

Introduction of Hetero Functional Group onto Molecular hexagons by Coordination  
Driven Self Assembly

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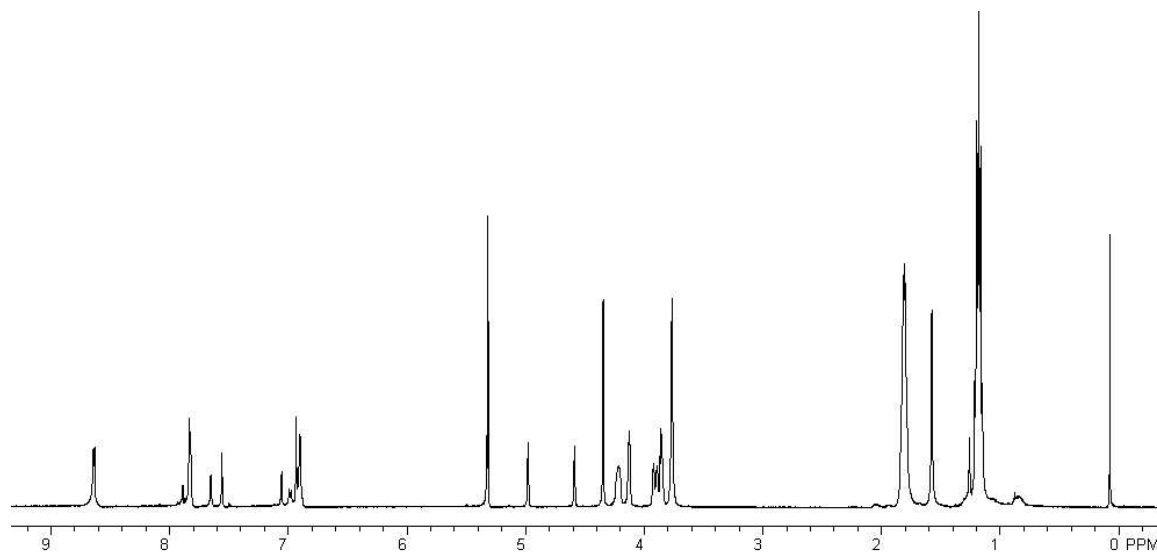
\* To whom correspondence should be addressed.

### **General Experimental Section:**

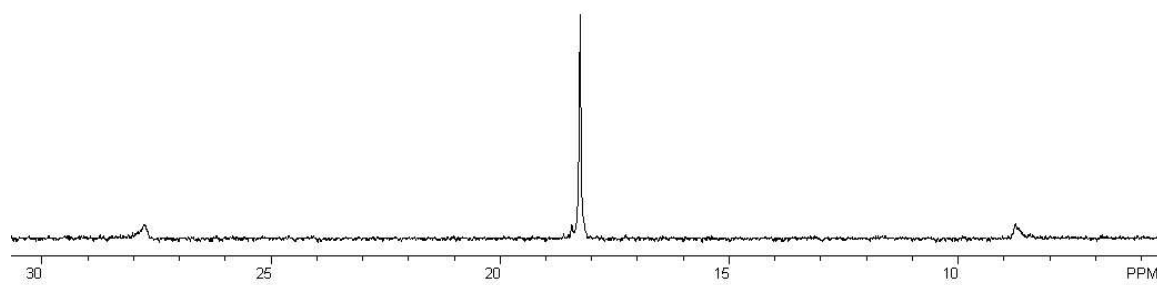
All reagents were purchased and used without further purification. NMR spectra were recorded on a 500 MHz spectrometer. The  $^1\text{H}$  NMR chemical shifts are reported relative to residual solvent signals, and  $^{31}\text{P}$  NMR resonances are referenced to an external unlocked sample of 85%  $\text{H}_3\text{PO}_4$  ( $\delta$  0.0). Mass spectra for **5**, **6**, **8** and **9** were recorded on a Quattro II triple-quadrupole mass spectrometer using electrospray ionization.

**Figure S1.** A)  $^1\text{H}$  and B)  $^{31}\text{P}$  NMR spectra of **5** in  $\text{CD}_2\text{Cl}_2$

A.

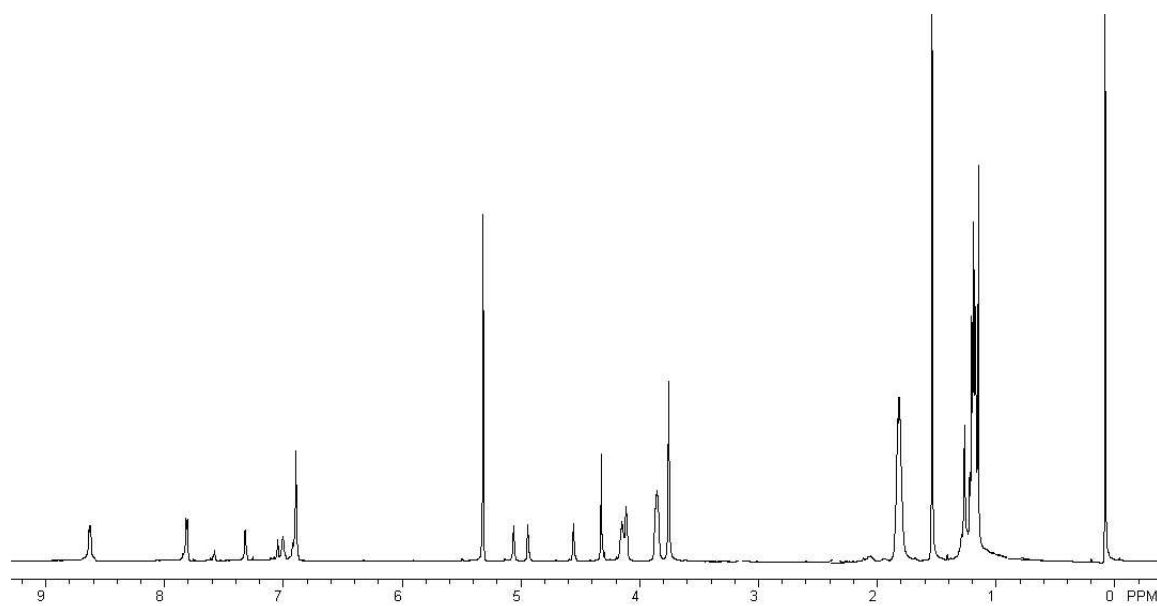


B.

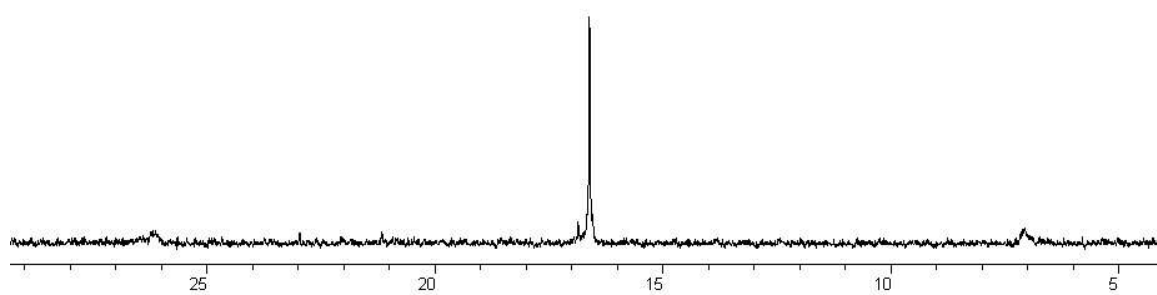


**Figure S2.** A)  $^1\text{H}$  and B)  $^{31}\text{P}$  NMR spectra of **6** in  $\text{CD}_2\text{Cl}_2$

**A.**

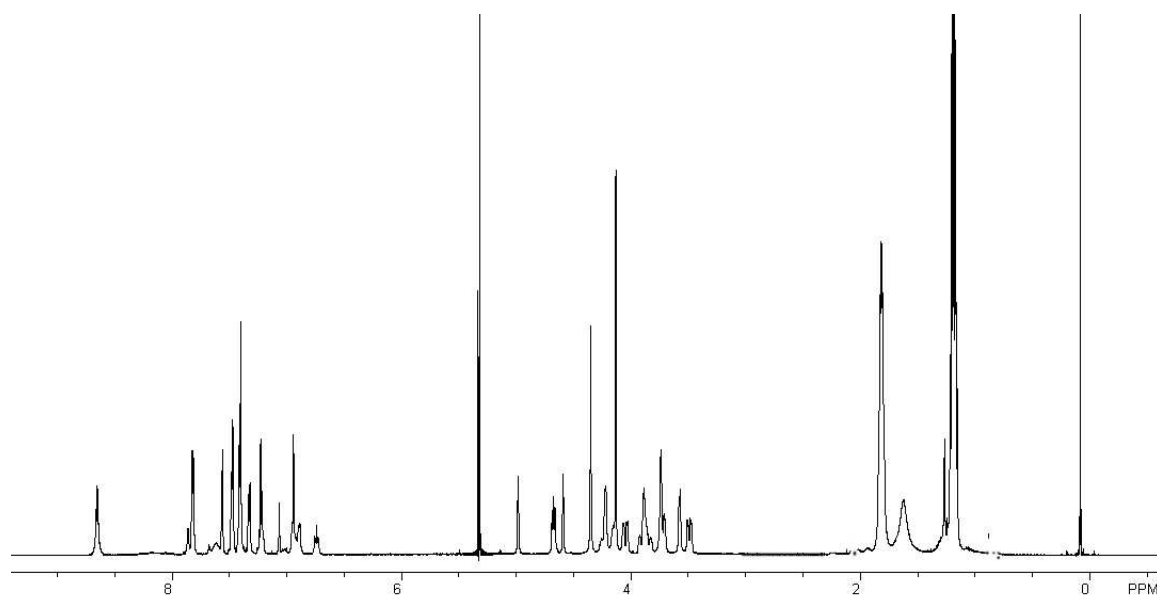


**B**

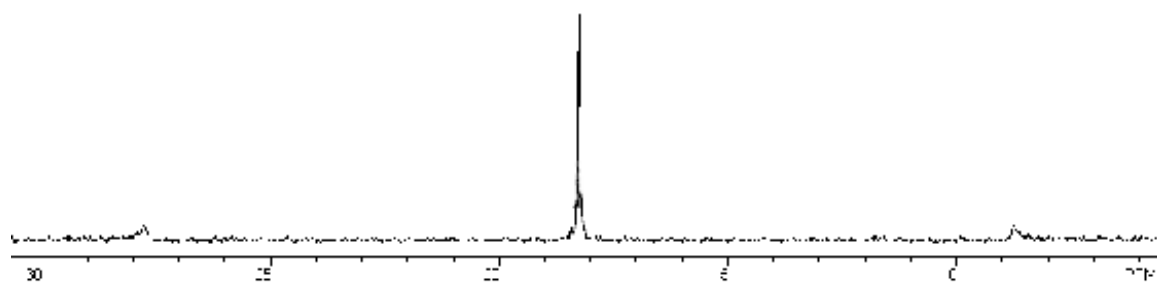


**Figure S3.** A)  $^1\text{H}$  and B)  $^{31}\text{P}$  NMR spectrum of **8** in  $\text{CD}_2\text{Cl}_2$ .

A.

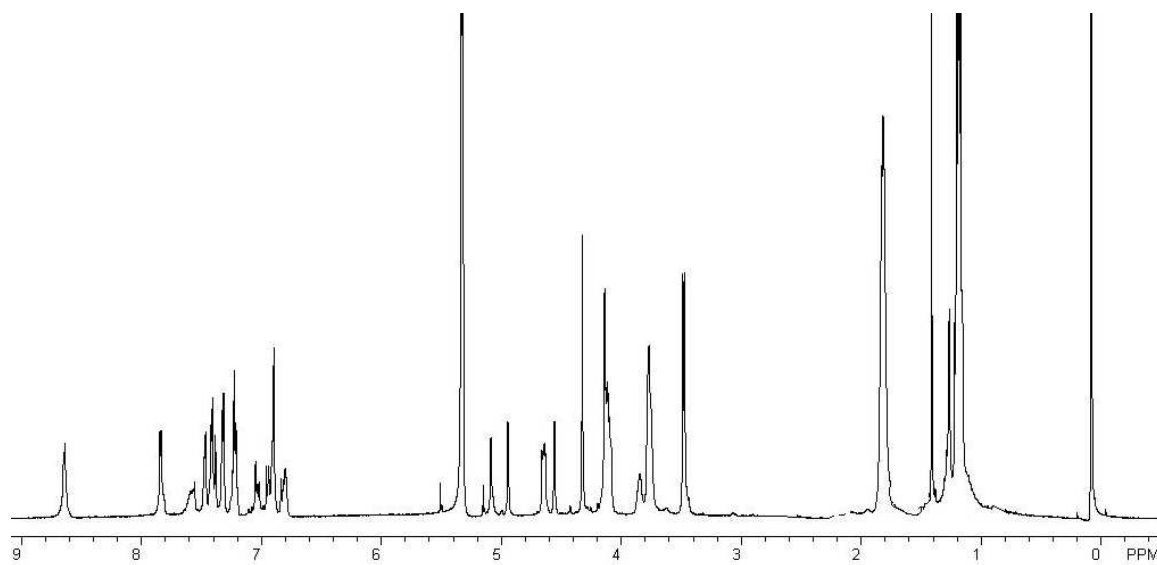


B.



**Figure S4.** A)  $^1\text{H}$  and B)  $^{31}\text{P}$  NMR spectra of **9** in  $\text{CD}_2\text{Cl}_2$ .

A.



B.

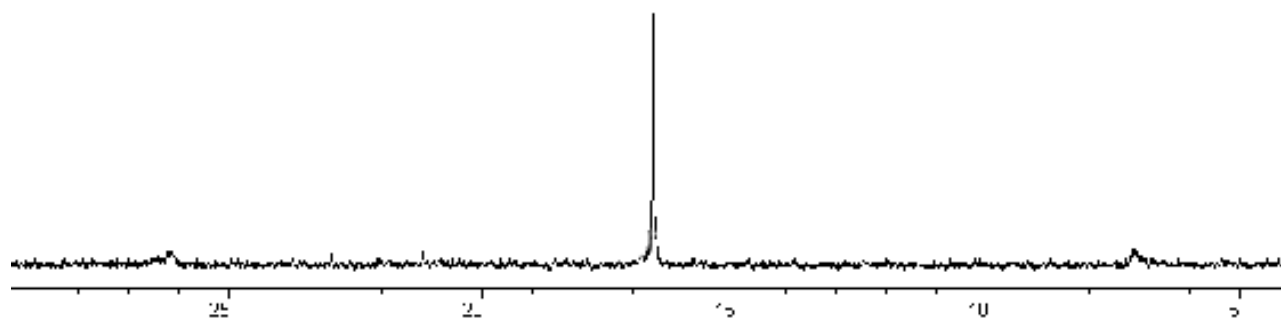
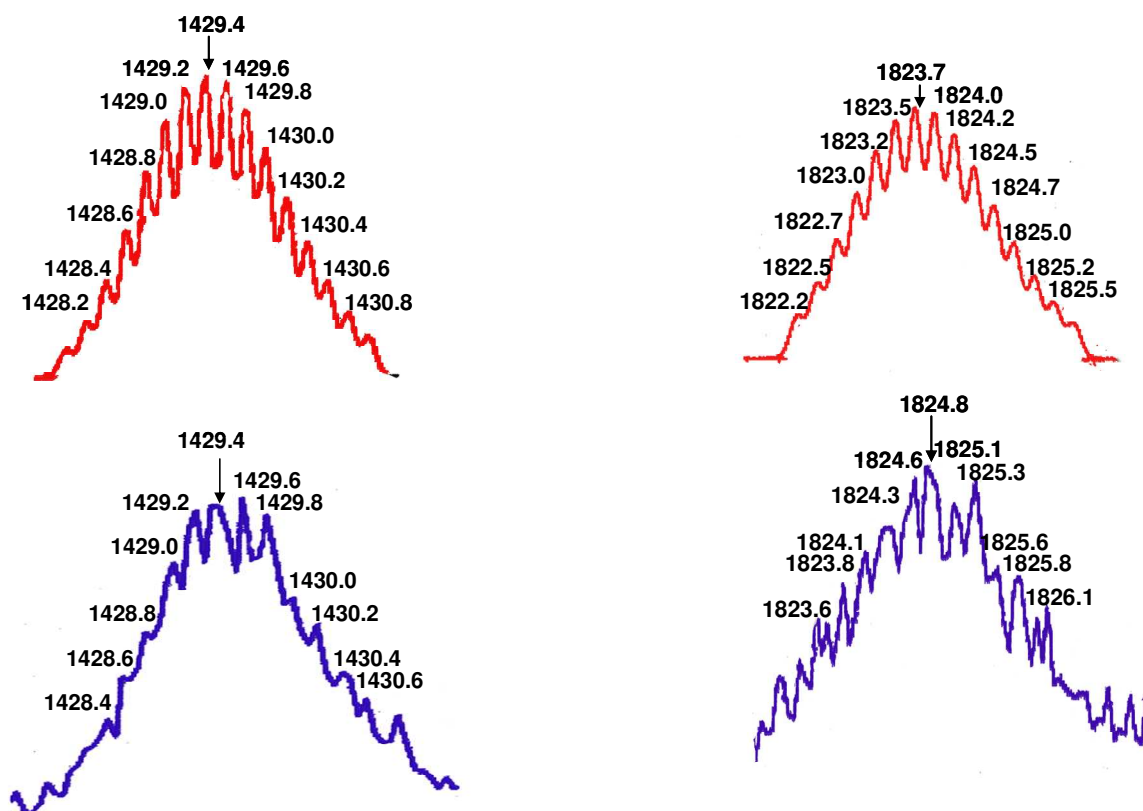
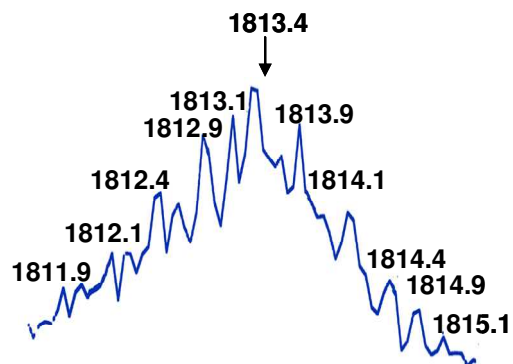
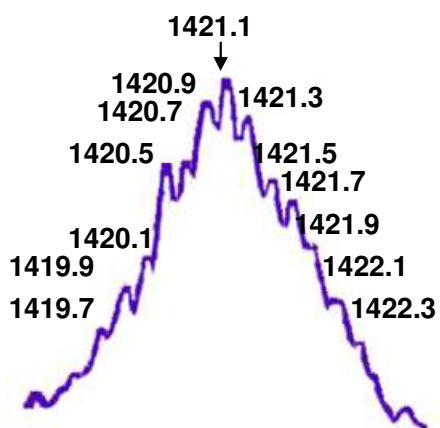
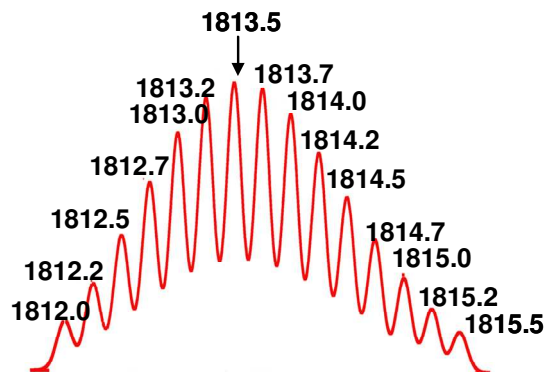


Figure S5. ESI-MS of **8**:



Calculated (top) and experimental (bottom) ESI-MS spectra of **8**.

Figure S6. ESI-MS of **9**:



A.  $[M-5OTf]^{5+}$

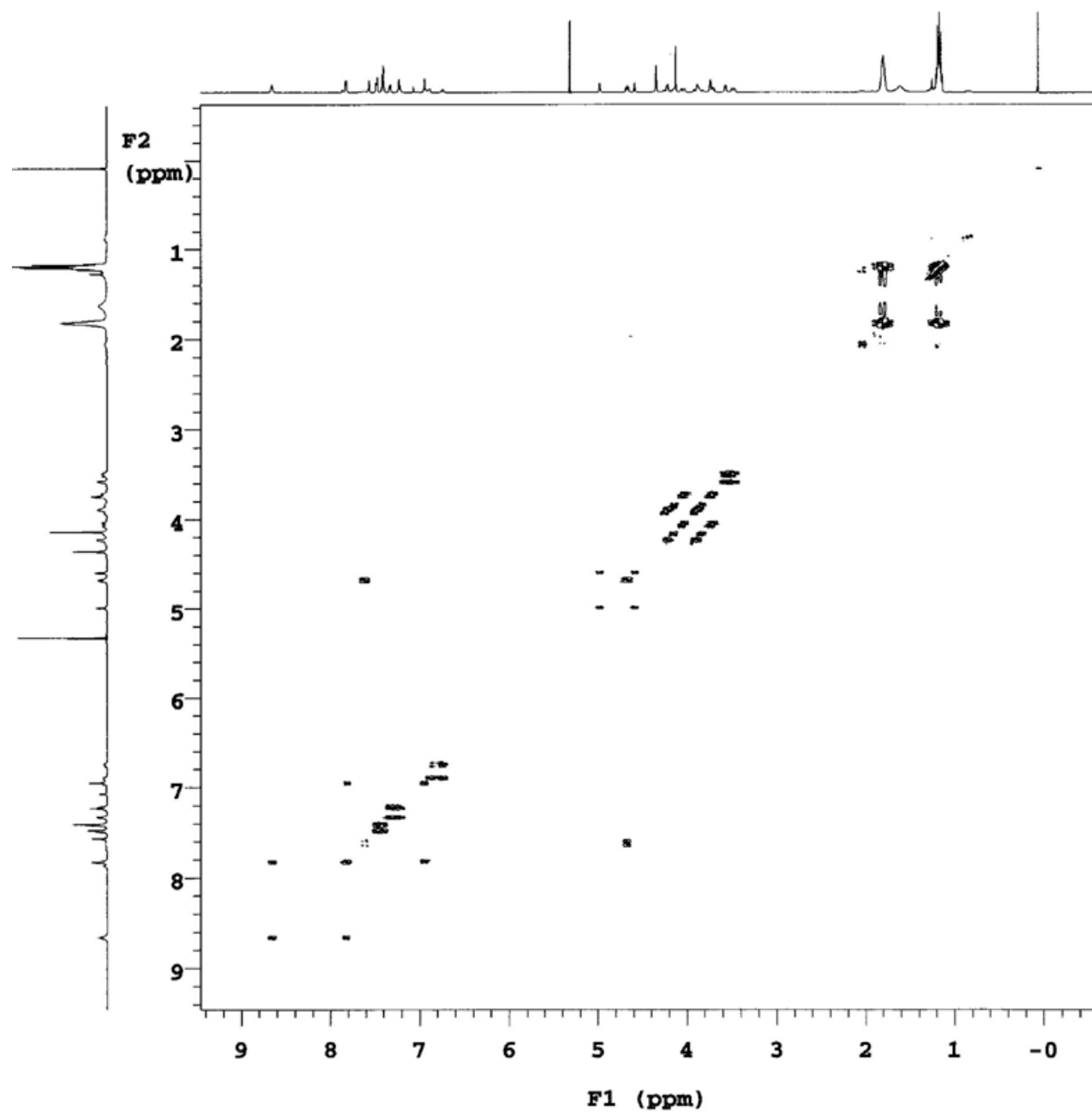
B.  $[M-4OTf]^{4+}$

Calculated (top) and experimental (bottom) ESI-MS spectra of **9**.

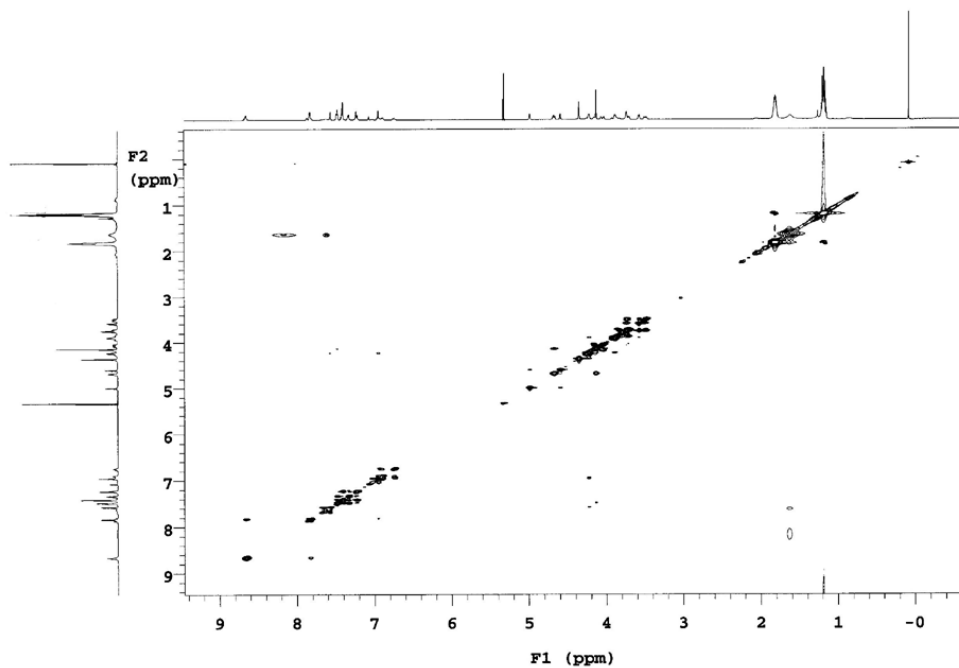


**Figure S7.**  $^1\text{H}$ - $^1\text{H}$  COSY and NOESY NMR spectra of **8**.

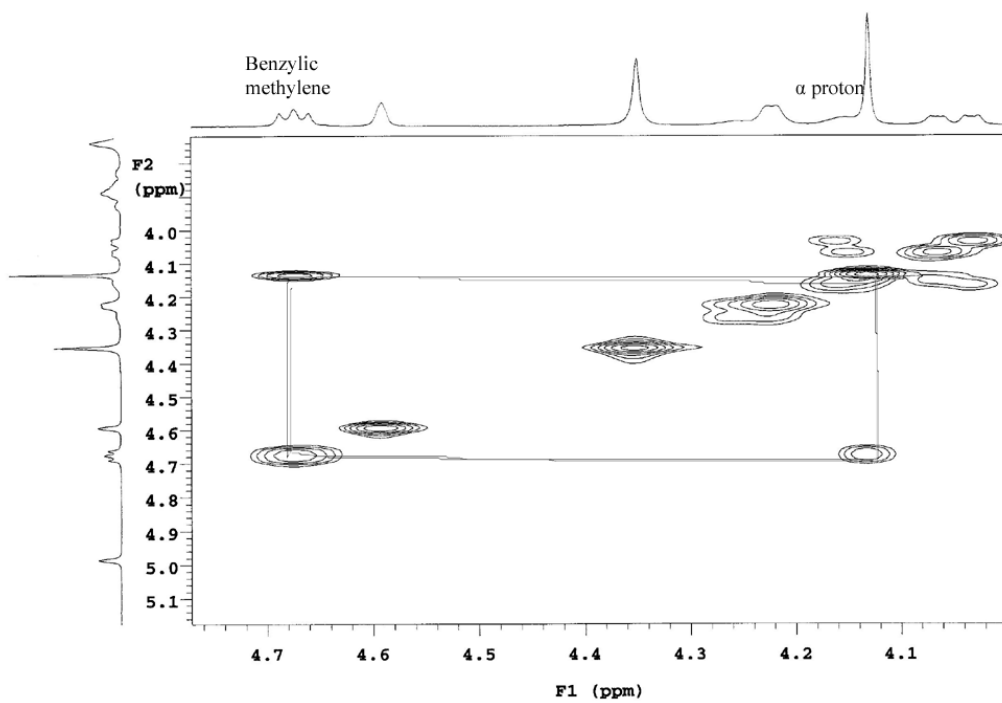
A. gDQCOSY of **8**:



B. NOESY of 8:

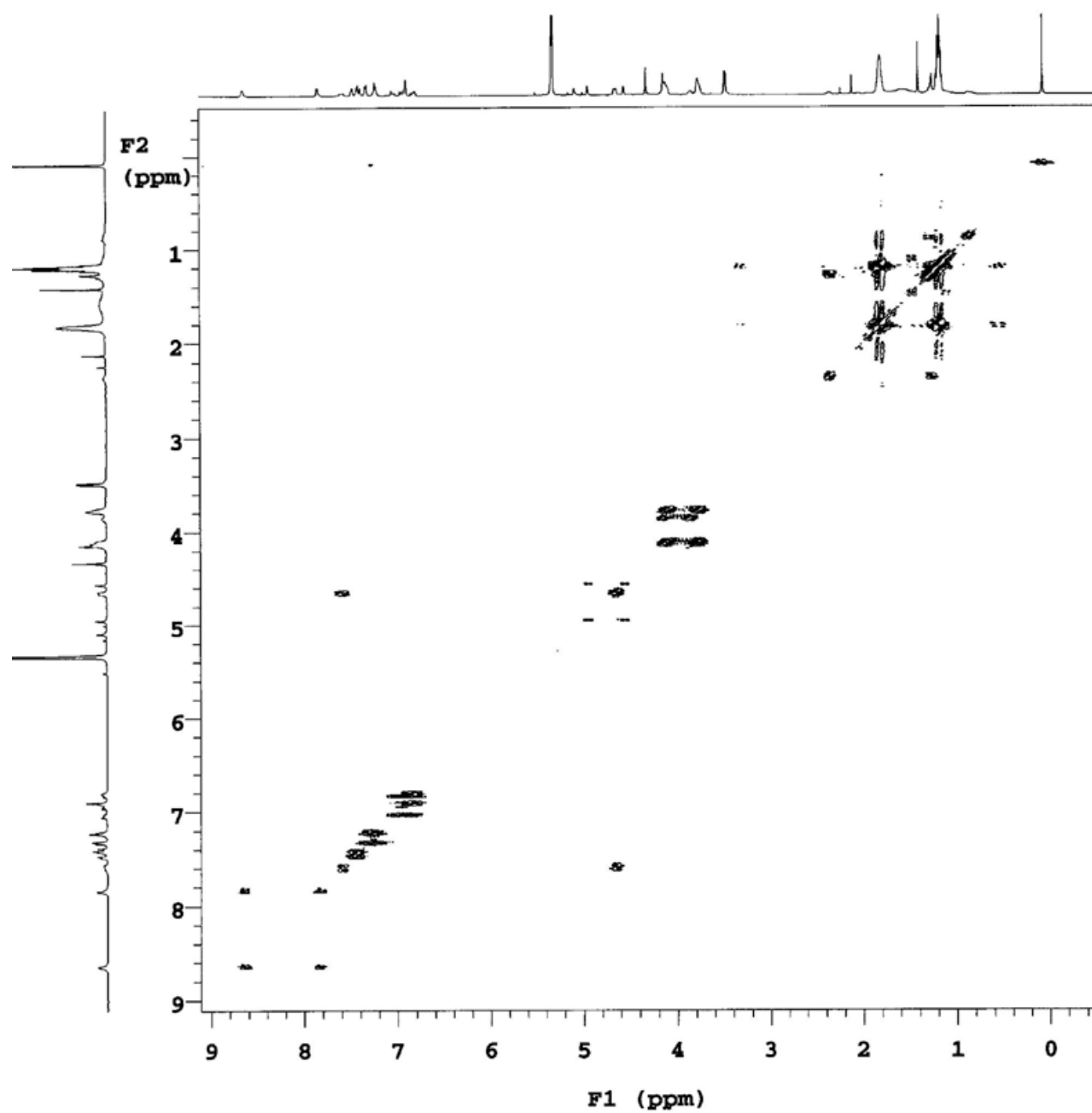


C. Expanded NOESY of 8:

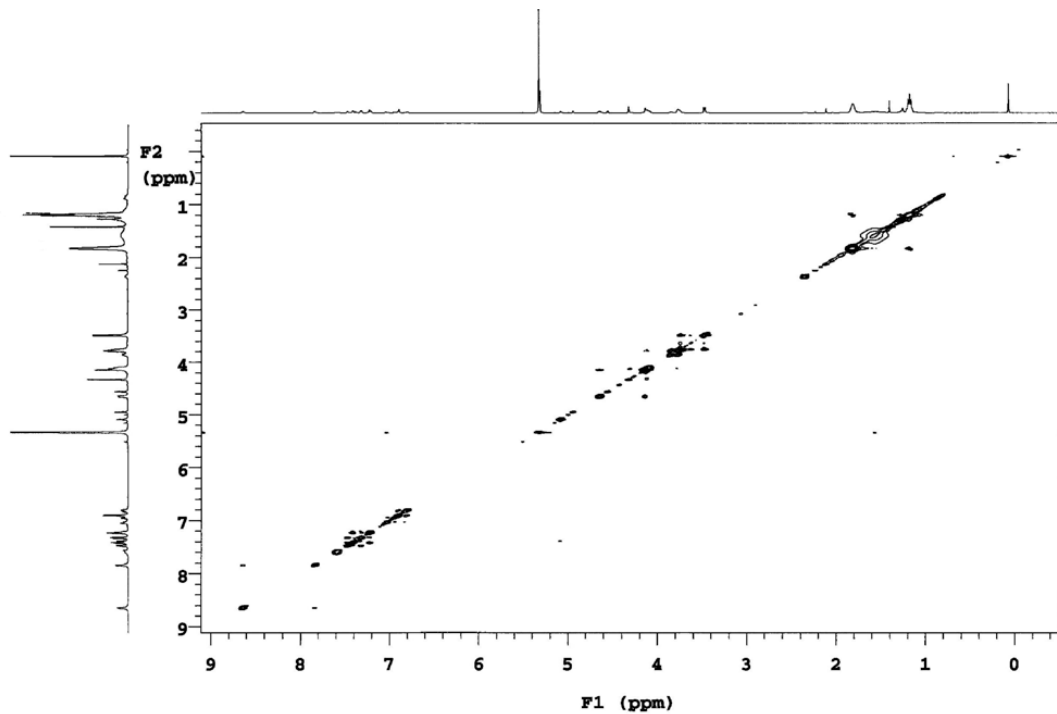


**Figure S8.**  $^1\text{H}$ - $^1\text{H}$  COSY and NOESY NMR spectra of **9**.

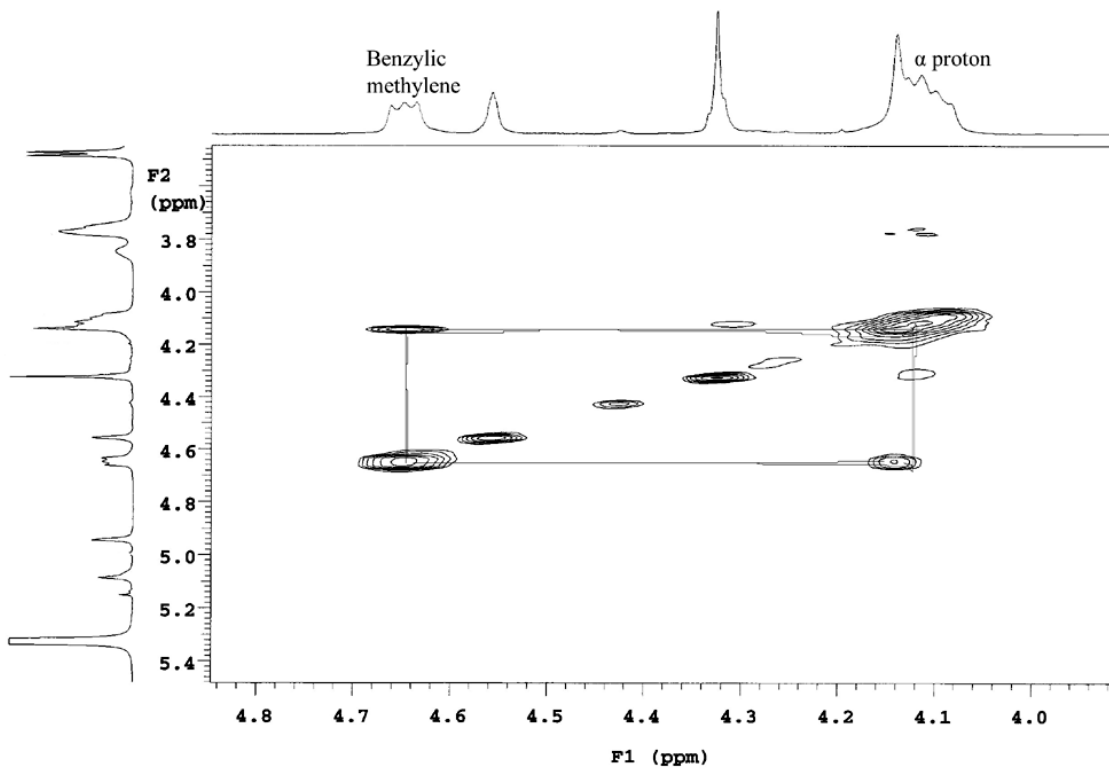
A. gDQCOSY of **9** :



B. NOESY of 9:



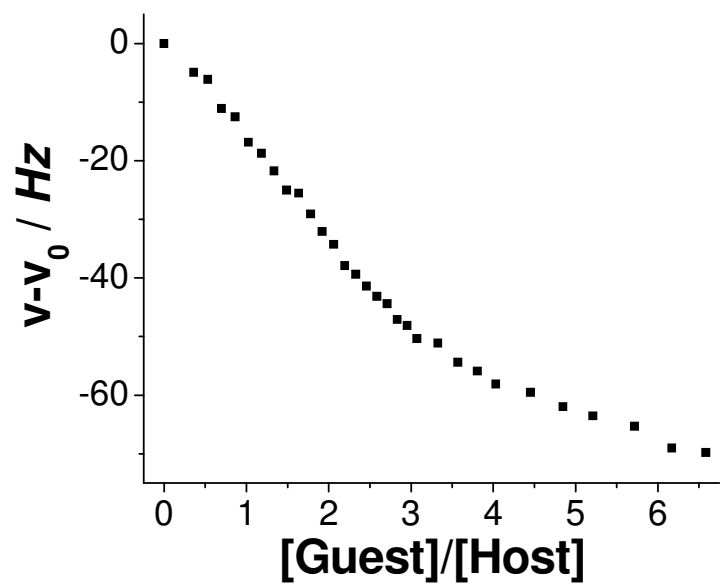
C. Expanded NOESY of 9



**Figure S9:** Experimental Data for  $^1\text{H}$  NMR Titration Experiments**A. NMR Titration Data for 8:**

	$\delta$	$[\delta - \delta_0]$ PPM	$[\delta - \delta_0]$ Hz	Guest:Host	V/mL	[Guest] $\times 10^{-3}$ M
0	$\delta_0=3.767$	0	0	0:1	0	0
1	3.7571	-0.0099	-4.95	0.181:1	0.759	0.13086
2	3.75477	-0.01223	-6.115	0.3598:1	0.768	0.25866
3	3.7448	-0.0222	-11.1	0.5306:1	0.777	0.38349
4	3.7419	-0.0251	-12.55	0.6993:1	0.786	0.50547
5	3.7332	-0.03377	-16.885	0.8642:1	0.795	0.62468
6	3.7295	-0.0375	-18.750	1.0258:1	0.804	0.74122
7	3.7235	-0.0435	-21.75	1.1832:1	0.813	0.85519
8	3.7169	-0.0501	-25.05	1.3374:1	0.822	0.96666
9	3.7159	-0.0511	-25.55	1.4883:1	0.831	1.0757
10	3.7088	-0.0582	-29.10	1.6359:1	0.84	1.18243
11	3.7028	-0.0642	-32.1	1.7804:1	0.849	1.28688
12	3.6984	-0.0686	-34.3	1.9219:1	0.858	1.38915
13	3.69115	-0.7585	-37.925	2.0604:1	0.867	1.48929
14	3.6882	-0.0788	-39.4	2.1961:1	0.876	1.58737
15	3.6842	-0.0828	-41.4	2.3291:1	0.885	1.68346
16	3.6807	-0.0863	-43.15	2.4593:1	0.894	1.77761
17	3.6781	-0.0889	-44.45	2.5870:1	0.903	1.86989
18	3.6727	-0.0943	-47.15	2.7122:1	0.912	1.96034
19	3.6707	-0.0963	-48.15	2.8344:1	0.921	2.04903
20	3.6662	-0.1008	-50.39	2.9552:1	0.930	2.136
21	3.6647	-0.1023	-51.15	3.0732:1	0.939	2.213
22	3.6581	-0.1089	-54.45	3.3275:1	0.959	2.40513
23	3.6552	-0.1118	-55.90	3.5715:1	0.979	2.58145
24	3.6507	-0.1163	-58.15	3.8056:1	0.999	2.75071
25	3.6479	-0.1191	-59.55	4.0306:1	1.019	2.91333
26	3.6430	-0.124	-62.0	4.4551:1	1.059	3.22014
27	3.6399	-0.1271	-63.55	4.8487:1	1.099	3.50461
28	3.6363	-0.1307	-65.35	5.2146:1	1.139	3.76910
29	3.6289	-0.1381	-69.05	5.7177:1	1.199	4.13275
30	3.6274	-0.1396	-69.80	6.1728:1	1.259	4.46173
31	3.6195	-0.1475	-73.75	6.5866:1	1.319	4.76079

[Host] =  $7.228 \times 10^{-4}$ M  
0.75ml solvent



The calculation of  $K_s$ :

$$K_{s,1} = (2.45 \pm 0.44) \times 10^3 \text{ M}^{-1}$$

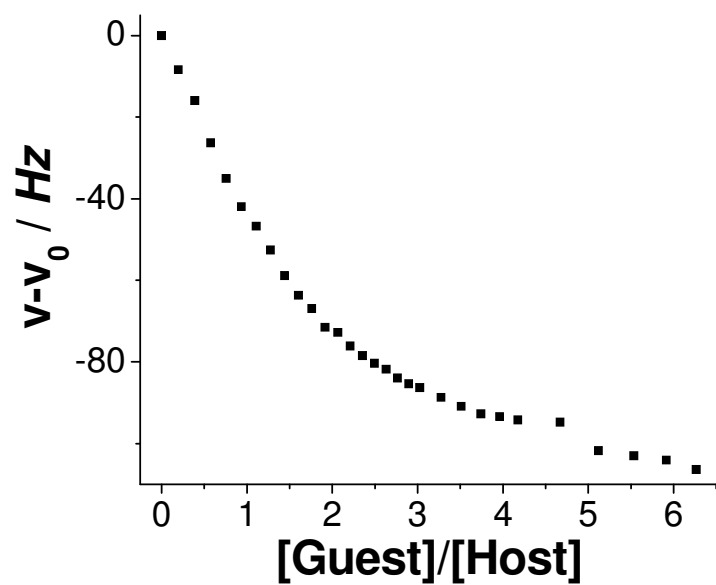
$$K_{s,2} = (1.66 \pm 0.19) \times 10^3 \text{ M}^{-1}$$

$$K_{s,3} = (4.02 \pm 0.19) \times 10^2 \text{ M}^{-1}$$

B. <sup>1</sup>H NMR Titration Experiment for **9**:

	$\delta$	$[\delta - \delta_0]$ PPM	$[\delta - \delta_0]$ Hz	Guest:Host	V/mL	[Guest]X10 <sup>-3</sup> M
0	$\delta_0=3.755$	0	0	0:1	0	0
1	3.7382	-0.0168	-8.40	0.1970:1	0.76	0.1423
2	3.7231	-0.0319	-15.95	0.3888:1	0.77	0.2808
3	3.7024	-0.0526	-26.30	0.5757:1	0.78	0.4158
4	3.68495	-0.07005	-35.025	0.7579:1	0.79	0.5474
5	3.6711	-0.0839	-41.95	0.9356:1	0.80	0.67575
6	3.6616	-0.09345	-46.725	1.1088:1	0.81	0.80089
7	3.6499	-0.1051	-52.55	1.2778:1	0.82	0.92298
8	3.6373	-0.1171	-58.85	1.4428:1	0.83	1.04212
9	3.6277	-0.1273	-63.65	1.6038:1	0.84	1.15843
10	3.6211	-0.1339	-66.95	1.7610:1	0.85	1.272
11	3.6119	-0.14309	-71.55	1.9146:1	0.86	1.38293
12	3.6075	-0.1455	-72.75	2.0647:1	0.87	1.49131
13	3.6029	-0.15215	-76.075	2.2113:1	0.88	1.59723
14	3.5980	-0.15702	-78.51	2.3547:1	0.89	1.70076
15	3.5942	-0.1608	-80.4	2.4948:1	0.90	1.802
16	3.5914	-0.1636	-81.8	2.6319:1	0.91	1.90101
17	3.5871	-0.1679	-83.95	2.7660:1	0.92	1.9979
18	3.5842	-0.1708	-85.4	2.8972:1	0.93	2.09265
19	3.5823	-0.1727	-86.35	3.0256:1	0.94	2.1854
20	3.5776	-0.1774	-88.7	3.2744:1	0.96	2.36513
21	3.5732	-0.1818	-90.9	3.5131:1	0.98	2.53751
22	3.5695	-0.1855	-92.75	3.7422:1	1.00	2.703
23	3.5682	-0.1868	-93.4	3.9623:1	1.02	2.8620
24	3.5665	-0.1885	-94.25	4.1740:1	1.04	3.01488
25	3.5654	-0.1896	-94.8	4.6692:1	1.09	3.37255
26	3.5515	-0.2035	-101.75	5.1209:1	1.14	3.69884
27	3.5489	-0.2061	-103.05	5.5347:1	1.19	3.99771
28	3.5468	-0.2082	-104.1	5.9151:1	1.24	4.27248
29	3.5422	-0.2128	-106.4	6.2660:1	1.29	4.5295
30	3.5396	-0.2154	-107.7	6.5908:1	1.34	4.76051

[Host] = 7.2230 X 10<sup>-4</sup> M  
0.75ml solvent



The calculation of  $Ks$ :

$$Ks_{.1} = (2.09 \pm 0.33) \times 10^4 \text{ M}^{-1}$$

$$Ks_{.2} = (1.83 \pm 0.06) \times 10^3 \text{ M}^{-1}$$

$$Ks_{.3} = (7.83 \pm 0.40) \times 10^1 \text{ M}^{-1}$$

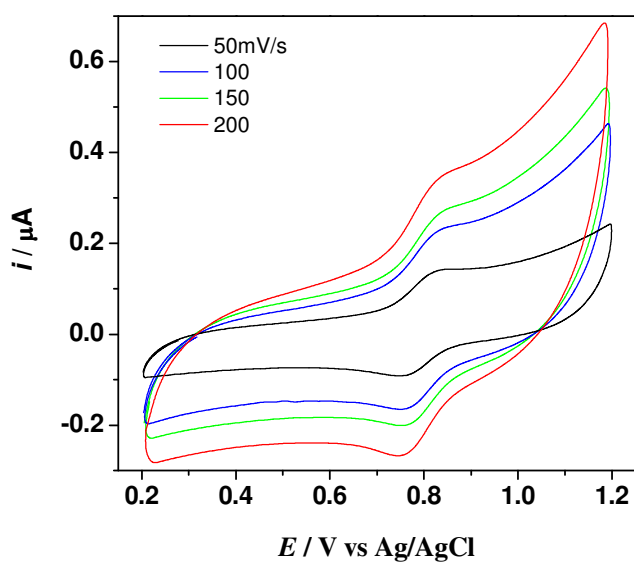


**Electrochemical Measurements:** Cyclic voltammetry (CV) was performed in a Faraday cage using a 3-electrode cell and a potentiostat. The working electrode was a platinum disk embedded in glass with surface area of about  $1 \text{ mm}^2$ . A Ag/AgCl electrode (Ag/AgCl wire soaked in 3M KCl solution) was used as reference electrode and a Pt wire as the counter. Voltammetric data were recorded using in-house virtual instrumentation. The CV measurements were carried out in a dichloromethane solution containing 0.1 M tetra-*n*-butylammonium hexafluorophosphate (TBAPF<sub>6</sub>,  $n\text{-Bu}_4\text{N}^+\text{PF}_6^-$ ) as the supporting electrolyte.

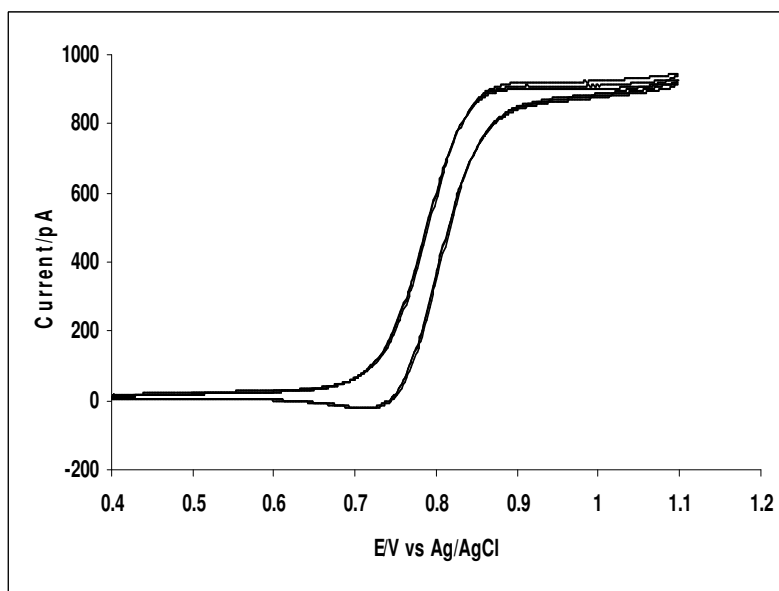
Steady-state voltammetric measurements were made using a two-electrode compartment with a micro-sized Pt disk (the diameter of  $25 \mu\text{m}$ ) as the working electrode and a Ag/AgCl electrode as the counter and reference. Potentiostat were used for potential generation and current measurement. The size of this micro-Pt disk was re-examined by steady-state voltammetric measurement using an acetonitrile solution containing 5.0 mM ferrocene and 0.1M TBAPF<sub>6</sub>.

Figure S10: Electrochemical Measurements of 5 (Solution: 0.2mM 5+0.1M *n*-Bu<sub>4</sub>NPF<sub>6</sub> in CH<sub>2</sub>Cl<sub>2</sub>):

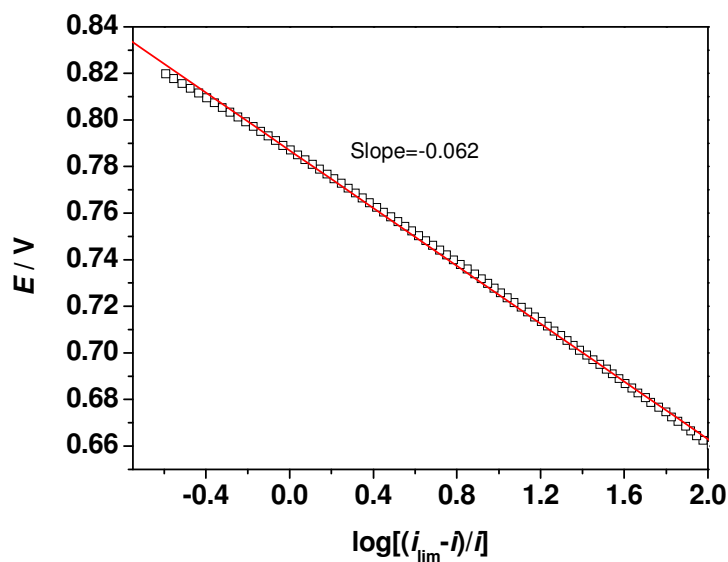
**A. Cyclic voltammetries at disk Pt electrode with  $1 \text{ mm}^2$  surface area.**



**B. Steady State Measurement using Microelectrode of 25  $\mu\text{m}$  diameter.**



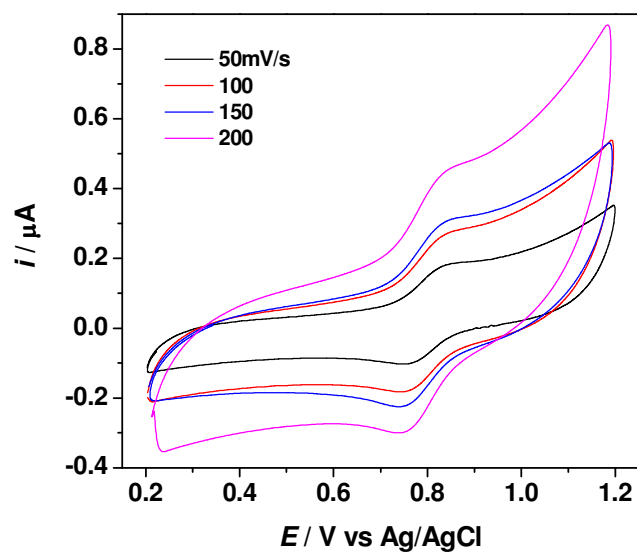
**B. E- $\log[(i_{\text{lim}}-i)/i]$  plot derived from the steady state measurement as obtained at micro electrode.**



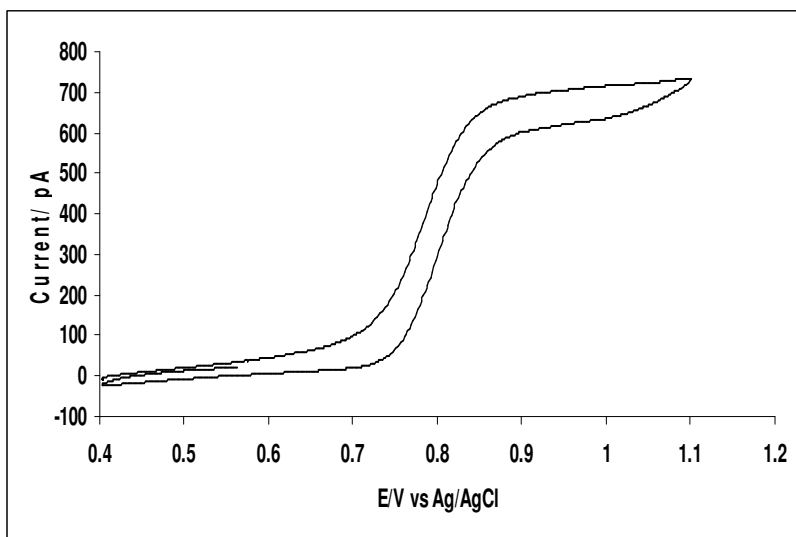
The slope (-0.062) is very close to -0.059, a theoretical value for one-electron-transfer reaction per redox molecule, indicating that one electron is transferred from each ferrocene group attached during its oxidation.

Figure S11: Electrochemical Measurements of 6 (Solution: 0.2mM 6+0.1M *n*-Bu<sub>4</sub>NPF<sub>6</sub> in CH<sub>2</sub>Cl<sub>2</sub>):

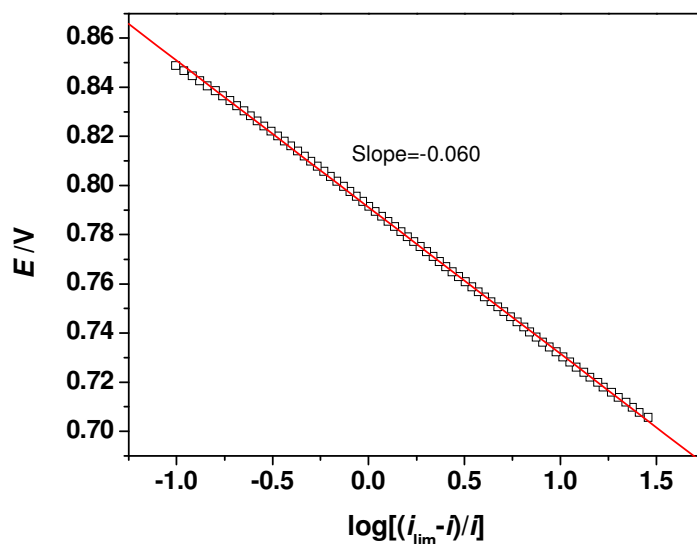
**A. Cyclic voltammograms at disk Pt electrode with 1mm<sup>2</sup> surface area**



**B. Steady State Measurement using 25  $\mu\text{m}$  electrode**



C. E-log[( $i_{lim}-i$ )/ $i$ ] plot derived from the steady state measurement as obtained at micro electrode.



The slope (-0.060) is very close to -0.059, a theoretical value for one-electron-transfer reaction per redox molecule, indicating that one electron is transferred from each ferrocene group attached during its oxidation.

**Figure S12: Electrochemical Measurements of 8 (Solution: 0.2mM 8+0.1M  $n$ -Bu<sub>4</sub>NPF<sub>6</sub> in CH<sub>2</sub>Cl<sub>2</sub>):**

**Cyclic voltammograms at disk Pt electrode with 1mm<sup>2</sup> surface area**

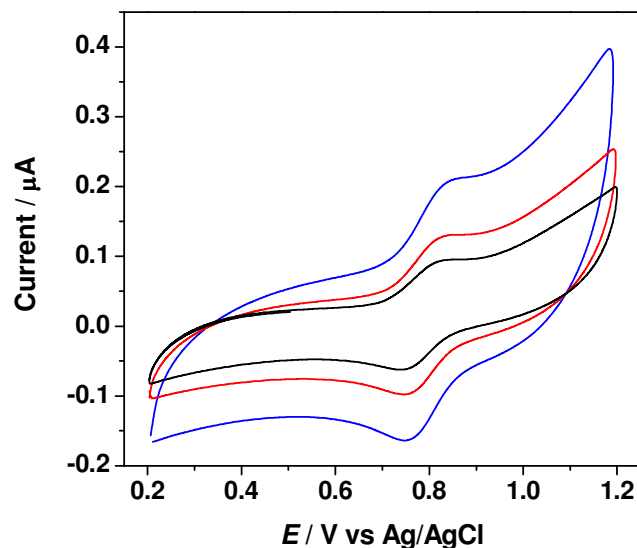
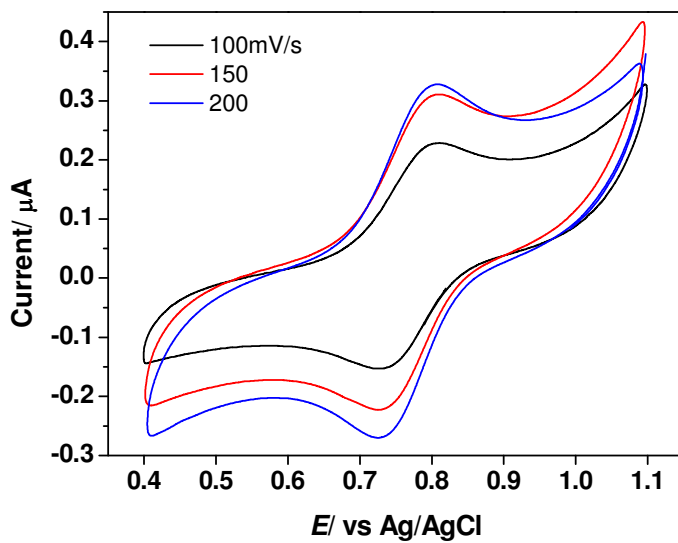


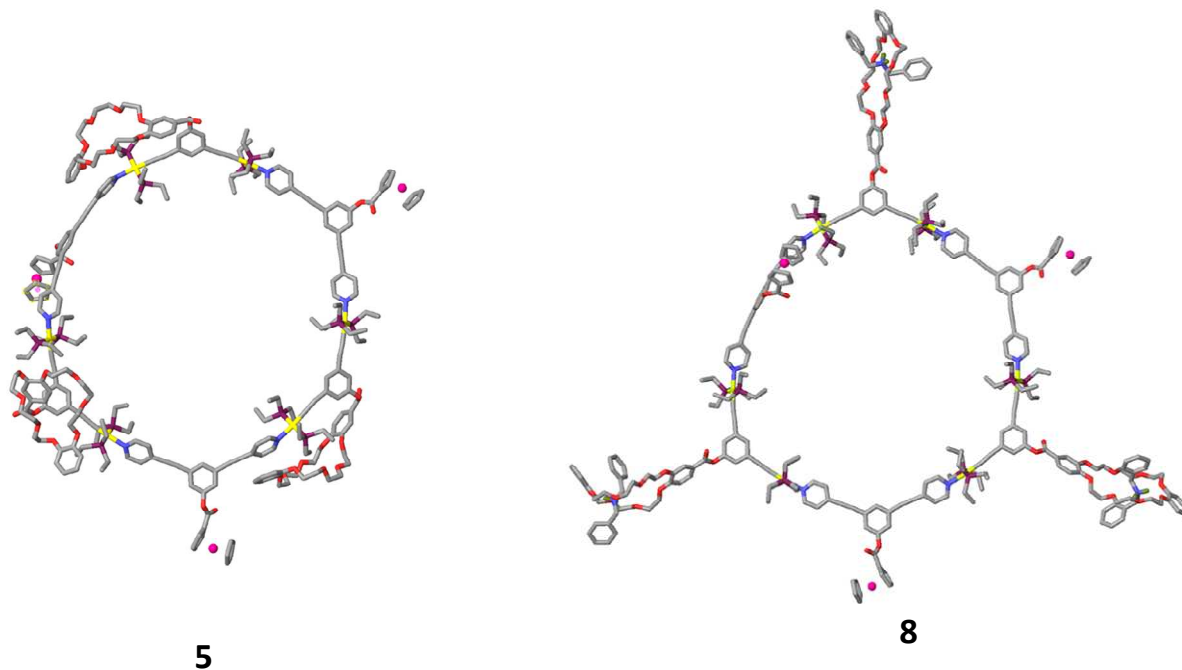
Figure S13: Electrochemical Measurements of **9** (Solution: 0.2mM **9**+0.1M *n*-Bu<sub>4</sub>NPF<sub>6</sub> in CH<sub>2</sub>Cl<sub>2</sub>):

Cyclic voltammtries at disk Pt electrode with 1mm<sup>2</sup> surface area



### Computational Procedures and Calculated Models for **5** and **8**:

The molecular structures of hexagonal tris-**DB24C8** hosts **5**, **6** as well as tris[2]pseudorotaxanes **8** and **9** were each constructed within the input mode of the program<sup>4</sup> Maestro v8.0.110 with the OPLS force-field. A 1.0 ns molecular dynamics simulation (0.05 fs timestep) at a simulation temperature of 300 K was used to equilibrate each structure. Following each molecular dynamics simulation a full energy minimization was used to obtain the final optimized structures.



Color scheme: C = gray, O = red, N = blue, P = purple, Pt = yellow, and  $R_2NH_2^+$  hydrogen atoms = green, Fe = purple all other hydrogen atoms have been removed for clarity.

## Molecular Modeling Atom Coordinates:

5:

C	41.64400	16.99610	-17.02060
C	41.95790	17.46540	-18.31590
C	42.38690	18.79000	-18.52650
C	42.44000	19.68450	-17.44110
C	42.18830	19.27290	-16.12410
C	41.77680	17.91040	-15.91390
C	42.43330	20.32030	-15.09320
C	41.24150	15.56470	-16.92110
C	40.97020	14.36010	-17.00320
C	42.73080	21.32670	-14.43570
C	43.23590	22.93430	-13.28150
C	40.62770	12.34830	-16.97430
C	44.78380	20.44150	-19.59210
C	46.12420	20.39280	-19.15350
C	46.70540	21.50610	-18.51550
C	44.07760	21.66220	-19.49440
C	44.63990	22.76810	-18.83110
C	45.95110	22.68460	-18.30300
O	43.84880	23.87620	-18.65130
C	44.35180	25.06920	-19.25550
C	43.22070	26.09210	-19.41730
O	42.86310	26.66700	-18.15970
C	41.86950	27.67640	-18.34030
C	41.50250	28.35920	-17.01410
O	40.74420	27.47560	-16.18050
O	46.41320	23.72800	-17.53520
C	47.81380	23.97970	-17.54590
C	48.04620	25.44100	-17.14810
O	47.69040	25.66090	-15.78190
C	47.97310	27.00760	-15.41150
C	47.72130	27.20660	-13.90800
O	46.33380	27.27520	-13.57220
C	45.69530	28.48390	-13.99510
C	44.83740	29.02490	-12.84340
O	43.76860	28.11630	-12.58910
C	39.85370	28.14680	-15.29430
C	40.59310	28.80670	-14.12130
O	41.12790	27.81010	-13.24300
C	42.81640	28.54110	-11.69410
C	41.45900	28.33230	-12.01880
C	43.15030	29.14200	-10.45800
C	42.13920	29.50620	-9.54850
C	40.78860	29.27420	-9.86680
C	40.44920	28.68760	-11.09960
P	42.15560	24.16400	-14.34880
P	44.36090	21.73260	-12.28650
C	43.30550	20.40750	-11.43770
C	42.37650	21.01300	-10.37330
C	45.57890	20.85780	-13.45120
C	46.36710	21.86440	-14.30750
C	45.46340	22.44870	-10.90880
C	46.23440	21.35890	-10.14450
C	40.66120	24.75050	-13.36000

C	39.76800	23.58120	-12.91700
C	43.21330	25.62180	-14.85850
C	44.49560	25.17470	-15.56390
C	41.44190	23.40630	-15.95030
C	40.60190	24.39380	-16.76580
P	39.02860	12.70480	-15.94620
C	39.49460	13.47490	-14.28170
C	40.31960	12.51200	-13.41270
C	37.91480	13.92490	-16.87020
C	37.54340	13.39920	-18.26650
C	37.90850	11.22270	-15.53830
C	36.69650	11.63360	-14.68600
P	42.19640	11.99570	-18.08690
C	43.63160	11.41020	-17.01260
C	43.98290	12.43300	-15.92080
C	41.86700	10.67350	-19.39600
C	40.75940	11.10670	-20.37280
C	42.83930	13.49090	-19.07630
C	43.96130	13.10970	-20.05700
C	44.10390	19.18460	-20.02480
C	37.95510	-1.91400	-18.80360
C	37.04290	-0.86570	-18.47350
C	35.70770	-1.26660	-18.79220
C	35.77900	-2.63520	-19.22070
C	37.16250	-3.02850	-19.24000
H	37.53430	-4.04090	-19.43720
C	38.14510	-1.20480	-22.20330
C	38.14010	-0.00980	-21.41590
C	36.80300	0.50070	-21.39360
C	35.98120	-0.37670	-22.17050
C	36.81150	-1.42900	-22.67400
H	36.50860	-2.19090	-23.40240
Fe	36.83330	-1.44960	-20.58010
C	37.37090	0.39630	-17.69160
O	36.66850	1.39650	-17.77630
O	38.47150	0.27110	-16.90720
C	38.75670	1.17530	-15.89810
C	38.88780	0.67850	-14.58190
C	38.97250	2.55690	-16.13540
C	39.29390	3.44390	-15.07890
C	39.20790	1.52440	-13.49620
C	39.40780	2.91400	-13.75690
C	39.32070	0.91960	-12.14720
C	39.38660	0.31830	-11.07320
C	39.50420	4.87840	-15.39290
C	39.67120	6.04950	-15.74040
C	39.46030	-0.37350	-9.76730
C	39.90490	7.45830	-16.13010
C	39.43380	0.37710	-8.57450
C	39.56580	-1.78430	-9.63920
C	39.66590	-2.39320	-8.35160
C	39.53930	-0.27530	-7.32340
C	40.78970	8.26110	-15.38120
C	40.97880	9.62210	-15.72390
N	40.33350	10.20650	-16.77500
C	39.26350	8.07170	-17.23770
C	39.49420	9.44680	-17.54230
C	46.58540	34.86690	-5.50000
C	47.46480	33.95200	-6.15560



C	48.74160	34.56490	-6.35380
C	48.69040	35.84470	-5.70470
C	47.36030	36.03520	-5.19140
C	45.70470	36.65360	-8.34990
C	45.77800	35.24840	-8.61020
C	47.05670	34.97130	-9.19070
C	47.77330	36.20600	-9.29310
C	46.93600	37.24660	-8.77690
H	47.14580	38.32180	-8.82800
Fe	47.31580	35.83400	-7.27820
C	47.19900	32.47670	-6.40940
O	47.79560	31.86540	-7.28770
O	46.28120	31.94350	-5.56390
C	46.13670	30.57500	-5.41090
C	45.78180	29.70950	-6.47700
C	46.29960	30.03410	-4.11610
C	46.13960	28.65360	-3.86050
C	45.61150	28.31850	-6.27020
C	45.79580	27.79890	-4.95180
C	45.24180	27.46910	-7.42870
C	44.92200	26.84770	-8.44440
C	46.33230	28.17530	-2.47020
C	46.50970	27.89870	-1.28200
C	44.49300	26.11570	-9.65760
C	46.69840	27.57510	0.14970
C	43.24050	25.46590	-9.70130
C	45.29980	26.02140	-10.81910
C	44.87450	25.24720	-11.93790
C	42.87570	24.69610	-10.83560
N	43.69600	24.56210	-11.91980
C	47.76640	28.10410	0.92010
C	47.95050	27.70350	2.27630
N	47.11290	26.79260	2.85630
C	45.80840	26.69800	0.80630
C	46.03900	26.32760	2.15470
N	39.66860	-1.62940	-7.21800
C	40.41810	-3.35910	-0.57630
C	39.62710	-4.44750	-0.14480
C	39.54410	-4.79020	1.21950
C	40.32540	-4.09090	2.15930
C	41.07310	-2.95930	1.80480
C	41.12910	-2.59680	0.41600
C	41.66640	-2.21720	2.94850
C	40.39610	-3.05790	-2.03310
C	40.24060	-2.88860	-3.24770
C	42.01080	-1.69570	4.01730
C	42.55000	-0.71980	5.72710
C	39.95190	-2.36400	-5.19720
C	37.45300	-4.84600	3.44390
C	36.62920	-3.75400	3.79390
C	36.80940	-3.09370	5.02560
C	38.36490	-5.35200	4.39830
C	38.58800	-4.65910	5.60780
C	37.82700	-3.51240	5.91270
O	39.58710	-5.01870	6.47740
C	39.70640	-6.41030	6.75640
C	40.36520	-6.59490	8.12940
O	41.73420	-6.18710	8.07310
C	42.53410	-6.77330	9.10390

C	42.37660	-6.05690	10.46280
O	43.17020	-4.87290	10.54790
O	38.14160	-2.82010	7.05760
C	37.03950	-2.35130	7.82760
C	37.48190	-2.19720	9.28690
O	38.42550	-1.13380	9.41900
C	38.67410	-0.85860	10.79610
C	39.68380	0.28960	10.91580
O	41.01060	-0.17960	10.67770
C	41.70750	-0.46050	11.89410
C	43.03860	-1.16120	11.60080
O	43.80150	-0.36180	10.69390
C	44.55020	-5.12650	10.80280
C	45.23530	-3.83830	11.27000
O	45.16010	-2.82080	10.26460
C	45.16310	-0.46990	10.83560
C	45.85200	-1.68660	10.60650
C	45.88690	0.68430	11.19640
C	47.28810	0.64010	11.31880
C	47.97520	-0.56150	11.07000
C	47.25990	-1.71910	10.71210
P	43.26670	-2.38290	6.49030
P	41.76120	0.89760	4.97730
C	42.83980	2.44260	5.19720
C	44.17390	2.32760	4.43700
C	41.39800	0.94580	3.09440
C	40.94910	2.33090	2.59340
C	40.08960	1.24500	5.78230
C	39.14230	0.04400	5.64240
C	45.15860	-2.34700	6.58440
C	45.74070	-3.66600	7.12050
C	42.65220	-2.55190	8.24220
C	41.12620	-2.53530	8.35960
C	42.78480	-4.02380	5.64550
C	43.63680	-4.42070	4.41810
P	38.01290	-2.46460	-4.99990
C	37.42930	-3.79350	-3.77510
C	37.87710	-5.20760	-4.18660
C	37.35320	-0.79950	-4.40100
C	37.98200	-0.34650	-3.07420
C	37.08590	-2.86270	-6.60930
C	35.58610	-3.09900	-6.36740
P	41.87300	-2.34790	-5.42480
C	42.60570	-4.01990	-4.93000
C	42.03080	-5.16010	-5.78620
C	42.53890	-1.99930	-7.17170
C	44.07590	-1.98390	-7.20700
C	42.62300	-1.01750	-4.30820
C	42.10160	0.38530	-4.65940
O	38.68120	-5.77060	1.64670
C	37.45140	-5.34890	2.03750
C	44.87490	7.31930	11.17200
C	45.49370	6.08760	10.78780
C	45.67340	8.40950	11.63020
C	47.06290	8.24670	11.70650
C	46.90410	5.97690	10.85910
C	47.69310	7.06200	11.29250
C	44.75050	4.92300	10.26580
C	44.30810	3.88960	9.76550

C	45.20950	9.75940	11.98140
C	45.19910	10.96040	12.23920
C	43.93360	2.65300	9.05610
C	45.45770	12.39720	12.40770
C	44.87660	1.99990	8.23380
C	42.64010	2.08520	9.13220
C	42.30460	0.96430	8.32250
C	44.48400	0.88860	7.44860
N	43.20050	0.42470	7.45140
C	46.55640	12.86980	13.16780
C	46.91900	14.24250	13.12800
N	46.22010	15.11060	12.34450
C	44.68630	13.34570	11.70780
C	45.09260	14.69970	11.69670
C	47.90410	21.50060	10.39680
C	48.14830	22.37330	11.47310
C	48.18820	23.77200	11.28510
C	48.10520	24.30650	9.98630
C	47.91410	23.47410	8.86490
C	47.79600	22.05940	9.07950
C	47.80990	24.15020	7.54730
C	47.70810	20.07200	10.74760
C	47.48050	18.94850	11.20710
C	47.72290	24.84200	6.52790
C	47.47900	25.85180	4.77530
C	46.91810	17.09100	11.82960
C	46.15390	23.78450	13.28950
C	45.33580	23.83160	12.13480
C	44.18480	23.02500	12.03470
C	45.74980	22.98300	14.37420
C	44.57090	22.21950	14.30070
C	43.80250	22.20340	13.11620
O	44.16050	21.55230	15.42290
C	43.03720	22.15980	16.08210
C	43.15910	23.68690	16.31650
O	42.91220	24.38450	15.09700
C	43.02660	25.79700	15.22180
C	42.71690	26.45300	13.86280
O	43.87160	26.53930	13.02350
O	42.72040	21.36290	13.03620
C	41.47750	21.97830	12.70100
C	40.85910	21.23370	11.50810
O	41.43150	21.68480	10.28090
C	40.60980	22.65980	9.64530
C	41.37270	23.34960	8.49740
O	42.41580	24.22020	8.93640
C	41.92880	25.41850	9.54420
C	43.08770	26.30770	9.99350
O	43.64570	27.01140	8.88390
C	44.52300	27.80540	13.10600
C	45.80070	27.80930	12.24410
O	45.53840	27.63280	10.84570
C	43.95350	28.31820	9.17370
C	44.89660	28.65560	10.17920
C	43.30470	29.33130	8.44020
C	43.58430	30.68510	8.69950
C	44.52400	31.02800	9.68730
C	45.17940	30.02160	10.42110
P	46.33400	27.18420	5.62640

P	48.67790	24.58780	3.94560
C	50.33720	24.55890	4.85570
C	51.02320	25.93420	4.81340
C	47.92120	22.85480	4.03760
C	46.58670	22.77690	3.27820
C	49.12520	24.84540	2.11280
C	50.04340	23.73270	1.58080
C	46.31990	28.86700	4.74270
C	45.51910	29.92090	5.52470
C	46.87070	27.58370	7.39840
C	48.32650	28.07470	7.48580
C	44.54980	26.56870	5.63530
C	44.38460	25.19400	6.30190
P	45.78980	17.83310	13.23770
C	46.51950	19.39850	14.01550
C	47.91640	19.16370	14.61660
C	44.08970	18.23500	12.52410
C	44.15610	19.10560	11.25950
C	45.50030	16.65890	14.70160
C	44.73350	17.35070	15.84070
P	48.09540	16.34220	10.49440
C	47.57020	16.95090	8.77590
C	46.16230	16.45430	8.40700
C	49.86950	16.91150	10.80820
C	50.37790	16.41550	12.17220
C	48.18650	14.45090	10.31440
C	49.06620	14.02940	9.12570
O	48.25270	24.64260	12.34700
C	47.41060	24.58740	13.43570
H	47.03230	36.87510	-4.56770
O	49.06620	7.00080	11.32040
C	49.76880	7.88660	10.57200
O	49.34010	8.44650	9.56150
C	51.05400	8.30960	11.22040
C	52.07050	9.06840	10.56040
C	53.18870	9.12150	11.45760
C	52.82600	8.43960	12.67180
C	51.48100	7.95630	12.53800
C	50.63080	11.73640	13.68980
C	51.41860	12.37240	12.68540
C	50.84760	12.06280	11.41770
C	49.69610	11.25150	11.64080
C	49.57590	11.02900	13.04380
H	50.94780	7.33090	13.25530
H	48.79980	10.45290	13.54830
Fe	51.53980	10.15950	12.40450
O	42.77340	19.21480	-19.77370
O	44.68120	18.12580	-20.26720
O	47.70050	25.15070	14.48170
O	36.56840	-5.11320	1.21470
H	41.90610	16.81170	-19.17710
H	42.73160	20.70610	-17.62470
H	41.56950	17.56850	-14.91110
H	46.70190	19.48450	-19.26760
H	47.72250	21.42000	-18.16120
H	43.06710	21.74190	-19.87200
H	45.15870	25.51010	-18.67180
H	44.75910	24.83760	-20.24220
H	43.56530	26.88040	-20.08980

H	42.35620	25.62470	-19.89190
H	42.25080	28.43800	-19.02370
H	40.97310	27.25850	-18.80210
H	42.39870	28.70160	-16.49590
H	40.92090	29.25020	-17.25910
H	48.33400	23.30900	-16.86140
H	48.22380	23.82150	-18.54580
H	49.10160	25.67690	-17.29850
H	47.47600	26.10070	-17.80470
H	49.02530	27.22160	-15.61020
H	47.39180	27.70970	-16.01120
H	48.17570	26.38270	-13.35760
H	48.22810	28.10890	-13.55990
H	46.41840	29.25340	-14.27390
H	45.08690	28.29430	-14.88030
H	45.46650	29.16160	-11.96380
H	44.43280	30.00200	-13.11520
H	39.26190	28.88640	-15.83750
H	39.13380	27.42550	-14.90860
H	41.38970	29.46380	-14.47250
H	39.87940	29.44680	-13.59900
H	44.17770	29.32980	-10.18570
H	42.39430	29.98260	-8.61180
H	40.00840	29.57860	-9.18090
H	39.40580	28.55020	-11.34970
H	42.71430	19.83590	-12.15120
H	43.95800	19.67230	-10.96580
H	42.93170	21.54870	-9.60160
H	41.63850	21.68920	-10.80120
H	41.81980	20.22350	-9.86400
H	46.29330	20.28040	-12.86580
H	45.10470	20.11590	-14.09140
H	45.73440	22.38650	-15.02580
H	46.89210	22.60780	-13.70550
H	47.13020	21.34860	-14.89500
H	46.21540	23.11840	-11.32620
H	44.89510	23.00160	-10.16340
H	46.86130	21.81010	-9.37260
H	45.57430	20.65590	-9.63620
H	46.90810	20.79080	-10.78660
H	40.93670	25.36950	-12.51040
H	40.06740	25.41460	-13.98930
H	40.27890	22.87340	-12.26900
H	38.90100	23.95800	-12.36920
H	39.37230	23.03590	-13.77600
H	42.65560	26.22200	-15.56940
H	43.42880	26.29770	-14.04180
H	44.27400	24.45880	-16.34970
H	44.97430	26.02650	-16.05220
H	45.23980	24.73090	-14.90970
H	42.23910	23.03740	-16.59680
H	40.77750	22.57170	-15.73250
H	39.77590	24.82430	-16.19950
H	41.20900	25.20940	-17.14540
H	40.16810	23.90700	-17.64100
H	40.03360	14.41300	-14.40590
H	38.58450	13.74740	-13.74510
H	39.78510	11.58070	-13.21740
H	41.28630	12.27510	-13.85270

H	40.51820	12.96340	-12.43820
H	36.99450	14.08150	-16.30660
H	38.34650	14.92130	-16.95220
H	36.85840	14.09420	-18.75920
H	38.40720	13.29920	-18.92340
H	37.02310	12.44090	-18.22370
H	37.50700	10.77350	-16.44660
H	38.42940	10.44600	-14.98050
H	36.98130	12.06060	-13.72400
H	36.04970	12.34960	-15.19520
H	36.07040	10.76580	-14.46730
H	43.44910	10.42970	-16.57740
H	44.51050	11.26850	-17.64490
H	44.83920	12.08380	-15.33910
H	44.27580	13.39210	-16.35260
H	43.16680	12.60810	-15.22300
H	42.77830	10.51890	-19.97700
H	41.67110	9.68600	-18.98570
H	40.56370	10.31700	-21.10270
H	39.81230	11.34780	-19.89500
H	41.06260	11.97980	-20.95530
H	42.03690	13.97140	-19.63810
H	43.26670	14.24530	-18.41710
H	44.80060	12.61410	-19.56790
H	43.61130	12.46480	-20.86430
H	44.36560	14.00200	-20.54050
H	39.03020	-1.92960	-18.60070
H	34.79380	-0.70440	-18.57240
H	34.92280	-3.29680	-19.39970
H	39.03160	-1.77050	-22.51160
H	39.02620	0.48940	-21.01370
H	36.48540	1.45730	-20.96770
H	34.93520	-0.20300	-22.44780
H	38.73570	-0.37910	-14.41350
H	38.88630	2.93520	-17.14470
H	39.65300	3.57550	-12.94000
H	39.33810	1.45740	-8.64230
H	39.57510	-2.39420	-10.54190
H	39.76370	-3.46480	-8.23250
H	39.54320	0.28840	-6.40250
H	41.30880	7.81400	-14.53740
H	41.62660	10.25470	-15.13560
H	38.58240	7.47650	-17.84480
H	38.98480	9.93400	-18.36210
H	45.57160	34.65580	-5.14660
H	49.63730	34.07830	-6.75460
H	49.54330	36.51350	-5.53720
H	44.81640	37.20250	-8.01730
H	44.95300	34.53870	-8.50190
H	47.38390	34.01110	-9.60090
H	48.73290	36.35410	-9.80140
H	45.64250	30.12440	-7.46570
H	46.55350	30.70500	-3.30640
H	45.66850	26.74130	-4.77650
H	42.57240	25.55860	-8.84930
H	46.25050	26.54810	-10.85600
H	45.51010	25.11740	-12.80050
H	41.95160	24.13790	-10.84880
H	48.45240	28.80920	0.45250

H	48.78280	28.06240	2.86800
H	44.95830	26.30730	0.25270
H	45.39250	25.62410	2.65900
H	39.03820	-5.02490	-0.84590
H	40.29690	-4.39320	3.19350
H	41.70710	-1.73560	0.11670
H	35.88270	-3.39170	3.09920
H	36.18360	-2.24450	5.25950
H	38.96880	-6.21530	4.15430
H	38.72090	-6.88110	6.77540
H	40.29360	-6.90980	5.98510
H	39.82500	-6.03500	8.89360
H	40.28370	-7.65140	8.39220
H	42.29450	-7.83250	9.21550
H	43.57360	-6.75830	8.78090
H	41.33430	-5.79000	10.63360
H	42.63430	-6.73830	11.27590
H	36.67130	-1.40160	7.43880
H	36.21390	-3.06550	7.78770
H	36.59700	-1.98960	9.89220
H	37.90750	-3.13280	9.65450
H	37.74100	-0.55580	11.27540
H	39.03130	-1.74600	11.32200
H	39.43910	1.06250	10.18740
H	39.60000	0.76550	11.89560
H	41.89110	0.46850	12.43670
H	41.10590	-1.09940	12.54380
H	43.57350	-1.31690	12.54050
H	42.84540	-2.14610	11.17690
H	44.66460	-5.87470	11.58970
H	45.04840	-5.51740	9.91640
H	44.76920	-3.48860	12.19240
H	46.27170	-4.07440	11.51560
H	45.36550	1.60370	11.41740
H	47.83980	1.51630	11.63170
H	49.05090	-0.60640	11.18490
H	47.80500	-2.63820	10.54410
H	42.30120	3.30730	4.80910
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H	44.75740	1.45070	4.71130
H	44.01850	2.28940	3.35760
H	44.79830	3.20310	4.62830
H	42.26450	0.63090	2.51210
H	40.57370	0.27460	2.85430
H	41.75060	3.06890	2.63010
H	40.63070	2.27400	1.55150
H	40.10130	2.72270	3.15660
H	40.17130	1.53270	6.82690
H	39.62220	2.10600	5.30450
H	38.92380	-0.19370	4.60060
H	39.53490	-0.85440	6.11630
H	38.18410	0.25460	6.12310
H	45.60770	-2.11580	5.61850
H	45.49110	-1.58960	7.28900
H	45.68310	-4.48150	6.40280
H	46.79750	-3.55170	7.36990
H	45.24040	-4.00250	8.02790
H	42.99810	-3.51300	8.61410
H	43.10110	-1.81790	8.89850

H	40.68150	-3.36020	7.80940
H	40.83020	-2.67890	9.40120
H	40.66390	-1.61220	8.02260
H	42.87440	-4.82740	6.37590
H	41.72630	-4.02730	5.38860
H	43.03970	-4.99540	3.70820
H	44.07570	-3.57690	3.88890
H	44.45750	-5.07930	4.70410
H	37.70980	-3.58480	-2.74450
H	36.33910	-3.78570	-3.73740
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H	37.51440	-5.48070	-5.17920
H	37.47620	-0.02690	-5.15900
H	36.27470	-0.88510	-4.25210
H	39.05060	-0.15520	-3.15560
H	37.51410	0.57990	-2.73390
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H	37.13060	-2.03930	-7.32040
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H	41.03250	0.48950	-4.48080
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C	34.61580	-1.68750	-17.17730
C	34.42000	-3.09650	-17.36880
C	35.64860	-3.76820	-17.04140
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C	37.68560	-1.47680	-19.33030

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C	37.34250	0.17340	-12.59730
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C	37.18290	0.21410	-9.00180
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C	54.03350	34.21920	-5.42290
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Fe	52.75290	34.98510	-6.91970
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C	35.26890	-1.99060	4.14420
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C	36.48120	-0.75720	0.76740
C	36.53690	-0.78000	-0.46140
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C	33.80040	-2.02410	6.85550
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O	48.63240	30.79560	5.89170
C	48.52430	32.11950	5.38000
C	48.95990	32.10460	3.90570
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C	43.45490	32.31020	4.73240
O	43.59150	31.88060	3.37700
C	42.75690	32.67520	2.53580
C	42.67770	32.09780	1.11830
O	43.88320	32.36650	0.40380
C	43.64320	32.87420	-0.90740
C	44.95510	33.34620	-1.54100
O	45.88580	32.26700	-1.64190
C	46.96170	31.95250	2.63620
C	47.27840	32.71690	1.34620
O	47.75330	31.80110	0.35780
C	47.17530	32.70380	-1.80670
C	48.12160	32.46720	-0.78490
C	47.55380	33.43110	-2.95690
C	48.86340	33.93220	-3.08120
C	49.80190	33.70860	-2.05660
C	49.43120	32.97770	-0.91240
P	46.27630	27.95670	0.82070
P	50.09090	28.44480	1.35800
C	50.90360	27.95990	3.00610
C	50.78800	29.02240	4.10570
C	50.99590	27.33450	0.11800
C	50.61790	25.85310	0.25460
C	50.62890	30.20530	0.93870
C	52.15840	30.36690	0.95040

C	45.44530	29.41250	-0.07270
C	44.02450	29.05540	-0.54520
C	45.12220	27.53390	2.27360
C	44.63550	28.75880	3.06740
C	46.06540	26.47590	-0.34780
C	46.48090	25.13700	0.28140
P	41.13890	16.02960	16.37070
C	41.43720	17.80290	16.96990
C	42.78490	17.97130	17.69790
C	39.29740	15.87810	15.98090
C	38.86940	16.71430	14.76630
C	41.48070	14.94280	17.88680
C	40.62080	15.35340	19.09420
P	43.26920	14.84510	13.33480
C	43.02400	15.87580	11.76430
C	41.57120	15.82160	11.26200
C	45.10160	14.89330	13.78210
C	45.36170	14.22780	15.14180
C	42.97280	13.05540	12.73460
C	43.78300	12.68970	11.47740
H	52.67540	34.84760	-9.81330
O	42.30820	8.58840	17.89150
C	43.64640	8.71470	17.69520
O	44.17260	8.76240	16.58060
C	44.40040	9.04930	18.94700
C	45.82620	9.07850	19.03390
C	46.14540	9.23910	20.42330
C	44.91520	9.38230	21.15590
C	43.82290	9.29950	20.22960
C	45.64640	13.16840	19.38810
C	45.69670	12.48220	18.14120
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C	43.53090	12.37690	18.93030
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H	43.94470	13.55700	20.79980
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C	37.73980	2.17190	7.86230
C	38.20220	3.49670	7.80220
C	37.43420	1.64540	9.14360
C	38.37030	4.22520	8.99780
C	37.61230	2.43310	10.31820
N	38.10910	3.69620	10.22800
C	36.59190	-0.75910	-1.93380
C	36.35230	-1.90510	-2.73630
C	36.90440	0.44300	-2.59580
C	36.43650	-1.82260	-4.15780
N	36.74820	-0.64020	-4.76720
C	36.98160	0.46720	-4.00600
C	41.61510	11.92520	-14.78690
C	41.68300	11.11720	-15.95180
C	41.02480	11.35510	-13.64230
C	41.18010	9.78180	-15.93780
N	40.62040	9.25710	-14.80590
C	40.54330	10.02680	-13.68270
C	45.90740	20.97080	-11.90010
C	46.70640	20.94070	-10.74240
C	47.08890	22.15670	-10.12960
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C	45.98490	23.43160	-11.77180
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N	42.87630	17.49040	14.39180
C	44.15600	17.90920	14.61490
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C	47.38850	26.04790	5.58730
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C	48.14070	26.05870	3.27170
O	41.22720	18.94070	-16.28160
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H	43.56700	23.40370	-16.27480
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H	39.74140	23.81530	-12.83640
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H	38.95450	25.69500	-6.83280
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H	39.58160	-0.16900	15.62170
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H	38.05630	4.90270	18.59230
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H	41.57670	2.85600	17.25040
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H	37.37070	8.12800	11.70860
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H	35.37760	3.69010	11.42600
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H	36.89880	5.62990	14.47120
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H	35.22690	7.34610	15.06930
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H	42.35480	4.76300	10.36580
H	40.93430	4.70160	9.40290
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H	32.54100	1.60980	-8.02530
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H	33.47080	-2.24950	-7.50510
H	34.87200	-2.71180	-6.55110
H	39.61880	10.28890	13.70180
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H	43.51200	24.31650	12.26000
H	45.12070	26.62040	9.01880
H	46.17260	22.48170	9.37470
H	41.89480	28.32250	9.51250
H	41.83000	29.26960	7.21870

H	46.10960	29.13310	9.74230
H	46.85730	32.01220	7.69500
H	47.20400	30.86790	8.96770
H	49.31410	31.42950	7.76270
H	48.91490	29.73980	7.61990
H	47.51080	32.50270	5.49440
H	49.18320	32.79510	5.92920
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H	49.98720	31.74880	3.85360
H	44.44230	32.06410	6.61120
H	45.38370	31.47380	5.25180
H	42.42260	32.21540	5.07510
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H	43.10620	33.70900	2.50630
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H	45.98960	29.77880	-0.93770
H	43.53090	29.93650	-0.95380
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H	46.20430	24.31250	-0.37890
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H	43.63460	17.51270	17.20130
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H	41.28300	13.88870	17.70990
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H	39.55320	15.23710	18.90320
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H	41.27680	14.80480	10.99630
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H	38.42580	3.92990	6.83240
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H	44.97620	22.29090	-13.33620
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H	41.02650	17.93130	13.52120
H	44.77970	17.29270	15.24760
H	45.69710	19.39570	14.14180
H	47.97340	24.26980	4.52630
H	46.95100	28.01920	6.34770

H	47.48870	29.19130	4.16620
H	48.47850	25.54160	2.38910
H	39.85800	19.54510	-14.85370
H	39.71340	20.31570	-16.41000
H	35.02320	-3.72560	6.31230
H	33.31380	-3.93450	6.03330
H	45.09870	27.98160	11.52240
H	43.51620	28.63270	11.84870

**8:**

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C	50.21540	18.47710	-17.94790
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C	49.38540	19.13430	-15.71280
C	49.13610	17.74380	-15.43590
C	49.09490	20.27090	-14.78420
C	49.21340	15.24950	-16.18820
C	49.08390	14.01800	-16.11860
C	48.88240	21.30030	-14.12690
C	48.44350	22.90980	-12.91910
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C	52.12900	19.37650	-21.57440
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C	50.31860	20.83700	-22.25200
C	50.95310	21.11180	-23.48480
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O	50.03730	23.42920	-27.67850
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C	47.30180	35.53110	-9.30230
C	48.69600	35.35680	-9.02950
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C	44.04690	29.24000	-1.69060
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C	43.45360	29.09740	-0.33820
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C	39.33020	-1.84290	2.47640
C	39.91590	-1.53280	1.20070
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C	41.38820	-2.19140	-2.20400
C	38.60210	-0.07360	4.42380
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C	39.46150	-7.57130	3.53000
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C	33.09960	-3.29900	-13.29700
C	34.23360	-4.02170	-12.78820
H	34.23310	-5.07490	-12.48180
C	35.00080	-4.02670	-16.57360
C	36.22830	-4.00230	-15.83700
C	36.52410	-2.63940	-15.51840
C	35.47550	-1.82250	-16.04850
C	34.53220	-2.67940	-16.69880
H	33.68040	-2.35660	-17.30870
Fe	34.66530	-3.21690	-14.67500
C	35.44730	-0.46650	-12.58850
O	35.19510	0.55600	-13.21650
O	36.25910	-0.52230	-11.49210
C	36.67190	0.61380	-10.80900
C	36.46060	0.65160	-9.41050
C	37.32440	1.70990	-11.43460
C	37.74700	2.84700	-10.70010
C	36.86030	1.75160	-8.61520
C	37.50490	2.85170	-9.28140
C	36.58200	1.68620	-7.14350
C	36.30420	1.54440	-5.94240
C	38.41660	3.96210	-11.44700
C	38.96170	4.83840	-12.13600
C	53.13220	33.34970	-10.92860
C	53.69730	32.04680	-11.07030
C	55.11490	32.15020	-11.21740

C	55.45200	33.52960	-11.00810
C	54.23000	34.26970	-10.84650
C	52.74060	32.78830	-14.04070
C	53.88470	31.95200	-14.23990
C	54.97650	32.78390	-14.64370
C	54.50510	34.13490	-14.69800
C	53.12470	34.13830	-14.31750
H	52.45250	35.00220	-14.37500
Fe	54.31060	33.39750	-12.75070
C	52.97410	30.72360	-10.85470
O	53.37410	29.67920	-11.35770
O	51.90070	30.81890	-10.01630
C	51.30940	29.70850	-9.42890
C	50.83560	28.59090	-10.16690
C	51.13850	29.72270	-8.02450
C	50.52750	28.65400	-7.32660
C	50.21920	27.48260	-9.53230
C	50.07240	27.53060	-8.10130
C	49.76210	26.34130	-10.39140
C	49.41590	25.43960	-11.16990
C	50.39860	28.77680	-5.83790
C	50.33180	28.97300	-4.61370
C	35.16250	2.55600	5.21340
C	34.45130	1.52020	5.85590
C	34.23000	1.51670	7.24830
C	34.73570	2.58960	8.02540
C	35.44640	3.65720	7.42660
C	35.65900	3.63050	6.01300
C	35.92650	4.75400	8.30110
C	35.34310	2.45950	3.74500
C	35.41840	2.25600	2.53170
C	36.27170	5.61660	9.11090
C	38.29930	10.47860	12.92020
C	35.95130	1.49080	-3.91060
C	32.50850	-0.92000	9.52590
C	31.27800	-1.13350	8.87890
C	30.46580	-2.22590	9.23960
C	32.90190	-1.81360	10.54520
C	32.10370	-2.91880	10.92200
C	30.85810	-3.13350	10.25740
O	32.63680	-3.68920	11.94320
C	31.97640	-4.86340	12.41630
C	32.82470	-5.48980	13.53330
O	32.33640	-6.77670	13.91420
C	33.15830	-7.36530	14.92340
C	32.86490	-8.86200	15.11370
O	31.61270	-9.06080	15.76150
O	30.07900	-4.22140	10.59190
C	28.68830	-4.21110	10.28890
C	28.05090	-5.45780	10.92390
O	28.07150	-5.37300	12.34620
C	26.91500	-4.77510	12.93170
C	25.75920	-5.78490	13.05740
O	26.24910	-6.98340	13.64360
C	25.21750	-7.89060	14.01850
C	25.79380	-9.31450	14.02050
O	26.89140	-9.41880	14.92500
C	31.40640	-10.43500	16.10020
C	30.18210	-10.59140	17.01310

O	29.00790	-10.26860	16.27800
C	26.66270	-9.87060	16.20930
C	27.79390	-10.31270	16.93470
C	25.38730	-9.88220	16.82640
C	25.24050	-10.33590	18.14960
C	26.36310	-10.77810	18.86920
C	27.63420	-10.76690	18.26760
P	36.53140	11.30260	12.86580
P	40.04290	9.61070	13.04970
C	40.20010	7.77600	12.58090
C	39.72720	6.82530	13.69850
C	41.27130	10.52980	11.94570
C	40.87390	10.51030	10.46280
C	40.73180	9.70530	14.81990
C	42.18790	9.21430	14.89850
C	36.04990	12.01290	14.56300
C	34.72480	12.79370	14.50700
C	36.56670	12.76720	11.67220
C	36.88430	12.36250	10.22570
C	35.04310	10.23680	12.35940
C	34.54780	9.31930	13.49510
P	37.74300	0.77890	-3.69020
C	38.29830	0.20270	-1.96570
C	37.82400	-1.21000	-1.58120
C	38.06760	-0.68120	-4.85700
C	36.92340	-1.71360	-4.88480
C	39.00190	2.10460	-4.16930
C	38.93450	3.34640	-3.26730
P	34.11730	2.12350	-4.14150
C	33.97510	3.93000	-3.61630
C	34.92480	4.83380	-4.41790
C	33.44040	2.04030	-5.92150
C	31.95080	2.41550	-6.00600
C	32.88430	1.11340	-3.13050
C	32.92530	-0.37570	-3.51630
C	40.70770	15.56330	14.23070
C	40.53480	14.23720	14.76830
C	41.64580	16.48550	14.81530
C	42.38720	16.05200	15.92730
C	41.31530	13.86360	15.88350
C	42.26390	14.74660	16.43220
C	39.65570	13.17430	14.20470
C	39.06900	12.15800	13.81370
C	41.99680	17.84590	14.31990
C	42.52420	18.92440	14.01800
C	47.64020	27.30330	8.57010
C	48.08450	28.43800	9.28920
C	48.70290	29.53150	8.63060
C	48.87910	29.47230	7.23280
C	48.46250	28.35820	6.47240
C	47.83720	27.27010	7.15470
C	48.70030	28.39310	5.00930
C	46.98250	26.21240	9.32870
C	46.43530	25.37800	10.05220
C	48.95670	28.54730	3.81360
C	50.12110	29.10510	-2.56740
C	43.46950	20.60980	13.32070
C	49.63350	32.08720	11.22350
C	49.10530	33.29050	10.71970

C	49.50350	34.52570	11.26880
C	50.57170	32.14640	12.27590
C	50.98190	33.37370	12.84450
C	50.42840	34.58990	12.34220
O	51.90950	33.25470	13.86670
C	52.26650	34.37760	14.67270
C	53.19980	33.91720	15.79910
O	53.40530	34.95900	16.75160
C	54.31100	34.55110	17.77590
C	54.31420	35.53510	18.95430
O	55.04320	36.71190	18.62340
O	50.82200	35.79460	12.88480
C	49.98580	36.93920	12.76110
C	50.27570	37.86940	13.95470
O	51.62280	38.33920	13.95870
C	51.85720	39.47790	13.13520
C	51.72420	40.77450	13.94950
O	52.86370	40.92720	14.78980
C	52.83880	42.15960	15.51220
C	54.25550	42.52310	15.96870
O	54.74490	41.54950	16.88630
C	55.18650	37.58450	19.74100
C	56.23070	38.66240	19.43420
O	55.73810	39.60630	18.48280
C	56.03750	41.70280	17.35160
C	56.55700	40.68600	18.19190
C	56.85100	42.82010	17.02710
C	58.16120	42.92670	17.52310
C	58.67840	41.91990	18.35110
C	57.88420	40.80920	18.68320
P	48.39810	30.00510	-2.79080
P	51.88490	28.28810	-2.35760
C	52.83890	28.96570	-0.87170
C	53.18680	30.45550	-1.03930
C	51.68810	26.43110	-2.08410
C	51.00030	25.73690	-3.27020
C	53.09610	28.50050	-3.81590
C	54.50970	27.99240	-3.48220
C	47.93120	30.56730	-4.55420
C	46.61680	31.36610	-4.59580
C	48.28830	31.57810	-1.75400
C	49.39230	32.58190	-2.12440
C	47.00570	28.85930	-2.23370
C	47.01300	27.52900	-3.00250
P	41.82260	21.57840	13.69600
C	41.88840	23.46390	13.50000
C	42.66220	24.15750	14.63810
C	40.43460	20.95850	12.57120
C	40.75580	21.10610	11.07720
C	41.24590	21.31500	15.48940
C	39.91120	22.02660	15.77180
P	45.13970	19.63690	13.02590
C	45.77770	19.81770	11.25220
C	44.78810	19.24620	10.22300
C	46.47140	20.27880	14.19410
C	45.94520	20.39310	15.63300
C	45.07720	17.75340	13.29420
C	46.41220	17.04990	12.99320
H	54.15830	35.33320	-10.58780

O	43.11920	14.34200	17.42300
C	44.28850	13.77770	17.04310
O	44.50860	13.36060	15.90270
C	45.35620	13.91120	18.08620
C	46.70680	13.48250	17.90820
C	47.34750	13.61460	19.18400
C	46.40150	14.17960	20.10870
C	45.16660	14.40310	19.41440
C	46.58810	17.81920	18.43490
C	47.79160	17.44970	17.76500
C	47.44340	16.64810	16.64010
C	46.02490	16.54580	16.60100
C	45.49440	17.24860	17.72390
H	44.23530	14.75020	19.86220
H	44.44750	17.36800	17.99810
Fe	46.81840	15.61260	18.54180
C	36.68860	6.67910	10.05170
C	36.55010	6.57320	11.46060
C	37.25600	7.86820	9.55500
C	36.98050	7.63210	12.31690
C	37.66580	8.88450	10.44920
N	37.53610	8.77060	11.80370
C	35.48850	2.01270	1.07410
C	35.08900	0.79080	0.47300
C	35.96650	3.01980	0.21290
C	35.18490	0.60820	-0.93940
N	35.66210	1.60130	-1.74790
C	36.04120	2.78400	-1.18070
C	42.25130	10.52980	-14.78810
C	41.93410	9.49100	-15.70200
C	41.85980	10.33550	-13.44780
C	41.25770	8.31260	-15.26330
N	40.89820	8.14970	-13.95510
C	41.19100	9.14570	-13.06650
C	46.94710	19.67390	-14.46110
C	47.12870	19.82400	-13.07070
C	47.67350	21.02300	-12.54750
N	48.04840	22.06670	-13.34540
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C	47.34430	20.76520	-15.27790
C	45.73890	24.37740	10.88980
C	44.72800	23.57560	10.32570
C	44.09240	22.58310	11.10790
N	44.41690	22.35650	12.41570
C	45.35940	23.15060	13.00470
C	46.03630	24.16480	12.26160
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C	48.99760	27.72040	1.45190
C	49.83540	29.94070	1.87000
C	50.10360	30.08210	0.47540
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C	49.28350	27.91450	0.07920
N	46.25550	15.54880	-31.51370
C	45.45190	14.58950	-30.74070
C	47.53610	15.91240	-30.89170
N	53.85300	38.99090	16.47850
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C	54.57970	38.03640	15.62840
N	29.35060	-8.07610	14.68890



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C	31.21290	-11.75130	11.76940
C	29.98460	-11.81210	12.45350
C	29.37600	-10.63060	12.91730
C	29.99770	-9.38070	12.70390
C	31.22530	-9.32410	12.00900
C	31.83220	-10.50740	11.54500
C	28.59990	-7.09880	19.56110
C	29.90040	-7.06060	19.02370
C	30.08520	-6.93220	17.63350
C	28.96770	-6.84550	16.77580
C	27.66580	-6.87250	17.32000
C	27.48320	-7.00280	18.70980
C	49.52790	18.83640	-33.39330
C	48.48530	19.23790	-32.53690
C	47.84840	18.29210	-31.71050
C	48.25100	16.93940	-31.74210
C	49.30430	16.54350	-32.59360
C	49.93840	17.49050	-33.42010
C	41.53820	14.03950	-32.52870
C	42.69490	13.68080	-33.24550
C	43.96580	13.85090	-32.66470
C	44.08550	14.38820	-31.36390
C	42.92190	14.73660	-30.64490
C	41.65120	14.56540	-31.22800
C	50.30330	41.64640	18.88920
C	49.77240	40.87410	17.83910
C	50.53450	39.83210	17.27610
C	51.83230	39.55860	17.76030
C	52.35600	40.33140	18.82030
C	51.59390	41.37440	19.37960
C	58.33830	39.83680	14.44200
C	57.14360	40.22210	13.80510
C	55.92340	39.62390	14.17410
C	55.89480	38.64120	15.18730
C	57.09630	38.25070	15.81640
C	58.31530	38.84940	15.44480
H	46.44180	15.17920	-32.44210
H	45.70560	16.39430	-31.65160
H	53.57350	39.78300	15.90470
H	54.49560	39.35680	17.17670
H	30.22830	-8.45570	15.04010
H	28.61790	-8.69610	15.02470
O	49.14420	30.68150	9.25910
C	49.14930	30.74410	10.68650
O	33.50900	0.44950	7.74970
C	33.36840	0.28630	9.16230
O	45.36020	14.69850	-19.60930
C	45.84300	15.76500	-20.42780
H	44.19180	13.00240	-18.12670
H	46.10800	16.84510	-18.05160
H	44.53470	15.16470	-14.40170
H	47.05000	13.49100	-21.38730
H	47.46730	12.85280	-23.72800
H	45.11220	17.09780	-22.73280
H	46.46770	16.36590	-26.95040
H	44.88630	15.56740	-26.84700
H	43.83930	17.88220	-26.98030

H	45.44710	18.54550	-27.23290
H	43.57690	19.09840	-28.93690
H	45.16790	19.19660	-29.65670
H	42.86470	17.44900	-30.71610
H	43.18330	19.08790	-31.22910
H	48.83760	14.07430	-25.44760
H	48.09380	12.63130	-26.11760
H	48.36380	15.27610	-27.65620
H	49.63960	14.10270	-27.67060
H	49.57630	12.50130	-29.27240
H	48.52720	11.61910	-28.17430
H	48.25630	10.70140	-30.39740
H	46.76010	11.53120	-29.99590
H	47.86230	10.92800	-32.65280
H	46.39460	11.88010	-32.50240
H	49.03270	12.90400	-33.67590
H	47.73200	12.21400	-34.65010
H	43.36940	16.69360	-33.11760
H	43.38340	18.42990	-33.32990
H	44.57990	17.53330	-35.16380
H	45.75570	18.34470	-34.12420
H	49.20170	13.67650	-35.75360
H	49.62200	15.20100	-37.60200
H	48.28180	17.27230	-37.86120
H	46.51430	17.81030	-36.27420
H	52.10610	22.22190	-10.61160
H	51.11090	23.45370	-9.90800
H	50.13190	20.62730	-10.67180
H	50.59230	21.13850	-9.06650
H	49.17520	21.84910	-9.80150
H	51.91080	21.21040	-13.16520
H	50.26540	20.81650	-13.34860
H	52.07800	22.46420	-15.15440
H	51.00260	21.17250	-15.60040
H	50.37460	22.79150	-15.28870
H	51.64980	24.76020	-13.89560
H	51.79250	25.36350	-12.27280
H	53.47670	23.05910	-13.37620
H	53.98910	24.70980	-13.13140
H	53.58830	23.71950	-11.74670
H	46.91830	25.31050	-9.95500
H	45.32980	25.19530	-10.62130
H	45.64240	23.39550	-8.98180
H	45.45760	22.66370	-10.55790
H	47.05970	22.78450	-9.80880
H	46.05480	26.75830	-13.09570
H	47.60390	27.02560	-12.39770
H	47.09080	25.75860	-15.16290
H	47.65950	27.37910	-14.85460
H	48.70420	26.02570	-14.47960
H	45.93170	23.67490	-14.44570
H	45.50750	22.65610	-13.07000
H	43.55760	23.85400	-13.90380
H	43.90230	24.40780	-12.28200
H	44.32110	25.40470	-13.67720
H	36.35170	8.08630	-11.99410
H	37.19290	6.83730	-11.13820
H	39.09760	8.42270	-10.67910
H	38.31890	9.65930	-11.68710

H	37.57980	9.13830	-10.19240
H	37.08800	9.20810	-14.39130
H	38.76140	9.50420	-14.27640
H	37.19100	8.06170	-16.44030
H	38.42980	9.26740	-16.63150
H	38.85790	7.59000	-16.28740
H	37.33120	5.68150	-15.24790
H	36.88060	4.99840	-13.71770
H	35.06530	6.67650	-13.42490
H	35.49840	7.43380	-14.95560
H	34.89990	5.79380	-14.92560
H	41.15540	4.96100	-10.33100
H	42.85400	5.01080	-10.66800
H	42.78610	7.54470	-10.77490
H	41.08360	7.47990	-10.27780
H	42.34010	6.88430	-9.21990
H	40.79330	3.14750	-12.93110
H	41.54930	3.69440	-14.39310
H	42.99760	2.91370	-11.79710
H	42.93160	1.99630	-13.28510
H	43.81920	3.49890	-13.24160
H	43.25530	7.37920	-13.36000
H	44.04010	5.92140	-12.96140
H	42.43130	5.89350	-15.56000
H	44.04090	6.61310	-15.48170
H	43.80280	4.93740	-15.08130
H	36.27240	-3.31610	-12.12890
H	32.81330	-1.09990	-13.72870
H	32.09190	-3.70770	-13.44220
H	34.57050	-4.90350	-17.07330
H	36.89120	-4.86110	-15.67950
H	37.45390	-2.28310	-15.06700
H	35.45750	-0.72910	-16.07150
H	35.97310	-0.20080	-8.95490
H	37.49330	1.66380	-12.50240
H	37.81710	3.70530	-8.69890
H	52.08280	33.58740	-10.73190
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H	56.46560	33.93320	-10.89280
H	51.72030	32.44920	-13.84270
H	53.89710	30.85860	-14.21730
H	55.95750	32.43850	-14.99020
H	55.06250	34.99220	-15.09540
H	50.95810	28.59740	-11.24200
H	51.49530	30.59110	-7.48590
H	49.60490	26.70020	-7.59410
H	34.05750	0.69400	5.28000
H	34.57290	2.60660	9.09300
H	36.20140	4.43560	5.54200
H	30.94960	-0.45910	8.10200
H	29.53640	-2.35470	8.70690
H	33.83730	-1.66070	11.06240
H	30.98690	-4.62630	12.80940
H	31.87030	-5.58270	11.60300
H	33.85120	-5.58500	13.17490
H	32.84620	-4.82440	14.39790
H	34.20780	-7.27480	14.63720
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H	32.90240	-9.39100	14.16190

H	33.65930	-9.28100	15.73420
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H	28.54510	-4.26220	9.20910
H	27.03800	-5.60650	10.54760
H	28.61790	-6.33970	10.62410
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H	24.96580	-5.35470	13.67150
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H	24.38930	-7.85470	13.30820
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H	26.16910	-9.54290	13.02280
H	31.29120	-11.03700	15.19740
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H	24.49900	-9.54730	16.31420
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H	26.24750	-11.13200	19.88480
H	28.46700	-11.11850	18.85740
H	39.74000	7.51850	11.63020
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H	38.84650	7.16140	14.24020
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H	40.50720	6.69230	14.45180
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H	40.70840	9.49570	10.09640
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H	40.71240	10.70380	15.24770
H	40.12580	9.09220	15.48850
H	42.87380	9.86190	14.35130
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H	35.94620	11.20700	15.29110
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H	34.44260	13.13660	15.50530
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H	33.88960	12.19460	14.14370
H	35.58460	13.24390	11.68110
H	37.26040	13.53700	12.01010
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H	36.73400	13.21710	9.56200
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H	45.77480	30.82430	-4.16450
H	47.32750	32.06040	-1.94030
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H	46.92920	27.68690	-4.07910
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H	42.88980	25.19460	14.38000
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H	40.98210	22.13990	10.81070
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H	53.98330	37.77400	14.75500
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