

Supplementary Information

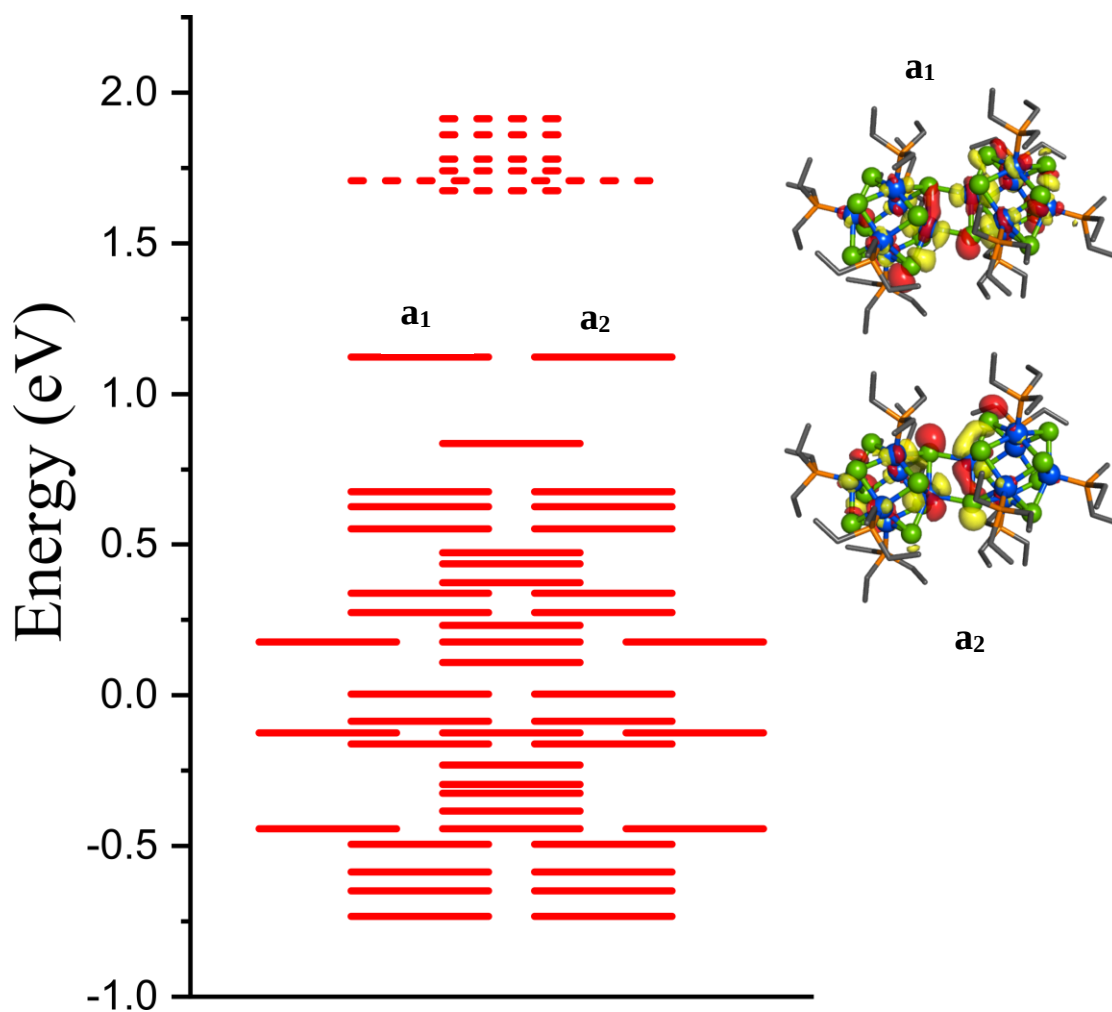
Interfacial Magnetism in a Fused Superatomic Cluster $[\text{Co}_6\text{Se}_8(\text{PEt}_3)_5]_2$

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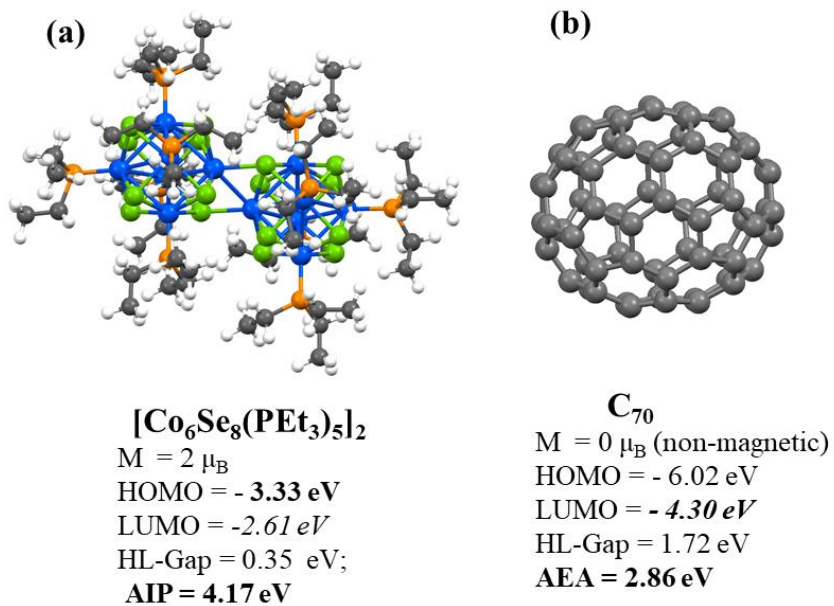
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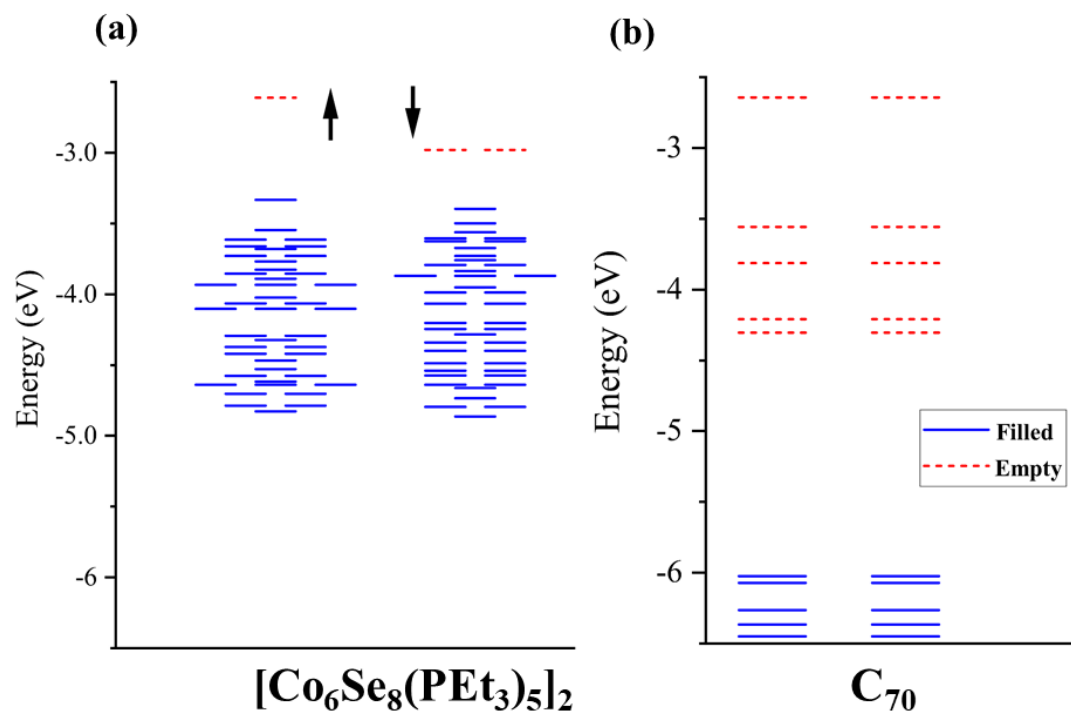
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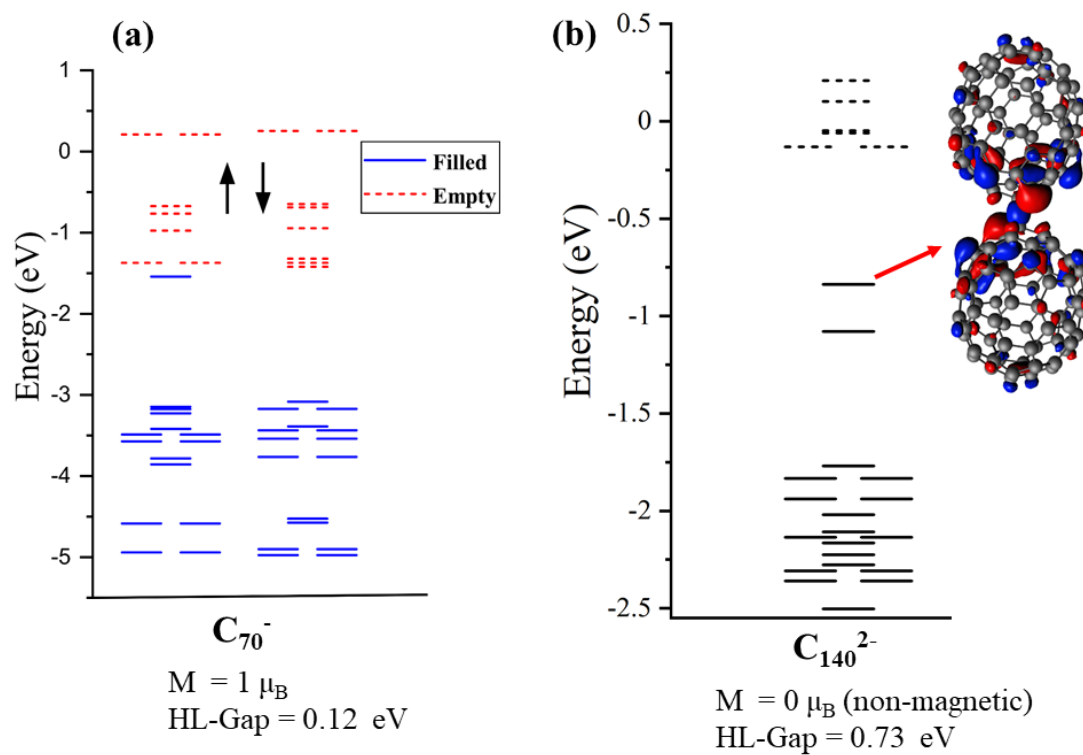
Supplementary Figure 1. One-electron energy levels of $[\text{Co}_6\text{Se}_8(\text{PEt}_3)_5]^{2-}$. The solid and dashed lines represent the occupied and unoccupied energy levels. Each energy level contains a pair of electrons. Molecular orbital surfaces of degenerate HOMO levels are shown. The gap is 0.53 eV.



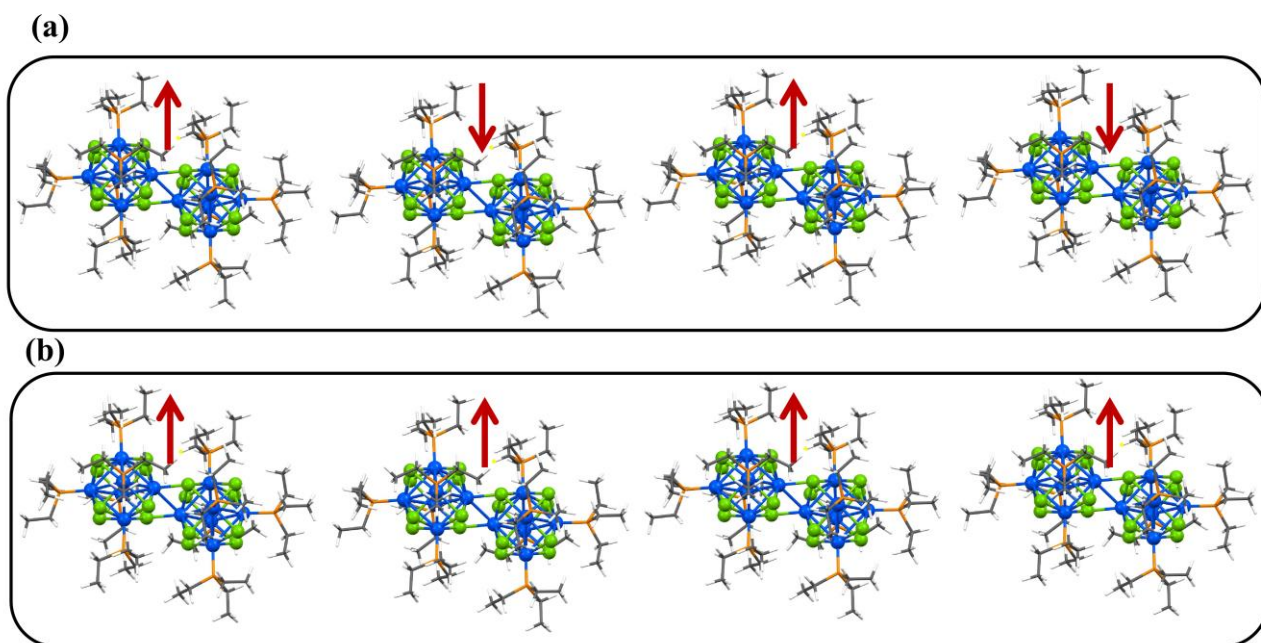
Supplementary Figure 2. Magnetic and Electronic Properties of **(a)** [Co₆Se₈(PEt₃)₅]₂
(b) C₇₀



Supplementary Figure 3. One-electron energy levels of **(a)** $[\text{Co}_6\text{Se}_8(\text{PEt}_3)_5]_2$ and **(b)** C_{70} . The solid and dashed lines represent the occupied and unoccupied energy levels. Each energy level contains one electron for (a) while a pair of electrons for (b).



Supplementary Figure 4. One-electron energy levels of **(a)** C_{70}^- and **(b)** C_{140}^{2-} . The solid and dashed lines represent the occupied and unoccupied energy levels. Each energy level contains one electron for (a) while a pair of electrons in (b).



Supplementary Figure 5. Schematic showing (a) antiferromagnetic-coupling between dimers in the cluster assembled solid $\{[\text{Co}_6\text{Se}_8(\text{PEt}_3)_5]_2(\text{Toluene})_2\text{C}_{140}\}_2$ (b) ferromagnetic-coupling between dimers in the solid. The red arrows show the direction of the spin-magnetic moment at the junction of the dimer. The antiferromagnetic coupling is more stable than ferromagnetic coupling by only 0.03 eV.

Cartesian-coordinates of optimized ground-state structures of [Co₆Se₈(PEt₃)₅]₂.

[Co₆Se₈(PEt₃)₅]₂

248

XYZ

Co	1.361432	1.840766	1.622095	H	2.942698	-4.3212	-1.554328
Co	1.473123	2.031212	5.922817	P	0.662909	-4.355582	-2.278533
Co	3.574852	2.27658	3.727954	H	-1.225309	-5.214097	-3.487605
Co	1.800256	-0.176303	3.835535	H	2.449345	-6.827378	-1.443741
Co	-0.710564	1.675439	3.79105	C	0.057058	-5.292022	-0.787879
Co	1.103929	4.069807	3.753099	H	0.17663	-6.366147	-1.000929
Se	3.351412	0.639849	5.437542	H	1.799032	-5.168602	0.524199
Se	2.868248	3.892765	5.357808	C	0.728754	-4.919406	0.526984
Se	-0.44111	3.396576	5.433319	H	-1.022809	-5.08838	-0.736653
Se	0.063476	0.138987	5.485993	H	0.262207	-5.458267	1.363567
Se	3.306962	0.505296	2.108954	H	0.635672	-3.843095	0.719664
Se	2.758192	3.767141	2.058193	H	-0.226706	2.844604	-7.765186
Se	-0.017685	-0.060532	2.233469	H	-1.996262	2.978135	-7.780582
Se	-0.481155	3.319327	2.099926	C	-1.149836	2.44978	-7.319211
Co	0.025846	-0.008078	-0.168631	H	-1.142289	2.692568	-6.249093
Co	-0.061866	-0.131779	-4.508162	H	1.764811	1.55219	-6.909356
Co	2.060078	0.234616	-2.362443	H	2.672197	1.047985	-9.217441
Co	-0.490585	2.051707	-2.359362	H	0.938388	1.390987	-9.308374
Co	-2.128866	-0.488518	-2.295452	C	1.680249	0.685192	-8.911023
Co	0.325028	-2.22968	-2.327082	C	1.60334	0.575528	-7.387651
Se	1.249933	1.799838	-4.013724	C	-1.279608	0.94299	-7.526884
Se	1.852792	-1.48634	-4.010056	H	-1.245099	0.691565	-8.598655
Se	-1.409137	-2.036144	-3.978787	H	2.393109	-0.080081	-6.991176
Se	-2.002363	1.179291	-3.98654	P	0.018401	-0.076378	-6.660931
Se	1.351645	1.93282	-0.775088	H	-2.242902	0.582984	-7.136593
Se	1.903661	-1.431455	-0.677672	H	1.517884	-0.28119	-9.407346
Se	-1.960079	1.270882	-0.655406	C	-0.205954	-1.698431	-7.558281
Se	-1.323377	-1.966516	-0.615797	H	-0.521425	-1.473208	-8.589237
H	1.38286	-5.33927	-5.147182	H	1.827148	-2.201087	-8.184889
H	-0.235421	-5.789024	-5.719717	C	1.020367	-2.609878	-7.56193
C	0.30946	-5.144371	-5.015173	H	-1.053137	-2.189376	-7.057666
H	0.11753	-4.101068	-5.292273	H	0.763196	-3.600717	-7.961815
H	2.829582	-4.366535	-3.301403	H	1.421054	-2.74634	-6.548889
H	3.874461	-6.486014	-2.436363	H	0.896112	5.973838	-4.41674
H	2.333117	-6.874607	-3.2143	H	2.354815	6.043788	-3.412917
C	2.786591	-6.3398	-2.368704	C	1.449955	5.455677	-3.622399
C	2.453902	-4.848532	-2.386872	H	1.764815	4.480606	-4.016324
C	-0.146694	-5.407463	-3.585737	H	-1.02307	4.473697	-4.846947
H	0.020968	-6.459593	-3.306031	H	-2.486009	6.488297	-5.095005

H	-1.163887	6.895828	-3.98976	H	6.966823	0.159716	-3.873364
C	-2.047042	6.254847	-4.114065	C	6.35679	0.940088	-4.34862
C	-1.699813	4.76771	-4.031739	C	4.860051	0.668711	-4.197555
C	0.614698	5.305127	-2.351764	C	5.292672	-0.635931	-1.619307
H	0.252431	6.288979	-2.01534	H	6.310753	-0.214654	-1.619399
H	-2.595756	4.142494	-4.152632	H	4.259362	1.436161	-4.708012
P	-0.874058	4.179615	-2.470207	P	4.179011	0.590376	-2.467044
H	1.22313	4.893469	-1.534178	H	4.946711	-0.658123	-0.57477
H	-2.779924	6.547378	-3.350614	H	6.646714	1.90472	-3.910134
C	-1.932337	4.939533	-1.13812	C	4.810016	2.153441	-1.683127
H	-1.811592	6.031579	-1.22014	H	5.908913	2.081468	-1.644621
H	-3.906299	4.882139	-2.089555	H	4.767053	3.52887	-3.385445
C	-3.410927	4.562668	-1.162054	C	4.37319	3.446783	-2.36291
H	-1.473455	4.630513	-0.186297	H	4.443148	2.122301	-0.646235
H	-3.937296	5.041011	-0.32322	H	4.729985	4.317244	-1.794425
H	-3.539762	3.477509	-1.062281	H	3.279419	3.50601	-2.419185
H	-4.473266	-3.906109	-1.113783	H	-1.097784	0.749872	9.21902
H	-4.46175	-4.775667	-2.661156	H	-2.077602	2.226899	9.29568
C	-4.148025	-3.847643	-2.161802	C	-1.218584	1.756733	8.79599
H	-3.050598	-3.806497	-2.16933	H	-1.460129	1.646188	7.731176
H	-4.311921	-1.636253	0.099708	H	1.016182	-0.321592	8.402487
H	-6.732971	-1.258052	0.705299	H	2.061192	-0.841573	10.63416
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C	-6.426089	-1.323902	-0.348849	C	1.899141	0.20288	10.33047
C	-4.948207	-0.961168	-0.491351	C	1.824324	0.30575	8.807168
C	-4.737806	-2.633623	-2.873425	C	0.037497	2.603503	8.98177
H	-5.838835	-2.665433	-2.854919	H	0.302507	2.685273	10.0481
H	-4.744872	0.047548	-0.103465	H	2.747106	-0.063075	8.335522
P	-4.216079	-0.976332	-2.20102	P	1.540624	1.991153	8.068295
H	-4.428706	-2.62352	-3.929052	H	-0.13128	3.624558	8.608725
H	-7.075513	-0.645955	-0.919489	H	2.728038	0.793935	10.7432
C	-5.382294	0.102343	-3.172686	C	2.833316	3.043633	8.8988
H	-6.371755	-0.381994	-3.165648	H	2.639704	3.015823	9.98297
H	-5.884773	1.610662	-1.670437	H	4.517235	1.648955	8.95188
C	-5.477582	1.546264	-2.689048	C	4.278563	2.660358	8.59467
H	-5.0097	0.06892	-4.207253	H	2.631682	4.070159	8.55804
H	-6.135341	2.131028	-3.347807	H	4.973277	3.358787	9.08279
H	-4.487771	2.020139	-2.688808	H	4.467879	2.690287	7.5136
H	5.691482	-2.048073	-3.241553	H	6.687893	4.873095	1.71407
H	5.895372	-2.721335	-1.612685	H	6.731628	3.98811	0.179918
C	5.284976	-2.038087	-2.220571	C	6.254721	4.022821	1.16987
H	4.263712	-2.437498	-2.261389	H	5.186229	4.227069	1.0254
H	4.57691	-0.286277	-4.664313	H	5.791898	4.914099	4.04807
H	6.63383	0.968289	-5.412455	H	8.121206	5.241524	4.96025

H	8.218334	4.458133	3.37606	H	-5.409813	0.149416	5.15753
C	7.865279	4.325915	4.40742	C	-5.088928	1.084854	5.635856
C	6.358594	4.072416	4.47268	C	-3.577883	1.291975	5.533037
C	6.475646	2.70377	1.906697	C	-3.51012	-0.131966	2.985055
H	7.553744	2.513493	2.027	H	-4.604342	-0.018564	2.919645
H	6.012092	3.987287	5.51268	H	-3.267807	2.219898	6.0356
P	5.708852	2.558404	3.605442	P	-2.845305	1.387985	3.825244
H	6.062669	1.862358	1.33099	H	-3.115494	-0.086281	1.95908
H	8.441704	3.503932	4.85251	H	-5.649772	1.907667	5.17207
C	6.789996	1.188707	4.28165	C	-3.899883	2.667234	2.979851
H	7.78894	1.312794	3.83508	H	-4.931283	2.280714	2.95617
H	7.370545	1.994026	6.23301	H	-4.271234	4.065461	4.6205
C	6.901715	1.098862	5.80249	C	-3.855026	4.058357	3.603381
H	6.367946	0.259821	3.8708	H	-3.536524	2.693212	1.9415
H	7.519159	0.234269	6.0859	H	-4.437202	4.770382	3.0007
H	5.916029	0.971652	6.26719	H	-2.822205	4.42386	3.659491
H	5.208991	-2.974681	4.126383	H	0.109717	7.288092	0.94445
H	5.488033	-3.04934	2.375489	H	1.763989	7.505066	0.33975
C	4.834165	-2.629219	3.152926	C	1.150052	6.95607	1.0678
H	4.929875	-1.535809	3.116168	H	1.1974	5.889082	0.814276
H	3.662824	-2.203719	5.9475	H	-1.342729	6.257377	2.72578
H	3.411747	-4.504739	6.964233	H	-2.35649	8.401701	3.538411
H	3.894677	-4.63874	5.266846	H	-0.768439	8.757716	2.8421
C	3.086457	-4.307055	5.932427	C	-1.277171	8.229263	3.659965
C	2.774824	-2.820986	5.751892	C	-0.979344	6.730495	3.649762
C	3.38584	-3.051674	2.91433	C	1.656172	7.196658	2.4868
H	3.283064	-4.146276	2.985029	H	1.571147	8.260021	2.7619
H	2.014455	-2.479358	6.469949	H	-1.502022	6.216593	4.469811
P	2.148057	-2.290022	4.080398	P	0.796118	6.195693	3.79958
H	3.058995	-2.75391	1.906576	H	2.718476	6.922024	2.56598
H	2.213485	-4.944072	5.737271	H	-0.97644	8.703671	4.603976
C	0.691601	-3.429163	3.822732	C	1.385908	7.122581	5.30463
H	1.095726	-4.423947	3.57986	H	1.232623	8.19576	5.108391
H	0.150258	-4.017557	5.860643	H	-0.34682	6.892618	6.620125
C	-0.295114	-3.526471	4.985084	C	0.737214	6.7135	6.623955
H	0.187634	-3.058459	2.919664	H	2.471405	6.949221	5.34363
H	-1.174402	-4.115169	4.687292	H	1.167338	7.287666	7.4572
H	-0.643484	-2.534863	5.30197	H	0.899088	5.645544	6.8221
H	-3.563317	-1.551484	4.650976				
H	-3.512434	-2.299938	3.041483				
C	-3.13969	-1.45739	3.641426				
H	-2.050632	-1.559732	3.720962				
H	-3.028173	0.48345	6.037181				
H	-5.395521	1.034468	6.69077				