Electronic Supplementary Material (ESI) for Dalton Transactions.

Site preferences in hetero-metallic [$Fe_{9-x}Ni_x$] clusters: a combined crystallographic, spectroscopic and theoretical analysis.

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Supporting Information

1. X-ray Fluorescence spectroscopy

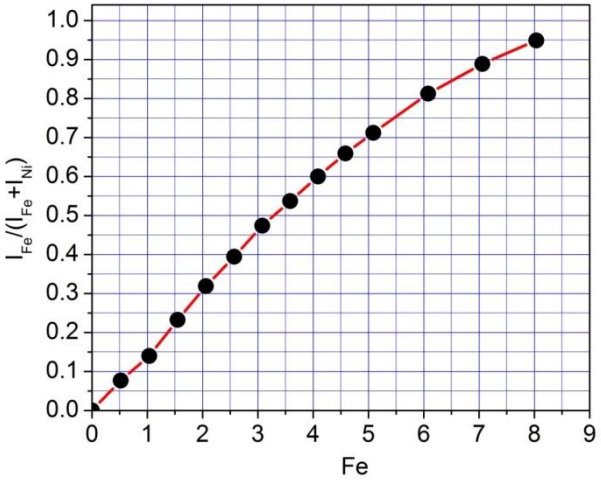

Figure S1. Calibration curve for XRF analysis. The horizontal axis represents the number of Fe atoms, while the total number of Fe and Ni atoms are constant and equal to 9. The vertical axis is the intensity ratio Fe/(Fe+Ni) of the corresponding Kα transition intensities. Solid line is a guide to the eye.

2. Mössbauer Spectroscopy

Simulation of the Mössbauer spectra.

In clusters with a high Fe content (**1**, **2**), the doublet assigned to the $Fe^{(8)}$ ion is visible only as a weak shoulder at $\delta \sim 3$ mm/s, making it difficult to simulate the spectra and identify accurate spectroscopic parameters. The data for cluster **1** are shown in Figure S2, along with two distinct simulation models. Model A yields the values listed in Table 3 in the main text: Doublet I: δ = 1.23(1) mm/s, ΔE_Q = 2.62(1) mm/s, Γ = 0.36 mm/s, Area = 90(4)%; Doublet II: δ = 1.35(3) mm/s, ΔE_Q = 3.18(4) mm/s, Γ = 0.28 mm/s. Area = 10.0(4) %. Model B yields: Doublet I: δ = 1.22(1) mm/s, ΔE_Q = 2.64 mm/s, Γ = 0.38 mm/s, Area = 91(4)%; Doublet II: δ = 1.48(4) mm/s, ΔE_Q = 2.92(5) mm/s, Γ = 0.34 mm/s. Area = 9.0(4) %. The two models differ primarily in the quadrupole splitting in doublet II, and yield fits of almost identical quality. The larger value of ΔE_Q for model A is more consistent with data for other clusters where doublet II is better resolved, so we have chosen to report this data set in Table 3. It should be noted that the slight differences in the bond lengths around the 6- and 8-coordinate sites in **1**-**5** due to

the presence of two crystallographically independent molecules (A and B) in the unit cell, cannot be identified by the Mössbauer spectra.

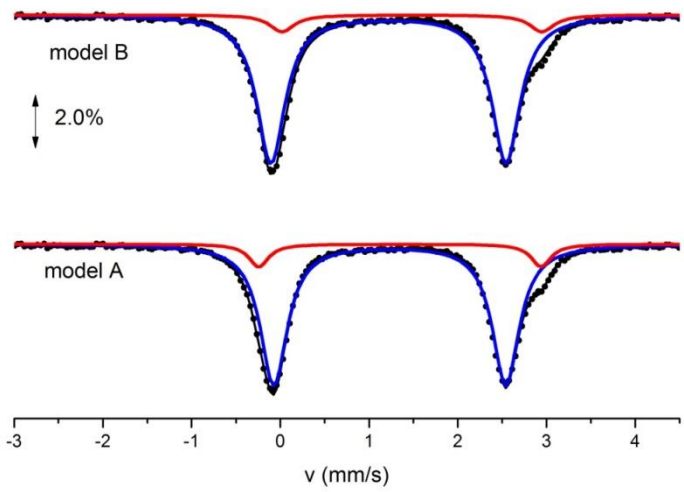

Figure S2. Simulation of the Mössbauer spectra sample **1** at 80 K assuming two models. The contribution of doublets I and II is shown in blue and red line respectively. The parameters in model A are listed in Table 3. Model B yields: Doublet I: δ = 1.22(1) mm/s, ΔE_Q = 2.64 mm/s, Γ = 0.38 mm/s, Area = 91(4)%; Doublet II: δ = 1.48(4) mm/s, ΔE_Q = 2.92(5) mm/s, Γ = 0.34 mm/s. Area = 9.0(4) %.

Temperature dependence of the Mössbauer spectra

Throughout the main text, we take the ratio of integrated intensities of the two Mössbauer doublets to be directly proportional to the ratio of the number of Fe^{II} ions in the respective coordination sites. This assumption is valid only if the two sites have equal Mössbauer-Lamb factors. For sample **3** a number of spectra at various temperatures are shown in Figure S3. The ratio $A_{(8)}/A_{(6)}$ is independent of temperature within experimental error especially below 100 K. Although no detailed temperature dependence was carried out for samples **4** and **5**, similar behavior was observed for the ratio $A_{(8)}/A_{(6)}$ (not shown). Therefore the relative ratio $A_{(8)}/A_{(6)}$ below 100 K is a reliable parameter which can be used in order to quantify the relative abundance of ions at the different sites.

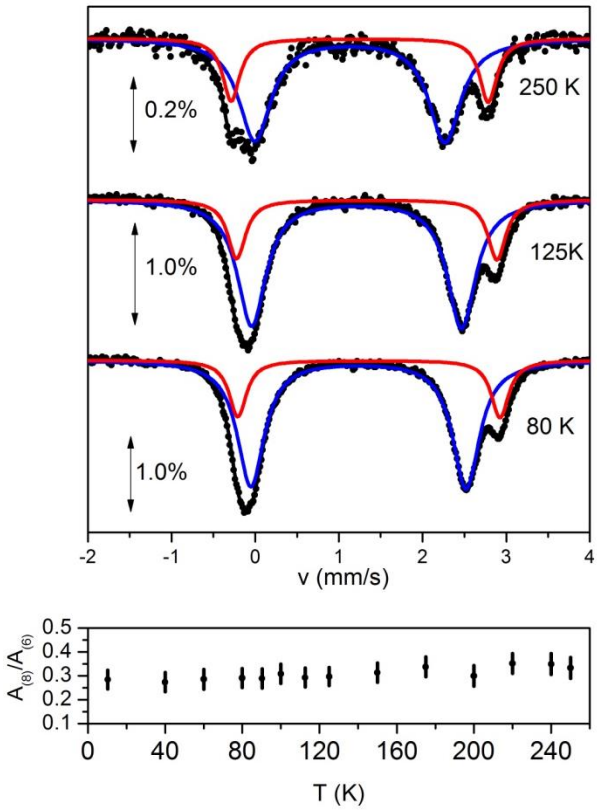

Figure S3. Upper panel. Experimental (•) and theoretical (black lines) Mössbauer spectra from powder sample of **3** at several temperatures as indicated in zero magnetic field. The contribution of doublets I and II is shown in blue and red lines respectively. Lower panel: temperature dependence of the ratio $A_{(8)}/A_{(6)}$.

Zero-field Mössbauer spectra at 4.2 K.

One possible outcome of our synthetic protocol is that the crystals contain a mixture of the homo-metallic [Fe_9] and [Ni_9] complexes rather than a hetero-metallic [$Fe_{9-x}Ni_x$] cluster. The [Fe_9] cluster shows a characteristic magnetic splitting at low temperature (Figure S4, **1**), so we measured the spectra for clusters **2 - 5** under the same conditions. Clusters **3 - 5** showed no sign of magnetic spitting at 4.2 K, confirming the absence of the [Fe_9] cluster. Cluster **2**, in contrast, does show magnetic splitting, and so we cannot conclude with certainty that this is a genuine hetero-metallic cluster.

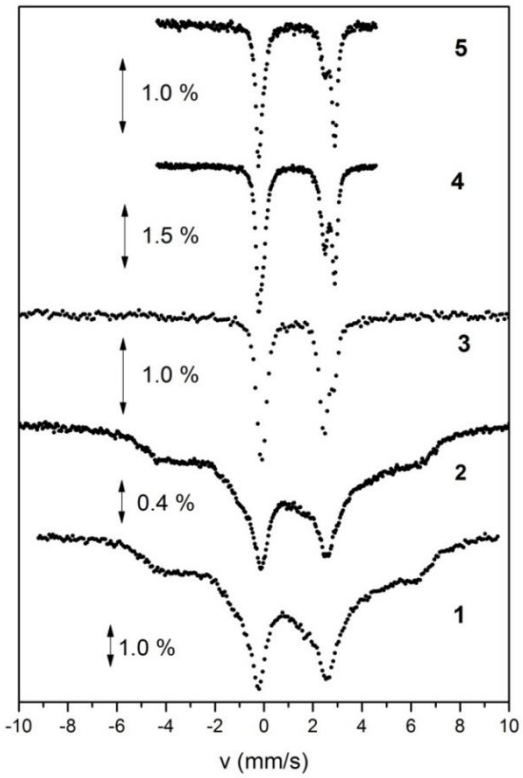

Figure S4. Zero field Mössbauer spectra at 4.2 K from powdered samples of **1** - **5**. The lack of magnetically split spectra for **3**, **4** and **5** is consistent with the absence of homo-metallic [Fe_9] clusters.

3. Density Functional Theory

The computed Mossbauer parameters for a range of high (D_4) symmetry clusters are collected in Table S1. The raw data, *i.e.* the computed isomer shift, δ, and quadrupole splitting, ΔE_Q for the Fe-containing clusters corroborate the assignment of the two doublets presented in the main text. The characteristic large value of ΔE_Q for the 8-coordinate site is found in both Fe@Fe_8 and Fe@Ni_8, and the components of the electric field gradient (EFG) are also very similar. In comparison, the components of the EFG in the isostructural Mn@Mn_8 cluster are very small, indicating that the valence contributions due to the anisotropy of the Fe^{II} ion dominate the lattice contribution that is common to all clusters. The strong axial anisotropy of the EFG arises because the crystal-field splitting in the 8-coordinate site places the d_{z^2} orbital below the other four orbitals (Figure S5), giving a $d_{z^2}{}^2 d_{xy}{}^1 d_{x^2-y^2}{}^1 d_{xz}{}^1 d_{yz}{}^1$ configuration.

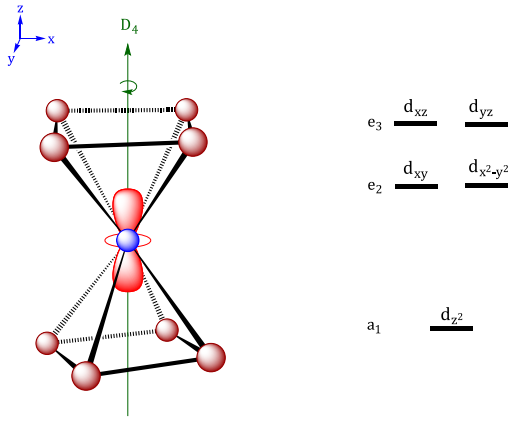

Figure S5: Coordination geometry and ligand-field splitting of the 8-coordinate site. Only the $\boldsymbol{d_{z^2}}$ orbital is doubly occupied in Fe^{II}.

Table S1. Computed Mössbauer parameters and components of the electric field gradient for high-symmetry clusters. The corresponding experimental data, where available, are shown in italics.

Cluster	**coordination number**	$\boldsymbol{\delta}$ **(mm/s)**	V_{XX} **(au)**	V_{YY} **(au)**	V_{ZZ} **(au)**	$\boldsymbol{\Delta E_Q}$ **(mm/s)**
$Fe@Ni_8$	8	1.26	+0.78	+0.78	–1.56	2.53
		(*1.33*)				(*3.12*)
$Fe@Fe_8$	6	1.23	–0.57	–0.87	+1.44	2.34
		(*1.23*)				(*2.62*)
	8	1.33	+0.83	+0.83	–1.66	2.69
		(*1.35*)				(*3.18*)
$Mn@Mn_8$	8		–0.20	–0.20	+0.40	
	6		+0.15	+0.25	–0.39	

Table S2: Total energies for the OH-capped clusters calculated using OPBE/TZP (both in au and in eV: 1au = 27.211385 eV).

	au	**eV**
	homonuclear clusters	
Fe@Fe$_8$	–39.6398728	–1078.66
Ni@Ni$_8$	–37.8966663	–1031.22
Zn@Zn$_8$	–37.1891406	–1011.97
Mn@Mn$_8$	–40.1950052	–1093.76
	Ni/Fe series	
Ni@Fe$_8$	–39.4236224	–1072.77
Fe@Ni$_8$	–38.1174119	–1037.23
	Ni/Zn series	
Ni@Zn$_8$	–37.2400878	–1013.35
Zn@Ni$_8$	–37.8425895	–1029.75
	Fe/Zn series	
Zn@Fe$_8$	–39.363354	–1071.13
Fe@Zn$_8$	–37.4622933	–1019.40
	Ni/Mn series	
Ni@Mn$_8$	–39.9015379	–1085.78
Mn@Ni$_8$	–38.1806799	–1038.95
	Fe/Mn series	
Fe@Mn$_8$	–40.1257598	–1091.88
Mn@Fe$_8$	–39.7036576	–1080.39

Sample calculations of ΔE for the isodesmic reactions shown in Figure 5a.

$$Ni@Ni_8 + 8\ Fe@Fe_8 \rightarrow 9Ni@Fe_8$$

ΔE = 9 x (–1072.77 eV) –(–1031.22 eV + 8 x (–1078.66 eV)) = +5.57 eV

$$Fe@Fe_8 + 8\ Ni@Ni_8 \rightarrow 9Fe@Ni_8$$

ΔE = 9 x (–1037.23 eV) –(–8 x (1031.22 eV) –1078.66 eV) = –6.65 eV

Table S3: Cartesian coordinates for Ni/Fe clusters calculated using OPBE/TZP

$Fe@Fe_8$			
Atom	X	Y	Z
1.Fe	0.000000	0.000000	0.000000
2.Fe	1.837600	1.304957	2.515134
3.Fe	1.304957	-1.837600	2.515134
4.Fe	-1.837600	-1.304957	2.515134
5.Fe	-1.304957	1.837600	2.515134
6.Fe	1.837600	-1.304957	-2.515134
7.Fe	-1.304957	-1.837600	-2.515134
8.Fe	-1.837600	1.304957	-2.515134
9.Fe	1.304957	1.837600	-2.515134
10.N	-3.485213	-1.924327	1.333793
11.N	-3.485213	1.924327	-1.333793
12.O	-1.998908	-0.206655	-1.105448
13.O	-1.998908	0.206655	1.105448
14.O	-1.723430	-2.993535	3.678071
15.O	0.494035	-3.095976	4.036073
16.O	0.000000	0.000000	3.114170
17.O	-3.095976	0.494035	-4.036073
18.O	-2.993535	-1.723430	-3.678071
19.O	0.000000	0.000000	-3.114170
20.C	-2.806943	0.000000	0.000000
21.C	-3.720739	-1.205381	0.231744
22.C	-4.776624	-1.485288	-0.620848
23.H	-4.923363	-0.875775	-1.506863
24.C	-5.640211	-2.520378	-0.309114
25.H	-6.487294	-2.746263	-0.953761
26.C	-5.407869	-3.252475	0.847888
27.H	-6.064094	-4.067665	1.144417

28.C	-4.314599	-2.937761	1.627026
29.H	-4.080384	-3.491790	2.530651
30.C	-3.720739	1.205381	-0.231744
31.C	-4.776624	1.485288	0.620848
32.H	-4.923363	0.875775	1.506863
33.C	-5.640211	2.520378	0.309114
34.H	-6.487294	2.746263	0.953761
35.C	-5.407869	3.252475	-0.847888
36.H	-6.064094	4.067665	-1.144417
37.C	-4.314599	2.937761	-1.627026
38.H	-4.080384	3.491790	-2.530651
39.C	-0.686177	-3.472713	4.226866
40.C	-0.895466	-4.591581	5.214242
41.H	-1.898810	-5.015906	5.128660
42.H	-0.770414	-4.189415	6.227158
43.H	-0.133578	-5.364523	5.074109
44.C	-3.472713	-0.686177	-4.226866
45.C	-4.591581	-0.895466	-5.214242
46.H	-5.015906	-1.898810	-5.128660
47.H	-4.189415	-0.770414	-6.227158
48.H	-5.364523	-0.133578	-5.074109
49.N	-1.924327	3.485213	1.333793
50.N	1.924327	3.485213	-1.333793
51.O	-0.206655	1.998908	-1.105448
52.O	0.206655	1.998908	1.105448
53.O	-2.993535	1.723430	3.678071
54.O	-3.095976	-0.494035	4.036073
55.O	0.494035	3.095976	-4.036073
56.O	-1.723430	2.993535	-3.678071
57.C	0.000000	2.806943	0.000000

58.C	-1.205381	3.720739	0.231744
59.C	-1.485288	4.776624	-0.620848
60.H	-0.875775	4.923363	-1.506863
61.C	-2.520378	5.640211	-0.309114
62.H	-2.746263	6.487294	-0.953761
63.C	-3.252475	5.407869	0.847888
64.H	-4.067665	6.064094	1.144417
65.C	-2.937761	4.314599	1.627026
66.H	-3.491790	4.080384	2.530651
67.C	1.205381	3.720739	-0.231744
68.C	1.485288	4.776624	0.620848
69.H	0.875775	4.923363	1.506863
70.C	2.520378	5.640211	0.309114
71.H	2.746263	6.487294	0.953761
72.C	3.252475	5.407869	-0.847888
73.H	4.067665	6.064094	-1.144417
74.C	2.937761	4.314599	-1.627026
75.H	3.491790	4.080384	-2.530651
76.C	-3.472713	0.686177	4.226866
77.C	-4.591581	0.895466	5.214242
78.H	-5.015906	1.898810	5.128660
79.H	-4.189415	0.770414	6.227158
80.H	-5.364523	0.133578	5.074109
81.C	-0.686177	3.472713	-4.226866
82.C	-0.895466	4.591581	-5.214242
83.H	-1.898810	5.015906	-5.128660
84.H	-0.770414	4.189415	-6.227158
85.H	-0.133578	5.364523	-5.074109
86.N	3.485213	1.924327	1.333793
87.N	3.485213	-1.924327	-1.333793

88.O	1.998908	0.206655	-1.105448
89.O	1.998908	-0.206655	1.105448
90.O	1.723430	2.993535	3.678071
91.O	-0.494035	3.095976	4.036073
92.O	3.095976	-0.494035	-4.036073
93.O	2.993535	1.723430	-3.678071
94.C	2.806943	0.000000	0.000000
95.C	3.720739	1.205381	0.231744
96.C	4.776624	1.485288	-0.620848
97.H	4.923363	0.875775	-1.506863
98.C	5.640211	2.520378	-0.309114
99.H	6.487294	2.746263	-0.953761
100.C	5.407869	3.252475	0.847888
101.H	6.064094	4.067665	1.144417
102.C	4.314599	2.937761	1.627026
103.H	4.080384	3.491790	2.530651
104.C	3.720739	-1.205381	-0.231744
105.C	4.776624	-1.485288	0.620848
106.H	4.923363	-0.875775	1.506863
107.C	5.640211	-2.520378	0.309114
108.H	6.487294	-2.746263	0.953761
109.C	5.407869	-3.252475	-0.847888
110.H	6.064094	-4.067665	-1.144417
111.C	4.314599	-2.937761	-1.627026
112.H	4.080384	-3.491790	-2.530651
113.C	0.686177	3.472713	4.226866
114.C	0.895466	4.591581	5.214242
115.H	1.898810	5.015906	5.128660
116.H	0.770414	4.189415	6.227158
117.H	0.133578	5.364523	5.074109

118.C	3.472713	0.686177	-4.226866
119.C	4.591581	0.895466	-5.214242
120.H	5.015906	1.898810	-5.128660
121.H	4.189415	0.770414	-6.227158
122.H	5.364523	0.133578	-5.074109
123.N	1.924327	-3.485213	1.333793
124.N	-1.924327	-3.485213	-1.333793
125.O	0.206655	-1.998908	-1.105448
126.O	-0.206655	-1.998908	1.105448
127.O	2.993535	-1.723430	3.678071
128.O	3.095976	0.494035	4.036073
129.O	-0.494035	-3.095976	-4.036073
130.O	1.723430	-2.993535	-3.678071
131.C	0.000000	-2.806943	0.000000
132.C	1.205381	-3.720739	0.231744
133.C	1.485288	-4.776624	-0.620848
134.H	0.875775	-4.923363	-1.506863
135.C	2.520378	-5.640211	-0.309114
136.H	2.746263	-6.487294	-0.953761
137.C	3.252475	-5.407869	0.847888
138.H	4.067665	-6.064094	1.144417
139.C	2.937761	-4.314599	1.627026
140.H	3.491790	-4.080384	2.530651
141.C	-1.205381	-3.720739	-0.231744
142.C	-1.485288	-4.776624	0.620848
143.H	-0.875775	-4.923363	1.506863
144.C	-2.520378	-5.640211	0.309114
145.H	-2.746263	-6.487294	0.953761
146.C	-3.252475	-5.407869	-0.847888
147.H	-4.067665	-6.064094	-1.144417

148.C	-2.937761	-4.314599	-1.627026
149.H	-3.491790	-4.080384	-2.530651
150.C	3.472713	-0.686177	4.226866
151.C	4.591581	-0.895466	5.214242
152.H	5.015906	-1.898810	5.128660
153.H	4.189415	-0.770414	6.227158
154.H	5.364523	-0.133578	5.074109
155.C	0.686177	-3.472713	-4.226866
156.C	0.895466	-4.591581	-5.214242
157.H	1.898810	-5.015906	-5.128660
158.H	0.770414	-4.189415	-6.227158
159.H	0.133578	-5.364523	-5.074109
160.H	0.000000	0.000000	-4.088132
161.H	0.000000	0.000000	4.088132

Ni@Fe_8

Atom	X	Y	Z	(Angstrom)
1.Ni	0.0000000	0.0000000	0.0000000	
2.Fe	1.8248510	1.2958220	2.4611270	
3.Fe	1.2958220	-1.8248510	2.4611270	
4.Fe	-1.8248510	-1.2958220	2.4611270	
5.Fe	-1.2958220	1.8248510	2.4611270	
6.Fe	1.8248510	-1.2958220	-2.4611270	
7.Fe	-1.2958220	-1.8248510	-2.4611270	
8.Fe	-1.8248510	1.2958220	-2.4611270	
9.Fe	1.2958220	1.8248510	-2.4611270	
10.N	-3.5130020	-1.9478780	1.3096070	
11.N	-3.5130020	1.9478780	-1.3096070	
12.O	-2.0725360	-0.2093190	-1.1107840	

13.O	-2.0725360	0.2093190	1.1107840
14.O	-1.7013320	-2.9842960	3.6372560
15.O	0.5148170	-3.0676850	4.0106770
16.O	0.0000000	0.0000000	3.0663080
17.O	-3.0676850	0.5148170	-4.0106770
18.O	-2.9842960	-1.7013320	-3.6372560
19.O	0.0000000	0.0000000	-3.0663080
20.C	-2.8691890	0.0000000	0.0000000
21.C	-3.7772210	-1.2084610	0.2290850
22.C	-4.8496660	-1.4826840	-0.6060560
23.H	-5.0165790	-0.8642060	-1.4824410
24.C	-5.7011410	-2.5251160	-0.2885410
25.H	-6.5619390	-2.7452920	-0.9171020
26.C	-5.4398250	-3.2755740	0.8502460
27.H	-6.0861890	-4.0979590	1.1482810
28.C	-4.3262500	-2.9708730	1.6053040
29.H	-4.0641520	-3.5399450	2.4918240
30.C	-3.7772210	1.2084610	-0.2290850
31.C	-4.8496660	1.4826840	0.6060560
32.H	-5.0165790	0.8642060	1.4824410
33.C	-5.7011410	2.5251160	0.2885410
34.H	-6.5619390	2.7452920	0.9171020
35.C	-5.4398250	3.2755740	-0.8502460
36.H	-6.0861890	4.0979590	-1.1482810
37.C	-4.3262500	2.9708730	-1.6053040
38.H	-4.0641520	3.5399450	-2.4918240
39.C	-0.6656290	-3.4506450	4.1964040
40.C	-0.8713370	-4.5618900	5.1932980
41.H	-1.8848080	-4.9660990	5.1368470

42.H	-0.7066090	-4.1604260	6.2005910
43.H	-0.1300140	-5.3511140	5.0339270
44.C	-3.4506450	-0.6656290	-4.1964040
45.C	-4.5618900	-0.8713370	-5.1932980
46.H	-4.9660990	-1.8848080	-5.1368470
47.H	-4.1604260	-0.7066090	-6.2005910
48.H	-5.3511140	-0.1300140	-5.0339270
49.N	-1.9478780	3.5130020	1.3096070
50.N	1.9478780	3.5130020	-1.3096070
51.O	-0.2093190	2.0725360	-1.1107840
52.O	0.2093190	2.0725360	1.1107840
53.O	-2.9842960	1.7013320	3.6372560
54.O	-3.0676850	-0.5148170	4.0106770
55.O	0.5148170	3.0676850	-4.0106770
56.O	-1.7013320	2.9842960	-3.6372560
57.C	0.0000000	2.8691890	0.0000000
58.C	-1.2084610	3.7772210	0.2290850
59.C	-1.4826840	4.8496660	-0.6060560
60.H	-0.8642060	5.0165790	-1.4824410
61.C	-2.5251160	5.7011410	-0.2885410
62.H	-2.7452920	6.5619390	-0.9171020
63.C	-3.2755740	5.4398250	0.8502460
64.H	-4.0979590	6.0861890	1.1482810
65.C	-2.9708730	4.3262500	1.6053040
66.H	-3.5399450	4.0641520	2.4918240
67.C	1.2084610	3.7772210	-0.2290850
68.C	1.4826840	4.8496660	0.6060560
69.H	0.8642060	5.0165790	1.4824410
70.C	2.5251160	5.7011410	0.2885410

71.H	2.7452920	6.5619390	0.9171020
72.C	3.2755740	5.4398250	-0.8502460
73.H	4.0979590	6.0861890	-1.1482810
74.C	2.9708730	4.3262500	-1.6053040
75.H	3.5399450	4.0641520	-2.4918240
76.C	-3.4506450	0.6656290	4.1964040
77.C	-4.5618900	0.8713370	5.1932980
78.H	-4.9660990	1.8848080	5.1368470
79.H	-4.1604260	0.7066090	6.2005910
80.H	-5.3511140	0.1300140	5.0339270
81.C	-0.6656290	3.4506450	-4.1964040
82.C	-0.8713370	4.5618900	-5.1932980
83.H	-1.8848080	4.9660990	-5.1368470
84.H	-0.7066090	4.1604260	-6.2005910
85.H	-0.1300140	5.3511140	-5.0339270
86.N	3.5130020	1.9478780	1.3096070
87.N	3.5130020	-1.9478780	-1.3096070
88.O	2.0725360	0.2093190	-1.1107840
89.O	2.0725360	-0.2093190	1.1107840
90.O	1.7013320	2.9842960	3.6372560
91.O	-0.5148170	3.0676850	4.0106770
92.O	3.0676850	-0.5148170	-4.0106770
93.O	2.9842960	1.7013320	-3.6372560
94.C	2.8691890	0.0000000	0.0000000
95.C	3.7772210	1.2084610	0.2290850
96.C	4.8496660	1.4826840	-0.6060560
97.H	5.0165790	0.8642060	-1.4824410
98.C	5.7011410	2.5251160	-0.2885410
99.H	6.5619390	2.7452920	-0.9171020

100.C	5.4398250	3.2755740	0.8502460
101.H	6.0861890	4.0979590	1.1482810
102.C	4.3262500	2.9708730	1.6053040
103.H	4.0641520	3.5399450	2.4918240
104.C	3.7772210	-1.2084610	-0.2290850
105.C	4.8496660	-1.4826840	0.6060560
106.H	5.0165790	-0.8642060	1.4824410
107.C	5.7011410	-2.5251160	0.2885410
108.H	6.5619390	-2.7452920	0.9171020
109.C	5.4398250	-3.2755740	-0.8502460
110.H	6.0861890	-4.0979590	-1.1482810
111.C	4.3262500	-2.9708730	-1.6053040
112.H	4.0641520	-3.5399450	-2.4918240
113.C	0.6656290	3.4506450	4.1964040
114.C	0.8713370	4.5618900	5.1932980
115.H	1.8848080	4.9660990	5.1368470
116.H	0.7066090	4.1604260	6.2005910
117.H	0.1300140	5.3511140	5.0339270
118.C	3.4506450	0.6656290	-4.1964040
119.C	4.5618900	0.8713370	-5.1932980
120.H	4.9660990	1.8848080	-5.1368470
121.H	4.1604260	0.7066090	-6.2005910
122.H	5.3511140	0.1300140	-5.0339270
123.N	1.9478780	-3.5130020	1.3096070
124.N	-1.9478780	-3.5130020	-1.3096070
125.O	0.2093190	-2.0725360	-1.1107840
126.O	-0.2093190	-2.0725360	1.1107840
127.O	2.9842960	-1.7013320	3.6372560
128.O	3.0676850	0.5148170	4.0106770

129.O	-0.5148170	-3.0676850	-4.0106770
130.O	1.7013320	-2.9842960	-3.6372560
131.C	0.0000000	-2.8691890	0.0000000
132.C	1.2084610	-3.7772210	0.2290850
133.C	1.4826840	-4.8496660	-0.6060560
134.H	0.8642060	-5.0165790	-1.4824410
135.C	2.5251160	-5.7011410	-0.2885410
136.H	2.7452920	-6.5619390	-0.9171020
137.C	3.2755740	-5.4398250	0.8502460
138.H	4.0979590	-6.0861890	1.1482810
139.C	2.9708730	-4.3262500	1.6053040
140.H	3.5399450	-4.0641520	2.4918240
141.C	-1.2084610	-3.7772210	-0.2290850
142.C	-1.4826840	-4.8496660	0.6060560
143.H	-0.8642060	-5.0165790	1.4824410
144.C	-2.5251160	-5.7011410	0.2885410
145.H	-2.7452920	-6.5619390	0.9171020
146.C	-3.2755740	-5.4398250	-0.8502460
147.H	-4.0979590	-6.0861890	-1.1482810
148.C	-2.9708730	-4.3262500	-1.6053040
149.H	-3.5399450	-4.0641520	-2.4918240
150.C	3.4506450	-0.6656290	4.1964040
151.C	4.5618900	-0.8713370	5.1932980
152.H	4.9660990	-1.8848080	5.1368470
153.H	4.1604260	-0.7066090	6.2005910
154.H	5.3511140	-0.1300140	5.0339270
155.C	0.6656290	-3.4506450	-4.1964040
156.C	0.8713370	-4.5618900	-5.1932980
157.H	1.8848080	-4.9660990	-5.1368470

158.H	0.7066090	-4.1604260	-6.2005910
159.H	0.1300140	-5.3511140	-5.0339270
160.H	0.0000000	0.0000000	-4.0404940
161.H	0.0000000	0.0000000	4.0404940

$Fe@Ni_8$

Atom	X	Y	Z	(Angstrom)
1.Fe	0.0000000	0.0000000	0.0000000	
2.Ni	1.8077760	1.2498070	2.4534470	
3.Ni	1.2498070	-1.8077760	2.4534470	
4.Ni	-1.8077760	-1.2498070	2.4534470	
5.Ni	-1.2498070	1.8077760	2.4534470	
6.Ni	1.8077760	-1.2498070	-2.4534470	
7.Ni	-1.2498070	-1.8077760	-2.4534470	
8.Ni	-1.8077760	1.2498070	-2.4534470	
9.Ni	1.2498070	1.8077760	-2.4534470	
10.N	-3.4319450	-1.8904650	1.3870390	
11.N	-3.4319450	1.8904650	-1.3870390	
12.O	-1.9543710	-0.2557000	-1.0927430	
13.O	-1.9543710	0.2557000	1.0927430	
14.O	-1.7279840	-2.9047670	3.6471890	
15.O	0.5083330	-3.0474800	3.9353940	
16.O	0.0000000	0.0000000	3.0743760	
17.O	-3.0474800	0.5083330	-3.9353940	
18.O	-2.9047670	-1.7279840	-3.6471890	
19.O	0.0000000	0.0000000	-3.0743760	
20.C	-2.7623140	0.0000000	0.0000000	
21.C	-3.6761250	-1.1973940	0.2762990	

22.C	-4.7414680	-1.5079970	-0.5579590
23.H	-4.8966940	-0.9342580	-1.4663360
24.C	-5.5963800	-2.5313620	-0.1960670
25.H	-6.4509860	-2.7798420	-0.8229770
26.C	-5.3516160	-3.2304410	0.9773660
27.H	-6.0059190	-4.0350390	1.3051330
28.C	-4.2452810	-2.8921480	1.7313520
29.H	-3.9836300	-3.4104470	2.6486200
30.C	-3.6761250	1.1973940	-0.2762990
31.C	-4.7414680	1.5079970	0.5579590
32.H	-4.8966940	0.9342580	1.4663360
33.C	-5.5963800	2.5313620	0.1960670
34.H	-6.4509860	2.7798420	0.8229770
35.C	-5.3516160	3.2304410	-0.9773660
36.H	-6.0059190	4.0350390	-1.3051330
37.C	-4.2452810	2.8921480	-1.7313520
38.H	-3.9836300	3.4104470	-2.6486200
39.C	-0.6819710	-3.3812440	4.1643060
40.C	-0.8730930	-4.4698830	5.1947730
41.H	-1.8930330	-4.8619870	5.1721480
42.H	-0.6823690	-4.0441540	6.1874220
43.H	-0.1453180	-5.2721110	5.0381020
44.C	-3.3812440	-0.6819710	-4.1643060
45.C	-4.4698830	-0.8730930	-5.1947730
46.H	-4.8619870	-1.8930330	-5.1721480
47.H	-4.0441540	-0.6823690	-6.1874220
48.H	-5.2721110	-0.1453180	-5.0381020
49.N	-1.8904650	3.4319450	1.3870390
50.N	1.8904650	3.4319450	-1.3870390

51.O	-0.2557000	1.9543710	-1.0927430
52.O	0.2557000	1.9543710	1.0927430
53.O	-2.9047670	1.7279840	3.6471890
54.O	-3.0474800	-0.5083330	3.9353940
55.O	0.5083330	3.0474800	-3.9353940
56.O	-1.7279840	2.9047670	-3.6471890
57.C	0.0000000	2.7623140	0.0000000
58.C	-1.1973940	3.6761250	0.2762990
59.C	-1.5079970	4.7414680	-0.5579590
60.H	-0.9342580	4.8966940	-1.4663360
61.C	-2.5313620	5.5963800	-0.1960670
62.H	-2.7798420	6.4509860	-0.8229770
63.C	-3.2304410	5.3516160	0.9773660
64.H	-4.0350390	6.0059190	1.3051330
65.C	-2.8921480	4.2452810	1.7313520
66.H	-3.4104470	3.9836300	2.6486200
67.C	1.1973940	3.6761250	-0.2762990
68.C	1.5079970	4.7414680	0.5579590
69.H	0.9342580	4.8966940	1.4663360
70.C	2.5313620	5.5963800	0.1960670
71.H	2.7798420	6.4509860	0.8229770
72.C	3.2304410	5.3516160	-0.9773660
73.H	4.0350390	6.0059190	-1.3051330
74.C	2.8921480	4.2452810	-1.7313520
75.H	3.4104470	3.9836300	-2.6486200
76.C	-3.3812440	0.6819710	4.1643060
77.C	-4.4698830	0.8730930	5.1947730
78.H	-4.8619870	1.8930330	5.1721480
79.H	-4.0441540	0.6823690	6.1874220

80.H	-5.2721110	0.1453180	5.0381020
81.C	-0.6819710	3.3812440	-4.1643060
82.C	-0.8730930	4.4698830	-5.1947730
83.H	-1.8930330	4.8619870	-5.1721480
84.H	-0.6823690	4.0441540	-6.1874220
85.H	-0.1453180	5.2721110	-5.0381020
86.N	3.4319450	1.8904650	1.3870390
87.N	3.4319450	-1.8904650	-1.3870390
88.O	1.9543710	0.2557000	-1.0927430
89.O	1.9543710	-0.2557000	1.0927430
90.O	1.7279840	2.9047670	3.6471890
91.O	-0.5083330	3.0474800	3.9353940
92.O	3.0474800	-0.5083330	-3.9353940
93.O	2.9047670	1.7279840	-3.6471890
94.C	2.7623140	0.0000000	0.0000000
95.C	3.6761250	1.1973940	0.2762990
96.C	4.7414680	1.5079970	-0.5579590
97.H	4.8966940	0.9342580	-1.4663360
98.C	5.5963800	2.5313620	-0.1960670
99.H	6.4509860	2.7798420	-0.8229770
100.C	5.3516160	3.2304410	0.9773660
101.H	6.0059190	4.0350390	1.3051330
102.C	4.2452810	2.8921480	1.7313520
103.H	3.9836300	3.4104470	2.6486200
104.C	3.6761250	-1.1973940	-0.2762990
105.C	4.7414680	-1.5079970	0.5579590
106.H	4.8966940	-0.9342580	1.4663360
107.C	5.5963800	-2.5313620	0.1960670
108.H	6.4509860	-2.7798420	0.8229770

109.C	5.3516160	-3.2304410	-0.9773660
110.H	6.0059190	-4.0350390	-1.3051330
111.C	4.2452810	-2.8921480	-1.7313520
112.H	3.9836300	-3.4104470	-2.6486200
113.C	0.6819710	3.3812440	4.1643060
114.C	0.8730930	4.4698830	5.1947730
115.H	1.8930330	4.8619870	5.1721480
116.H	0.6823690	4.0441540	6.1874220
117.H	0.1453180	5.2721110	5.0381020
118.C	3.3812440	0.6819710	-4.1643060
119.C	4.4698830	0.8730930	-5.1947730
120.H	4.8619870	1.8930330	-5.1721480
121.H	4.0441540	0.6823690	-6.1874220
122.H	5.2721110	0.1453180	-5.0381020
123.N	1.8904650	-3.4319450	1.3870390
124.N	-1.8904650	-3.4319450	-1.3870390
125.O	0.2557000	-1.9543710	-1.0927430
126.O	-0.2557000	-1.9543710	1.0927430
127.O	2.9047670	-1.7279840	3.6471890
128.O	3.0474800	0.5083330	3.9353940
129.O	-0.5083330	-3.0474800	-3.9353940
130.O	1.7279840	-2.9047670	-3.6471890
131.C	0.0000000	-2.7623140	0.0000000
132.C	1.1973940	-3.6761250	0.2762990
133.C	1.5079970	-4.7414680	-0.5579590
134.H	0.9342580	-4.8966940	-1.4663360
135.C	2.5313620	-5.5963800	-0.1960670
136.H	2.7798420	-6.4509860	-0.8229770
137.C	3.2304410	-5.3516160	0.9773660

138.H	4.0350390	-6.0059190	1.3051330
139.C	2.8921480	-4.2452810	1.7313520
140.H	3.4104470	-3.9836300	2.6486200
141.C	-1.1973940	-3.6761250	-0.2762990
142.C	-1.5079970	-4.7414680	0.5579590
143.H	-0.9342580	-4.8966940	1.4663360
144.C	-2.5313620	-5.5963800	0.1960670
145.H	-2.7798420	-6.4509860	0.8229770
146.C	-3.2304410	-5.3516160	-0.9773660
147.H	-4.0350390	-6.0059190	-1.3051330
148.C	-2.8921480	-4.2452810	-1.7313520
149.H	-3.4104470	-3.9836300	-2.6486200
150.C	3.3812440	-0.6819710	4.1643060
151.C	4.4698830	-0.8730930	5.1947730
152.H	4.8619870	-1.8930330	5.1721480
153.H	4.0441540	-0.6823690	6.1874220
154.H	5.2721110	-0.1453180	5.0381020
155.C	0.6819710	-3.3812440	-4.1643060
156.C	0.8730930	-4.4698830	-5.1947730
157.H	1.8930330	-4.8619870	-5.1721480
158.H	0.6823690	-4.0441540	-6.1874220
159.H	0.1453180	-5.2721110	-5.0381020
160.H	0.0000000	0.0000000	-4.0487540
161.H	0.0000000	0.0000000	4.0487540

$Ni@Ni_8$

Atom	X	Y	Z	(Angstrom)
1.Ni	0.0000000	0.0000000	0.0000000	

2.Ni	1.7976440	1.2564230	2.4336920
3.Ni	1.2564230	-1.7976440	2.4336920
4.Ni	-1.7976440	-1.2564230	2.4336920
5.Ni	-1.2564230	1.7976440	2.4336920
6.Ni	1.7976440	-1.2564230	-2.4336920
7.Ni	-1.2564230	-1.7976440	-2.4336920
8.Ni	-1.7976440	1.2564230	-2.4336920
9.Ni	1.2564230	1.7976440	-2.4336920
10.N	-3.4236470	-1.9006420	1.3755450
11.N	-3.4236470	1.9006420	-1.3755450
12.O	-1.9612010	-0.2477250	-1.0954470
13.O	-1.9612010	0.2477250	1.0954470
14.O	-1.7111570	-2.9167820	3.6264680
15.O	0.5251950	-3.0352740	3.9263360
16.O	0.0000000	0.0000000	3.0586780
17.O	-3.0352740	0.5251950	-3.9263360
18.O	-2.9167820	-1.7111570	-3.6264680
19.O	0.0000000	0.0000000	-3.0586780
20.C	-2.7666420	0.0000000	0.0000000
21.C	-3.6778620	-1.1988250	0.2717540
22.C	-4.7509370	-1.5039760	-0.5543800
23.H	-4.9136470	-0.9245480	-1.4578320
24.C	-5.6032690	-2.5291450	-0.1914330
25.H	-6.4636940	-2.7729470	-0.8122230
26.C	-5.3482680	-3.2360420	0.9749990
27.H	-6.0000980	-4.0421320	1.3039340
28.C	-4.2341150	-2.9039720	1.7205430
29.H	-3.9641950	-3.4287600	2.6316990
30.C	-3.6778620	1.1988250	-0.2717540

31.C	-4.7509370	1.5039760	0.5543800
32.H	-4.9136470	0.9245480	1.4578320
33.C	-5.6032690	2.5291450	0.1914330
34.H	-6.4636940	2.7729470	0.8122230
35.C	-5.3482680	3.2360420	-0.9749990
36.H	-6.0000980	4.0421320	-1.3039340
37.C	-4.2341150	2.9039720	-1.7205430
38.H	-3.9641950	3.4287600	-2.6316990
39.C	-0.6629880	-3.3809140	4.1503460
40.C	-0.8471400	-4.4686950	5.1826770
41.H	-1.8662980	-4.8631390	5.1649930
42.H	-0.6515760	-4.0426260	6.1742300
43.H	-0.1185040	-5.2695480	5.0221760
44.C	-3.3809140	-0.6629880	-4.1503460
45.C	-4.4686950	-0.8471400	-5.1826770
46.H	-4.8631390	-1.8662980	-5.1649930
47.H	-4.0426260	-0.6515760	-6.1742300
48.H	-5.2695480	-0.1185040	-5.0221760
49.N	-1.9006420	3.4236470	1.3755450
50.N	1.9006420	3.4236470	-1.3755450
51.O	-0.2477250	1.9612010	-1.0954470
52.O	0.2477250	1.9612010	1.0954470
53.O	-2.9167820	1.7111570	3.6264680
54.O	-3.0352740	-0.5251950	3.9263360
55.O	0.5251950	3.0352740	-3.9263360
56.O	-1.7111570	2.9167820	-3.6264680
57.C	0.0000000	2.7666420	0.0000000
58.C	-1.1988250	3.6778620	0.2717540
59.C	-1.5039760	4.7509370	-0.5543800

60.H	-0.9245480	4.9136470	-1.4578320
61.C	-2.5291450	5.6032690	-0.1914330
62.H	-2.7729470	6.4636940	-0.8122230
63.C	-3.2360420	5.3482680	0.9749990
64.H	-4.0421320	6.0000980	1.3039340
65.C	-2.9039720	4.2341150	1.7205430
66.H	-3.4287600	3.9641950	2.6316990
67.C	1.1988250	3.6778620	-0.2717540
68.C	1.5039760	4.7509370	0.5543800
69.H	0.9245480	4.9136470	1.4578320
70.C	2.5291450	5.6032690	0.1914330
71.H	2.7729470	6.4636940	0.8122230
72.C	3.2360420	5.3482680	-0.9749990
73.H	4.0421320	6.0000980	-1.3039340
74.C	2.9039720	4.2341150	-1.7205430
75.H	3.4287600	3.9641950	-2.6316990
76.C	-3.3809140	0.6629880	4.1503460
77.C	-4.4686950	0.8471400	5.1826770
78.H	-4.8631390	1.8662980	5.1649930
79.H	-4.0426260	0.6515760	6.1742300
80.H	-5.2695480	0.1185040	5.0221760
81.C	-0.6629880	3.3809140	-4.1503460
82.C	-0.8471400	4.4686950	-5.1826770
83.H	-1.8662980	4.8631390	-5.1649930
84.H	-0.6515760	4.0426260	-6.1742300
85.H	-0.1185040	5.2695480	-5.0221760
86.N	3.4236470	1.9006420	1.3755450
87.N	3.4236470	-1.9006420	-1.3755450
88.O	1.9612010	0.2477250	-1.0954470

89.O	1.9612010	-0.2477250	1.0954470
90.O	1.7111570	2.9167820	3.6264680
91.O	-0.5251950	3.0352740	3.9263360
92.O	3.0352740	-0.5251950	-3.9263360
93.O	2.9167820	1.7111570	-3.6264680
94.C	2.7666420	0.0000000	0.0000000
95.C	3.6778620	1.1988250	0.2717540
96.C	4.7509370	1.5039760	-0.5543800
97.H	4.9136470	0.9245480	-1.4578320
98.C	5.6032690	2.5291450	-0.1914330
99.H	6.4636940	2.7729470	-0.8122230
100.C	5.3482680	3.2360420	0.9749990
101.H	6.0000980	4.0421320	1.3039340
102.C	4.2341150	2.9039720	1.7205430
103.H	3.9641950	3.4287600	2.6316990
104.C	3.6778620	-1.1988250	-0.2717540
105.C	4.7509370	-1.5039760	0.5543800
106.H	4.9136470	-0.9245480	1.4578320
107.C	5.6032690	-2.5291450	0.1914330
108.H	6.4636940	-2.7729470	0.8122230
109.C	5.3482680	-3.2360420	-0.9749990
110.H	6.0000980	-4.0421320	-1.3039340
111.C	4.2341150	-2.9039720	-1.7205430
112.H	3.9641950	-3.4287600	-2.6316990
113.C	0.6629880	3.3809140	4.1503460
114.C	0.8471400	4.4686950	5.1826770
115.H	1.8662980	4.8631390	5.1649930
116.H	0.6515760	4.0426260	6.1742300
117.H	0.1185040	5.2695480	5.0221760

118.C	3.3809140	0.6629880	-4.1503460
119.C	4.4686950	0.8471400	-5.1826770
120.H	4.8631390	1.8662980	-5.1649930
121.H	4.0426260	0.6515760	-6.1742300
122.H	5.2695480	0.1185040	-5.0221760
123.N	1.9006420	-3.4236470	1.3755450
124.N	-1.9006420	-3.4236470	-1.3755450
125.O	0.2477250	-1.9612010	-1.0954470
126.O	-0.2477250	-1.9612010	1.0954470
127.O	2.9167820	-1.7111570	3.6264680
128.O	3.0352740	0.5251950	3.9263360
129.O	-0.5251950	-3.0352740	-3.9263360
130.O	1.7111570	-2.9167820	-3.6264680
131.C	0.0000000	-2.7666420	0.0000000
132.C	1.1988250	-3.6778620	0.2717540
133.C	1.5039760	-4.7509370	-0.5543800
134.H	0.9245480	-4.9136470	-1.4578320
135.C	2.5291450	-5.6032690	-0.1914330
136.H	2.7729470	-6.4636940	-0.8122230
137.C	3.2360420	-5.3482680	0.9749990
138.H	4.0421320	-6.0000980	1.3039340
139.C	2.9039720	-4.2341150	1.7205430
140.H	3.4287600	-3.9641950	2.6316990
141.C	-1.1988250	-3.6778620	-0.2717540
142.C	-1.5039760	-4.7509370	0.5543800
143.H	-0.9245480	-4.9136470	1.4578320
144.C	-2.5291450	-5.6032690	0.1914330
145.H	-2.7729470	-6.4636940	0.8122230
146.C	-3.2360420	-5.3482680	-0.9749990

147.H	-4.0421320	-6.0000980	-1.3039340
148.C	-2.9039720	-4.2341150	-1.7205430
149.H	-3.4287600	-3.9641950	-2.6316990
150.C	3.3809140	-0.6629880	4.1503460
151.C	4.4686950	-0.8471400	5.1826770
152.H	4.8631390	-1.8662980	5.1649930
153.H	4.0426260	-0.6515760	6.1742300
154.H	5.2695480	-0.1185040	5.0221760
155.C	0.6629880	-3.3809140	-4.1503460
156.C	0.8471400	-4.4686950	-5.1826770
157.H	1.8662980	-4.8631390	-5.1649930
158.H	0.6515760	-4.0426260	-6.1742300
159.H	0.1185040	-5.2695480	-5.0221760
160.H	0.0000000	0.0000000	-4.0323780
161.H	0.0000000	0.0000000	4.0323780