



Supporting Information

for

A heterobimetallic tetrahedron from a linear platinum(II)-bis(acetylide) metalloligand

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Beilstein J. Org. Chem. **2020**, *16*, 2701–2708. doi:10.3762/bjoc.16.220

Collection of the different NMR spectra recorded from heterobimetallic metallosupramolecular tetrahedron 4 and details regarding the energy-minimized structures of 4

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NMR spectra of metallocsupramolecular tetrahedron 4

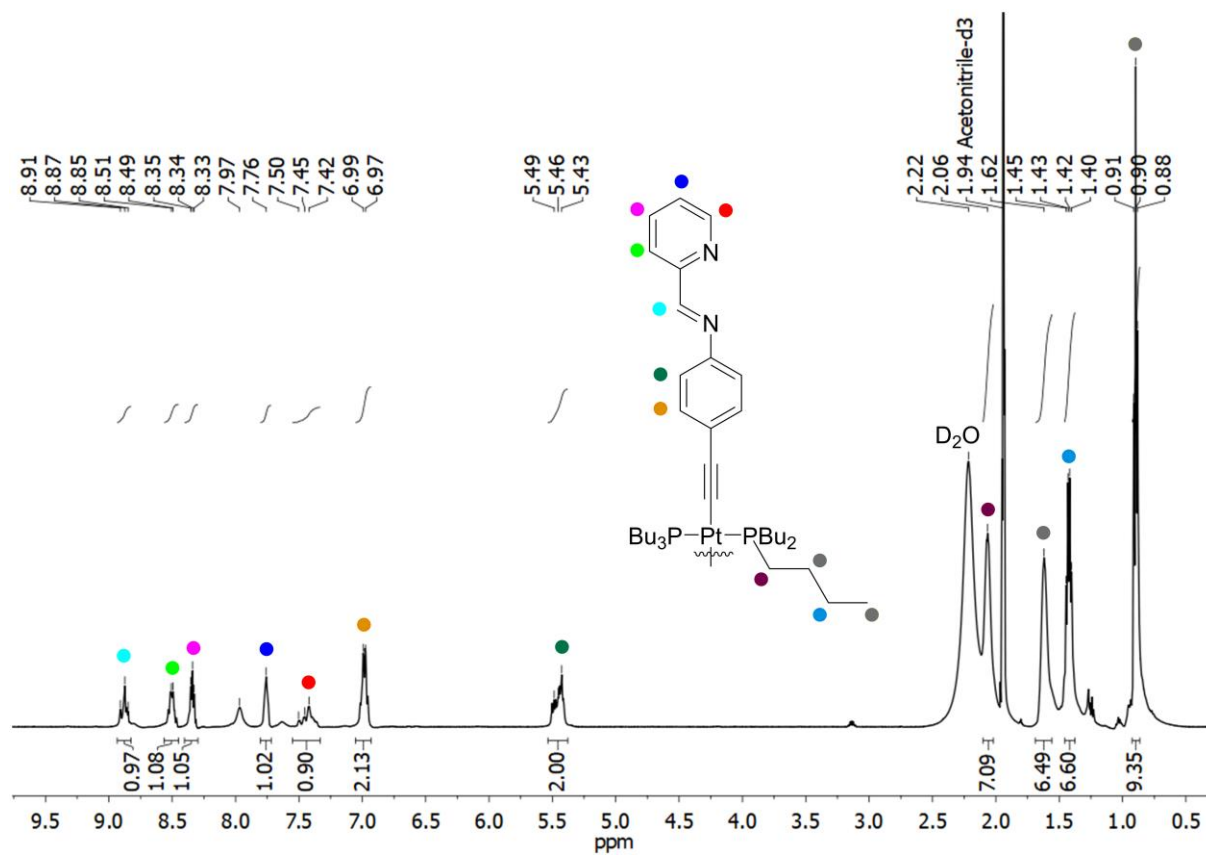


Figure S1. ^1H NMR spectrum of **4** (500 MHz, acetonitrile- d_3 , 298 K).

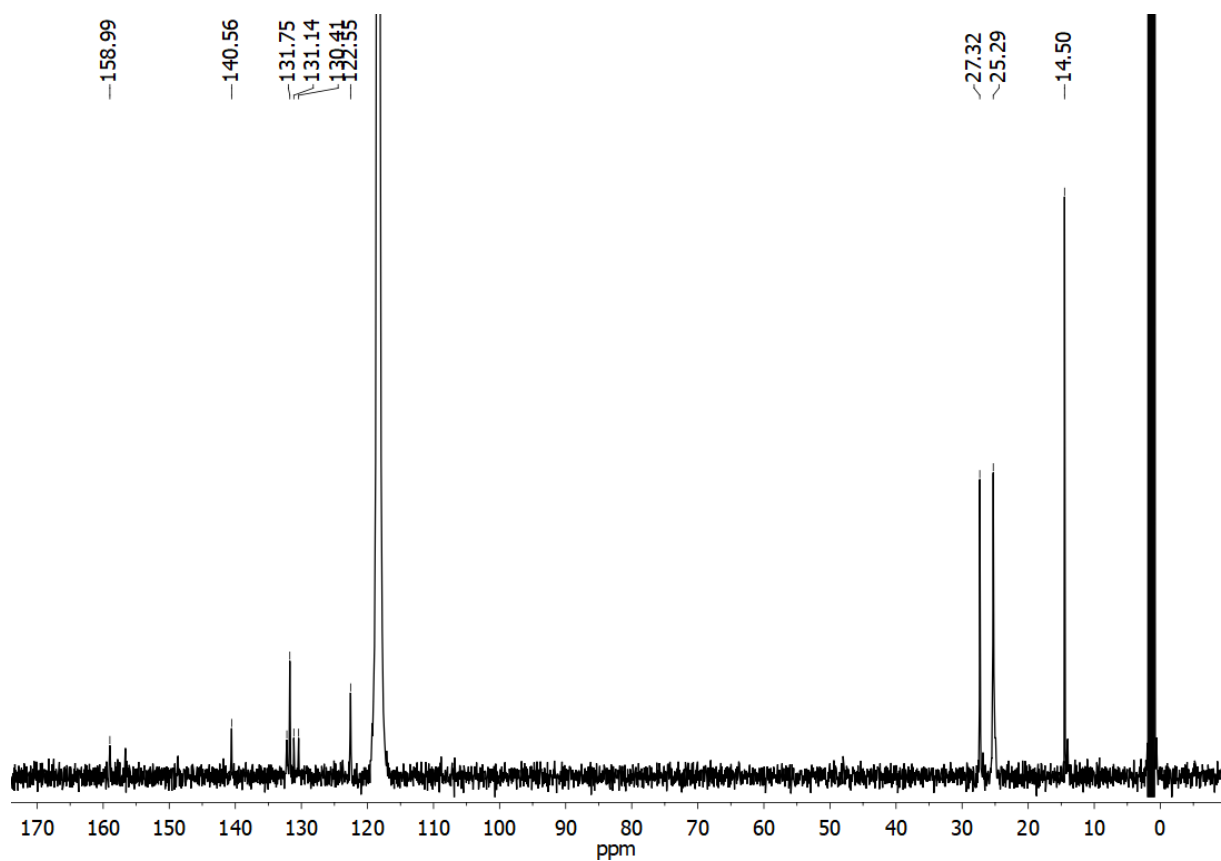


Figure S2. ¹³C NMR spectrum of **4** (126 MHz, acetonitrile-*d*₃, 298 K).

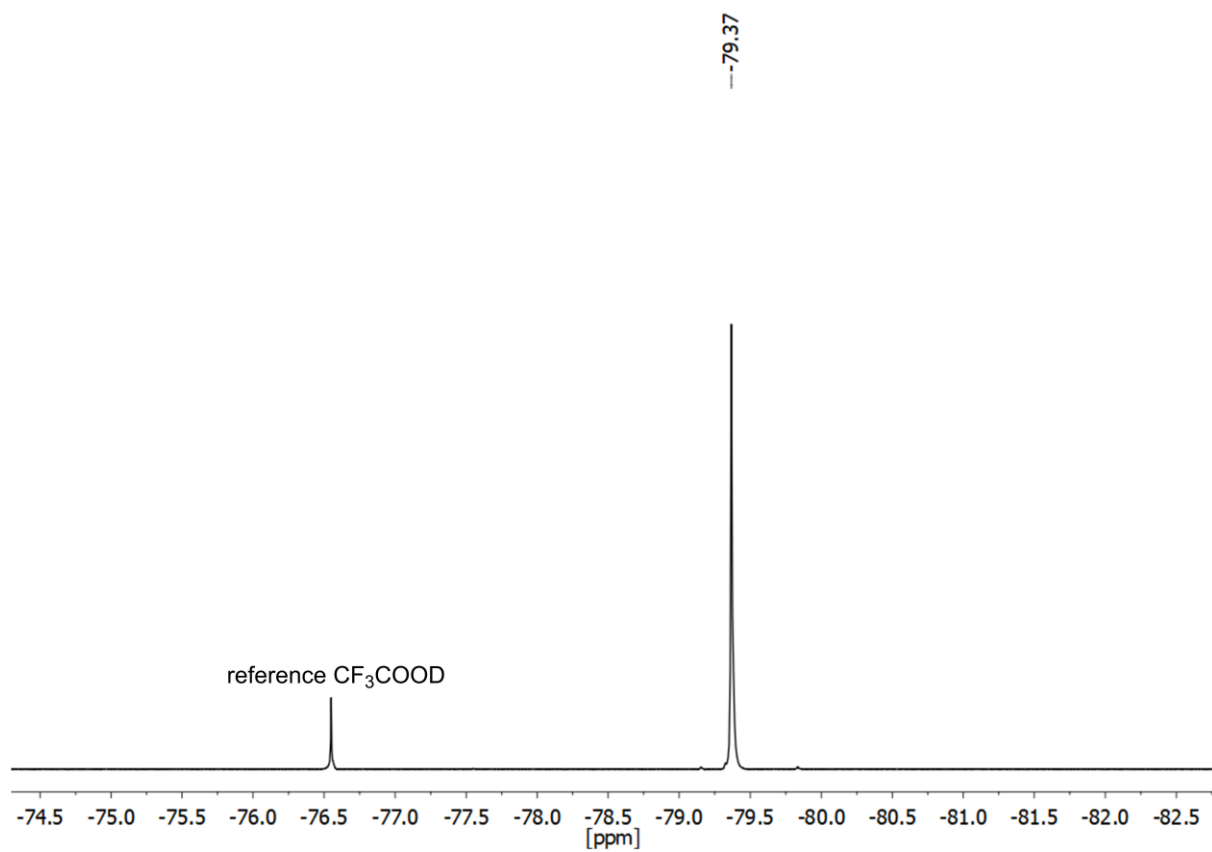


Figure S3. ¹⁹F NMR spectrum of **4** (470 MHz, acetonitrile-*d*₃, 298 K).

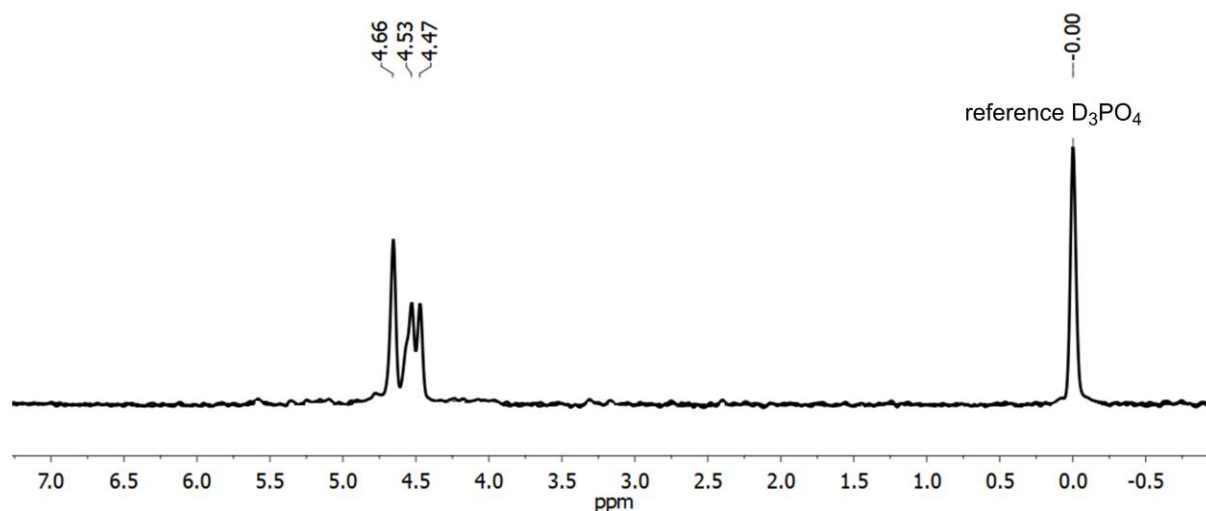


Figure S4. ^{31}P NMR spectrum of **4** (202 MHz, acetonitrile- d_3 , 298 K).

Symmetry	T	S_4	C_3
^1H -NMR	one signal	three signals (1:1:1)	four signals (1:1:1:1)
^{31}P -NMR	one signal 	two signals (1:2) 	two signals (1:1)

Scheme S1. Schematic representation of symmetry-considerations concerning possible diastereomeric tetrahedra. The table summarizes the cage symmetries and the expected observations in the ^1H - and ^{31}P -NMR spectra, looking at one chemically equivalent position. The coloured dots represent chemically and magnetically equivalent positions.

The ^1H NMR spectrum of **4** shows signals that clearly indicate the presence of various diastereomeric cages, but unfortunately the superposition of these signals makes it impossible to differentiate between these diastereomers. However, looking at the expected signal integrals with different configurations of the stereogenic centers (Scheme S1) it is clear, that all three possible diastereomers must be present in solution, as the observed signals cannot be explained with only one or two of these diastereomers.

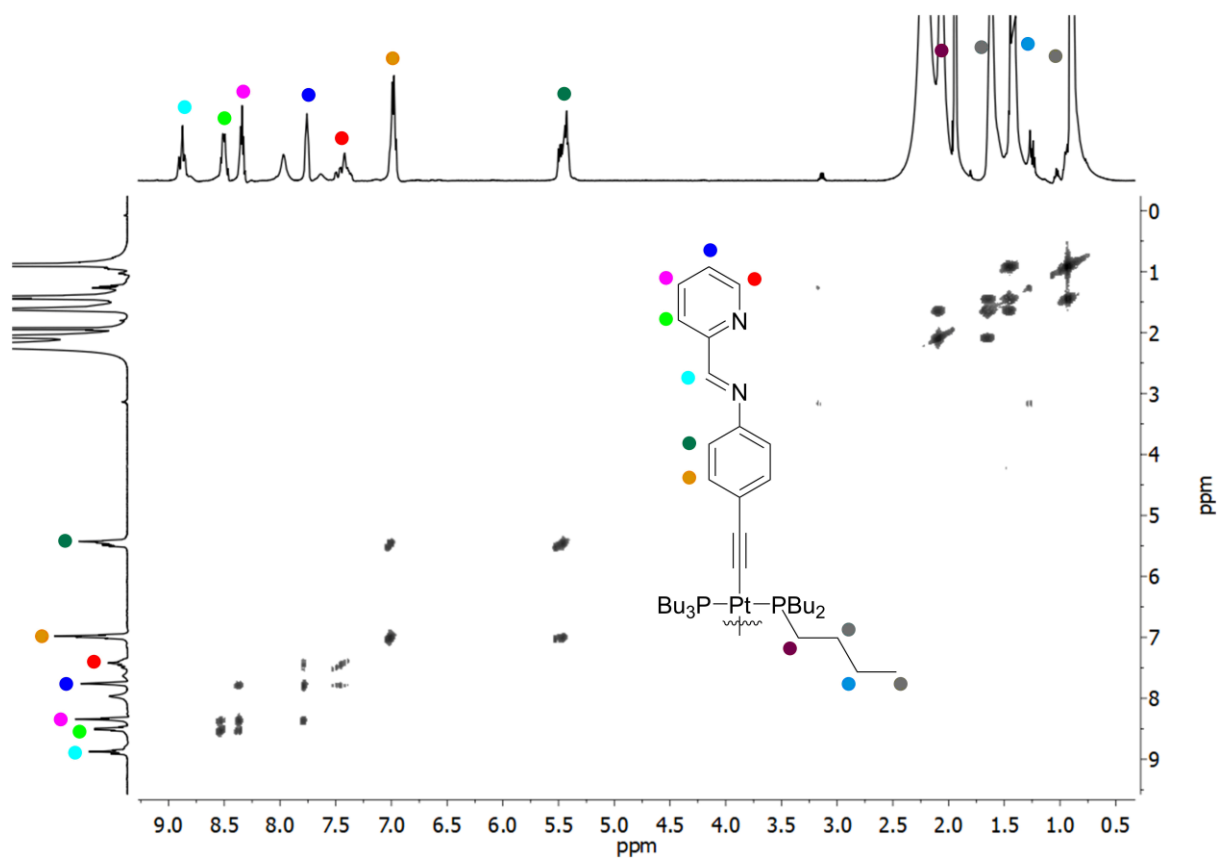


Figure S5. ^1H - ^1H -COSY spectrum of **4** (500 MHz, acetonitrile- d_3 , 298 K).

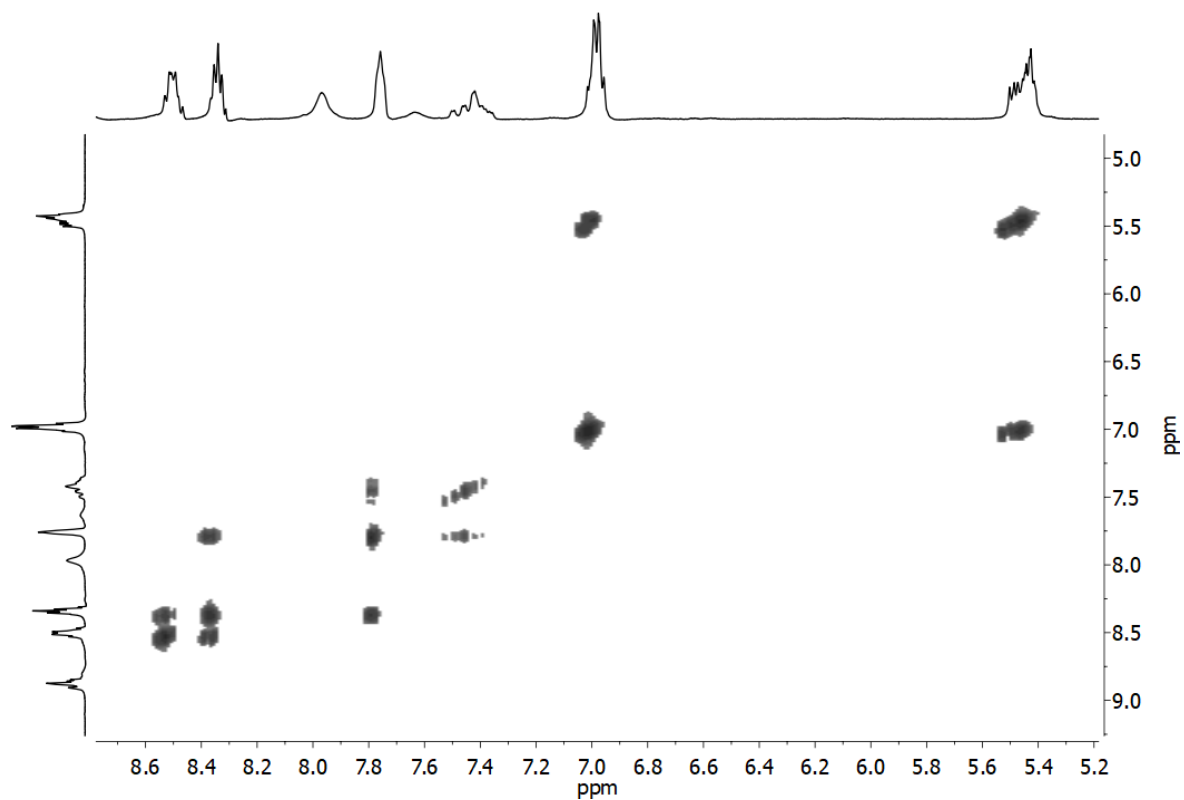


Figure S6. Aromatic region of the ^1H - ^1H -COSY spectrum of **4** (500 MHz, acetonitrile- d_3 , 298 K).

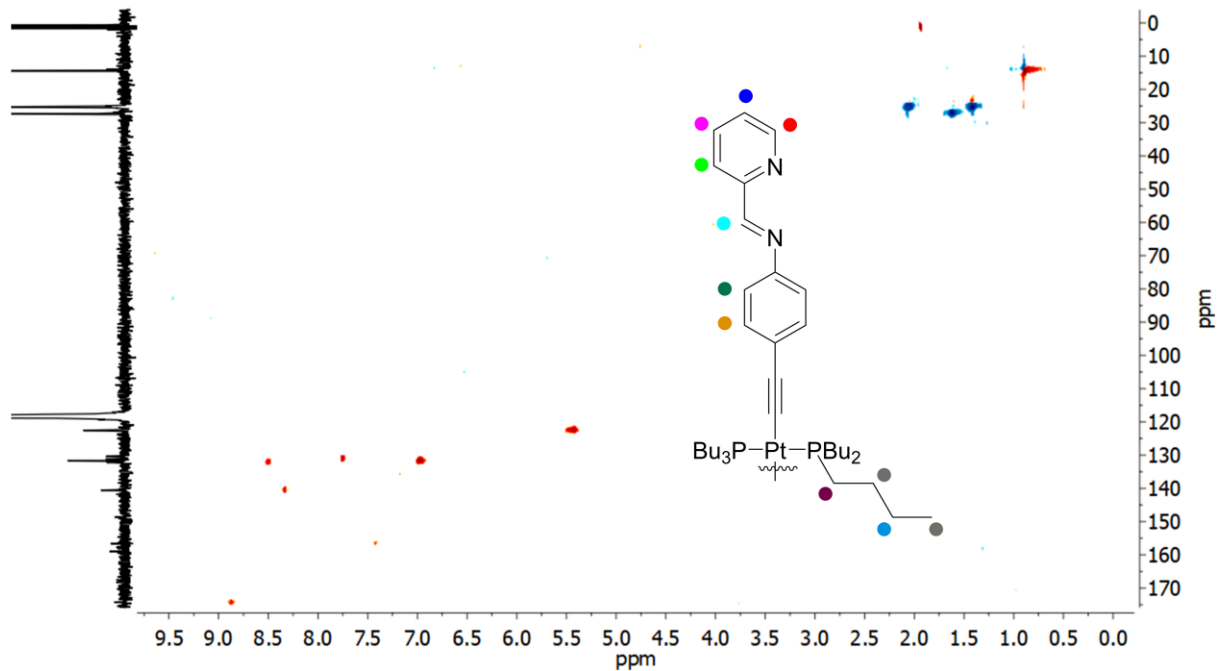


Figure S7. ^1H - ^{13}C -HSQC spectrum of **4** (500 MHz, 126 MHz, acetonitrile- d_3 , 298 K). Blue signals = CH_2 ; red signals = CH , CH_3

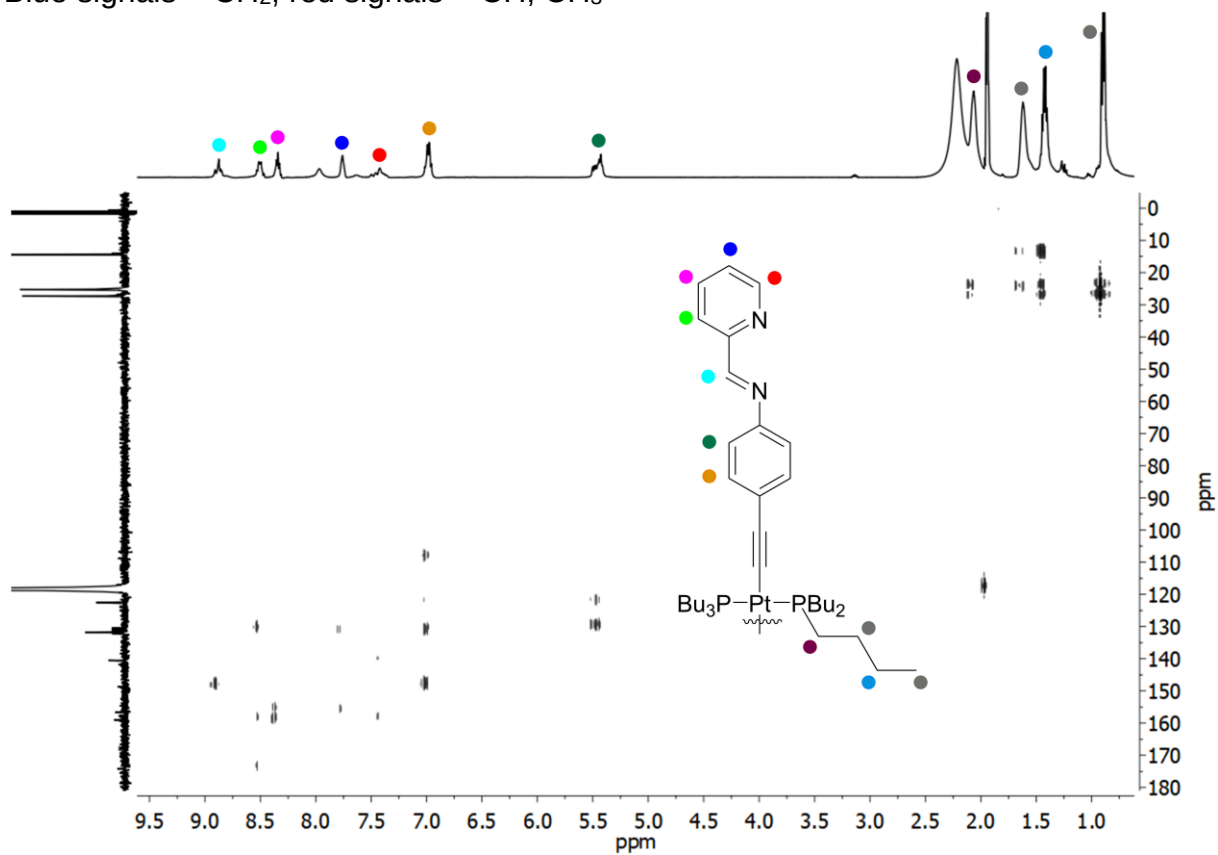


Figure S8. ^1H - ^{13}C -HMBC spectrum of **4** (500 MHz, 126 MHz, acetonitrile- d_3 , 298 K).

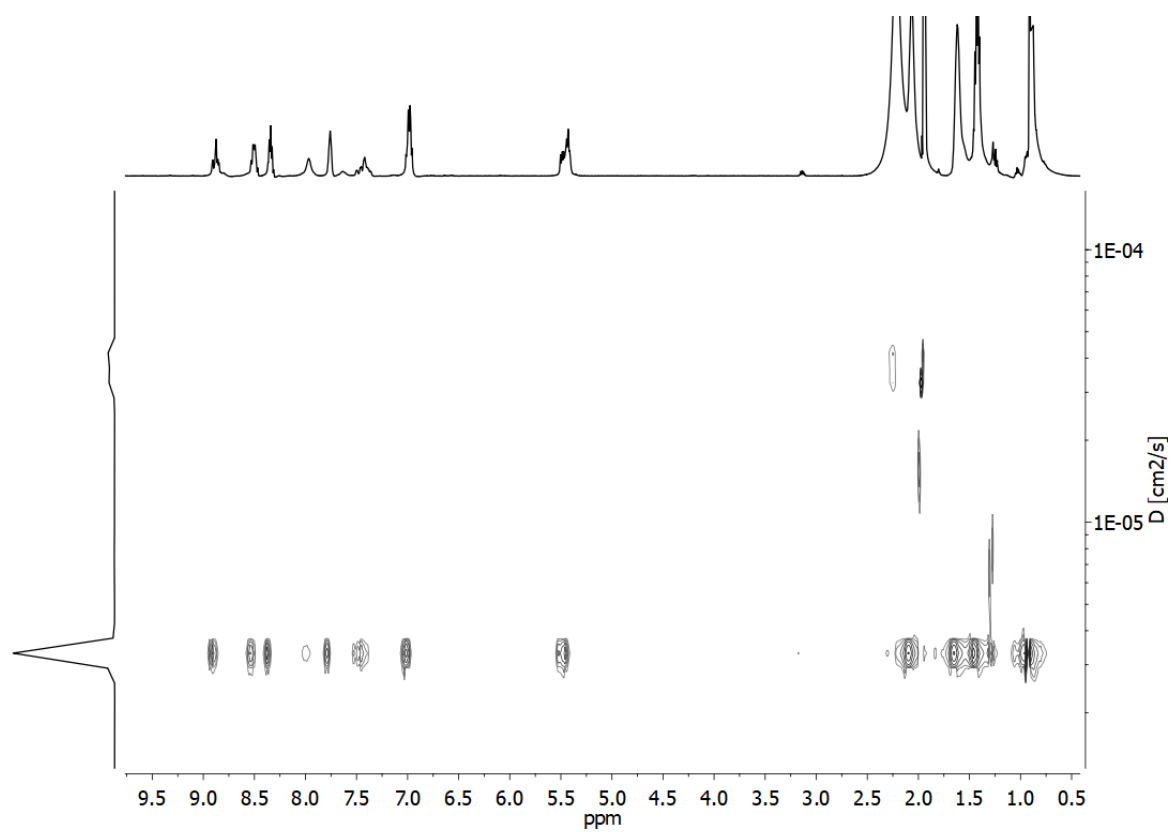


Figure S9. ^1H -2D-DOSY spectrum of **4** (500 MHz, acetonitrile- d_3 , 298 K, $\tau = 150$ ms).
 $D = 3.33 \cdot 10^{-10} \text{ m}^2/\text{s}$, $d_h = 33 \text{ \AA}$, $r_h = 1.65 \text{ nm}$.

Selected isotopic pattern from the mass spectrum of metallosupramolecular tetrahedron **4**

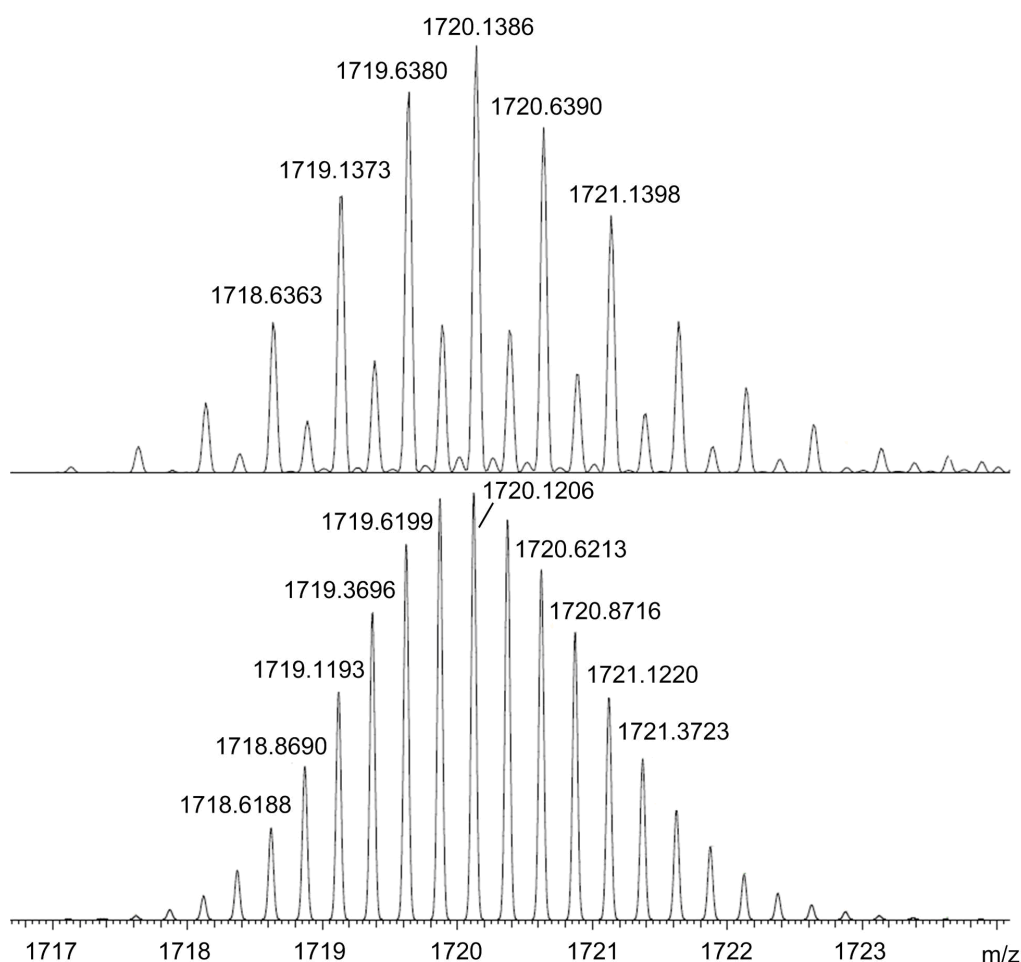


Figure S10. Isotopic pattern of the $[4 - 4 \text{ OTf}]^{4+}$ peak from the mass spectrum of **4**. Top: measured spectrum; bottom: calculated spectrum.

The isotopic pattern of the $[4 - 4 \text{ OTf}]^{4+}$ peak from the mass spectrum of **4** shows the presence of the expected four times positively charged species next to the doubly charged fragment $[\text{Fe}_2\text{Pt}_3\text{L}_6 + 2 \text{ OTf}]^{2+}$. The superposition of these two peaks is a commonly found phenomenon with ESI mass spectrometry with rather labile metallosupramolecular architectures.

Atom coordinates of energy-minimized cages 4

We performed computational calculations for all possible diastereomers of the cationic unit of metallocupramolecular cage **4**. Please note, that these calculations do not include any solvent molecules or counter anions. The models were minimized regarding symmetry considerations, and therefore, the calculations yield reasonable molecular structures of the presented cages and can be used to verify spectroscopic and spectrometric findings, e.g. the size and shape. However, these calculations do not give reasonable insights into energy differences between the diastereomers, and therefore, these are not discussed herein.

(all- Δ)-T-4

	x-coord.	y.coord.	z-coord.				
Fe	69.062	65.995	-77.615	H	95.076	109.111	-68.919
N	65.928	69.171	-96.511	H	53.052	108.757	-60.190
C	59.413	70.205	-123.605	H	74.905	120.969	-60.006
C	65.542	80.825	-103.001	C	49.521	83.454	-69.920
C	63.094	57.867	-103.380	H	40.111	87.949	-66.837
C	59.814	58.096	-116.927	C	64.284	45.891	-95.567
C	62.364	81.737	-116.457	H	63.216	36.152	-100.286
H	67.878	89.750	-97.305	C	84.998	58.716	-56.653
H	57.661	48.784	-122.021	H	88.792	56.173	-46.781
H	62.237	91.453	-121.235	N	72.766	62.527	-58.543
H	56.905	70.667	-134.132	N	66.851	47.142	-82.929
N	87.958	61.909	-79.629	N	50.132	71.525	-75.003
C	114.621	53.852	-79.005	C	37.843	65.189	-77.666
C	93.693	57.956	-68.049	C	12.507	53.074	-79.526
C	95.343	61.928	-90.741	C	26.515	72.763	-81.080
C	108.636	58.014	-90.822	C	36.476	51.307	-76.479
C	107.003	53.853	-67.457	C	24.045	45.396	-77.244
H	90.528	65.188	-99.892	C	14.112	66.814	-81.967
H	114.189	58.257	-100.114	H	27.503	83.346	-83.199
H	111.185	50.768	-57.954	H	45.132	45.134	-74.557
H	124.992	50.732	-78.820	H	23.116	34.681	-75.856
N	72.611	84.656	-73.260	H	0.5440	72.825	-84.442
C	74.215	110.817	-63.718	C	70.181	35.401	-75.838
C	61.615	91.034	-68.687	C	76.688	11.714	-62.102
C	84.230	91.225	-73.246	C	78.483	25.772	-81.753
C	85.412	104.237	-68.633	C	65.533	33.219	-62.843
C	62.136	104.081	-63.787	C	68.623	21.570	-56.166
H	92.912	85.983	-77.075	C	81.687	14.165	-74.994
				H	82.672	27.630	-91.579

H	59.203	40.531	-58.041	H	-125.343	-25.618	-101.615
H	64.736	19.928	-46.175	H	-120.227	0.8445	-76.005
H	88.156	0.6842	-79.679	H	-127.078	-0.0876	-98.195
C	64.840	64.582	-47.059	C	-111.266	-0.6610	-54.943
C	49.493	67.242	-23.622	H	-112.301	0.3834	-52.099
C	51.363	60.860	-46.891	C	-107.632	-46.075	-30.977
C	70.394	70.270	-35.506	H	-105.381	-51.358	-21.740
C	62.833	71.609	-24.031	C	-85.244	-41.351	-71.034
C	43.885	62.017	-35.385	H	-75.981	-41.788	-76.715
H	46.732	56.734	-55.723	N	-88.922	-30.652	-64.701
H	80.602	73.913	-35.676	N	-98.466	-43.308	-39.711
H	67.241	76.101	-15.209	N	-106.983	-15.603	-46.641
H	33.528	58.814	-35.370	C	-105.237	-11.619	-33.244
C	41.492	68.106	-12.007	C	-100.633	-0.1880	-0.7258
C	33.877	68.594	-0.2502	C	-114.042	-0.2375	-27.412
C	79.360	-0.0185	-54.941	C	-94.662	-16.593	-25.557
C	80.983	-10.241	-48.245	C	-92.350	-11.752	-12.868
C	-0.0263	47.035	-79.106	C	-111.774	0.2390	-14.665
C	-11.178	41.713	-78.160	H	-122.805	0.0898	-32.888
Fe	-105.865	-33.387	-55.087	H	-87.954	-23.994	-29.661
N	-122.777	-36.666	-46.080	H	-83.903	-15.459	-0.7171
C	-144.669	-40.991	-29.372	H	-118.590	0.9619	-10.342
C	-135.096	-33.328	-49.973	C	-85.726	-48.999	-37.546
C	-121.156	-42.261	-33.883	C	-60.585	-60.107	-31.394
C	-131.919	-44.512	-25.314	C	-84.724	-62.029	-32.444
C	-146.222	-35.351	-41.963	C	-73.970	-41.926	-40.247
H	-136.164	-28.920	-59.821	C	-61.662	-47.324	-37.106
H	-130.139	-49.025	-15.630	C	-72.400	-67.456	-29.448
H	-155.999	-32.501	-45.639	H	-93.691	-67.964	-31.075
H	-153.211	-42.646	-22.920	H	-74.436	-31.998	-44.497
N	-105.483	-50.645	-63.999	H	-52.670	-41.551	-38.953
C	-100.536	-75.061	-76.491	H	-71.802	-77.517	-25.455
C	-93.922	-52.767	-70.668	C	-81.232	-19.035	-66.880
C	-114.504	-60.467	-63.583	C	-63.922	0.2761	-71.079
C	-112.418	-72.726	-69.695	C	-78.540	-0.9995	-56.558
C	-91.172	-64.891	-76.980	C	-75.978	-16.444	-79.632
H	-123.729	-58.509	-58.233	C	-67.505	-0.5758	-81.665
H	-120.098	-80.334	-69.098	C	-70.021	0.0659	-58.610
H	-81.773	-66.136	-82.215	H	-82.803	-11.496	-46.747
H	-98.672	-84.569	-81.335	H	-78.737	-22.787	-87.978
N	-113.944	-24.124	-70.165	H	-63.423	-0.3967	-91.545
C	-123.394	-0.7344	-90.327	H	-67.858	0.7432	-50.430
C	-114.934	-10.792	-68.159	C	-54.013	12.712	-72.717
C	-117.653	-29.078	-81.989	C	-44.818	20.642	-73.810
C	-122.423	-21.064	-92.236	C	-47.998	-65.332	-27.556
C	-119.598	-0.2168	-78.074	C	-37.167	-69.563	-23.900
H	-116.837	-39.803	-83.355	C	-97.146	0.3750	0.5223

C	-92.723	0.8790	15.405	H	43.903	-91.675	68.299
Fe	67.219	-101.212	32.283	H	55.437	-70.370	32.848
N	76.347	-101.639	49.451	H	49.460	-49.267	43.531
C	89.161	-97.964	73.927	H	37.881	-70.448	79.019
C	76.207	-111.228	58.728	C	78.028	-75.458	19.370
C	82.895	-90.128	52.153	C	81.367	-57.514	-0.2061
C	89.369	-88.014	64.318	C	90.643	-70.043	16.489
C	82.481	-109.779	70.998	C	67.283	-72.313	11.000
H	70.949	-120.396	56.310	C	68.908	-63.432	0.0593
H	94.500	-78.631	66.035	C	92.269	-61.264	0.5962
H	82.095	-117.898	78.150	H	99.226	-73.004	22.413
H	94.124	-96.593	83.456	H	57.510	-76.547	12.815
N	82.535	-108.202	22.531	H	60.381	-60.902	-0.5600
C	103.177	-115.417	0.5230	H	102.081	-57.169	0.3858
C	80.770	-107.832	0.9138	C	45.530	-99.262	10.006
C	94.349	-112.193	27.286	C	19.797	-93.500	0.0018
C	104.827	-115.892	19.009	C	37.199	-90.139	16.562
C	90.934	-111.337	0.0256	C	40.382	-106.237	-0.1049
H	95.522	-112.497	38.059	C	27.811	-103.366	-0.5963
H	114.184	-119.109	23.406	C	24.642	-87.323	11.657
H	89.058	-110.870	-10.401	H	40.680	-84.905	25.337
H	111.235	-118.228	-0.1442	H	46.234	-114.089	-0.5694
N	58.747	-118.536	34.524	H	24.087	-108.732	-14.610
C	43.012	-141.277	38.089	H	18.440	-80.047	16.744
C	46.829	-117.769	40.860	C	0.7400	-89.369	-0.5398
C	62.822	-130.430	30.047	C	-0.2933	-84.718	-0.9890
C	55.297	-141.952	31.654	C	82.542	-48.024	-12.488
C	38.753	-128.974	42.764	C	82.877	-39.734	-21.416
H	72.429	-130.820	25.038	C	38.504	-46.026	67.545
H	59.110	-151.353	27.869	C	33.945	-35.438	71.531
H	29.290	-127.877	47.916	Fe	-28.054	65.767	102.473
H	36.948	-150.147	39.458	N	-19.232	82.725	106.120
C	43.649	-104.657	45.727	C	-0.3514	105.633	108.651
H	34.614	-103.107	51.579	C	-24.692	94.423	109.512
C	82.904	-80.754	41.290	C	-0.5893	82.227	104.016
H	88.469	-71.451	42.152	C	0.2198	93.528	105.166
C	67.545	-104.085	0.5069	C	-17.210	106.003	110.902
H	65.063	-103.945	-0.5517	H	-35.393	94.603	111.234
N	58.827	-101.202	14.231	H	12.842	92.629	103.376
N	76.336	-83.861	30.561	H	-22.158	115.207	113.736
N	51.859	-94.980	43.076	H	0.2541	114.558	109.654
C	49.469	-82.653	49.515	N	-26.389	59.161	120.664
C	42.828	-58.270	61.948	C	-24.332	45.919	145.115
C	44.781	-82.412	62.738	C	-31.241	46.631	122.166
C	51.519	-70.498	42.912	C	-20.623	65.056	131.156
C	48.140	-58.566	48.945	C	-19.439	58.807	143.468
C	41.555	-70.455	68.824	C	-30.333	39.774	134.271

H	-16.842	75.118	129.740	C	-65.697	33.304	81.042
H	-14.712	64.078	151.660	C	-48.873	40.420	65.367
H	-34.386	29.757	135.007	H	-31.913	50.239	73.487
H	-23.519	40.827	154.642	H	-61.945	37.851	101.577
N	-45.846	73.073	105.217	H	-75.316	28.760	83.113
C	-71.927	82.914	105.039	H	-45.227	41.288	55.189
C	-51.370	77.773	93.818	C	-68.538	28.715	56.959
C	-53.128	73.306	116.397	C	-74.554	24.210	47.375
C	-66.108	78.149	116.708	C	14.489	0.9678	88.797
C	-64.401	82.717	93.433	C	19.002	-0.0801	84.522
H	-48.474	69.544	125.437	C	0.1477	74.078	37.811
H	-71.547	78.155	126.070	C	0.8363	72.643	27.877
H	-68.409	86.380	84.061	Pt	-83.806	16.682	31.369
H	-82.064	86.733	105.028	Pt	-28.302	31.706	-76.032
C	-42.567	77.534	82.494	Pt	-19.871	-76.913	-17.035
H	-46.050	81.381	72.936	Pt	21.007	70.434	12.561
C	-0.0913	69.126	101.020	Pt	82.135	-25.505	-35.385
H	0.9764	67.690	99.538	Pt	26.267	-18.172	77.886
C	-37.691	41.429	110.456	P	59.224	-24.459	-34.064
H	-42.532	31.697	110.818	P	104.974	-25.262	-38.005
N	-37.674	48.694	99.725	P	0.9668	87.193	0.1683
N	-0.9347	59.298	100.326	P	30.018	52.736	24.052
N	-30.615	72.777	84.060	P	-63.559	17.517	20.484
C	-21.842	73.854	73.065	P	-104.200	16.260	41.965
C	-0.6142	74.546	49.709	P	-12.184	-55.923	-11.672
C	-22.496	84.824	64.340	P	-28.369	-97.762	-21.769
C	-12.574	63.734	70.373	P	0.4906	-25.435	73.211
C	-0.4999	63.987	58.880	P	46.798	-10.006	84.045
C	-14.781	85.142	52.892	P	-18.010	12.455	-82.955
H	-28.930	93.227	66.680	P	-38.873	50.405	-67.979
H	-11.500	55.388	77.111	C	-44.815	-100.088	-13.628
H	0.1859	55.845	56.806	H	-42.935	-102.959	-0.3234
H	-15.442	93.663	46.223	H	-49.351	-90.134	-13.282
C	-0.3923	46.379	98.789	C	-54.876	-109.797	-19.933
C	0.8305	21.720	92.861	H	-50.788	-119.926	-20.169
C	0.8552	43.069	104.315	H	-56.964	-106.765	-30.234
C	-10.642	36.704	91.239	C	-67.950	-109.807	-11.933
C	-0.4579	24.731	88.173	H	-65.868	-112.696	-0.1582
C	14.508	30.958	101.429	H	-72.098	-99.660	-11.788
H	13.495	49.963	111.061	C	-78.125	-119.442	-17.999
H	-20.530	38.679	87.399	H	-74.197	-129.610	-18.032
H	-0.9765	17.576	81.898	H	-80.458	-116.584	-28.265
H	24.157	28.569	105.749	H	-87.328	-119.298	-12.166
C	-45.648	44.216	88.970	C	-31.210	-98.913	-40.008
C	-61.153	34.055	67.769	H	-22.724	-93.825	-44.684
C	-41.350	45.507	75.729	H	-39.874	-92.477	-41.864
C	-58.110	38.272	91.447	C	-33.304	-112.506	-46.896

H	-39.622	-110.853	-55.686	H	-19.463	-0.1162	-0.9860
H	-38.666	-119.412	-40.354	C	-14.278	-53.011	0.6481
C	-20.126	-118.848	-51.443	H	-0.7863	-60.139	11.730
H	-15.319	-112.284	-58.774	H	-11.167	-42.979	0.9451
H	-13.308	-119.815	-42.937	C	-28.870	-55.658	10.505
C	-22.492	-132.609	-57.628	H	-31.138	-66.166	0.8527
H	-13.031	-136.885	-60.932	H	-35.623	-49.709	0.4281
H	-29.155	-131.846	-66.223	C	-31.605	-52.651	25.270
H	-26.992	-139.346	-50.327	H	-24.651	-58.362	31.498
H	-0.8965	-111.981	-22.678	H	-41.723	-56.090	27.626
C	-17.729	-111.753	-16.124	C	-30.510	-37.789	28.692
H	-13.995	-108.699	-0.6287	H	-20.308	-34.156	27.368
C	-23.748	-125.804	-14.920	H	-33.364	-36.158	39.090
H	-28.025	-129.005	-24.443	H	-37.132	-31.893	22.326
H	-31.775	-125.733	-0.7493	C	50.596	0.4641	73.319
C	-12.971	-135.837	-10.659	H	40.841	0.8704	70.558
H	-0.8750	-132.753	-0.1031	H	54.747	0.0435	64.104
H	-0.4865	-135.765	-18.023	C	59.639	16.105	78.107
C	-18.735	-149.931	-0.9507	H	63.960	20.875	69.241
H	-10.937	-156.909	-0.6470	H	67.954	12.203	84.015
H	-22.771	-153.190	-19.096	C	52.243	26.757	86.275
H	-26.729	-150.201	-0.2098	H	59.691	33.552	90.525
C	0.5597	-52.237	-15.901	H	46.913	22.092	94.608
H	0.6883	-41.753	-18.713	C	42.343	34.895	77.935
H	0.7406	-58.077	-24.977	H	38.069	42.881	84.010
C	16.236	-56.135	-0.5512	H	34.150	28.670	74.306
H	25.152	-59.585	-10.860	H	47.347	39.389	69.340
H	12.681	-64.502	0.0543	C	61.041	-21.614	82.122
C	20.207	-44.495	0.3593	H	58.940	-27.450	73.096
H	11.770	-41.650	0.9959	H	60.576	-28.684	90.470
H	22.785	-35.807	-0.2560	C	75.187	-15.793	81.058
C	32.178	-48.115	12.367	H	77.542	-0.9807	89.889
H	40.904	-50.322	0.6201	H	75.842	-0.9250	72.312
H	29.971	-56.892	18.451	C	85.469	-27.086	79.739
H	34.634	-39.823	19.009	H	83.171	-33.053	70.838
C	-21.186	-41.838	-19.777	H	84.718	-33.682	88.446
H	-16.505	-40.112	-29.521	C	99.666	-21.554	78.722
H	-31.203	-45.710	-21.890	H	106.800	-29.741	77.804
C	-22.842	-28.471	-12.448	H	102.149	-15.772	87.624
H	-27.664	-30.068	-0.2763	H	100.642	-15.087	69.993
H	-29.690	-22.368	-18.440	C	46.291	-0.5213	101.843
C	-0.9882	-20.608	-10.406	H	41.176	-13.560	106.746
H	-0.2992	-26.300	-0.4098	H	39.459	0.3299	102.620
H	-0.4994	-18.980	-20.068	C	59.340	-0.2261	109.349
C	-12.707	-0.7152	-0.3739	H	65.094	0.5362	104.045
H	-0.3445	-0.1574	-0.2347	H	65.423	-11.337	109.817
H	-17.317	-0.8668	0.6031	C	56.603	0.2771	123.581

H	66.111	0.6095	127.854	H	-100.035	31.413	60.186
H	49.952	11.464	123.126	C	-112.401	-0.0300	41.262
C	50.530	-0.7911	132.651	H	-108.533	-0.6281	49.573
H	49.613	-0.4023	142.789	H	-108.833	-0.5085	32.089
H	56.884	-16.769	132.909	C	-115.255	18.985	69.266
H	40.605	-10.840	129.200	H	-111.394	19.916	79.479
C	0.0847	-38.904	85.142	H	-119.215	0.8845	68.248
H	0.1017	-34.394	95.111	C	-126.483	29.210	67.343
H	0.9509	-45.580	84.820	H	-122.267	39.319	67.499
C	-12.056	-47.035	83.388	H	-131.246	27.736	57.606
H	-13.770	-49.346	72.832	C	-137.042	27.872	78.298
H	-20.547	-41.105	86.899	H	-132.619	29.596	88.113
C	-11.537	-60.141	91.348	H	-141.426	17.891	78.161
H	-0.8292	-58.075	101.591	H	-144.973	35.175	76.726
H	-21.667	-64.245	91.836	C	-127.749	-0.0602	41.345
C	-0.2295	-70.526	85.004	H	-131.641	0.4699	50.071
H	0.8054	-67.068	84.851	H	-131.554	0.4443	32.414
H	-0.5379	-72.636	74.748	C	-132.801	-15.068	41.560
H	-0.2700	-79.796	90.719	H	-128.898	-20.131	50.448
C	-0.8004	-12.315	75.351	H	-128.987	-20.364	32.761
H	-0.4237	-0.3546	69.977	C	-148.064	-15.558	41.674
H	-0.7828	-0.9626	85.961	H	-151.977	-10.476	50.489
C	-22.461	-14.941	70.998	H	-151.452	-25.913	41.849
H	-22.875	-16.658	60.196	H	-152.119	-10.714	32.784
H	-26.386	-23.856	75.951	H	-125.767	27.679	37.673
C	-31.288	-0.2910	74.554	C	-115.719	27.875	33.410
H	-27.419	0.6022	69.518	H	-116.499	24.378	23.066
H	-30.766	-0.1110	85.342	C	-110.310	42.232	33.441
C	-45.842	-0.5147	70.489	H	-100.225	42.320	29.183
H	-46.599	-0.7034	59.768	H	-109.557	45.865	43.737
H	-51.782	0.3684	72.865	C	-119.445	51.508	25.379
H	-50.030	-13.698	75.799	H	-120.132	47.846	15.082
H	0.2792	-24.786	48.976	H	-129.507	51.292	29.675
C	0.1001	-32.523	56.498	C	-114.184	65.842	25.392
H	-0.9623	-35.074	55.944	H	-120.833	72.252	19.610
C	0.9442	-44.926	53.281	H	-104.216	66.272	20.973
H	19.325	-41.783	49.840	H	-113.635	69.700	35.579
H	10.902	-50.878	62.336	C	-52.852	0.3838	26.942
C	0.2828	-53.762	42.697	H	-56.956	-0.5268	22.465
H	0.2490	-48.466	33.116	H	-55.200	0.3170	37.607
H	-0.7475	-55.919	45.707	C	-37.590	0.3872	25.197
C	10.388	-66.929	41.098	H	-34.747	0.8188	15.572
H	20.717	-65.096	38.099	H	-34.175	-0.6542	25.186
H	0.5557	-73.112	33.529	C	-30.431	11.299	36.502
H	10.488	-72.436	50.516	H	-32.892	0.6538	46.038
C	-103.319	20.976	59.817	H	-33.900	21.653	37.032
H	-94.909	15.112	63.685	C	-15.289	11.179	34.570

H	-11.522	0.0942	34.312	H	0.3396	91.910	-28.476
H	-10.467	16.449	42.807	C	19.408	104.188	-36.081
H	-12.566	16.111	25.226	H	25.686	112.435	-32.564
C	-64.453	15.313	0.2100	H	26.036	95.861	-38.725
H	-66.987	25.054	-0.2205	C	11.612	108.593	-48.450
H	-73.251	0.8986	0.0564	H	18.495	111.926	-56.222
C	-52.801	0.9145	-0.5700	H	0.4890	116.821	-46.012
H	-43.945	15.541	-0.5151	H	0.5699	100.311	-52.384
H	-50.196	-0.0598	-0.1456	H	-0.4135	74.734	-13.757
C	-56.843	0.7328	-20.382	C	-0.6311	80.085	-0.4460
H	-59.342	17.093	-24.652	H	-0.9085	72.430	0.2852
H	-65.837	0.1096	-20.928	C	-18.269	89.456	-0.6491
C	-45.695	0.0867	-28.565	H	-15.656	97.639	-13.242
H	-36.453	0.6597	-27.683	H	-21.145	93.813	0.3120
H	-48.471	0.0408	-39.096	C	-30.159	81.771	-12.343
H	-43.822	-0.9291	-25.069	H	-27.573	78.288	-22.400
H	-62.746	41.217	22.314	H	-32.177	72.934	-0.6189
C	-54.883	33.651	23.129	C	-42.663	90.505	-13.006
H	-51.721	33.792	33.600	H	-40.813	99.371	-19.074
C	-43.211	37.552	13.965	H	-45.616	93.713	-0.3011
H	-47.084	40.150	0.4062	H	-50.898	84.911	-17.445
H	-36.356	29.138	12.696	C	32.888	55.370	42.168
C	-35.186	49.367	19.577	H	39.888	47.986	46.179
H	-26.691	51.193	12.904	H	23.292	53.883	47.218
H	-31.143	46.654	29.393	C	37.882	69.528	45.354
C	-43.395	62.189	20.825	H	47.840	71.030	41.100
H	-48.000	64.733	11.272	H	31.190	76.818	40.710
H	-36.930	70.427	23.861	C	38.292	71.842	60.484
H	-51.270	61.084	28.283	H	45.108	64.607	65.083
C	0.5366	101.138	12.967	H	28.305	70.115	64.669
H	14.107	102.553	19.408	C	42.862	86.028	63.806
H	-0.2591	97.444	19.504	H	52.853	87.842	59.842
C	18.270	94.543	-12.964	H	43.102	87.447	74.610
H	24.884	102.453	-0.9291	H	36.029	93.345	59.481
H	24.832	86.597	-16.654	C	17.861	38.734	23.127
C	0.1509	114.682	0.6873	H	15.536	37.833	12.468
H	10.075	118.700	0.1389	H	0.8674	42.290	27.891
H	-0.6722	113.524	-0.0222	C	21.375	24.755	28.451
C	-0.2564	124.742	17.712	H	31.390	21.818	25.170
H	0.5214	125.175	25.401	H	14.312	17.710	23.900
H	-0.3215	134.631	13.083	C	20.360	23.453	43.683
C	-16.007	121.408	24.162	H	28.449	29.040	48.470
H	-18.795	129.297	31.143	H	10.879	27.750	47.101
H	-15.536	111.992	29.669	C	21.167	0.8836	48.082
H	-23.801	120.586	16.572	H	20.091	0.8120	58.906
C	10.027	99.791	-24.773	H	30.766	0.4489	45.271
H	0.3822	108.246	-21.696	H	13.231	0.2943	43.460

H	43.753	42.544	0.7220	H	133.324	-45.406	-0.9276
C	45.712	45.355	17.624	C	148.005	-54.684	-22.096
H	48.451	36.244	23.019	H	148.481	-59.806	-31.709
C	57.410	55.284	17.966	H	151.583	-61.469	-14.357
H	54.107	64.940	14.023	H	154.610	-46.018	-22.447
H	60.629	56.816	28.305	C	54.947	-0.8204	-26.181
C	69.179	50.139	0.9625	H	56.907	-0.0779	-33.981
H	65.927	48.802	-0.0755	H	62.573	-0.6464	-18.542
H	72.326	40.357	13.413	C	41.049	-0.5744	-20.093
C	80.951	59.856	10.087	H	33.447	-11.935	-24.938
H	77.982	69.628	0.6255	H	38.300	0.4708	-21.881
H	89.163	56.082	0.3994	C	40.901	-0.8336	-0.4993
H	84.494	61.090	20.323	H	48.374	-0.1958	-0.0159
C	109.207	-30.019	-55.447	H	43.646	-18.737	-0.2977
H	99.616	-29.348	-60.660	C	27.156	-0.5451	0.1012
H	111.914	-40.618	-55.530	H	19.586	-11.817	-0.3590
C	119.487	-21.969	-63.607	H	24.363	0.4969	-0.0627
H	119.075	-11.380	-60.896	H	27.235	-0.7376	11.745
H	116.494	-22.684	-74.119	C	51.118	-23.788	-50.647
C	133.826	-27.159	-62.324	H	53.804	-33.101	-55.724
H	134.099	-37.751	-65.076	H	56.102	-15.813	-56.235
H	137.204	-26.332	-51.958	C	35.925	-21.831	-51.309
C	143.326	-19.286	-71.325	H	33.452	-11.357	-49.307
H	153.463	-23.142	-70.289	H	30.910	-27.912	-43.717
H	143.319	-0.8730	-68.575	C	30.686	-25.841	-65.138
H	140.325	-20.169	-81.769	H	33.565	-36.195	-67.213
C	111.058	-0.8122	-34.708	H	35.315	-19.502	-72.767
H	105.243	-0.4651	-26.104	C	15.502	-24.561	-65.935
H	107.813	-0.1973	-43.164	H	11.973	-27.710	-75.754
C	125.925	-0.5756	-31.864	H	12.517	-14.200	-64.321
H	128.805	-11.050	-22.740	H	10.697	-30.774	-58.359
H	132.044	-0.9596	-40.048	C	49.729	-37.356	-24.653
C	128.713	0.9215	-30.125	H	55.724	-39.617	-15.781
H	122.690	13.093	-21.838	H	40.170	-33.383	-21.147
H	125.680	14.534	-39.213	C	46.939	-50.395	-32.271
C	143.520	11.763	-27.380	H	39.962	-48.444	-40.471
H	146.645	0.6659	-18.267	H	41.944	-57.290	-25.362
H	145.310	22.444	-26.171	C	59.512	-57.120	-37.815
H	149.612	0.8128	-35.658	H	66.365	-59.412	-29.612
H	107.809	-45.628	-25.986	H	64.709	-50.214	-44.536
C	114.008	-36.618	-26.566	C	56.041	-69.934	-45.344
H	113.596	-32.049	-16.620	H	65.116	-74.557	-49.220
C	128.402	-40.781	-29.774	H	49.388	-67.784	-53.714
H	128.717	-45.747	-39.510	H	51.083	-77.032	-38.703
H	134.900	-32.015	-30.256	C	-27.740	0.1525	-94.204
C	133.680	-50.362	-19.037	H	-36.413	-0.2076	-88.592
H	127.183	-59.170	-18.534	H	-22.006	-0.7246	-97.328

C	-32.612	0.9411	-106.450	H	-18.047	47.988	-24.920
H	-24.018	13.001	-112.193	H	-34.887	45.989	-19.812
H	-38.181	18.192	-103.029	C	-50.810	58.038	-79.846
C	-41.557	0.0803	-115.406	H	-45.023	63.274	-87.516
H	-49.963	-0.3016	-109.498	H	-57.106	65.471	-74.867
H	-35.861	-0.7817	-119.025	C	-59.554	47.374	-86.594
C	-46.869	0.8841	-127.251	H	-53.098	40.323	-91.909
H	-38.627	12.609	-133.310	H	-64.984	41.675	-78.982
H	-52.780	17.319	-123.762	C	-69.459	53.679	-96.413
H	-53.178	0.2534	-133.506	H	-63.958	59.522	-103.853
C	-14.790	0.1879	-68.070	H	-76.089	60.520	-91.024
H	-10.671	-0.7897	-70.680	C	-77.741	42.948	-103.448
H	-24.518	0.0185	-63.356	H	-71.260	36.172	-109.029
C	-0.5597	0.9146	-58.174	H	-84.723	47.593	-110.404
H	0.4474	0.9858	-62.397	H	-83.419	37.110	-96.183
H	-0.9250	19.354	-56.707	H	-21.408	66.133	-72.581
C	-0.4953	0.2016	-44.640	C	-27.466	64.303	-63.647
H	-0.2177	-0.8474	-46.112	H	-20.537	60.596	-56.032
H	-14.850	0.2197	-39.951	C	-33.711	77.494	-58.970
C	0.5219	0.8721	-35.421	H	-40.342	75.770	-50.437
H	15.168	0.8467	-39.898	H	-39.712	81.807	-67.031
H	0.5637	0.3551	-25.830	C	-22.756	87.406	-54.883
H	0.2490	19.131	-33.631	H	-17.032	83.217	-46.522
C	-0.1632	14.495	-91.187	H	-15.839	88.817	-63.256
H	-0.3293	20.577	-100.133	C	-28.679	100.879	-50.817
H	0.4469	20.633	-84.488	H	-20.742	107.665	-47.694
C	0.6085	0.1810	-94.945	H	-35.650	99.647	-42.521
H	0.0481	-0.3947	-102.365	H	-34.019	105.390	-59.181
H	0.7395	-0.4518	-86.116				
C	19.835	0.5463	-100.643				
H	18.510	11.679	-109.554				
H	25.351	11.386	-93.249				
C	27.870	-0.7008	-104.251				
H	22.555	-12.969	-111.671				
H	29.545	-13.173	-95.404				
H	37.549	-0.4157	-108.370				
C	-49.218	47.655	-52.751				
H	-59.405	45.463	-56.077				
H	-49.748	56.797	-46.788				
C	-44.623	35.891	-44.040				
H	-45.515	26.718	-49.920				
H	-51.461	35.065	-35.518				
C	-30.235	36.924	-38.923				
H	-23.502	38.733	-47.362				
H	-27.428	27.268	-34.576				
C	-28.386	47.819	-28.388				
H	-30.783	57.628	-32.491				

($\Delta,\Delta,\Lambda,\Lambda$)S₄-4

	x-coord.	y-coord.	z-coord.
Fe	-0.487	-1.364	-12.441
Fe	-10.907	-4.987	4.893
N	-1.836	-2.368	-13.458
C	-3.681	-4.094	-14.658
C	-2.703	-1.923	-14.372
C	-1.873	-3.680	-13.136
C	-2.785	-4.563	-13.716
C	-3.630	-2.747	-14.990
H	-2.662	-0.873	-14.632
H	-2.771	-5.605	-13.421
H	-4.397	-4.759	-15.126
N	0.965	-1.749	-13.679
C	3.280	-2.133	-15.186
C	2.112	-1.106	-13.362
C	0.967	-2.569	-14.731
C	2.097	-2.786	-15.504
C	3.283	-1.278	-14.098
H	0.036	-3.071	-14.971
H	2.041	-3.462	-16.347
H	4.176	-0.739	-13.808
H	4.176	-2.285	-15.776
N	-0.995	0.282	-13.348
C	-2.020	2.652	-14.402
C	-2.023	0.919	-12.745
C	-0.480	0.815	-14.458
C	-0.962	1.991	-15.011
C	-2.556	2.104	-13.250
H	0.342	0.289	-14.928
H	-3.381	2.577	-12.733
H	-2.417	3.570	-14.818
N	-11.015	-5.987	6.569
C	-11.003	-7.088	9.136
C	-11.609	-7.157	6.817
C	-10.400	-5.355	7.595
C	-10.381	-5.878	8.886
C	-11.624	-7.735	8.077
H	-12.095	-7.654	5.985
H	-9.878	-5.330	9.673
H	-12.124	-8.685	8.218
H	-11.006	-7.518	10.131
N	-11.969	-6.337	3.919

C	-13.115	-8.408	2.432
C	-13.293	-6.431	3.778
C	-11.200	-7.280	3.331
C	-11.742	-8.322	2.581
C	-13.899	-7.443	3.049
H	-13.902	-5.679	4.266
H	-11.080	-9.051	2.130
H	-14.978	-7.468	2.974
H	-13.564	-9.208	1.857
N	-12.514	-3.939	5.265
C	-14.877	-2.457	5.352
C	-12.920	-3.216	4.195
C	-13.265	-3.914	6.367
C	-14.444	-3.189	6.449
C	-14.097	-2.471	4.209
H	-12.920	-4.492	7.217
H	-15.013	-3.205	7.370
H	-14.383	-1.914	3.325
H	-15.798	-1.889	5.390
C	1.990	-0.229	-12.231
H	2.818	0.415	-11.941
C	-0.887	-4.090	-12.182
H	-0.853	-5.137	-11.896
C	-2.495	0.274	-11.554
H	-3.328	0.709	-11.005
C	-9.793	-7.124	3.571
H	-9.094	-7.852	3.164
C	-9.782	-4.112	7.220
H	-9.274	-3.505	7.966
C	-12.001	-3.262	3.089
H	-12.192	-2.692	2.183
N	-10.916	-3.941	3.256
N	-9.396	-6.135	4.302
N	-9.863	-3.743	5.985
N	-0.063	-3.209	-11.697
N	0.872	-0.236	-11.582
N	-1.913	-0.815	-11.165
C	-2.322	-1.324	-9.912
C	-3.134	-2.271	-7.389
C	-2.496	-2.692	-9.690
C	-2.559	-0.431	-8.856
C	-2.944	-0.898	-7.617
C	-2.902	-3.156	-8.454
H	-2.352	-3.394	-10.500
H	-2.398	0.631	-9.001
H	-3.109	-0.197	-6.807
H	-3.055	-4.219	-8.304

C	0.720	0.751	-10.575	H	-7.632	-6.272	2.342
C	0.497	2.745	-8.606	H	-5.195	-6.024	2.533
C	0.317	0.421	-9.281	H	-5.587	-5.488	6.774
C	0.991	2.089	-10.886	C	-3.811	-5.536	4.761
C	0.873	3.069	-9.920	C	-2.606	-5.364	4.815
C	0.223	1.401	-8.311	C	-7.275	1.177	5.061
H	0.098	-0.605	-9.019	C	-6.743	2.267	4.948
H	1.267	2.352	-11.901	C	-7.151	-3.818	-0.929
H	1.076	4.103	-10.176	C	-6.317	-3.710	-1.810
H	-0.068	1.126	-7.303	C	0.389	3.726	-7.589
C	0.963	-3.680	-10.863	C	0.288	4.536	-6.686
C	2.858	-4.616	-8.988	H	-0.509	2.377	-15.916
C	1.389	-5.022	-10.874	H	-4.303	-2.327	-15.726
C	1.596	-2.803	-9.978	C	3.684	-5.078	-7.941
C	2.523	-3.253	-9.065	C	4.321	-5.434	-6.964
C	2.303	-5.479	-9.950	C	-3.604	-2.716	-6.131
H	1.017	-5.714	-11.620	C	-4.081	-3.037	-5.057
H	1.338	-1.757	-9.991	Fe	-0.108	12.371	2.770
H	2.992	-2.549	-8.387	Fe	9.665	-5.453	4.141
H	2.598	-6.521	-9.960	N	0.947	13.220	4.176
C	-9.201	-2.531	5.661	C	2.263	14.185	6.440
C	-7.911	-0.079	5.227	C	1.741	14.290	4.102
C	-9.888	-1.474	5.063	C	0.806	12.609	5.375
C	-7.856	-2.370	6.012	C	1.447	13.070	6.522
C	-7.219	-1.165	5.787	C	2.410	14.798	5.204
C	-9.253	-0.264	4.858	H	1.847	14.764	3.133
H	-10.934	-1.588	4.805	H	1.298	12.549	7.460
H	-7.313	-3.202	6.444	H	2.772	14.567	7.317
H	-6.178	-1.048	6.065	N	-1.706	13.427	3.171
H	-9.803	0.562	4.424	C	-4.097	14.856	3.341
C	-9.981	-3.951	2.198	C	-2.695	13.235	2.268
C	-8.109	-3.892	0.113	C	-1.907	14.309	4.151
C	-8.649	-3.636	2.464	C	-3.082	15.036	4.270
C	-10.377	-4.249	0.891	C	-3.897	13.937	2.325
C	-9.451	-4.225	-0.135	H	-1.107	14.445	4.870
C	-7.733	-3.604	1.433	H	-3.190	15.738	5.087
H	-8.342	-3.393	3.473	H	-4.656	13.753	1.575
H	-11.407	-4.525	0.694	H	-5.022	15.417	3.410
H	-9.763	-4.464	-1.145	N	0.467	13.661	1.399
H	-6.702	-3.361	1.645	C	1.520	15.179	-0.695
C	-7.996	-5.998	4.446	C	1.526	13.220	0.686
C	-5.213	-5.708	4.665	C	-0.055	14.849	1.082
C	-7.408	-5.776	5.692	C	0.440	15.631	0.051
C	-7.181	-6.108	3.313	C	2.071	13.954	-0.367
C	-5.814	-5.955	3.420	H	-0.895	15.197	1.671
C	-6.036	-5.642	5.800	H	2.920	13.555	-0.907
H	-8.023	-5.751	6.582	H	1.924	15.772	-1.507

N	10.768	-4.498	5.426	N	1.494	11.389	2.153
C	12.008	-2.860	7.308	C	2.073	10.163	2.557
C	12.098	-4.402	5.476	C	3.375	7.783	3.289
C	10.035	-3.791	6.313	C	2.398	9.918	3.893
C	10.629	-2.960	7.263	C	2.389	9.202	1.589
C	12.750	-3.602	6.399	C	3.010	8.027	1.954
H	12.665	-4.985	4.758	C	3.048	8.752	4.250
H	10.001	-2.410	7.953	H	2.196	10.671	4.644
H	13.832	-3.565	6.400	H	2.120	9.375	0.554
H	12.495	-2.224	8.037	H	3.236	7.285	1.196
N	11.167	-5.990	3.034	H	3.329	8.591	5.284
C	13.165	-6.502	1.161	C	-0.963	10.662	0.388
C	11.836	-7.145	3.049	C	-0.467	8.773	-1.623
C	11.481	-5.072	2.091	C	-0.576	9.366	0.729
C	12.476	-5.302	1.143	C	-1.080	11.021	-0.958
C	12.837	-7.434	2.136	C	-0.831	10.090	-1.947
H	11.568	-7.862	3.817	C	-0.333	8.436	-0.267
H	12.697	-4.537	0.409	H	-0.495	9.086	1.773
H	13.352	-8.384	2.196	H	-1.342	12.041	-1.218
H	13.945	-6.705	0.436	H	-0.921	10.374	-2.989
N	9.620	-7.075	5.217	H	-0.032	7.430	0.003
C	9.125	-9.449	6.595	C	-1.431	10.010	4.195
C	8.797	-8.015	4.702	C	-3.124	7.790	4.404
C	10.197	-7.314	6.397	C	-0.923	8.781	4.623
C	9.978	-8.482	7.109	C	-2.778	10.122	3.845
C	8.528	-9.209	5.371	C	-3.613	9.029	3.959
H	10.861	-6.552	6.789	C	-1.758	7.684	4.714
H	10.478	-8.626	8.059	H	0.130	8.695	4.867
H	7.862	-9.933	4.917	H	-3.177	11.079	3.535
H	8.936	-10.369	7.135	H	-4.664	9.129	3.717
C	-2.389	12.234	1.281	H	-1.359	6.731	5.041
H	-3.109	11.989	0.503	C	6.800	-5.103	5.316
C	-0.063	11.463	5.335	C	3.996	-5.385	5.313
H	-0.272	10.895	6.239	C	6.080	-5.120	6.522
C	2.058	11.968	1.144	C	6.106	-5.341	4.125
H	2.949	11.557	0.673	C	4.735	-5.482	4.123
C	10.740	-3.848	2.209	C	4.706	-5.251	6.517
H	10.985	-2.995	1.580	H	6.604	-5.045	7.467
C	8.621	-4.005	6.211	H	6.635	-5.375	3.185
H	7.955	-3.491	6.900	H	4.216	-5.646	3.186
C	8.292	-7.696	3.399	H	4.165	-5.239	7.456
H	7.683	-8.423	2.867	C	8.278	-6.374	1.516
N	8.609	-6.552	2.876	C	7.381	-6.147	-1.144
N	9.808	-3.793	3.105	C	7.842	-5.142	1.017
N	8.179	-4.817	5.301	C	8.362	-7.465	0.636
N	-0.592	11.153	4.200	C	7.922	-7.352	-0.666
N	-1.262	11.615	1.390	C	7.390	-5.036	-0.283

H	7.820	-4.272	1.661	H	-5.224	-0.697	-5.095
H	8.794	-8.399	0.977	H	-6.595	0.047	-4.304
H	7.983	-8.207	-1.329	C	-6.806	-0.162	-6.443
H	7.019	-4.083	-0.642	H	-6.511	-0.868	-7.225
C	9.258	-2.526	3.393	H	-7.896	-0.083	-6.451
C	8.210	0.017	3.992	C	-6.196	1.210	-6.748
C	7.888	-2.357	3.606	H	-5.105	1.150	-6.662
C	10.106	-1.416	3.517	H	-6.548	1.936	-6.007
C	9.590	-0.168	3.811	C	-6.571	1.684	-8.150
C	7.376	-1.110	3.896	H	-6.198	0.986	-8.901
H	7.218	-3.201	3.515	H	-6.138	2.666	-8.342
H	11.176	-1.548	3.411	H	-7.654	1.757	-8.252
H	10.259	0.680	3.904	C	-7.238	-3.355	-6.023
H	6.309	-0.991	4.046	H	-6.412	-3.210	-6.725
C	7.628	1.290	4.200	H	-7.170	-4.396	-5.693
C	7.025	2.348	4.271	C	-8.581	-3.143	-6.734
C	2.583	-5.386	5.265	H	-8.702	-2.091	-7.001
C	1.374	-5.298	5.143	H	-9.399	-3.414	-6.061
C	6.814	-6.067	-2.438	C	-8.677	-3.982	-8.016
C	6.266	-6.040	-3.527	H	-7.811	-3.771	-8.652
C	-0.256	7.820	-2.653	H	-9.572	-3.665	-8.559
C	-0.114	7.039	-3.576	C	-8.765	-5.482	-7.744
H	-0.022	16.588	-0.157	H	-7.853	-5.852	-7.274
H	3.040	15.672	5.086	H	-8.908	-6.017	-8.683
C	-3.984	6.671	4.525	H	-9.609	-5.703	-7.089
C	-4.717	5.698	4.576	C	-8.432	-2.127	-3.604
C	4.094	6.609	3.624	H	-8.948	-3.093	-3.597
C	4.761	5.622	3.879	H	-8.149	-1.931	-2.565
Pt	-5.137	-3.414	-3.397	C	-9.396	-1.028	-4.064
Pt	5.296	-5.795	-5.263	H	-9.719	-1.205	-5.092
Pt	0.106	5.788	-5.136	H	-8.893	-0.057	-4.033
Pt	5.903	3.997	4.114	C	-10.624	-0.987	-3.147
Pt	-0.613	-5.260	4.954	H	-11.131	-1.957	-3.179
Pt	-5.767	4.007	4.724	H	-10.298	-0.817	-2.114
P	0.051	7.648	-6.481	C	-11.593	0.114	-3.569
P	0.252	4.071	-3.644	H	-11.938	-0.051	-4.590
P	6.270	-7.687	-6.135	H	-11.108	1.090	-3.520
P	4.468	-3.839	-4.406	H	-12.459	0.123	-2.907
P	-6.844	-2.358	-4.520	C	-3.429	-5.282	-0.866
P	-3.313	-4.506	-2.545	H	-4.015	-6.200	-0.983
P	-0.808	-7.210	6.155	H	-4.034	-4.614	-0.246
P	-0.562	-3.278	3.786	C	-2.115	-5.597	-0.139
P	7.259	5.079	5.618	H	-1.630	-4.664	0.165
P	4.734	3.032	2.391	H	-1.424	-6.121	-0.805
P	-6.266	4.445	6.917	C	-2.359	-6.466	1.099
P	-5.298	3.179	2.627	H	-2.899	-7.373	0.807
C	-6.317	-0.670	-5.082	H	-2.985	-5.921	1.813

C	-1.043	-6.852	1.767	H	-4.095	6.015	1.982
H	-0.492	-5.963	2.076	H	-2.993	4.865	2.727
H	-0.417	-7.427	1.084	C	-2.355	5.566	0.795
H	-1.233	-7.455	2.653	H	-2.034	6.583	1.043
C	-2.945	-5.881	-3.727	H	-2.752	5.586	-0.225
H	-2.721	-5.395	-4.682	C	-1.144	4.637	0.863
H	-3.919	-6.362	-3.866	H	-0.367	4.973	0.175
C	-1.912	-6.983	-3.454	H	-1.423	3.617	0.594
H	-2.135	-7.805	-4.142	H	-0.729	4.627	1.872
H	-2.027	-7.375	-2.440	C	-6.880	2.665	1.802
C	-0.464	-6.542	-3.687	H	-7.232	3.519	1.214
H	-0.169	-5.800	-2.938	H	-7.591	2.550	2.624
H	-0.386	-6.070	-4.672	C	-6.951	1.394	0.949
C	0.497	-7.727	-3.615	H	-8.010	1.202	0.741
H	1.519	-7.389	-3.790	H	-6.576	0.540	1.520
H	0.244	-8.472	-4.369	C	-6.204	1.499	-0.381
H	0.451	-8.198	-2.632	H	-5.129	1.598	-0.198
C	-1.769	-3.476	-2.500	H	-6.533	2.398	-0.913
H	-0.913	-4.073	-2.178	C	-6.458	0.273	-1.255
H	-1.578	-3.167	-3.532	H	-5.900	0.356	-2.188
C	-1.848	-2.226	-1.614	H	-7.519	0.188	-1.491
H	-0.837	-1.812	-1.522	H	-6.143	-0.640	-0.748
H	-2.180	-2.498	-0.606	C	-5.376	3.162	7.908
C	-2.778	-1.154	-2.185	H	-4.421	3.013	7.394
H	-2.516	-0.962	-3.230	H	-5.932	2.228	7.784
H	-3.808	-1.516	-2.170	C	-5.095	3.415	9.393
C	-2.691	0.143	-1.388	H	-4.481	4.313	9.504
H	-3.359	0.889	-1.817	H	-6.028	3.576	9.938
H	-1.676	0.539	-1.405	C	-4.356	2.218	10.001
H	-2.978	-0.023	-0.348	H	-3.418	2.058	9.457
C	-4.339	1.603	2.828	H	-4.966	1.316	9.881
H	-4.255	1.101	1.861	C	-4.061	2.444	11.482
H	-4.918	0.956	3.491	H	-3.438	3.329	11.616
C	-2.925	1.771	3.399	H	-3.535	1.583	11.894
H	-2.362	2.488	2.793	H	-4.988	2.585	12.038
H	-2.417	0.803	3.315	C	-5.741	6.099	7.547
C	-2.902	2.213	4.862	H	-4.653	6.069	7.663
H	-3.544	1.554	5.454	H	-5.938	6.801	6.731
H	-3.308	3.222	4.945	C	-6.390	6.638	8.829
C	-1.485	2.201	5.428	H	-6.232	5.945	9.659
H	-1.496	2.522	6.470	H	-7.468	6.742	8.678
H	-0.842	2.877	4.862	C	-5.796	8.004	9.191
H	-1.059	1.198	5.380	H	-4.715	7.900	9.340
C	-4.334	4.011	1.257	H	-5.952	8.698	8.359
H	-5.030	4.410	0.514	C	-6.439	8.563	10.458
H	-3.716	3.267	0.745	H	-6.002	9.532	10.701
C	-3.454	5.154	1.778	H	-6.276	7.889	11.299

H	-7.512	8.691	10.317	H	10.608	6.975	3.273
C	-8.070	4.266	7.271	H	11.495	5.858	4.320
H	-8.551	5.215	7.012	C	11.815	7.942	4.779
H	-8.439	3.530	6.550	H	12.155	7.765	5.800
C	-8.502	3.833	8.678	H	11.268	8.885	4.753
H	-8.136	4.541	9.426	H	12.687	8.028	4.132
H	-8.075	2.852	8.906	C	5.624	1.576	1.686
C	-10.030	3.753	8.763	H	6.673	1.888	1.688
H	-10.457	4.734	8.529	H	5.553	0.776	2.430
H	-10.397	3.042	8.015	C	5.295	1.007	0.305
C	-10.481	3.317	10.155	H	4.347	0.461	0.333
H	-10.137	4.027	10.908	H	5.198	1.805	-0.437
H	-10.079	2.332	10.397	C	6.419	0.052	-0.113
H	-11.569	3.269	10.196	H	6.634	-0.637	0.711
C	6.560	6.664	6.259	H	7.330	0.627	-0.307
H	5.496	6.471	6.428	C	6.046	-0.751	-1.353
H	6.607	7.384	5.435	H	5.146	-1.340	-1.169
C	7.156	7.285	7.528	H	6.856	-1.433	-1.608
H	8.227	7.462	7.402	H	5.863	-0.090	-2.201
H	7.026	6.599	8.370	C	4.541	4.204	0.978
C	6.462	8.615	7.843	H	3.929	5.033	1.345
H	5.388	8.440	7.978	H	4.021	3.768	0.121
H	6.583	9.296	6.994	C	5.917	4.742	0.558
C	7.043	9.254	9.102	H	6.514	4.944	1.452
H	8.107	9.452	8.973	H	6.446	3.980	-0.022
H	6.914	8.595	9.961	C	5.794	6.028	-0.262
H	6.537	10.197	9.309	H	5.326	6.803	0.354
C	7.740	4.053	7.078	H	5.140	5.850	-1.122
H	7.757	3.020	6.716	C	7.159	6.513	-0.743
H	6.924	4.110	7.805	H	7.815	6.706	0.106
C	9.075	4.351	7.774	H	7.048	7.435	-1.314
H	9.896	4.223	7.062	H	7.628	5.763	-1.381
H	9.098	5.383	8.131	C	3.015	2.477	2.802
C	9.282	3.403	8.960	H	3.109	1.740	3.606
H	9.262	2.367	8.603	H	2.513	3.346	3.240
H	8.459	3.527	9.671	C	2.149	1.898	1.680
C	10.611	3.682	9.660	H	2.637	1.022	1.247
H	11.443	3.545	8.969	H	2.019	2.637	0.883
H	10.739	3.000	10.500	C	0.776	1.479	2.217
H	10.636	4.705	10.036	H	0.249	2.358	2.600
C	8.811	5.491	4.701	H	0.909	0.782	3.051
H	8.497	5.709	3.676	C	-0.059	0.812	1.128
H	9.401	4.571	4.646	H	0.437	-0.089	0.764
C	9.689	6.647	5.198	H	-0.203	1.492	0.286
H	10.008	6.470	6.228	H	-1.038	0.529	1.516
H	9.116	7.578	5.178	C	1.482	8.727	-6.027
C	10.927	6.794	4.305	H	2.360	8.315	-6.532

H	1.642	8.561	-4.957	H	5.443	5.514	-3.405
C	1.384	10.237	-6.277	H	4.906	6.561	-4.726
H	0.542	10.639	-5.706	H	4.850	4.801	-4.912
H	1.200	10.441	-7.334	C	0.517	2.370	-4.324
C	2.663	10.963	-5.838	H	1.436	2.394	-4.917
H	2.906	10.682	-4.808	H	-0.290	2.220	-5.048
H	2.461	12.039	-5.849	C	0.549	1.190	-3.337
C	3.854	10.672	-6.749	H	-0.043	0.369	-3.755
H	4.710	11.271	-6.439	H	0.082	1.468	-2.387
H	3.613	10.922	-7.783	C	1.966	0.684	-3.060
H	4.139	9.620	-6.703	H	2.442	0.394	-4.003
C	-1.491	8.624	-6.197	H	2.568	1.483	-2.617
H	-1.382	9.110	-5.221	C	1.948	-0.512	-2.112
H	-2.291	7.886	-6.077	H	2.966	-0.838	-1.900
C	-1.925	9.652	-7.249	H	1.398	-1.345	-2.552
H	-1.134	10.387	-7.415	H	1.472	-0.245	-1.168
H	-2.116	9.146	-8.199	C	-1.291	3.927	-2.637
C	-3.198	10.375	-6.795	H	-1.452	4.917	-2.200
H	-3.008	10.873	-5.838	H	-1.201	3.215	-1.812
H	-3.994	9.640	-6.635	C	-2.497	3.572	-3.516
C	-3.646	11.404	-7.830	H	-2.493	4.207	-4.407
H	-2.870	12.154	-7.984	H	-2.414	2.533	-3.850
H	-4.551	11.905	-7.489	C	-3.812	3.765	-2.757
H	-3.855	10.919	-8.784	H	-3.927	4.822	-2.495
C	0.170	7.325	-8.297	H	-3.780	3.195	-1.822
H	0.803	6.437	-8.393	C	-5.006	3.310	-3.593
H	-0.825	7.025	-8.641	H	-5.051	3.866	-4.530
C	0.727	8.424	-9.210	H	-5.934	3.475	-3.046
H	1.745	8.678	-8.901	H	-4.924	2.246	-3.825
H	0.118	9.328	-9.138	C	6.592	-8.940	-4.814
C	0.747	7.944	-10.666	H	7.328	-8.503	-4.133
H	1.350	7.032	-10.738	H	5.654	-8.968	-4.249
H	-0.273	7.693	-10.978	C	6.974	-10.389	-5.156
C	1.319	9.016	-11.591	H	6.301	-10.771	-5.929
H	2.341	9.263	-11.303	H	6.797	-10.987	-4.255
H	0.716	9.923	-11.543	C	8.423	-10.600	-5.603
H	1.325	8.657	-12.620	H	8.643	-9.984	-6.479
C	1.556	4.279	-2.341	H	8.527	-11.646	-5.908
H	1.480	3.482	-1.595	C	9.440	-10.308	-4.501
H	1.341	5.222	-1.829	H	9.421	-9.256	-4.210
C	2.987	4.323	-2.897	H	10.443	-10.544	-4.856
H	3.683	4.223	-2.057	H	9.233	-10.914	-3.619
H	3.157	3.469	-3.561	C	7.871	-7.272	-6.958
C	3.292	5.618	-3.653	H	7.634	-6.610	-7.797
H	3.146	6.473	-2.985	H	8.350	-8.160	-7.375
H	2.589	5.730	-4.481	C	8.843	-6.553	-6.015
C	4.714	5.623	-4.207	H	8.394	-5.612	-5.678

H	9.020	-7.165	-5.125	C	5.704	-2.472	-4.605
C	10.174	-6.277	-6.720	H	5.389	-1.576	-4.064
H	9.999	-5.629	-7.585	H	5.725	-2.217	-5.669
H	10.589	-7.220	-7.088	C	7.114	-2.891	-4.172
C	11.176	-5.616	-5.777	H	7.419	-3.770	-4.746
H	10.788	-4.662	-5.414	H	7.104	-3.184	-3.118
H	12.114	-5.432	-6.299	C	8.121	-1.759	-4.390
H	11.375	-6.258	-4.918	H	7.756	-0.845	-3.909
C	5.263	-8.541	-7.429	H	8.211	-1.555	-5.461
H	4.674	-7.759	-7.921	C	9.490	-2.122	-3.819
H	4.544	-9.188	-6.917	H	9.872	-3.026	-4.293
C	6.010	-9.343	-8.504	H	9.421	-2.298	-2.744
H	6.649	-8.671	-9.084	H	10.197	-1.312	-3.995
H	6.653	-10.097	-8.043	C	-1.750	-6.922	7.714
C	5.012	-10.032	-9.441	H	-1.887	-7.851	8.272
H	4.369	-9.274	-9.903	H	-2.742	-6.559	7.428
H	4.371	-10.701	-8.859	C	-1.065	-5.869	8.597
C	5.734	-10.827	-10.527	H	-0.876	-4.975	7.996
H	6.363	-10.170	-11.129	H	-0.095	-6.246	8.936
H	5.008	-11.309	-11.180	C	-1.921	-5.489	9.810
H	6.364	-11.597	-10.080	H	-1.445	-4.638	10.308
C	2.989	-3.019	-5.175	H	-2.909	-5.163	9.467
H	3.240	-2.893	-6.232	C	-2.071	-6.631	10.813
H	2.853	-2.019	-4.754	H	-1.092	-6.988	11.134
C	1.689	-3.824	-5.064	H	-2.620	-7.467	10.377
H	1.899	-4.875	-5.288	H	-2.617	-6.283	11.689
H	1.311	-3.769	-4.038	C	-1.747	-8.523	5.250
C	0.603	-3.331	-6.028	H	-1.032	-9.087	4.644
H	0.955	-3.437	-7.059	H	-2.404	-7.999	4.551
H	-0.276	-3.973	-5.911	C	-2.598	-9.493	6.081
C	0.194	-1.880	-5.782	H	-1.978	-10.016	6.814
H	1.024	-1.199	-5.974	H	-3.363	-8.934	6.627
H	-0.137	-1.743	-4.751	C	-3.276	-10.518	5.165
H	-0.629	-1.609	-6.444	H	-2.511	-11.077	4.617
C	4.091	-3.840	-2.590	H	-3.895	-9.991	4.430
H	5.045	-3.815	-2.056	C	-4.142	-11.487	5.968
H	3.532	-2.946	-2.301	H	-3.535	-12.032	6.691
C	3.329	-5.100	-2.162	H	-4.614	-12.206	5.299
H	3.909	-5.981	-2.446	H	-4.923	-10.947	6.506
H	2.370	-5.155	-2.685	C	0.782	-7.984	6.677
C	3.083	-5.106	-0.652	H	1.355	-8.179	5.764
H	4.043	-5.044	-0.128	H	1.339	-7.214	7.221
H	2.496	-4.222	-0.381	C	0.708	-9.260	7.522
C	2.339	-6.362	-0.206	H	0.244	-10.063	6.942
H	2.904	-7.257	-0.469	H	0.093	-9.088	8.410
H	1.361	-6.416	-0.686	C	2.112	-9.697	7.956
H	2.194	-6.348	0.875	H	2.729	-9.864	7.066

H	2.577	-8.892	8.536
C	2.058	-10.972	8.794
H	3.065	-11.264	9.092
H	1.614	-11.787	8.222
H	1.462	-10.813	9.693
C	0.591	-3.116	2.334
H	0.436	-2.129	1.884
H	0.301	-3.851	1.579
C	2.075	-3.297	2.688
H	2.369	-4.327	2.473
H	2.236	-3.138	3.758
C	2.964	-2.325	1.909
H	2.745	-1.301	2.229
H	2.743	-2.390	0.838
C	4.442	-2.626	2.145
H	4.706	-3.601	1.732
H	4.661	-2.634	3.213
H	5.065	-1.871	1.667
C	-0.119	-1.726	4.720
H	0.898	-1.444	4.434
H	-0.771	-0.905	4.407
C	-0.152	-1.859	6.248
H	0.300	-0.957	6.674
H	0.460	-2.713	6.548
C	-1.568	-2.026	6.802
H	-1.963	-2.997	6.488
H	-2.218	-1.247	6.388
C	-1.583	-1.934	8.326
H	-1.268	-0.942	8.652
H	-0.905	-2.670	8.759
H	-2.588	-2.122	8.703
C	-2.137	-2.871	2.893
H	-1.930	-2.202	2.052
H	-2.484	-3.821	2.475
C	-3.256	-2.280	3.755
H	-3.340	-2.844	4.687
H	-3.010	-1.245	4.010
C	-4.609	-2.322	3.039
H	-5.319	-1.714	3.609
H	-4.981	-3.352	3.043
C	-4.543	-1.816	1.598
H	-4.135	-2.578	0.934
H	-3.916	-0.928	1.527
H	-5.540	-1.557	1.243

($\Delta,\Delta,\Delta,\Lambda$)-C₃-4

	x-coord.	y-coord.	z-coord.
Fe	9.139	6.710	3.008
Fe	-4.369	-6.810	8.912
Fe	-8.249	7.136	-5.533
Fe	4.181	-8.467	-9.119
N	-3.781	-7.229	10.746
C	-2.685	-8.094	13.164
C	-4.444	-7.092	11.889
C	-2.552	-7.793	10.792
C	-1.978	-8.239	11.985
C	-3.942	-7.503	13.113
H	-5.422	-6.639	11.829
H	-0.998	-8.688	11.972
H	-4.528	-7.367	14.007
H	-2.272	-8.432	14.101
N	-4.651	-8.731	8.483
C	-4.828	-11.317	7.457
C	-4.851	-8.939	7.164
C	-4.576	-9.791	9.281
C	-4.661	-11.095	8.819
C	-4.933	-10.224	6.619
H	-4.459	-9.596	10.336
H	-4.600	-11.916	9.514
H	-5.083	-10.344	5.558
H	-4.889	-12.321	7.068
N	-6.239	-6.560	9.431
C	-8.789	-5.898	10.361
C	-7.228	-7.449	9.421
C	-6.510	-5.321	9.897
C	-7.776	-4.960	10.369
C	-8.507	-7.170	9.872
H	-6.991	-8.431	9.044
H	-7.943	-3.961	10.738
H	-9.265	-7.935	9.847
H	-9.774	-5.655	10.726
N	9.281	8.608	2.577
C	8.846	11.292	1.967
C	10.009	9.564	3.143
C	8.354	8.968	1.665
C	8.104	10.306	1.347
C	9.833	10.910	2.870
H	10.774	9.243	3.833

H	7.339	10.548	0.626
H	10.455	11.644	3.355
H	8.676	12.334	1.748
N	10.758	6.229	2.101
C	13.137	5.194	1.078
C	11.052	4.915	2.220
C	11.628	7.010	1.471
C	12.823	6.543	0.948
C	12.235	4.366	1.717
H	11.362	8.051	1.381
H	13.495	7.223	0.452
H	12.429	3.312	1.840
H	14.064	4.805	0.688
N	10.080	6.985	4.689
C	11.152	7.800	7.137
C	11.338	6.708	5.014
C	9.329	7.656	5.591
C	9.837	8.082	6.821
C	11.914	7.089	6.215
H	11.919	6.161	4.288
H	9.201	8.622	7.503
H	12.941	6.837	6.422
H	11.577	8.119	8.074
N	-10.121	6.606	-5.702
C	-12.653	5.517	-6.155
C	-11.217	7.352	-5.611
C	-10.273	5.298	-6.010
C	-11.526	4.723	-6.242
C	-12.493	6.859	-5.828
H	-11.073	8.391	-5.356
H	-11.596	3.676	-6.489
H	-13.344	7.514	-5.744
H	-13.634	5.107	-6.334
N	-8.040	7.476	-7.456
C	-7.538	8.394	-10.044
C	-6.922	8.184	-7.739
C	-8.880	7.215	-8.452
C	-8.675	7.647	-9.752
C	-6.645	8.660	-9.024
H	-9.760	6.641	-8.204
H	-9.394	7.409	-10.518
H	-5.747	9.229	-9.200
H	-7.358	8.754	-11.044
N	-8.717	9.046	-5.219
C	-9.135	11.683	-4.404
C	-9.006	9.999	-6.099
C	-8.662	9.386	-3.913

C	-8.858	10.699	-3.475	H	10.125	3.092	3.011
C	-9.223	11.321	-5.744	C	-9.042	4.569	-6.062
H	-9.086	9.698	-7.132	H	-9.057	3.505	-6.282
H	-8.797	10.925	-2.423	C	-8.444	8.288	-3.023
H	-9.461	12.049	-6.502	H	-8.438	8.475	-1.953
H	-9.293	12.705	-4.099	C	-6.051	8.355	-6.617
N	6.026	-8.827	-9.786	H	-5.118	8.901	-6.724
C	8.740	-9.252	-10.322	C	6.377	-8.777	-7.475
C	6.470	-8.980	-11.030	H	7.023	-8.883	-6.607
C	6.935	-8.893	-8.787	C	1.625	-9.227	-8.575
C	8.297	-9.101	-9.022	H	0.555	-9.209	-8.390
C	7.802	-9.193	-11.346	C	4.095	-6.180	-10.719
H	5.734	-8.941	-11.817	H	4.150	-5.164	-11.099
H	8.982	-9.146	-8.190	N	4.415	-6.468	-9.499
H	8.096	-9.316	-12.375	N	5.100	-8.606	-7.360
H	9.783	-9.418	-10.537	N	2.367	-8.175	-8.469
N	3.495	-8.425	-11.019	N	-7.938	5.209	-5.839
C	2.876	-8.023	-13.719	N	-8.339	7.095	-3.512
C	3.635	-7.212	-11.594	N	-6.391	7.772	-5.512
C	3.057	-9.421	-11.784	N	9.026	4.831	3.355
C	2.737	-9.272	-13.124	N	8.072	6.666	1.344
C	3.332	-6.978	-12.940	N	7.603	7.304	4.069
H	2.963	-10.390	-11.322	N	-4.262	-4.837	9.417
H	2.390	-10.121	-13.690	N	-2.479	-7.300	8.510
H	3.464	-5.990	-13.351	N	-4.918	-6.596	6.990
H	2.640	-7.878	-14.761	C	-1.885	-7.421	7.256
N	3.641	-10.325	-8.992	C	-0.607	-7.628	4.767
C	2.448	-12.843	-9.071	C	-1.713	-6.294	6.450
C	2.300	-10.464	-8.842	C	-1.428	-8.660	6.789
C	4.371	-11.421	-9.158	C	-0.817	-8.764	5.562
C	3.825	-12.694	-9.203	C	-1.076	-6.392	5.235
C	1.676	-11.713	-8.882	H	-2.028	-5.335	6.827
H	5.436	-11.276	-9.264	H	-1.587	-9.544	7.391
H	4.465	-13.550	-9.341	H	-0.481	-9.727	5.205
H	0.605	-11.779	-8.767	H	-0.920	-5.506	4.636
H	1.996	-13.821	-9.113	C	-3.224	-3.926	9.273
C	-1.901	-7.871	9.519	C	-1.101	-2.174	8.685
H	-0.937	-8.365	9.431	C	-3.469	-2.590	8.905
C	-5.400	-4.421	9.875	C	-1.894	-4.339	9.408
H	-5.537	-3.414	10.258	C	-0.855	-3.481	9.131
C	-5.032	-7.745	6.400	C	-2.433	-1.740	8.610
H	-5.298	-7.829	5.350	H	-4.486	-2.250	8.774
C	7.725	7.866	1.009	H	-1.693	-5.339	9.750
H	7.054	8.063	0.177	H	0.164	-3.820	9.239
C	7.972	7.843	5.185	H	-2.641	-0.730	8.289
H	7.277	8.366	5.834	C	-5.304	-5.465	6.280
C	10.035	4.168	2.896	C	-6.005	-3.185	4.778

C	-6.423	-5.475	5.430	H	-5.558	1.598	-4.427
C	-4.576	-4.278	6.389	C	-8.111	6.041	-2.637
C	-4.914	-3.165	5.661	C	-7.557	3.856	-0.958
C	-6.766	-4.361	4.701	C	-7.246	6.177	-1.540
H	-7.044	-6.358	5.379	C	-8.748	4.810	-2.830
H	-3.710	-4.261	7.023	C	-8.487	3.744	-2.002
H	-4.330	-2.262	5.755	C	-6.957	5.104	-0.734
H	-7.633	-4.386	4.057	H	-6.760	7.123	-1.358
C	7.535	5.606	0.615	H	-9.487	4.724	-3.610
C	6.504	3.480	-0.924	H	-9.003	2.805	-2.146
C	8.352	4.540	0.222	H	-6.261	5.215	0.084
C	6.195	5.596	0.202	C	-5.565	7.895	-4.401
C	5.687	4.549	-0.529	C	-3.853	8.085	-2.192
C	7.853	3.509	-0.540	C	-5.051	9.136	-4.004
H	9.400	4.564	0.468	C	-5.224	6.753	-3.671
H	5.543	6.404	0.494	C	-4.366	6.846	-2.602
H	4.645	4.548	-0.816	C	-4.227	9.232	-2.907
H	8.510	2.713	-0.858	H	-5.338	10.026	-4.546
C	6.292	7.482	3.646	H	-5.613	5.798	-3.986
C	3.635	7.799	2.824	H	-4.079	5.959	-2.058
C	5.673	8.738	3.706	H	-3.855	10.196	-2.594
C	5.565	6.389	3.165	C	4.615	-5.411	-8.624
C	4.253	6.540	2.789	C	4.816	-3.369	-6.713
C	4.376	8.898	3.281	C	5.606	-5.454	-7.639
H	6.241	9.593	4.047	C	3.777	-4.286	-8.683
H	6.039	5.423	3.126	C	3.865	-3.295	-7.739
H	3.688	5.684	2.450	C	5.711	-4.448	-6.708
H	3.917	9.875	3.300	H	6.310	-6.270	-7.651
C	7.971	4.130	3.933	H	2.998	-4.242	-9.429
C	5.797	2.760	5.064	H	3.172	-2.467	-7.763
C	7.499	4.471	5.205	H	6.486	-4.480	-5.956
C	7.358	3.076	3.246	C	4.569	-8.502	-6.075
C	6.278	2.421	3.791	C	3.458	-8.274	-3.506
C	6.443	3.790	5.764	C	3.448	-9.257	-5.713
H	8.004	5.245	5.760	C	5.150	-7.662	-5.115
H	7.712	2.818	2.258	C	4.588	-7.529	-3.867
H	5.792	1.632	3.237	C	2.917	-9.161	-4.449
H	6.106	4.041	6.758	H	3.034	-9.954	-6.422
C	-6.765	4.456	-5.791	H	6.018	-7.077	-5.376
C	-4.458	2.847	-5.783	H	5.024	-6.850	-3.148
C	-6.722	3.267	-5.050	H	2.079	-9.781	-4.166
C	-5.624	4.841	-6.501	C	1.785	-6.956	-8.110
C	-4.500	4.044	-6.511	C	0.662	-4.498	-7.347
C	-5.584	2.497	-5.024	C	0.729	-6.403	-8.838
H	-7.581	2.976	-4.466	C	2.258	-6.274	-6.986
H	-5.654	5.745	-7.089	C	1.685	-5.086	-6.594
H	-3.642	4.334	-7.099	C	0.195	-5.185	-8.477

H	0.361	-6.920	-9.714	H	1.812	-12.681	3.922
H	3.060	-6.702	-6.413	H	2.492	-11.707	5.228
H	2.046	-4.584	-5.707	C	3.594	-13.504	4.799
H	-0.594	-4.750	-9.072	H	4.520	-13.165	5.256
C	2.881	-8.145	-2.229	H	3.841	-14.135	3.950
C	2.376	-8.048	-1.126	H	3.056	-14.107	5.525
C	0.130	-3.242	-6.987	C	4.332	-10.054	0.502
C	-0.307	-2.151	-6.668	H	4.381	-9.461	-0.417
C	-7.242	2.758	-0.139	H	3.758	-10.956	0.263
C	-6.952	1.821	0.585	C	5.750	-10.425	0.928
C	-3.365	1.959	-5.844	H	6.329	-9.518	1.112
C	-2.489	1.114	-5.908	H	5.742	-11.017	1.842
C	-2.958	8.153	-1.109	C	6.443	-11.236	-0.168
C	-2.163	8.188	-0.187	H	6.458	-10.654	-1.094
C	0.064	-7.725	3.533	H	5.873	-12.147	-0.359
C	0.660	-7.799	2.473	C	7.867	-11.606	0.228
C	-0.056	-1.338	8.254	H	8.463	-10.714	0.405
C	0.822	-0.631	7.794	H	8.343	-12.184	-0.560
C	-6.280	-2.064	3.977	H	7.869	-12.205	1.134
C	-6.430	-1.082	3.271	C	4.394	-7.920	2.571
C	2.316	7.950	2.362	H	3.733	-7.132	2.946
C	1.184	8.075	1.928	H	5.041	-7.466	1.813
C	4.709	2.071	5.633	C	5.227	-8.447	3.736
C	3.777	1.469	6.137	H	5.891	-9.246	3.411
Pt	-1.311	-0.472	-6.243	H	4.567	-8.843	4.510
P	0.615	0.631	-5.600	C	6.073	-7.323	4.337
P	-3.243	-1.419	-7.068	H	5.417	-6.504	4.647
Pt	1.528	-7.937	0.673	H	6.750	-6.936	3.573
P	3.282	-9.081	1.665	C	6.885	-7.809	5.532
P	-0.480	-7.156	-0.193	H	7.478	-6.999	5.949
Pt	-6.651	0.380	1.936	H	7.561	-8.606	5.235
P	-4.645	-0.241	0.945	H	6.231	-8.193	6.311
P	-8.774	0.889	2.688	C	-1.317	-5.824	0.778
Pt	2.305	0.430	6.989	H	-0.742	-4.905	0.634
Pt	-0.559	8.175	0.978	H	-1.186	-6.120	1.821
C	5.990	2.423	-1.701	C	-2.800	-5.588	0.476
C	5.502	1.526	-2.365	H	-2.901	-4.781	-0.254
C	4.856	-2.377	-5.718	H	-3.251	-6.482	0.043
C	4.845	-1.500	-4.873	C	-3.585	-5.219	1.738
Pt	5.079	-0.010	-3.581	H	-3.042	-4.448	2.286
C	2.613	-10.277	2.899	H	-4.551	-4.803	1.445
H	1.692	-10.668	2.451	C	-3.834	-6.412	2.654
H	2.312	-9.680	3.766	H	-2.901	-6.867	2.977
C	3.482	-11.454	3.332	H	-4.427	-7.166	2.140
H	4.413	-11.105	3.777	H	-4.377	-6.089	3.539
H	3.726	-12.074	2.468	C	-0.721	-6.534	-1.917
C	2.746	-12.317	4.358	H	0.020	-5.743	-2.067

H	-1.715	-6.081	-1.973	H	-5.260	-7.099	-9.025
C	-0.569	-7.582	-3.014	H	-6.083	-5.591	-9.410
H	-1.344	-8.343	-2.910	H	-6.059	-6.183	-7.749
H	0.402	-8.070	-2.916	C	-4.637	-1.389	-5.846
C	-0.687	-6.938	-4.395	H	-4.594	-2.348	-5.319
H	0.109	-6.200	-4.521	H	-4.377	-0.608	-5.125
H	-1.642	-6.411	-4.465	C	-6.046	-1.131	-6.365
C	-0.598	-7.965	-5.517	H	-6.335	-1.898	-7.082
H	-0.726	-7.477	-6.481	H	-6.077	-0.164	-6.870
H	-1.372	-8.720	-5.406	C	-7.063	-1.128	-5.224
H	0.373	-8.456	-5.505	H	-7.112	-2.124	-4.779
C	-1.621	-8.588	-0.016	H	-6.736	-0.433	-4.445
H	-2.463	-8.511	-0.709	C	-8.448	-0.724	-5.713
H	-2.002	-8.539	1.007	H	-8.801	-1.414	-6.475
C	-0.878	-9.911	-0.219	H	-8.421	0.275	-6.145
H	0.097	-9.857	0.295	H	-9.162	-0.729	-4.893
H	-0.679	-10.059	-1.282	C	0.493	2.443	-5.282
C	-1.653	-11.112	0.324	H	1.441	2.795	-4.863
H	-1.178	-12.025	-0.038	H	-0.282	2.566	-4.519
H	-2.673	-11.096	-0.068	C	0.108	3.249	-6.518
C	-1.692	-11.156	1.847	H	-0.707	2.735	-7.036
H	-0.681	-11.160	2.252	H	0.958	3.315	-7.201
H	-2.197	-12.059	2.181	C	-0.351	4.659	-6.150
H	-2.219	-10.300	2.262	H	0.418	5.150	-5.549
C	-3.625	-0.366	-8.548	H	-1.255	4.590	-5.540
H	-2.644	0.078	-8.768	C	-0.632	5.498	-7.391
H	-4.261	0.454	-8.204	H	-1.376	5.014	-8.020
C	-4.175	-0.972	-9.843	H	0.273	5.628	-7.979
H	-3.815	-1.993	-9.973	H	-1.001	6.482	-7.112
H	-3.773	-0.390	-10.675	C	1.417	0.094	-4.019
C	-5.697	-0.945	-9.959	H	1.099	0.776	-3.225
H	-6.151	-1.522	-9.153	H	2.516	0.178	-4.125
H	-6.046	0.086	-9.862	C	1.033	-1.338	-3.654
C	-6.157	-1.510	-11.298	H	1.699	-1.696	-2.865
H	-5.835	-2.543	-11.411	H	1.172	-1.982	-4.525
H	-5.744	-0.933	-12.121	C	-0.416	-1.437	-3.186
H	-7.240	-1.482	-11.373	H	-1.084	-1.091	-4.002
C	-3.160	-3.173	-7.629	H	-0.570	-0.779	-2.326
H	-2.602	-3.701	-6.848	C	-0.795	-2.866	-2.818
H	-2.522	-3.172	-8.518	H	-0.667	-3.518	-3.678
C	-4.466	-3.912	-7.906	H	-1.834	-2.920	-2.501
H	-5.058	-3.389	-8.654	H	-0.169	-3.235	-2.008
H	-5.058	-3.977	-6.991	C	1.985	0.482	-6.817
C	-4.185	-5.329	-8.409	H	2.656	1.338	-6.699
H	-3.578	-5.862	-7.672	H	2.544	-0.427	-6.574
H	-3.609	-5.275	-9.336	C	1.446	0.407	-8.244
C	-5.476	-6.097	-8.663	H	0.810	-0.481	-8.332

H	0.823	1.280	-8.452	C	-5.103	-1.164	-0.578
C	2.564	0.339	-9.282	H	-4.222	-1.662	-0.992
H	3.229	-0.497	-9.047	H	-5.473	-0.437	-1.305
H	3.156	1.257	-9.237	C	-6.220	-2.157	-0.259
C	2.014	0.167	-10.692	H	-5.844	-2.938	0.405
H	1.433	-0.751	-10.765	H	-7.010	-1.615	0.284
H	2.822	0.122	-11.416	C	-6.823	-2.801	-1.506
H	1.368	1.001	-10.954	H	-7.673	-3.414	-1.203
C	-8.856	2.669	3.175	H	-7.198	-2.020	-2.171
H	-8.363	2.731	4.152	C	-5.829	-3.678	-2.260
H	-8.213	3.186	2.454	H	-5.402	-4.426	-1.596
C	-10.204	3.381	3.217	H	-5.021	-3.084	-2.682
H	-10.858	2.933	3.963	H	-6.330	-4.196	-3.074
H	-10.690	3.308	2.243	C	-3.359	0.961	0.366
C	-10.022	4.859	3.562	H	-2.416	0.418	0.249
H	-9.525	4.948	4.530	H	-3.230	1.694	1.166
H	-9.377	5.329	2.813	C	-3.703	1.687	-0.931
C	-11.360	5.586	3.615	H	-3.670	0.983	-1.765
H	-12.002	5.151	4.376	H	-4.716	2.093	-0.868
H	-11.872	5.521	2.657	C	-2.715	2.818	-1.215
H	-11.215	6.636	3.855	H	-1.693	2.443	-1.113
C	-9.349	-0.142	4.103	H	-2.848	3.615	-0.479
H	-9.427	-1.152	3.684	C	-2.902	3.379	-2.619
H	-8.509	-0.169	4.805	H	-2.678	2.619	-3.366
C	-10.632	0.243	4.848	H	-2.245	4.230	-2.785
H	-11.147	-0.670	5.154	H	-3.931	3.701	-2.767
H	-11.312	0.787	4.195	C	-3.573	-1.477	1.798
C	-10.358	1.076	6.100	H	-2.831	-1.846	1.082
H	-9.745	0.491	6.791	H	-4.219	-2.308	2.088
H	-9.791	1.971	5.838	C	-2.888	-0.925	3.044
C	-11.653	1.481	6.792	H	-3.658	-0.557	3.727
H	-12.225	0.603	7.081	H	-2.241	-0.088	2.777
H	-12.272	2.086	6.133	C	-2.055	-1.999	3.744
H	-11.444	2.060	7.687	H	-1.294	-2.373	3.054
C	-9.912	0.596	1.253	H	-2.707	-2.836	4.005
H	-9.335	-0.088	0.618	C	-1.380	-1.480	5.008
H	-9.970	1.542	0.711	H	-0.890	-2.290	5.542
C	-11.307	-0.009	1.460	H	-2.111	-1.032	5.677
H	-11.299	-0.678	2.321	H	-0.628	-0.728	4.779
H	-11.532	-0.623	0.585	P	5.928	1.370	-5.226
C	-12.444	1.001	1.614	P	4.504	-1.375	-1.787
H	-12.237	1.690	2.433	C	4.876	2.889	-5.248
H	-13.349	0.449	1.873	H	5.166	3.459	-4.363
C	-12.716	1.797	0.342	H	3.859	2.520	-5.060
H	-11.864	2.416	0.063	C	4.865	3.775	-6.489
H	-13.571	2.450	0.490	H	5.865	4.162	-6.685
H	-12.940	1.127	-0.485	H	4.549	3.186	-7.352

C	3.906	4.959	-6.334	H	5.006	-3.685	-2.241
H	3.827	5.462	-7.299	H	3.584	-3.155	-3.113
H	2.912	4.592	-6.068	C	3.161	-3.900	-1.139
C	4.367	5.974	-5.294	H	2.819	-4.822	-1.618
H	5.371	6.323	-5.524	H	2.271	-3.306	-0.921
H	4.368	5.549	-4.293	C	3.848	-4.277	0.171
H	3.703	6.835	-5.294	H	4.335	-3.399	0.600
C	5.970	0.668	-6.933	H	4.622	-5.020	-0.027
H	4.928	0.584	-7.257	C	2.857	-4.832	1.185
H	6.336	-0.356	-6.796	H	3.349	-5.012	2.137
C	6.807	1.344	-8.016	H	2.427	-5.786	0.830
H	7.847	1.417	-7.700	H	2.042	-4.130	1.352
H	6.445	2.351	-8.221	H	2.302	-1.032	-0.812
C	6.756	0.535	-9.313	C	3.322	-0.841	-0.469
H	5.720	0.458	-9.654	H	3.513	-1.454	0.412
H	7.116	-0.479	-9.121	C	3.464	0.636	-0.120
C	7.603	1.179	-10.403	H	4.506	0.862	0.109
H	7.558	0.594	-11.317	H	3.190	1.236	-0.991
H	8.643	1.245	-10.093	C	2.604	1.044	1.076
H	7.248	2.183	-10.623	H	1.550	0.862	0.856
H	8.321	1.259	-5.514	H	2.729	2.118	1.227
C	7.685	1.807	-4.816	C	3.000	0.308	2.351
H	7.841	1.364	-3.827	H	2.636	-0.716	2.344
C	8.104	3.280	-4.754	H	2.603	0.798	3.237
H	8.892	3.373	-4.003	H	4.084	0.284	2.441
H	7.268	3.890	-4.408	P	0.183	10.147	0.046
C	8.643	3.844	-6.070	P	-1.294	6.556	2.437
H	8.705	4.930	-5.978	P	1.266	2.272	7.908
H	7.953	3.619	-6.883	P	3.436	-1.533	6.500
C	10.027	3.311	-6.422	C	1.968	10.240	-0.429
H	10.743	3.561	-5.643	H	2.020	10.011	-1.498
H	10.372	3.753	-7.352	H	2.452	9.415	0.104
H	10.024	2.230	-6.546	C	2.725	11.531	-0.123
C	6.100	-1.507	-0.876	H	2.615	11.781	0.933
H	6.257	-0.552	-0.370	H	2.330	12.358	-0.712
H	6.068	-2.301	-0.126	C	4.213	11.369	-0.434
C	7.236	-1.753	-1.870	H	4.337	11.129	-1.493
H	7.165	-1.007	-2.681	H	4.609	10.528	0.146
H	7.112	-2.739	-2.324	C	4.994	12.636	-0.107
C	8.621	-1.671	-1.231	H	6.041	12.529	-0.384
H	9.356	-2.052	-1.942	H	4.937	12.862	0.955
H	8.653	-2.315	-0.349	H	4.591	13.482	-0.657
C	9.014	-0.252	-0.841	C	-0.767	10.864	-1.359
H	8.974	0.399	-1.712	H	-0.933	10.035	-2.056
H	10.028	-0.240	-0.449	H	-1.746	11.130	-0.949
H	8.349	0.148	-0.078	C	-0.161	12.045	-2.112
C	4.058	-3.153	-2.128	H	0.784	11.750	-2.570

H	0.034	12.876	-1.436	C	-3.006	5.861	2.290
C	-1.109	12.525	-3.213	H	-3.697	6.673	2.529
H	-1.319	11.697	-3.896	H	-3.131	5.645	1.223
H	-2.055	12.836	-2.764	C	-3.323	4.609	3.106
C	-0.515	13.692	-3.992	H	-3.336	4.848	4.169
H	0.421	13.403	-4.465	H	-2.549	3.860	2.935
H	-0.319	14.533	-3.331	C	-4.666	3.977	2.736
H	-1.201	14.023	-4.766	H	-5.474	4.693	2.899
C	-0.091	11.245	1.506	H	-4.669	3.708	1.677
H	0.735	11.051	2.197	C	-4.911	2.728	3.578
H	-1.004	10.848	1.980	H	-5.110	2.993	4.613
C	-0.265	12.747	1.289	H	-4.038	2.077	3.554
H	0.624	13.171	0.822	H	-5.774	2.160	3.194
H	-1.117	12.931	0.634	C	1.512	2.138	9.731
C	-0.509	13.463	2.619	H	2.497	2.570	9.938
H	0.335	13.284	3.289	H	1.575	1.065	9.945
H	-1.402	13.051	3.095	C	0.462	2.753	10.654
C	-0.687	14.963	2.420	H	0.363	3.823	10.472
H	0.200	15.400	1.968	H	-0.506	2.283	10.473
H	-0.860	15.453	3.373	C	0.845	2.540	12.120
H	-1.538	15.166	1.774	H	1.814	3.004	12.314
C	-1.189	7.463	4.045	H	0.945	1.470	12.316
H	-0.124	7.493	4.296	C	-0.194	3.134	13.062
H	-1.483	8.489	3.787	H	-0.292	4.205	12.901
C	-2.004	7.005	5.250	H	0.096	2.972	14.095
H	-1.766	5.967	5.486	H	-1.167	2.673	12.904
H	-3.070	7.072	5.023	C	-0.552	2.229	7.578
C	-1.706	7.860	6.486	H	-0.645	1.887	6.540
H	-0.633	7.839	6.689	H	-0.932	1.419	8.207
H	-2.213	7.412	7.344	C	-1.398	3.484	7.768
C	-2.168	9.306	6.350	H	-1.021	4.292	7.139
H	-1.596	9.838	5.593	H	-1.362	3.816	8.805
H	-2.035	9.828	7.294	C	-2.854	3.194	7.397
H	-3.222	9.349	6.086	H	-2.912	2.919	6.340
C	-0.195	5.068	2.534	H	-3.205	2.338	7.978
H	0.772	5.389	2.137	C	-3.766	4.383	7.671
H	-0.609	4.350	1.821	H	-3.457	5.252	7.095
C	0.025	4.418	3.902	H	-3.741	4.647	8.725
H	0.665	5.075	4.495	H	-4.794	4.145	7.408
H	-0.918	4.300	4.433	C	1.875	3.950	7.430
C	0.685	3.042	3.775	H	2.952	3.827	7.272
H	1.065	2.724	4.751	H	1.439	4.172	6.452
H	1.541	3.113	3.102	C	1.635	5.120	8.380
C	-0.282	1.976	3.272	H	2.146	4.943	9.327
H	-1.151	1.918	3.925	H	0.572	5.240	8.586
H	0.205	1.005	3.267	C	2.165	6.420	7.773
H	-0.620	2.189	2.259	H	3.233	6.314	7.565

H	1.664	6.603	6.818
C	1.940	7.605	8.704
H	2.307	8.523	8.252
H	2.462	7.456	9.645
H	0.881	7.729	8.919
C	4.761	-1.567	7.772
H	5.579	-0.936	7.416
H	5.139	-2.582	7.916
C	4.212	-0.991	9.079
H	3.395	-1.617	9.448
H	3.802	0.016	8.868
C	5.280	-0.871	10.162
H	6.106	-0.260	9.791
H	5.677	-1.862	10.392
C	4.717	-0.245	11.433
H	3.897	-0.843	11.825
H	4.346	0.758	11.234
H	5.486	-0.181	12.197
C	4.302	-1.753	4.883
H	4.511	-0.740	4.529
H	3.573	-2.197	4.199
C	5.599	-2.560	4.874
H	5.454	-3.541	5.324
H	6.361	-2.038	5.455
C	6.107	-2.743	3.444
H	6.225	-1.762	2.975
H	5.364	-3.300	2.868
C	7.436	-3.486	3.409
H	7.772	-3.628	2.384
H	7.339	-4.463	3.876
H	8.200	-2.929	3.945
C	2.478	-3.088	6.775
H	1.530	-2.956	6.243
H	2.240	-3.089	7.841
C	3.094	-4.427	6.383
H	3.234	-4.470	5.301
H	4.066	-4.559	6.862
C	2.173	-5.573	6.809
H	1.159	-5.374	6.452
H	2.137	-5.615	7.900
C	2.638	-6.918	6.267
H	2.602	-6.923	5.179
H	1.993	-7.716	6.628
H	3.656	-7.129	6.586