
N	1.54419200	-1.51920600	-0.75083600
H	4.14941100	-3.54621500	-0.31102900
H	2.00212300	-4.73942800	-1.45679900
C	-2.35757800	-0.13863800	-1.31766700
C	-3.33252300	-1.17595900	-1.57929600
C	-2.64178800	-2.32575300	-1.80686300
C	-1.24449100	-2.02630700	-1.59779700
N	-1.10090800	-0.69885100	-1.28594400
H	-4.40040000	-1.01865000	-1.60957200
H	-3.02435900	-3.30247700	-2.06737900
C	2.53596000	2.53056200	-0.41771900
C	3.87380900	2.81457800	0.04764400
C	4.42544700	1.62374100	0.41519900
C	3.44215400	0.60190900	0.13775900
N	2.28930200	1.18324200	-0.32382200
H	4.31740300	3.80049300	0.07270700
H	5.41849900	1.43044700	0.79577600
C	0.29821100	3.23186700	-1.14868700
C	-0.67760300	4.22981900	-1.50938600
C	-1.88854700	3.60206400	-1.55475600
C	-1.65552700	2.21101400	-1.25938200
N	-0.32303900	2.00885600	-1.00229400
H	-0.44950200	5.26965000	-1.69858900
H	-2.85663500	4.01953200	-1.79480600
C	3.71699000	-0.76935700	0.16711300
C	-2.65338000	1.22906600	-1.28746200
C	-0.22039600	-2.97206700	-1.67794600

C	1.64323200	3.50385200	-0.88014000
Fe	0.57863800	0.21099600	-0.76987100
Cl	1.17182600	0.38695400	-3.03764600
O	0.19773900	0.13106600	0.89832400
H	-0.41112100	-0.66764500	1.55734600
C	-0.25756500	1.73508700	5.53174200
C	0.83572800	0.91389000	5.19192000
C	0.68554200	-0.15020500	4.29708300
C	-0.57114900	-0.39321700	3.72946500
C	-1.68108900	0.42221400	4.09194300
C	-1.52411700	1.48732400	4.98857700
H	-0.12217600	2.54854000	6.23975300
H	1.80803000	1.10562700	5.63881700
H	1.53060500	-0.77973300	4.03628600
H	-2.37541500	2.10327600	5.27085300
C	-0.97344400	-1.35456800	2.67397200
C	-2.41700500	-1.14336900	2.52729600
C	-3.34213600	-1.77460500	1.68336800
C	-4.64853400	-1.30662300	1.62535900
C	-5.03563200	-0.22039900	2.42820600
C	-4.15315400	0.39846400	3.31597900
C	-2.84098500	-0.05571200	3.34882200
H	-3.02854600	-2.59379300	1.04684300
H	-5.37412300	-1.74429700	0.95153200
H	-4.49564600	1.22946700	3.92042400
C	-0.51938800	-4.30721500	-2.28825400
C	-0.26192400	-4.48296700	-3.66470700
C	-1.03986100	-5.36313400	-1.51856400
C	-0.53587700	-5.72382300	-4.24630900
C	-1.29923800	-6.58963200	-2.14156400
C	-1.05768900	-6.78859700	-3.50317400
H	-0.33471900	-5.86348700	-5.30685700
H	-1.69700900	-7.40861900	-1.54519200
C	-4.08652700	1.65823200	-1.33120300
C	-4.66733200	2.22486600	-0.17188200
C	-4.87782300	1.45795300	-2.48052000
C	-6.04231700	2.45406600	-0.13886000
C	-6.25516100	1.70705000	-2.40607900
C	-6.86200100	2.16064000	-1.23429900
H	-6.49464900	2.82517500	0.77743100
H	-6.86789900	1.52694300	-3.28744400
C	2.16134600	4.88662000	-1.13013200
C	1.99668700	5.91686900	-0.18562900
C	2.82742600	5.14308600	-2.34775900

C	2.48804900	7.19492000	-0.47151100
C	3.30144800	6.43452500	-2.59709000
C	3.13882800	7.47484600	-1.67629200
H	2.36143000	7.98865000	0.26228700
H	3.81270500	6.63336800	-3.53708400
C	5.08024800	-1.20679900	0.61381000
C	5.34292700	-1.43331100	1.97820900
C	6.10617200	-1.36371300	-0.34274600
C	6.62779200	-1.83144300	2.36503800
C	7.37404900	-1.76695800	0.08592200
C	7.65418700	-2.01168100	1.43450900
H	6.83082000	-2.00235200	3.42062600
H	8.16568600	-1.88544200	-0.65151900
C	-1.32490700	-5.17466100	-0.04888000
H	-0.50526100	-4.66324200	0.46108700
H	-2.22168500	-4.56072200	0.10356400
H	-1.49164000	-6.13227800	0.45285500
C	0.31035700	-3.35317200	-4.49010800
H	-0.30392400	-2.44840400	-4.42039700
H	1.30638300	-3.06330800	-4.13548800
H	0.39087400	-3.63639500	-5.54420600
C	-1.37288000	-8.10959400	-4.16629200
H	-1.40713200	-8.92743400	-3.43851200
H	-2.34909900	-8.07672800	-4.66851200
H	-0.62700400	-8.36384500	-4.92791200
C	4.26068600	-1.25901400	3.02025800
H	3.69676300	-0.33320000	2.86322300
H	3.53657400	-2.08142600	2.98459100
H	4.68538700	-1.23640400	4.02912700
C	5.84372400	-1.09044200	-1.80630000
H	5.09614500	-1.78020200	-2.21464300
H	5.44590600	-0.08032200	-1.95717800
H	6.75967600	-1.19122000	-2.39650400
C	9.02563600	-2.47620500	1.86676200
H	9.81452600	-2.01480600	1.26218400
H	9.21909600	-2.23648000	2.91782200
H	9.12733400	-3.56410400	1.75539600
C	1.30616500	5.65407700	1.13453200
H	0.25488500	5.37517500	0.97767400
H	1.80758000	4.84134700	1.67916500
H	1.32068300	6.53953700	1.77727900
C	3.63388900	8.86745000	-1.99037800
H	2.93076200	9.39695000	-2.64694500
H	3.75069500	9.46848400	-1.08235700

H	4.60002300	8.84183600	-2.50681900
C	3.04359300	4.03577500	-3.35386400
H	3.79568900	3.32320100	-2.99295400
H	2.13403500	3.45037600	-3.52472300
H	3.38920600	4.43629900	-4.31187300
C	-3.82718100	2.60524300	1.02741000
H	-3.10835500	1.81767700	1.27183700
H	-3.26657300	3.52902100	0.82767500
H	-4.45957300	2.77229300	1.90282800
C	-4.27681000	0.99184600	-3.79030600
H	-3.23923200	1.32225600	-3.89840300
H	-4.27096000	-0.10121900	-3.87509200
H	-4.85305600	1.38389500	-4.63506200
C	-8.35823000	2.31894800	-1.11700300
H	-8.63309100	3.33597000	-0.81119600
H	-8.86607900	2.09912400	-2.06163200
H	-8.74473100	1.63473000	-0.35124900
C	-0.36505700	-2.72031600	2.68145500
C	0.95612100	-2.91263000	2.25363200
C	-1.06614700	-3.82129000	3.20225400
C	1.56967100	-4.16171300	2.36336100
H	1.49094300	-2.07680500	1.81887400
C	-0.45522500	-5.07078300	3.30900800
H	-2.09043300	-3.68739100	3.53846200
C	0.86819700	-5.24524500	2.89576900
H	2.58918600	-4.28707500	2.01118900
H	-1.01332100	-5.90865700	3.71918000
K	-0.06984900	2.45347900	2.00630400
H	1.34327300	-6.21919200	2.97666100
N	-6.37666700	0.33017300	2.27951900
O	-7.16230400	-0.23580100	1.51579700
O	-6.65111900	1.36209800	2.90729700

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C	2.46943900	0.31492700	-1.32498300
C	3.57008000	-0.51802000	-1.76654000
C	3.03492500	-1.69850400	-2.18785100
C	1.61486000	-1.63376100	-1.91942600
N	1.30236400	-0.39836300	-1.41902200
H	4.60820900	-0.22157200	-1.76134100
H	3.54314800	-2.56027900	-2.59794700
C	-2.34494700	-2.04571000	-0.36867800
C	-2.45592200	-3.47975100	-0.54547100
C	-1.36906600	-3.87841300	-1.26469800

C	-0.54304600	-2.70656500	-1.46098900
N	-1.16289600	-1.61580200	-0.91496300
H	-3.27759300	-4.08208400	-0.18437200
H	-1.11620500	-4.87139900	-1.60962900
C	-0.59862900	3.28117200	-0.95851200
C	0.27371800	4.43344600	-1.00005600
C	1.55252700	3.96277400	-0.91930700
C	1.46871200	2.51968200	-0.89460300
N	0.15805000	2.13589100	-0.89843500
H	-0.06439600	5.45826700	-1.07107700
H	2.47816900	4.52206700	-0.92290300
C	-2.77126000	2.21907200	-0.52499500
C	-4.15672800	2.27107500	-0.11877100
C	-4.50350800	1.00680800	0.26629500
C	-3.34914500	0.16675300	0.04084700
N	-2.30839800	0.93066000	-0.41127700
H	-4.76607000	3.16465400	-0.12800800
H	-5.46026900	0.65164700	0.62419800
C	2.57971100	1.66694500	-0.96613400
C	-3.35151800	-1.22994000	0.16247500
C	0.74189400	-2.72344500	-2.01659800
C	-1.99389300	3.33969500	-0.84980900
Fe	-0.48305000	0.23766300	-0.86818500
Cl	-1.06313600	0.48433600	-3.13843700
O	-0.08600600	0.11461400	0.81198200
H	0.43807600	-0.95554100	1.21805900
C	4.65751700	-0.22454600	3.06795100
C	3.55314700	-0.23643200	3.92370800
C	3.44138600	-1.45464100	1.41755400
C	4.62000200	-0.84445100	1.81757900
H	3.62653500	0.25797500	4.88614000
H	5.48981400	-0.80771800	1.17397000
C	1.01650500	-1.98970800	1.76162100
C	2.29744500	-1.44586000	2.23569600
C	2.37084200	-0.84068700	3.51241200
C	1.12758500	-0.79336200	4.37717900
H	1.09878200	-2.64099100	0.89203600
H	1.40174500	-0.76959900	5.43874200
H	0.61721900	0.17240600	4.19360200
H	3.38441100	-1.91285900	0.43806400
C	0.10019000	-2.48386200	2.81051900
C	-0.82905200	-3.50460300	2.54961700
C	-1.68218700	-3.96696500	3.54844700
C	-1.61293800	-3.42161400	4.83376200

C	-0.69454300	-2.40441000	5.10317300
C	0.15500100	-1.92331200	4.10399200
H	-0.88117500	-3.92608100	1.55090300
H	-2.40049200	-4.75082800	3.32506500
H	-2.26763100	-3.78569400	5.62084100
H	-0.63258400	-1.98234100	6.10471800
C	1.20814900	-3.95775800	-2.72566900
C	1.03429500	-4.02189300	-4.12432300
C	1.80802700	-5.02736000	-2.03381700
C	1.46226200	-5.16587300	-4.80488900
C	2.22223600	-6.15329400	-2.75406000
C	2.05458000	-6.24330800	-4.13880700
H	1.33002600	-5.21534300	-5.88408700
H	2.68921400	-6.97843600	-2.21955300
C	3.92080400	2.21644100	-0.59491900
C	4.15661400	2.46901300	0.78048500
C	4.94754000	2.43534200	-1.53055500
C	5.43431200	2.83537300	1.19720500
C	6.22056600	2.80247600	-1.06709800
C	6.49240600	2.97496700	0.28948500
H	5.62360000	2.98850000	2.25762000
H	7.01871200	2.94932200	-1.79279000
C	-4.51099700	-1.86688100	0.86137600
C	-4.54641300	-1.82899600	2.27093800
C	-5.56147100	-2.47196900	0.14207300
C	-5.59990200	-2.45716100	2.94172400
C	-6.60089500	-3.08260700	0.85238900
C	-6.63011500	-3.10195000	2.25038100
H	-5.61905800	-2.43787900	4.02997400
H	-7.41329600	-3.54883600	0.29806200
C	-2.67924900	4.65496900	-1.05272800
C	-3.14501400	4.97371300	-2.34623200
C	-2.85722100	5.56496000	0.00499100
C	-3.77580700	6.20463300	-2.54967100
C	-3.49405500	6.78649400	-0.23869800
C	-3.96164400	7.12396600	-1.51161200
H	-4.13010400	6.45372000	-3.54812800
H	-3.62576400	7.48955800	0.58168000
C	0.40896000	-2.86704400	-4.87261500
H	-0.56062600	-2.58411200	-4.44862500
H	1.03115300	-1.96674100	-4.80785900
H	0.26943900	-3.11171500	-5.93023800
C	2.01446700	-4.96693300	-0.53778900
H	2.63517800	-4.10870500	-0.25530000

H	1.06228400	-4.85943100	-0.00517200
H	2.50594100	-5.87196000	-0.16775700
C	2.47609400	-7.48280800	-4.89368600
H	1.63954600	-8.18737700	-4.99484000
H	2.81788600	-7.23916900	-5.90574700
H	3.28648600	-8.01117700	-4.37968300
C	3.04389900	2.35423900	1.80188500
H	2.33839400	3.19026600	1.68943800
H	2.47911300	1.42429000	1.67677500
H	3.44840000	2.38409200	2.81704200
C	4.71588500	2.30010600	-3.02126900
H	5.14067200	1.37027300	-3.41948600
H	3.65121900	2.30144200	-3.26936400
H	5.19511300	3.12734800	-3.55721900
C	7.87725800	3.29604200	0.79721000
H	7.90923100	4.28344600	1.27546800
H	8.18052600	2.56033000	1.55183800
H	8.61710100	3.28961100	-0.00980100
C	-2.36933900	5.23369900	1.39850900
H	-2.88036400	4.33861900	1.78266200
H	-1.28628800	5.04835800	1.39924300
H	-2.56794600	6.05180400	2.09772300
C	-2.96674200	3.99583800	-3.48405400
H	-1.92029400	3.69433700	-3.60114200
H	-3.51943900	3.06747100	-3.29948400
H	-3.31600800	4.42244700	-4.42940300
C	-4.67130100	8.43468400	-1.76055200
H	-5.76036400	8.29596500	-1.78615600
H	-4.45214300	9.16734900	-0.97659800
H	-4.37934500	8.87019500	-2.72280500
C	-5.58861300	-2.43666500	-1.36991800
H	-5.36727700	-1.43132200	-1.74511800
H	-4.83576400	-3.10199000	-1.80744200
H	-6.56856000	-2.73995400	-1.75155300
C	-3.49269500	-1.07489100	3.05328900
H	-2.48646000	-1.27016600	2.67116300
H	-3.67725300	0.00775800	2.97992000
H	-3.50936900	-1.35174800	4.11032900
C	-7.73933500	-3.81051900	2.99278500
H	-8.67669800	-3.79339900	2.42597800
H	-7.48627000	-4.86469300	3.16951300
H	-7.92568100	-3.35308800	3.97073200
N	5.84392100	0.53033200	3.44883700
O	6.87127700	0.37726800	2.78434000

O	5.74526300	1.31695000	4.39913900
K	-0.91302100	2.00479300	2.21382500

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C	-0.73487000	-2.88450600	-0.78372600
C	-1.64637600	-3.94916300	-0.42902800
C	-2.77272100	-3.35852800	0.05743000
C	-2.57379000	-1.92751000	-0.03866000
N	-1.30476700	-1.66895000	-0.50123600
H	-1.43578600	-5.00268400	-0.54943100
H	-3.67954000	-3.83024500	0.40955200
C	-2.58562500	2.35094600	-0.55562100
C	-3.99050200	2.55701100	-0.29857700
C	-4.51738000	1.33992800	0.02220300
C	-3.43542500	0.38428900	-0.04366000
N	-2.26582500	1.02600600	-0.37448000
H	-4.49617800	3.50934800	-0.37868100
H	-5.54416800	1.09131200	0.25184300
C	2.44714100	-0.09776100	-1.45110100
C	3.45758700	-1.07289400	-1.80387600
C	2.83060000	-2.27680200	-1.91128000
C	1.44953200	-2.06177800	-1.54229100
N	1.24014700	-0.72996700	-1.29176700
H	4.50419800	-0.84984600	-1.94932900
H	3.25428100	-3.23791500	-2.16774900
C	1.64310200	2.21934700	-1.28702900
C	1.84804000	3.64692700	-1.41876700
C	0.62220400	4.22970100	-1.33950500
C	-0.33432800	3.16206600	-1.12913700
N	0.31247700	1.95435600	-1.12364300
H	2.81131300	4.11408000	-1.56980800
H	0.36725100	5.27815300	-1.40631800
C	0.52851600	-3.09342500	-1.34571900
C	-1.69524700	3.37303600	-0.90041800
C	-3.59262000	-0.99152800	0.17185100
C	2.67724700	1.28157600	-1.35797200
Fe	-0.47583300	0.14127100	-0.78251100
Cl	-1.16937300	0.06588900	-3.02129200
O	0.02680700	0.28237100	0.86392300
C	-4.97366300	-1.49215600	0.47740900
C	-5.51433300	-1.39001800	1.77243700
C	-5.75152300	-2.04316700	-0.56712300
C	-6.80662100	-1.86716500	2.01996300
C	-7.03885300	-2.50456900	-0.27939600

C	-7.58441200	-2.43157900	1.00717200
H	-7.21404200	-1.79379000	3.02666000
H	-7.63585400	-2.92944700	-1.08430100
C	0.88731800	-4.47251000	-1.81187200
C	0.64890800	-4.79438500	-3.16550500
C	1.43332000	-5.43349100	-0.94036100
C	0.96504600	-6.07845200	-3.61917800
C	1.73455100	-6.70720000	-1.43564200
C	1.51094400	-7.04825700	-2.77228100
H	0.77699500	-6.32828200	-4.66169800
H	2.15394500	-7.44980100	-0.75947400
C	4.09164000	1.76173500	-1.24564400
C	4.97761700	1.76006300	-2.33893900
C	4.54403000	2.17242700	0.03199100
C	6.32810200	2.06484100	-2.11532500
C	5.89653100	2.46459400	0.20996400
C	6.81216100	2.38617300	-0.84592500
H	7.01685500	2.04455300	-2.95799600
H	6.25157000	2.74654800	1.19915300
C	-2.22879800	4.76760500	-1.01484500
C	-2.57087300	5.27597900	-2.28460000
C	-2.38447500	5.56742100	0.13257400
C	-3.07141700	6.57841300	-2.37629400
C	-2.88564800	6.86624500	-0.00047200
C	-3.23898000	7.38851100	-1.24807700
H	-3.33569500	6.97190700	-3.35599400
H	-2.99896000	7.48514900	0.88775900
C	-5.21144900	-2.13276100	-1.97697700
H	-4.70350800	-1.20978100	-2.27581600
H	-4.46894700	-2.93436000	-2.06808300
H	-6.01580700	-2.33491600	-2.69105800
C	-4.73013900	-0.74361700	2.89174700
H	-3.68908300	-1.08098900	2.89280800
H	-4.73736300	0.35154800	2.78472000
H	-5.16018900	-0.97888200	3.87084700
C	-8.98534300	-2.92937700	1.27732200
H	-9.20094900	-2.96501100	2.35024400
H	-9.73434800	-2.27704800	0.80978100
H	-9.13711400	-3.93556100	0.86885000
C	-2.38598300	4.42915400	-3.52263300
H	-1.32346300	4.23595100	-3.71245800
H	-2.85732000	3.44612900	-3.41382500
H	-2.80625800	4.92160900	-4.40495600
C	-2.01886000	5.03055400	1.49957600

H	-2.73233300	4.25273100	1.80975300
H	-1.01497200	4.58743500	1.49245700
H	-2.03866200	5.82042900	2.25714000
C	-3.80975100	8.78195400	-1.37589000
H	-3.46853200	9.27135600	-2.29486900
H	-4.90721800	8.75794700	-1.41046400
H	-3.52302200	9.41403400	-0.52856100
C	4.49788000	1.44758800	-3.74085800
H	4.46880700	0.36950700	-3.93944400
H	3.48334800	1.82370700	-3.90764300
H	5.16025600	1.90093500	-4.48568900
C	8.27632000	2.65619500	-0.59347800
H	8.63666400	2.05007300	0.24635500
H	8.88824800	2.42659700	-1.47196900
H	8.44911300	3.70790100	-0.33050600
C	3.58647900	2.32339500	1.19329400
H	2.93266500	3.19155500	1.04472600
H	2.93053300	1.45398200	1.30035200
H	4.13168200	2.46927900	2.12914000
C	1.69409400	-5.10711400	0.51211200
H	2.40945300	-4.28248400	0.61306900
H	0.77545800	-4.79811400	1.02456600
H	2.10282300	-5.97039400	1.04620100
C	0.06631500	-3.76694500	-4.10903700
H	-0.85855400	-3.33039600	-3.71636600
H	0.75279100	-2.92443100	-4.25313300
H	-0.14481500	-4.20709900	-5.08857700
C	1.87356800	-8.41801700	-3.29747600
H	1.16857200	-8.75165900	-4.06714400
H	2.87277700	-8.41465000	-3.75346200
H	1.88265400	-9.16653700	-2.49782000
K	-1.63605100	1.26899900	2.52267200
C	-1.81620900	-2.25147100	4.33956600
C	-0.94107500	-2.37662800	3.25846900
C	-0.28241900	-0.70930400	5.40930200
C	-1.49548300	-1.40646000	5.40948800
H	-2.74887600	-2.80736800	4.34476800
H	-1.20455700	-2.99984900	2.40762700
H	-2.17242500	-1.30669600	6.25328000
C	0.59177300	-0.85849300	4.33075800
C	0.27760000	-1.67988800	3.23027500
C	1.16948800	-1.65827000	2.05783600
H	1.07281000	-2.50504800	1.38153700
H	0.66149500	-0.70042100	1.33998300

H	0.01140400	-0.07261400	6.23863900
C	2.77628300	-0.42904000	3.48818200
C	4.01514600	0.13792700	3.74176800
C	5.04701700	-0.10550500	2.83218900
C	4.87457800	-0.93128200	1.72137100
C	3.62404100	-1.49162400	1.49942400
C	2.54086900	-1.23199000	2.35297800
H	4.16632700	0.78617700	4.59498200
H	5.69481100	-1.08054700	1.03140800
H	3.45743600	-2.09496100	0.61605600
N	6.31159900	0.60570200	2.99341800
O	7.26660900	0.25810400	2.29592500
O	6.34312300	1.54369400	3.79748200
O	1.76098100	-0.12768300	4.37793000

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C	1.90395300	2.66306000	-0.50694300
C	3.23017400	3.21115200	-0.32961200
C	4.05920700	2.16346100	-0.07452700
C	3.25224800	0.96348600	-0.13452800
N	1.94273000	1.29635800	-0.38088900
H	3.47030800	4.26347700	-0.38678300
H	5.12354500	2.17664600	0.11366900
C	1.41395800	-2.87847200	-0.74885400
C	2.59272400	-3.68201600	-0.50090400
C	3.59209500	-2.82140400	-0.17001900
C	3.03044200	-1.48746800	-0.22076100
N	1.70632900	-1.55247400	-0.55956900
H	2.63011900	-4.75920700	-0.58533000
H	4.62196900	-3.04428900	0.07086900
C	-2.19994500	1.47970900	-0.96579600
C	-2.76896500	2.81067100	-0.94108600
C	-1.72922300	3.68418700	-0.84833700
C	-0.52193500	2.89148900	-0.77983500
N	-0.83460600	1.55737200	-0.81517900
H	-3.82501000	3.02662400	-1.02332100
H	-1.75311700	4.76504200	-0.83291900
C	-2.38465400	-0.95009300	-1.34254000
C	-3.12578400	-2.12656400	-1.73587600
C	-2.24746500	-3.17064700	-1.72232600
C	-0.96902500	-2.63608500	-1.31626800
N	-1.07810000	-1.28584600	-1.08237400
H	-4.17362700	-2.13204700	-2.00194300
H	-2.42820700	-4.20625600	-1.97524400

C	0.76281300	3.43926200	-0.71902400
C	0.18432600	-3.40901000	-1.14449000
C	3.78064000	-0.32425800	-0.02301000
C	-2.94552400	0.32993500	-1.24323400
Fe	0.44071300	0.00921100	-0.67586200
Cl	0.82273900	0.11571900	-2.98289800
O	0.15896300	-0.15867700	1.02308200
C	5.25607300	-0.47201700	0.20604500
C	5.76898400	-0.60337000	1.50974700
C	6.12587800	-0.48652100	-0.90379300
C	7.14906300	-0.74535200	1.68781100
C	7.49953900	-0.62875500	-0.68326100
C	8.03102400	-0.76238500	0.60338900
H	7.54407200	-0.84354200	2.69738200
H	8.17146300	-0.63592400	-1.53944500
C	0.92395500	4.90412300	-0.99789000
C	0.92535000	5.31994000	-2.34773400
C	1.08328600	5.84975600	0.03312000
C	1.09359800	6.67763500	-2.63616100
C	1.24704700	7.19897500	-0.30052400
C	1.25402200	7.63357000	-1.62845800
H	1.10331500	6.99572300	-3.67706300
H	1.37307500	7.92738200	0.49833000
C	-4.39956800	0.48598100	-1.57870800
C	-4.76179400	0.95539200	-2.86108300
C	-5.39875500	0.15806400	-0.64233600
C	-6.11756600	1.10375600	-3.16740000
C	-6.74437900	0.32640500	-0.98690100
C	-7.12453000	0.79837800	-2.24532200
H	-6.39561100	1.46673600	-4.15517400
H	-7.51064500	0.08318600	-0.25326600
C	0.10414600	-4.87584900	-1.43897800
C	0.50447900	-5.34306000	-2.70887800
C	-0.36936800	-5.78039200	-0.47127200
C	0.41224900	-6.71046400	-2.98363100
C	-0.44191300	-7.14237600	-0.78282900
C	-0.05530200	-7.62688700	-2.03520000
H	0.71307700	-7.07052900	-3.96570100
H	-0.80812500	-7.83965200	-0.03154000
C	5.58193600	-0.34810800	-2.30703400
H	4.85293200	-1.13549800	-2.53062800
H	5.05400800	0.60352800	-2.43806300
H	6.38444200	-0.40089700	-3.04919100
C	4.84017500	-0.58638700	2.70085900

H	4.29770300	0.36361900	2.76385200
H	4.08266100	-1.37510700	2.62463800
H	5.38937300	-0.72757400	3.63728700
C	9.51592300	-0.95016400	0.81248400
H	9.83483100	-0.57556100	1.79132900
H	9.79120300	-2.01246500	0.76450600
H	10.09816600	-0.42995900	0.04392600
C	1.03044700	-4.38056500	-3.74879500
H	0.35937000	-3.52598800	-3.88735700
H	1.99601200	-3.96103900	-3.44170200
H	1.16641300	-4.87773500	-4.71417400
C	-0.81288200	-5.29204700	0.89050900
H	-0.06793100	-4.61470600	1.32726900
H	-1.76728100	-4.75077600	0.81297500
H	-0.96386500	-6.12481100	1.58441400
C	-0.11282200	-9.10305800	-2.35342700
H	-0.45712000	-9.27761400	-3.37913000
H	0.87884500	-9.56611000	-2.26299700
H	-0.78682200	-9.63616000	-1.67453900
C	-3.70806900	1.29564700	-3.89130800
H	-3.19354800	2.23099500	-3.63990300
H	-2.93247400	0.52439600	-3.94722700
H	-4.15447600	1.41257700	-4.88372400
C	-8.58197900	0.94632200	-2.61590200
H	-9.21392500	1.05519300	-1.72806900
H	-8.74541600	1.81887000	-3.25829900
H	-8.94051500	0.06689200	-3.16750700
C	-5.04235900	-0.39906000	0.71577100
H	-4.82976700	-1.47570900	0.64985000
H	-4.15449700	0.09865700	1.11898100
H	-5.85504700	-0.27286700	1.43667300
C	1.06714100	5.43180100	1.48573600
H	0.08938600	5.02270100	1.76912300
H	1.81137000	4.65433800	1.69075400
H	1.27437700	6.28130100	2.14401400
C	0.73448300	4.32059400	-3.46664200
H	1.35361800	3.42703200	-3.33508500
H	-0.30275500	3.96456000	-3.50070500
H	0.96862800	4.76890000	-4.43730600
C	1.40413500	9.09841100	-1.96817000
H	1.98291700	9.23890300	-2.88795400
H	0.42503000	9.57017000	-2.12684700
H	1.90523200	9.64871500	-1.16451900
K	-1.80719100	-1.77699600	1.76548500

C	-1.04560700	-1.80220200	5.75649400
C	-2.23513200	-1.23715600	5.34344500
C	-2.22535100	-0.12003200	4.46515200
C	-0.96464900	0.43112800	4.05377800
C	0.25149200	-0.20920200	4.45087800
C	0.19026600	-1.30388000	5.29634600
C	-3.40871800	0.49251400	3.93378400
C	-0.92955600	1.55970600	3.15184400
C	-2.12553200	2.17354100	2.77253600
C	-3.35684300	1.64797600	3.16660400
C	0.32659700	1.89304800	2.51483500
C	1.58335200	1.65307900	3.32586200
C	1.58315300	0.21900800	3.86492400
H	1.79456600	-0.45250600	3.02202600
H	1.63271100	2.37283600	4.15829600
H	-1.06305600	-2.64865500	6.43788300
H	-3.17867200	-1.64923600	5.67652900
H	1.11287000	-1.78983500	5.60477900
H	-4.28476400	2.07454500	2.80319800
H	-2.09875800	3.01060700	2.08149800
H	0.31189900	2.79551800	1.91074700
H	0.30774000	0.90312000	1.62266500
N	-4.68878500	-0.18756700	3.97701400
O	-4.68022900	-1.43168000	3.90601700
O	-5.71906900	0.48718800	3.99011400
H	2.38155200	0.07039600	4.60087700
H	2.46642800	1.82059300	2.70097800

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C	-2.55118500	1.85901300	-0.72062700
C	-2.99766200	3.22013500	-0.53526300
C	-1.88408800	4.00102600	-0.51613500
C	-0.75011300	3.12071400	-0.69909000
N	-1.18290200	1.81854100	-0.79366500
H	-4.03287200	3.51608100	-0.44372700
H	-1.81642400	5.07504600	-0.41401600
C	2.92544700	0.95617300	-1.29673800
C	3.79678800	2.10391500	-1.40091500
C	3.01085000	3.21124500	-1.25126400
C	1.65833100	2.73977600	-1.05676300
N	1.63114600	1.36667900	-1.08448200
H	4.86153300	2.05141000	-1.58222200
H	3.29933600	4.25291100	-1.28613200
C	-1.70067600	-2.32259300	-1.22554400

C	-3.07117100	-2.76185900	-1.36853500
C	-3.85500900	-1.65566800	-1.27466000
C	-2.97076600	-0.53281300	-1.05531100
N	-1.66516900	-0.96387200	-1.02898800
H	-3.36884900	-3.78925700	-1.52150000
H	-4.93163400	-1.58174200	-1.33512000
C	0.72055300	-2.74376600	-1.26827900
C	1.86259200	-3.62827200	-1.36118600
C	2.97061100	-2.84107400	-1.36977700
C	2.51178100	-1.46994900	-1.29337700
N	1.14132700	-1.44310200	-1.21340000
H	1.79932200	-4.70520800	-1.42612800
H	4.00763200	-3.13701600	-1.44280100
C	-3.41827300	0.77516500	-0.87414200
C	3.36884900	-0.36981400	-1.35322100
C	0.56176000	3.57983400	-0.83003200
C	-0.60509900	-3.18386100	-1.30190400
Fe	-0.03269900	0.17365400	-0.96542900
Cl	-0.15630900	0.37051600	-3.29496500
O	0.21809000	0.05827600	0.74694600
C	0.79956400	5.05981800	-0.79666400
C	1.06618800	5.72057100	0.41642100
C	0.73625400	5.79288600	-2.00089400
C	1.27078400	7.10512900	0.41264400
C	0.95078600	7.17342600	-1.96388800
C	1.22200900	7.84898100	-0.76878700
H	1.46901900	7.61376600	1.35435700
H	0.89865200	7.73859800	-2.89252400
C	-4.89115700	1.04850000	-0.95238900
C	-5.46067100	1.29709500	-2.22067500
C	-5.69259100	1.07333400	0.20414000
C	-6.83015200	1.55912700	-2.30703100
C	-7.06012900	1.34701200	0.07144800
C	-7.64839000	1.58661500	-1.17195100
H	-7.26875700	1.75289000	-3.28421700
H	-7.67864500	1.37283300	0.96674700
C	-0.85751300	-4.64801500	-1.50087600
C	-1.13919700	-5.13372000	-2.79481700
C	-0.80086300	-5.53055100	-0.40576600
C	-1.38009100	-6.50071700	-2.96308400
C	-1.04873600	-6.89101800	-0.61817300
C	-1.34073100	-7.39544900	-1.88836000
H	-1.60200000	-6.87681800	-3.96013500
H	-1.01239200	-7.57134100	0.23068600

C	4.83706300	-0.62019300	-1.52565000
C	5.36888500	-0.72662500	-2.82825300
C	5.67717900	-0.76565000	-0.40572400
C	6.73663400	-0.96901900	-2.98135400
C	7.04050400	-1.01410400	-0.60133400
C	7.59017800	-1.11362400	-1.88170800
H	7.14641400	-1.05483700	-3.98597600
H	7.68444800	-1.13794000	0.26734400
C	0.43072700	5.09387400	-3.30536200
H	1.17025200	4.31553000	-3.52516100
H	-0.54106700	4.58855300	-3.26574600
H	0.41732300	5.80175700	-4.13969300
C	1.14761400	4.95623300	1.71999100
H	0.33512200	4.22710700	1.81554800
H	2.10476100	4.41595100	1.79181700
H	1.09953300	5.62977700	2.58131100
C	1.47434000	9.33885900	-0.76440800
H	1.31129000	9.77221000	0.22807200
H	2.50870900	9.56499800	-1.05576200
H	0.81906800	9.85774100	-1.47301600
C	4.46902400	-0.58961400	-4.03470700
H	3.67765200	-1.34799800	-4.02742900
H	3.96091400	0.38142100	-4.04674800
H	5.03607400	-0.69285500	-4.96494800
C	5.13425200	-0.64935900	1.00101400
H	5.06307600	0.40855900	1.30236300
H	4.13892500	-1.09761100	1.08381300
H	5.78112400	-1.14102000	1.73302200
C	9.06954300	-1.35143800	-2.07826100
H	9.26091300	-1.98504200	-2.95149000
H	9.60356100	-0.40568500	-2.24134700
H	9.51910900	-1.83370000	-1.20375000
C	-1.18534800	-4.19446600	-3.97876500
H	-2.04262900	-3.51347600	-3.91623700
H	-0.29409800	-3.55850200	-4.02111600
H	-1.26059000	-4.74941900	-4.91910900
C	-1.57511500	-8.87272000	-2.10497100
H	-1.90605000	-9.36674100	-1.18504400
H	-2.33268000	-9.04991500	-2.87673100
H	-0.65537300	-9.37533300	-2.43343500
C	-0.45426700	-5.02146800	0.97307300
H	0.60895100	-4.75225600	1.03183600
H	-1.02603800	-4.12498900	1.22480700
H	-0.65324100	-5.77523400	1.74003100

C	-5.11236100	0.79482000	1.57146900
H	-4.98961700	-0.28220800	1.73835800
H	-4.12758900	1.24971100	1.70366800
H	-5.76662200	1.17365900	2.36288700
C	-4.60111600	1.28301200	-3.46434400
H	-3.77996000	2.00534500	-3.39189200
H	-4.13056800	0.30462300	-3.61557000
H	-5.19153300	1.52097200	-4.35458500
C	-9.13141000	1.84905700	-1.29770500
H	-9.33898100	2.62777300	-2.04065900
H	-9.66731800	0.94592000	-1.61925900
H	-9.56658300	2.16590500	-0.34390400
K	2.23499400	1.43119100	1.74619400
C	-2.38294600	-4.14184200	3.83511900
C	-1.54101500	-3.02856400	3.81323800
C	-1.74523100	-1.98663100	2.89003500
C	-2.82096300	-2.09915700	1.99636500
C	-3.65829300	-3.21176000	2.01199100
C	-3.44455900	-4.24022500	2.93398700
H	-2.20808800	-4.93158200	4.56129000
H	-0.72702100	-2.96265500	4.52904000
H	-2.98661700	-1.30404600	1.28236300
H	-4.46714800	-3.27669200	1.29074500
H	-4.09519500	-5.11030100	2.94594300
C	-0.92176900	-0.73119400	2.90023400
C	-1.70067300	0.50003700	3.30965400
C	-1.52679600	1.72941200	2.65066300
C	-2.61769700	0.44251300	4.37307200
C	-2.23428000	2.86540800	3.04925400
C	-3.32002300	1.57897700	4.77688000
H	-2.78159000	-0.50410900	4.88008000
C	-3.12989400	2.79667000	4.11845000
H	-2.11226700	3.78992500	2.49208300
H	-4.02365600	1.51014800	5.60258900
H	-3.68918100	3.67708100	4.42327000
H	-0.49003800	-0.43170700	1.59626600
C	0.43981700	-0.87001200	3.46906900
C	1.30242100	-1.87337500	2.95397500
C	0.97038100	0.02284600	4.42960900
C	2.62999200	-1.95688300	3.34205500
H	0.92013400	-2.55385800	2.20053300
C	2.30383600	-0.05005100	4.82961400
C	3.13207100	-1.02518300	4.26339000
H	3.29449900	-2.70229500	2.92240400

H	0.32042900	0.77350500	4.86806800
H	2.71099100	0.63004500	5.56924800
N	4.55098300	-1.04446600	4.60543800
O	5.24216900	-1.95992700	4.14976100
O	4.98433000	-0.13010400	5.31369500
H	-0.88524900	1.76932700	1.77774100

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C	-3.24055500	1.89464000	-0.02832800
C	-4.60830700	2.02340000	-0.48022300
C	-5.18660200	0.79068600	-0.34706400
C	-4.15766800	-0.10736100	0.12517300
N	-2.98391000	0.58519000	0.29736200
H	-5.06741000	2.94975300	-0.79731200
H	-6.20883700	0.50138300	-0.55004400
C	-1.23570700	-3.17321000	0.82229100
C	-2.10157700	-4.30714800	0.58308100
C	-3.35870200	-3.81337500	0.40869700
C	-3.25672500	-2.37031100	0.48505200
N	-1.95555300	-2.01460000	0.73541700
H	-1.77368100	-5.33766000	0.59653100
H	-4.27854700	-4.35520900	0.23728500
C	0.50433000	2.05100400	2.06424000
C	0.57397700	3.49080100	2.16132100
C	-0.43320900	3.98823200	1.39123900
C	-1.15843900	2.85233800	0.86318700
N	-0.55684000	1.69057000	1.27556000
H	1.32143800	4.03015100	2.72577700
H	-0.69597300	5.02129900	1.21167200
C	1.38483500	-0.20181800	2.46028600
C	2.40262200	-1.11376400	2.92944200
C	2.08434900	-2.34441600	2.44609000
C	0.82932600	-2.21017900	1.73486400
N	0.44040500	-0.89574500	1.74422100
H	3.25509500	-0.82472600	3.52736200
H	2.63266700	-3.26761300	2.55972800
C	-2.36440500	2.97126800	0.16562600
C	0.10258300	-3.28785000	1.20957700
C	-4.32135600	-1.49448900	0.25261300
C	1.42105000	1.17907400	2.65711300
Fe	-1.20622100	-0.16157100	0.93575000
Cl	-2.15484700	-0.13357300	3.09973400
O	-0.64305600	-0.22597300	-0.70137300
H	0.45998900	-0.11318700	-1.21523300

C	1.47727500	0.12103000	-2.14183900
C	2.46896800	-0.97638300	-1.91088500
C	2.94673100	-1.82910900	-2.92644000
C	2.93803600	-1.19280800	-0.60135600
C	3.77160300	-2.90859300	-2.63805700
H	2.67015300	-1.64334300	-3.95721800
C	3.77277300	-2.25709900	-0.29759300
H	2.60579800	-0.53398100	0.19018200
C	4.14775400	-3.13606800	-1.31411100
H	4.11137100	-3.58266900	-3.41470200
H	4.09305000	-2.44204200	0.71762400
C	0.65810400	0.05683900	-3.39043200
C	0.09277800	-1.16397600	-3.83356000
C	0.33719100	1.21730400	-4.12757800
C	-0.72222000	-1.22225300	-4.96498000
H	0.29897600	-2.07362000	-3.27999600
C	-0.49952200	1.16383400	-5.24731800
H	0.76022800	2.16810000	-3.82046400
C	-1.03361000	-0.05513800	-5.68011000
H	-1.11593900	-2.18241400	-5.29124100
H	-0.71939400	2.07838000	-5.79265500
C	1.89670700	1.50016200	-1.74245200
C	3.11845900	2.06042800	-1.91525800
H	1.10098900	2.10630400	-1.31362900
C	4.19857000	1.32615800	-2.64346200
C	5.32825400	0.84569900	-1.96605600
C	4.08968300	1.10168600	-4.02249800
C	6.30459300	0.11816800	-2.64505800
H	5.42000300	1.01948500	-0.89823300
C	5.07519000	0.38809600	-4.70698700
H	3.21756400	1.47428100	-4.55230200
C	6.18040900	-0.11400800	-4.01797100
H	7.16102200	-0.27247800	-2.10215000
H	4.97483100	0.21815800	-5.77595100
H	6.94214000	-0.68149500	-4.54571600
C	3.42633900	3.43859200	-1.45814800
C	4.48678100	4.16420700	-2.03145900
C	2.66635200	4.06621100	-0.45447900
C	4.76313200	5.47026400	-1.62563600
H	5.09308600	3.70276900	-2.80411800
C	2.94006900	5.36930800	-0.05134000
H	1.87213600	3.52285400	0.03887700
C	3.99142200	6.08174600	-0.63579900
H	5.58621700	6.01070700	-2.08610100

H	2.33786800	5.81941600	0.73361900
H	4.21215600	7.09669200	-0.31633400
C	-5.70017900	-2.06474400	0.11847100
C	-6.49231700	-2.18848000	1.27999300
C	-6.20177600	-2.48716600	-1.12605100
C	-7.77541300	-2.73089800	1.16564500
C	-7.49069600	-3.02695700	-1.19875600
C	-8.29461400	-3.15372400	-0.06297800
H	-8.38483500	-2.83138700	2.06176300
H	-7.87314700	-3.35910300	-2.16215100
C	-2.78794200	4.33689600	-0.28096100
C	-2.25753600	4.87147700	-1.47237300
C	-3.69026600	5.09526300	0.49467200
C	-2.67013100	6.14006500	-1.89330700
C	-4.07392200	6.36092500	0.03975200
C	-3.58036300	6.89947300	-1.15300500
H	-2.26430600	6.54796200	-2.81728300
H	-4.77161400	6.94480400	0.63718800
C	2.48339200	1.75825000	3.53921500
C	3.78865300	1.97245500	3.05824800
C	2.14575400	2.10173900	4.86691100
C	4.74197100	2.53461900	3.91622700
C	3.13001900	2.65435500	5.68992700
C	4.43429500	2.87852000	5.23399700
H	5.74842800	2.70946100	3.54052900
H	2.87206800	2.91964400	6.71363400
C	0.82381600	-4.58931300	1.03920800
C	1.26842600	-4.92607400	-0.25898900
C	1.16962600	-5.40437000	2.13354900
C	2.16364900	-5.98357200	-0.41807000
C	2.07227700	-6.45714300	1.93091700
C	2.62228800	-6.72680100	0.67523000
H	2.55696400	-6.20005500	-1.40881700
H	2.37059100	-7.06420600	2.78349100
C	-4.22010400	4.56269200	1.80713600
H	-4.90433000	3.71994400	1.65580400
H	-3.40676400	4.18946600	2.43938000
H	-4.75752800	5.34042000	2.35842900
C	-1.22502100	4.10980100	-2.27375500
H	-0.26272700	4.07833500	-1.74765300
H	-1.51905700	3.06732600	-2.43939000
H	-1.05664400	4.57496800	-3.25054500
C	-3.98949100	8.28248500	-1.60448800
H	-3.37627600	9.05370000	-1.11937300

H	-3.87047800	8.40415300	-2.68649100
H	-5.03435500	8.49436400	-1.35180000
C	4.18318900	1.58948000	1.64990800
H	4.49424100	0.53743400	1.59791100
H	3.35773100	1.70956500	0.94556800
H	5.01781700	2.20277300	1.29510600
C	0.73960000	1.89483200	5.38353400
H	0.04501100	2.61799600	4.93838600
H	0.34805200	0.90564700	5.12370300
H	0.69909900	2.01321600	6.47094400
C	5.48338000	3.45674100	6.15549900
H	5.87916900	2.68996000	6.83484300
H	6.33008500	3.86623300	5.59434100
H	5.07076000	4.25765200	6.77982100
C	0.78580800	-4.15137600	-1.46239200
H	-0.27613400	-4.35236100	-1.65483400
H	0.88084600	-3.07431500	-1.30280200
H	1.35455200	-4.41876200	-2.35674400
C	0.59080600	-5.14989500	3.50888600
H	1.07739300	-4.30753000	4.01422800
H	-0.47470400	-4.90261400	3.44933300
H	0.70490200	-6.03174900	4.14742400
C	3.71105500	-7.75385700	0.48277300
H	3.47493600	-8.44534700	-0.33500700
H	4.64834400	-7.24678500	0.22032100
H	3.88124300	-8.34213000	1.39038000
C	-5.36672400	-2.35910900	-2.38131300
H	-5.25528200	-1.30170900	-2.66556100
H	-4.36619500	-2.78573000	-2.23682600
H	-5.83432800	-2.87315800	-3.22681400
C	-5.95280900	-1.75047700	2.62171100
H	-5.04224300	-2.30040500	2.88485300
H	-5.66721300	-0.69265900	2.61444900
H	-6.69172900	-1.90486400	3.41404300
C	-9.69547900	-3.71270700	-0.15602400
H	-10.44305600	-2.90831600	-0.15160900
H	-9.83953900	-4.28946300	-1.07580800
H	-9.92187900	-4.36708400	0.69339200
H	-1.66281700	-0.10105100	-6.56477800
N	4.89304800	-4.34387900	-0.97311400
O	5.25558300	-4.49354200	0.19602600
O	5.09622400	-5.17077600	-1.86870600
K	-2.53195300	-0.03798500	-2.49648000