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## Supplementary Materials

# Synthetic and DFT Modeling Studies on Suzuki–Miyaura Reactions of 4,5-Dibromo-2-methylpyridazin-3(2H)-one with Ferrocene boronates, Accompanied by Hydrodebromination and a Novel Bridge-Forming Annulation In Vitro Cytotoxic Activity of the Ferrocenyl–Pyridazinone Products

Nour-Eddine El Alaoui <sup>1</sup>, Mohammed Boulhaoua <sup>1</sup>, Dániel Hutai <sup>1</sup>, Rita Oláh-Szabó <sup>2</sup>, Szilvia Bősze <sup>2</sup>, Ferenc Hudecz <sup>1,2</sup> and Antal Csámpai <sup>1,\*</sup>

- <sup>1</sup> Department of Organic Chemistry, Institute of Chemistry, Eötvös Loránd University (ELTE), H-1117 Budapest, Hungary; nour-eddine1990@live.fr (N.-E.E.A.); mboulhaoua@student.elte.hu (M.B.); hutaidani@gmail.com (D.H.); ferenc.hudecz@ttk.elte.hu (F.H.)
- <sup>2</sup> ELKH-ELTE Research Group of Peptide Chemistry, Eötvös Loránd Research Network (ELKH), Eötvös Loránd University (ELTE), Budapest Pázmány P. Sétány 1/A, H-1117 Budapest, Hungary; rita.szabo@ttk.elte.hu (R.O.-S.); szilvia.bosze@ttk.elte.hu (S.B.)
- \* Correspondence: csampai@caesar.elte.hu; Tel.: +36-1-372-2500-6591

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S.1. Copies of the 1D- and 2D-NMR spectra pp. 2 – 14

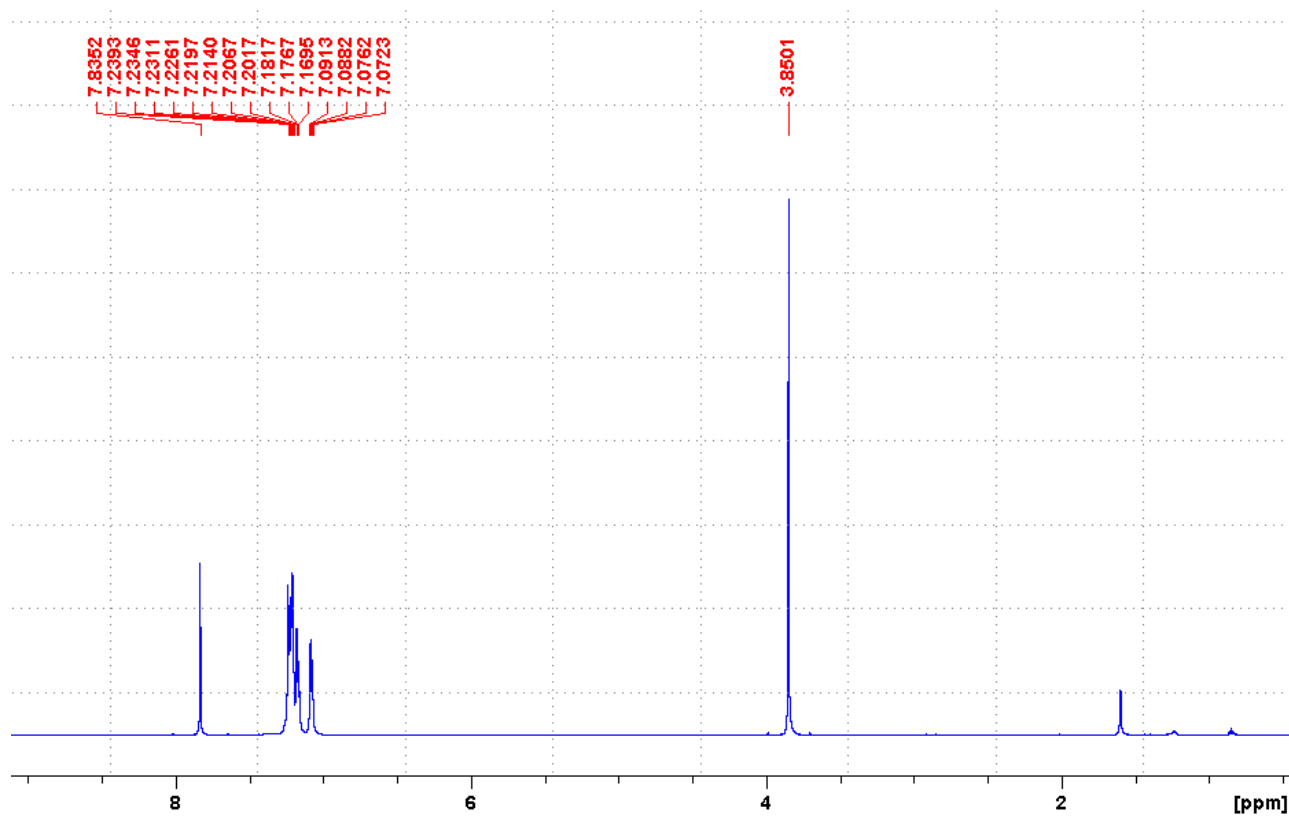
S.2. Copies of the <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of the deuterated products. pp. 15 – 16.

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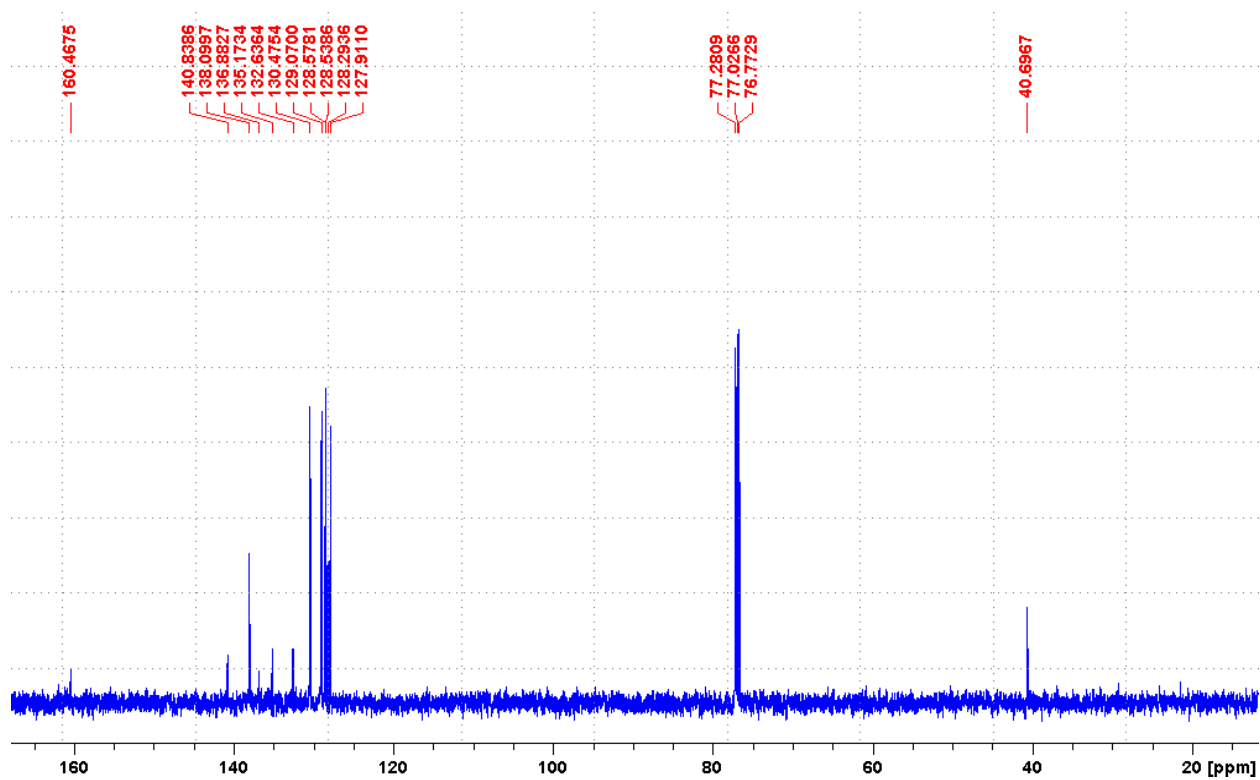
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## S.1. Copies of the 1D- and 2D-NMR spectra

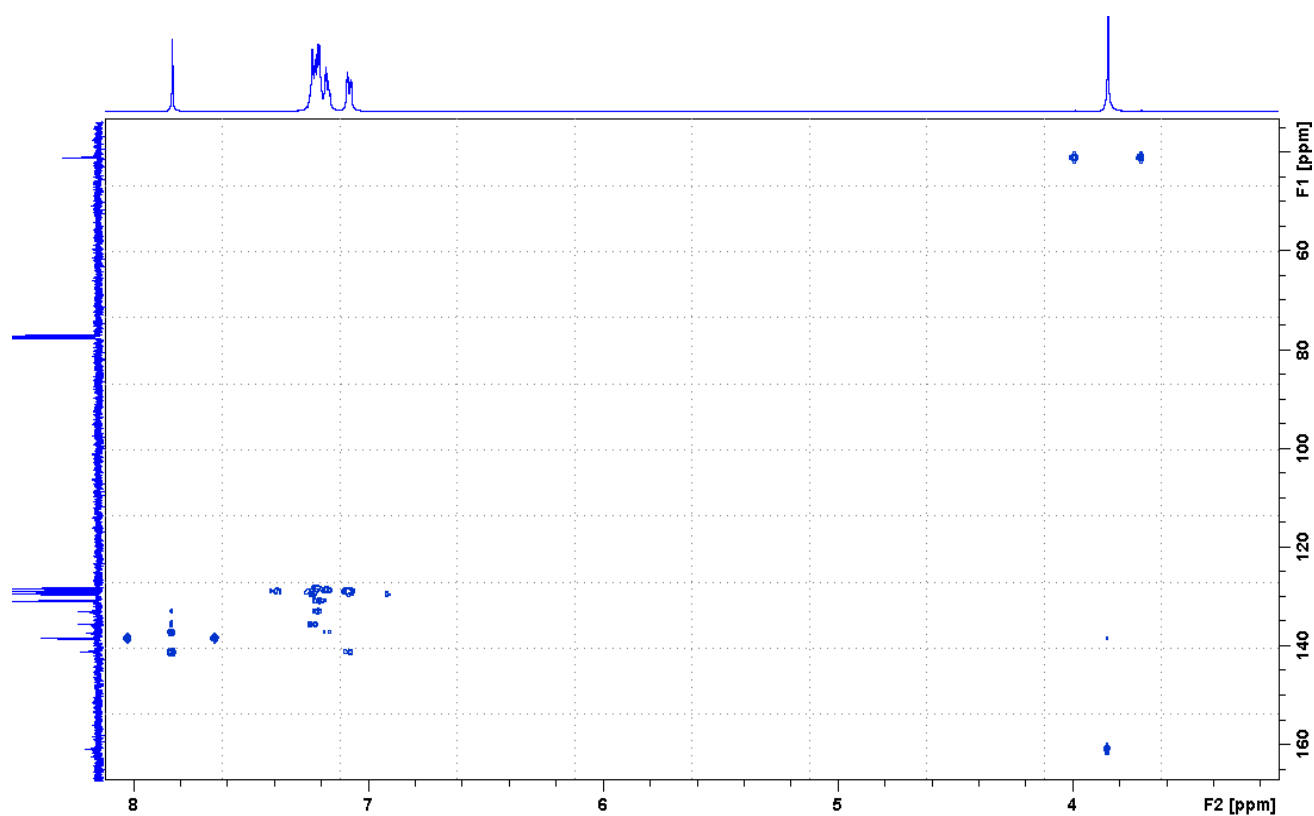
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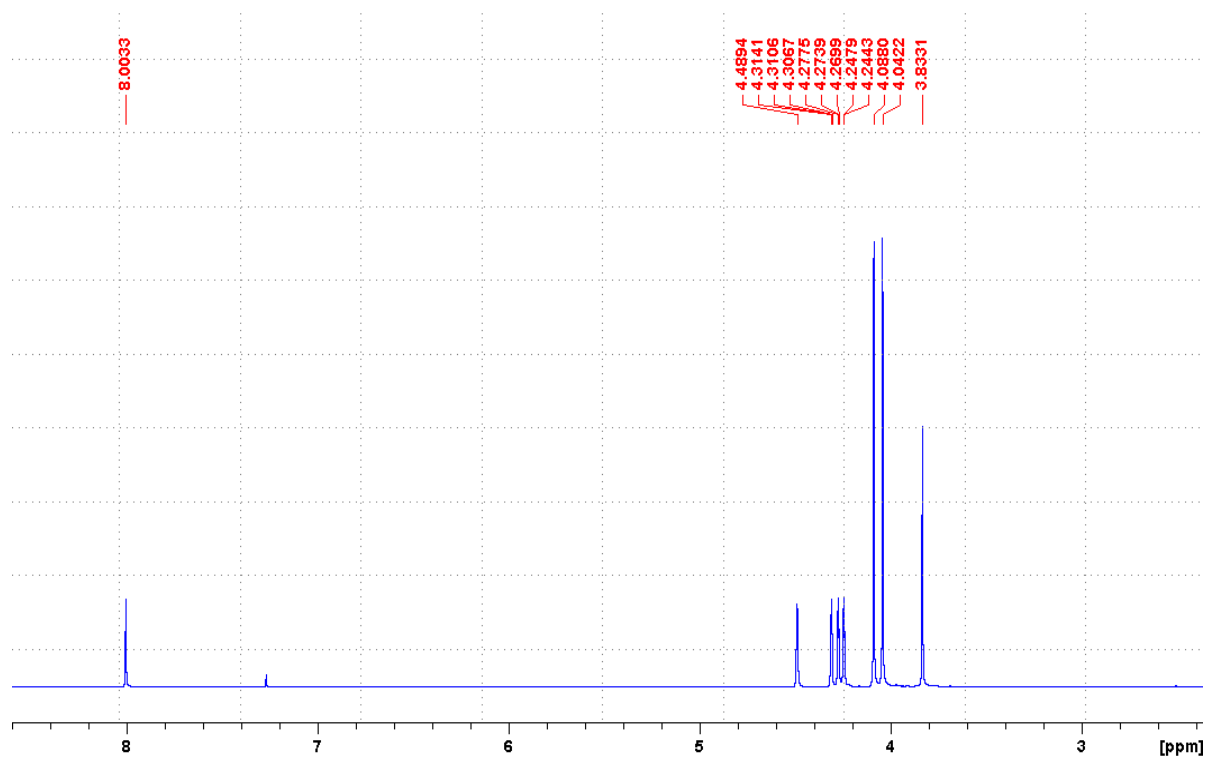
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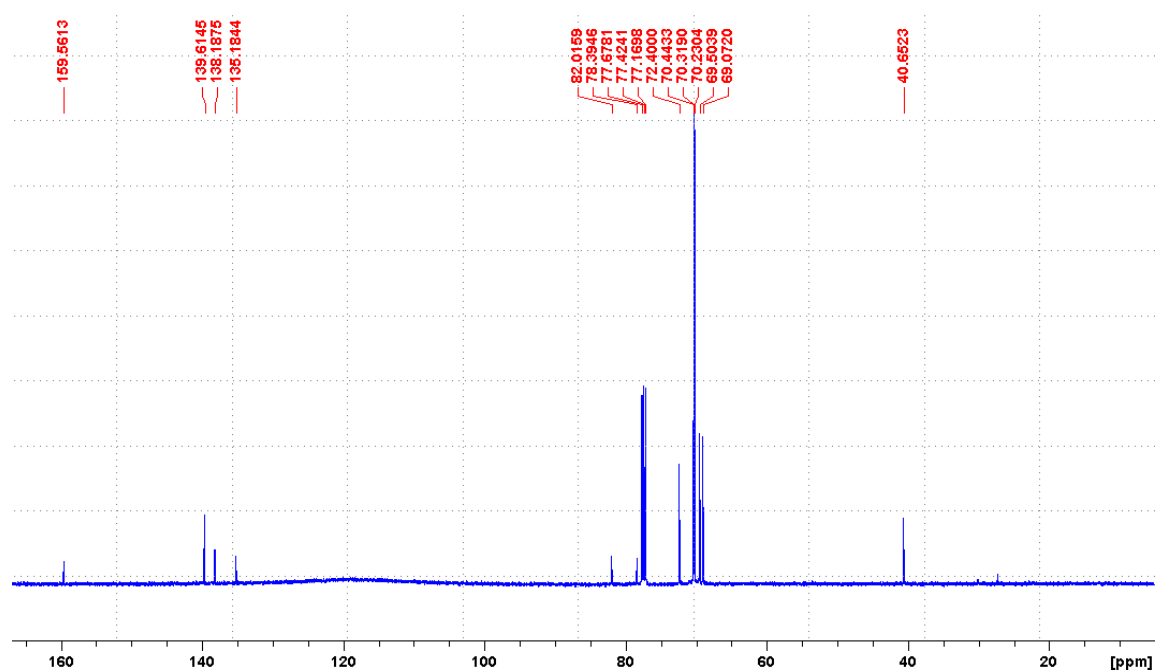
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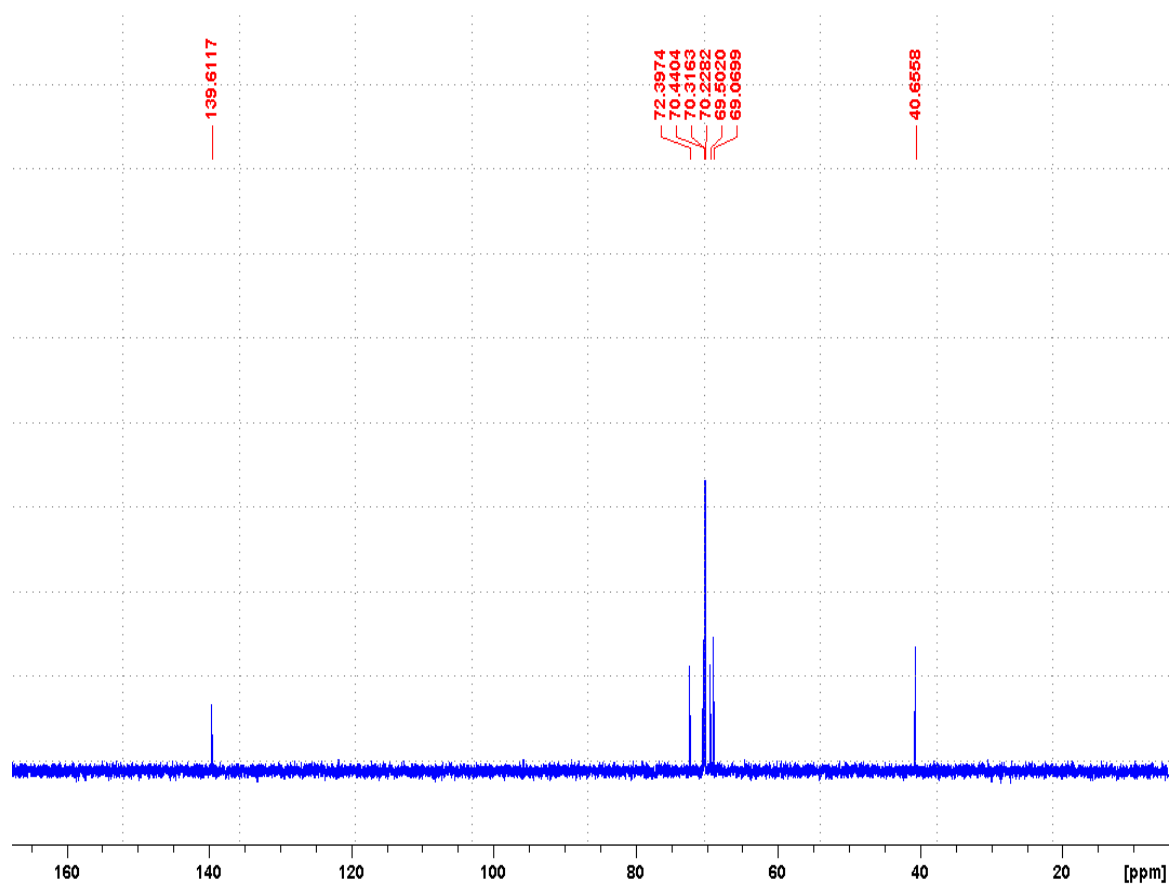
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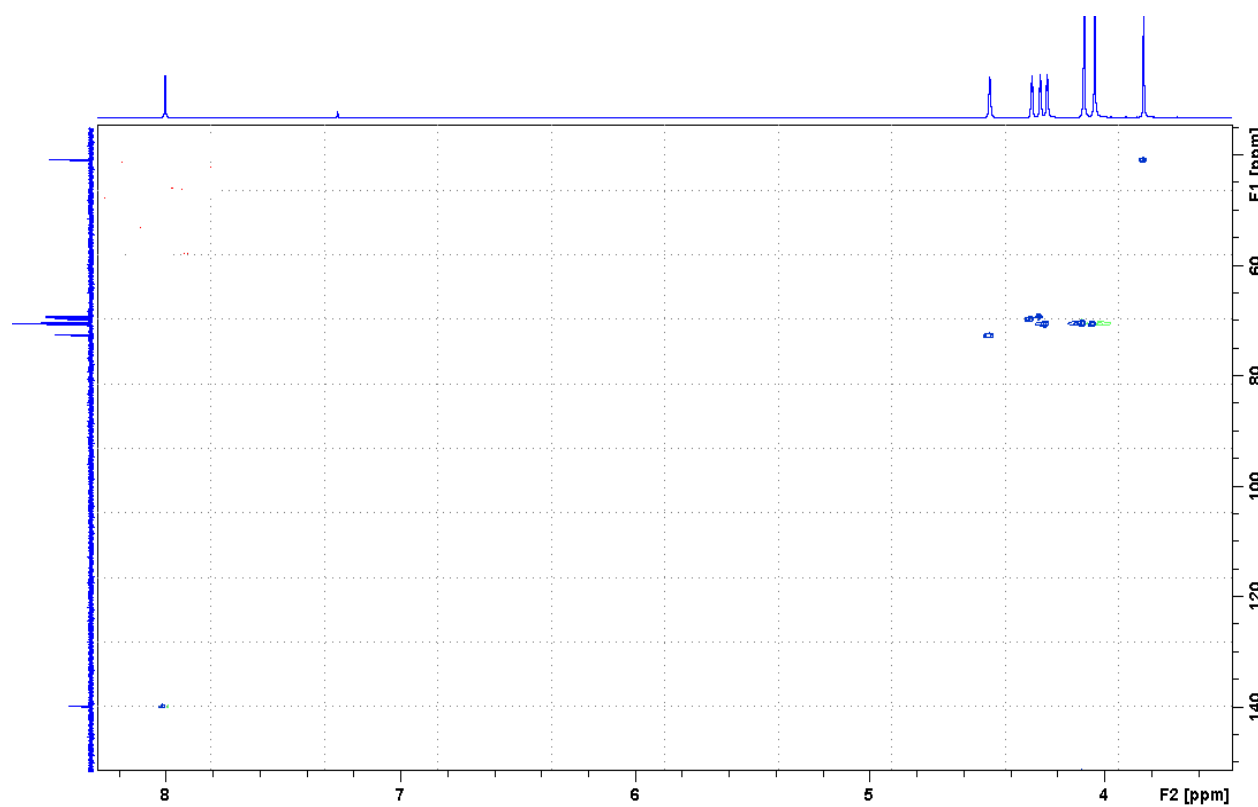
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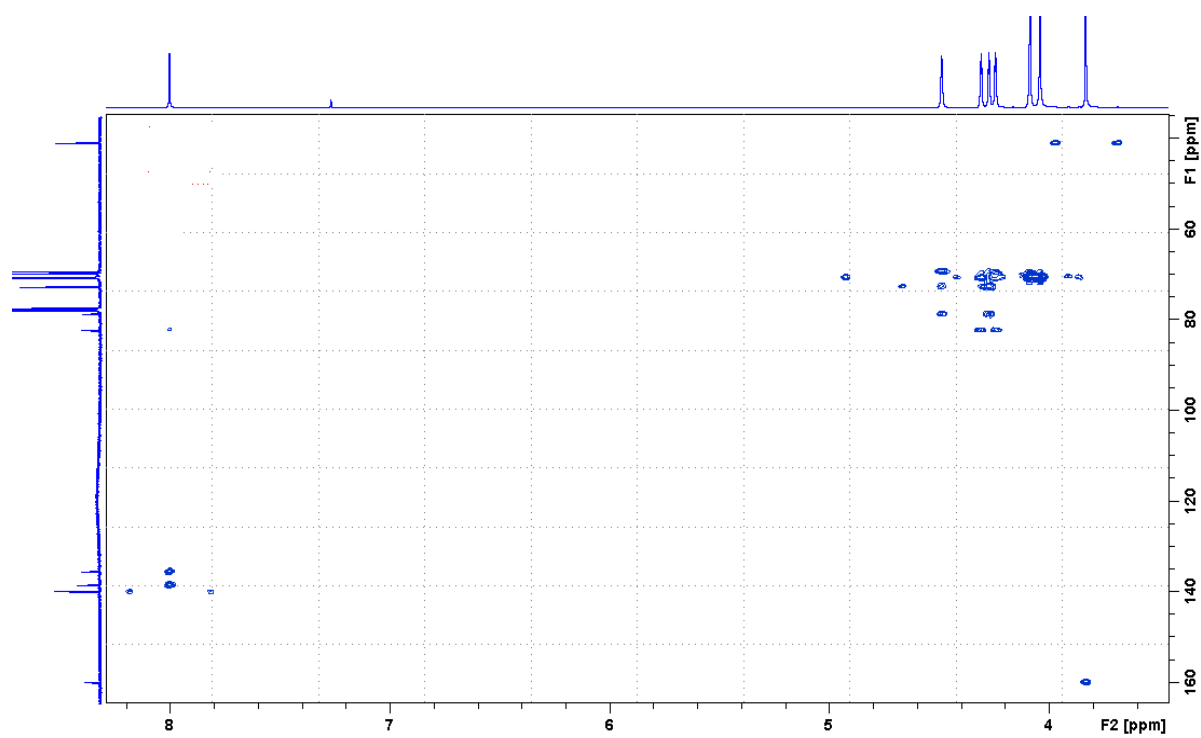
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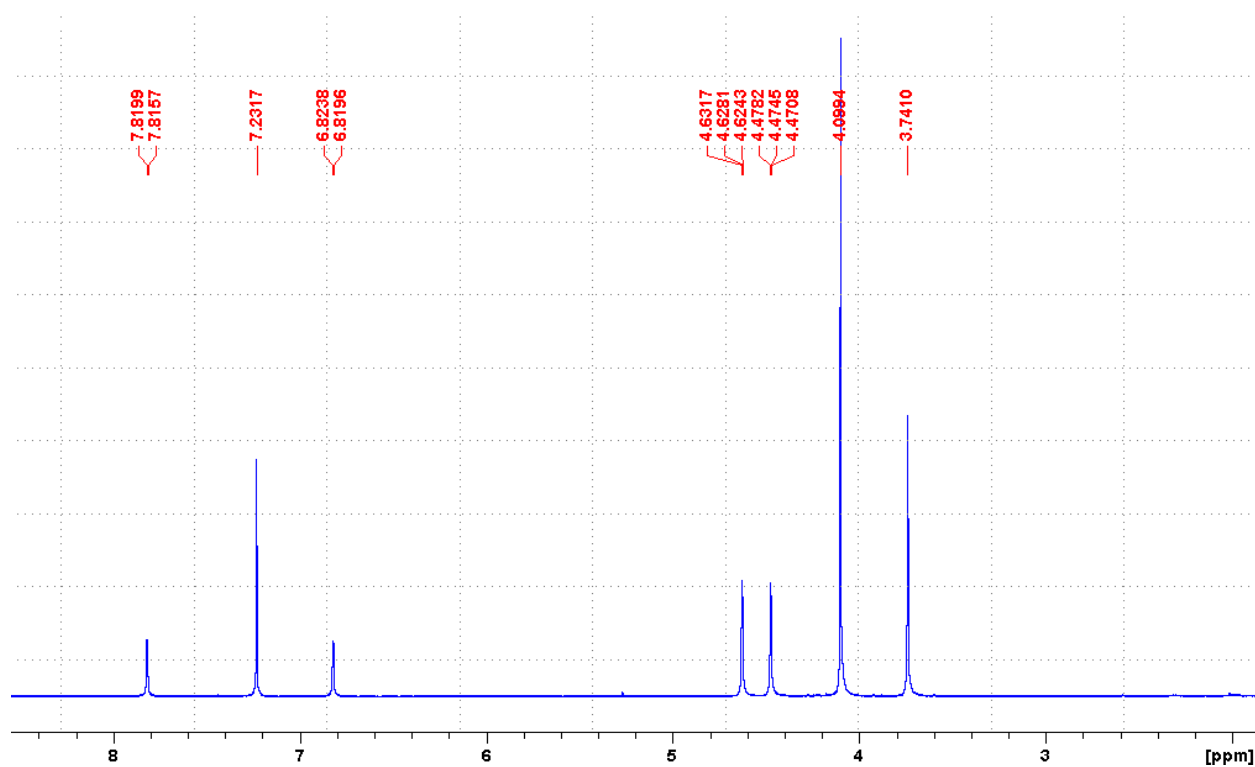
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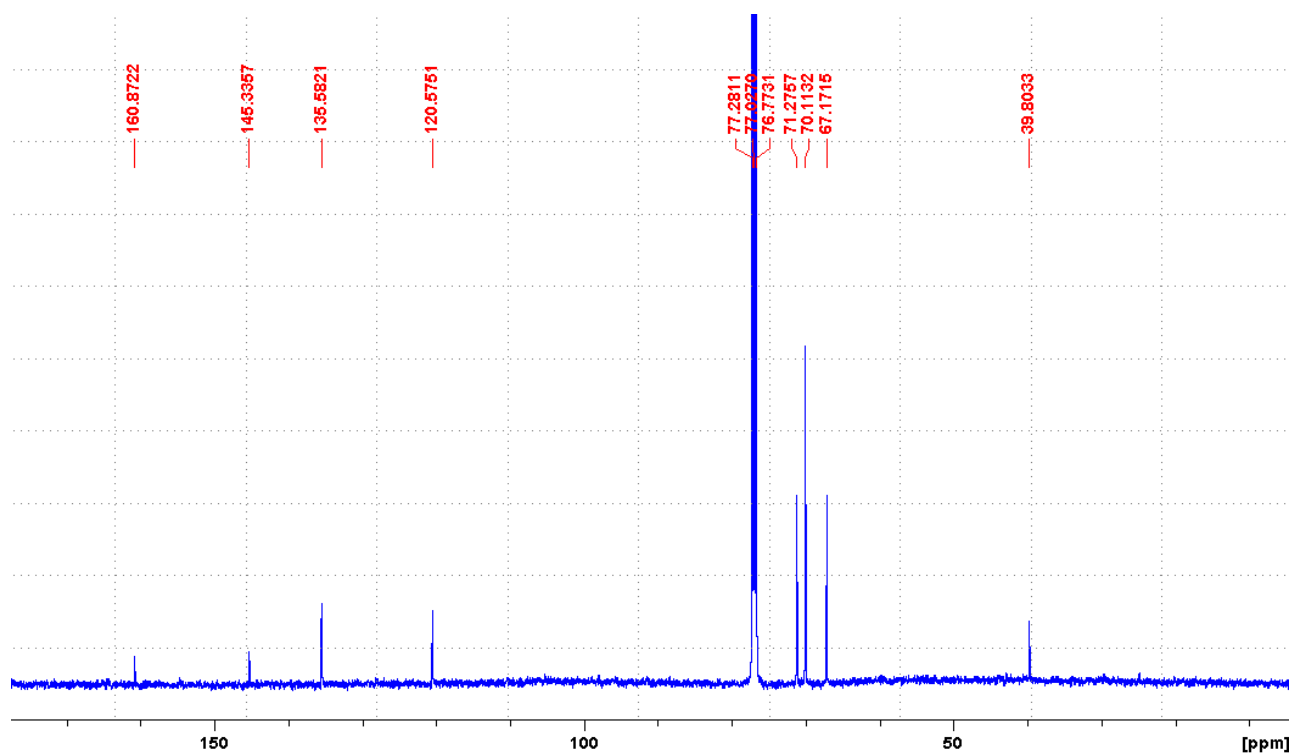
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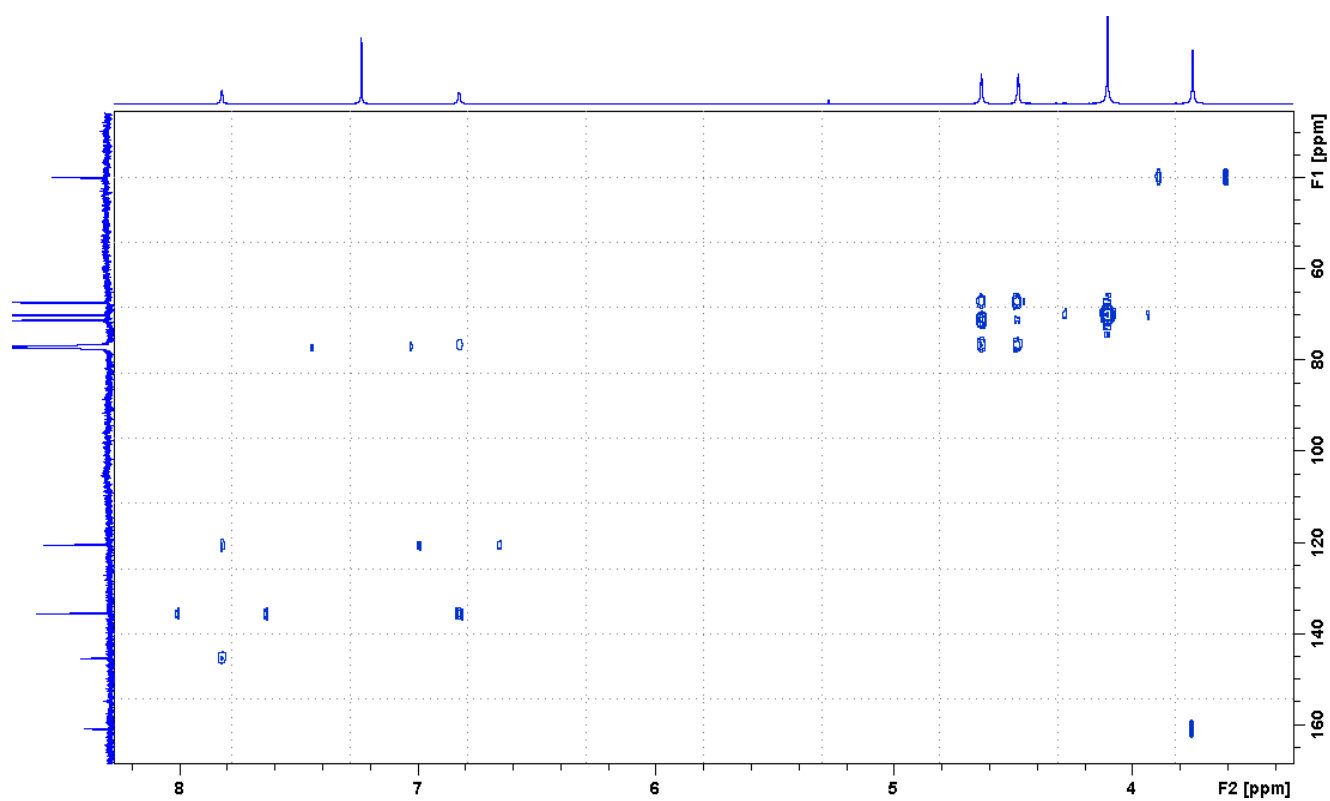
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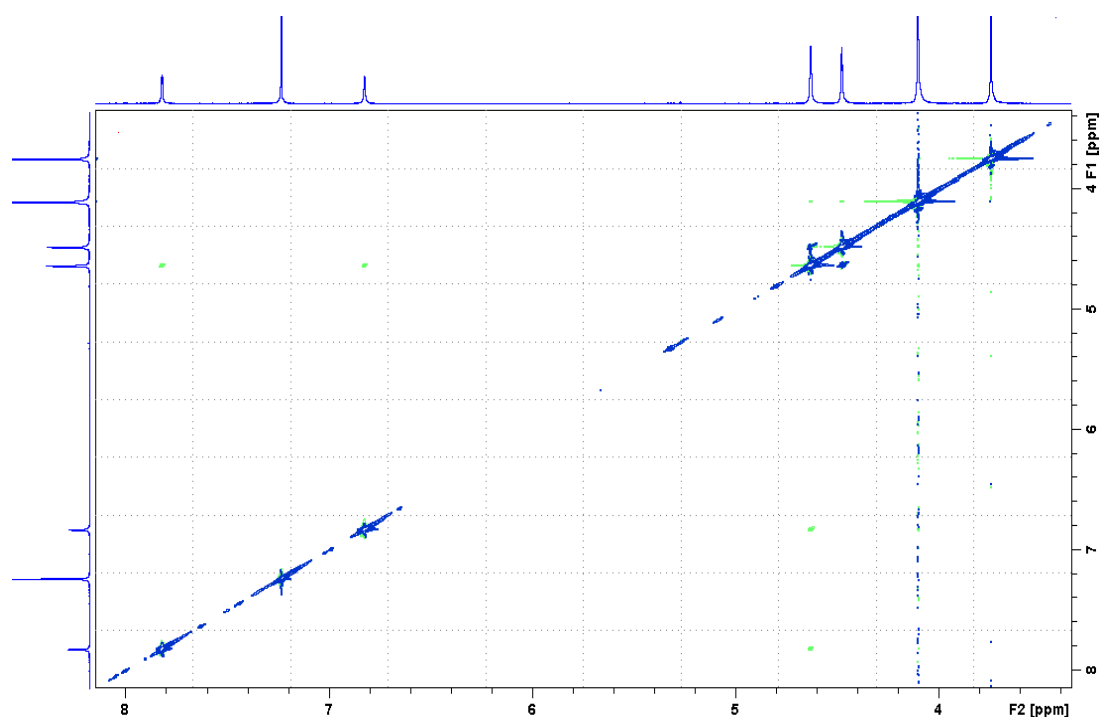
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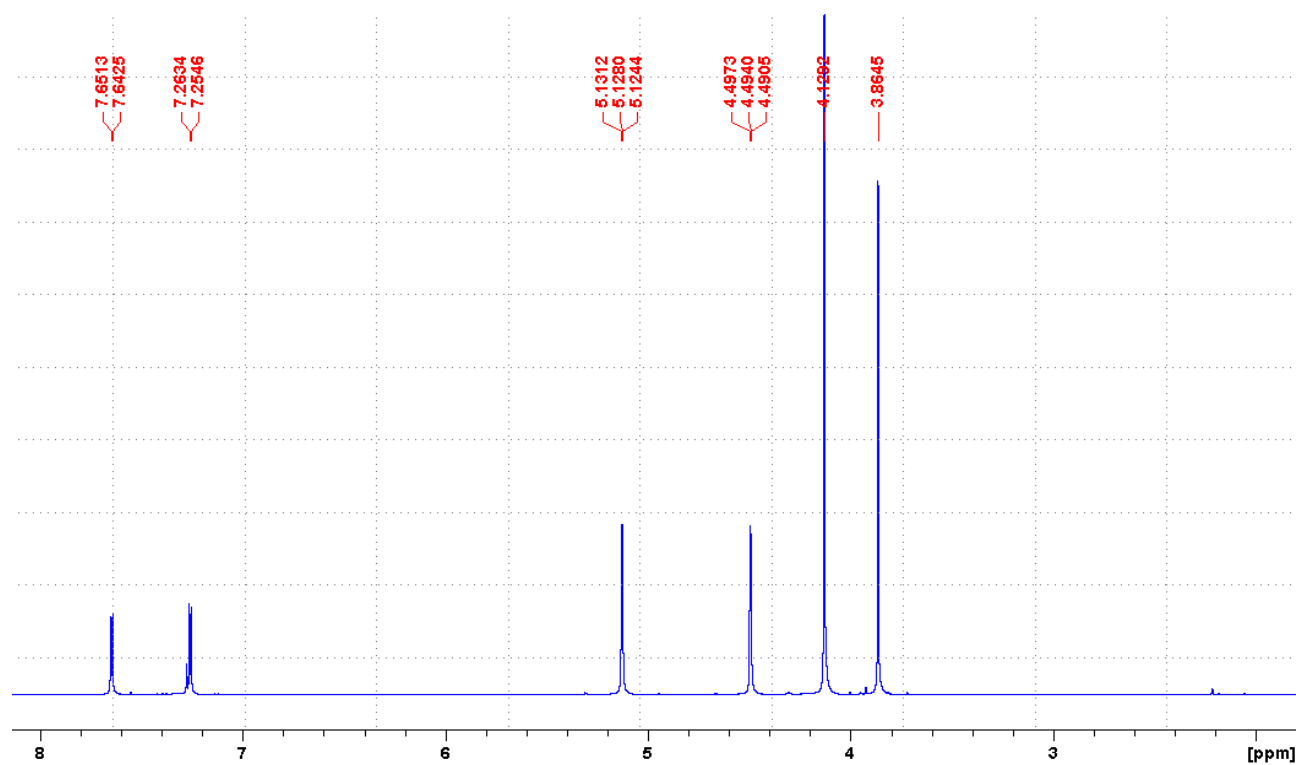
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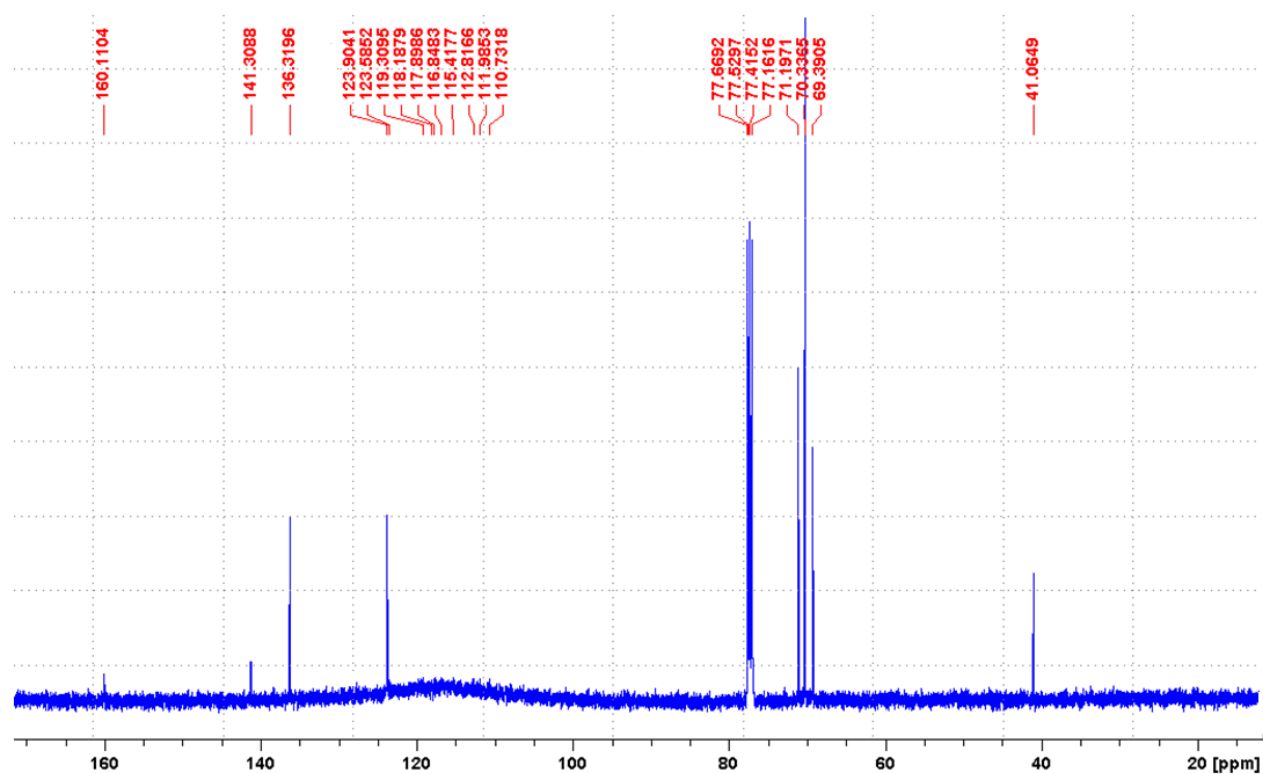
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<sup>1</sup>H NMR 9

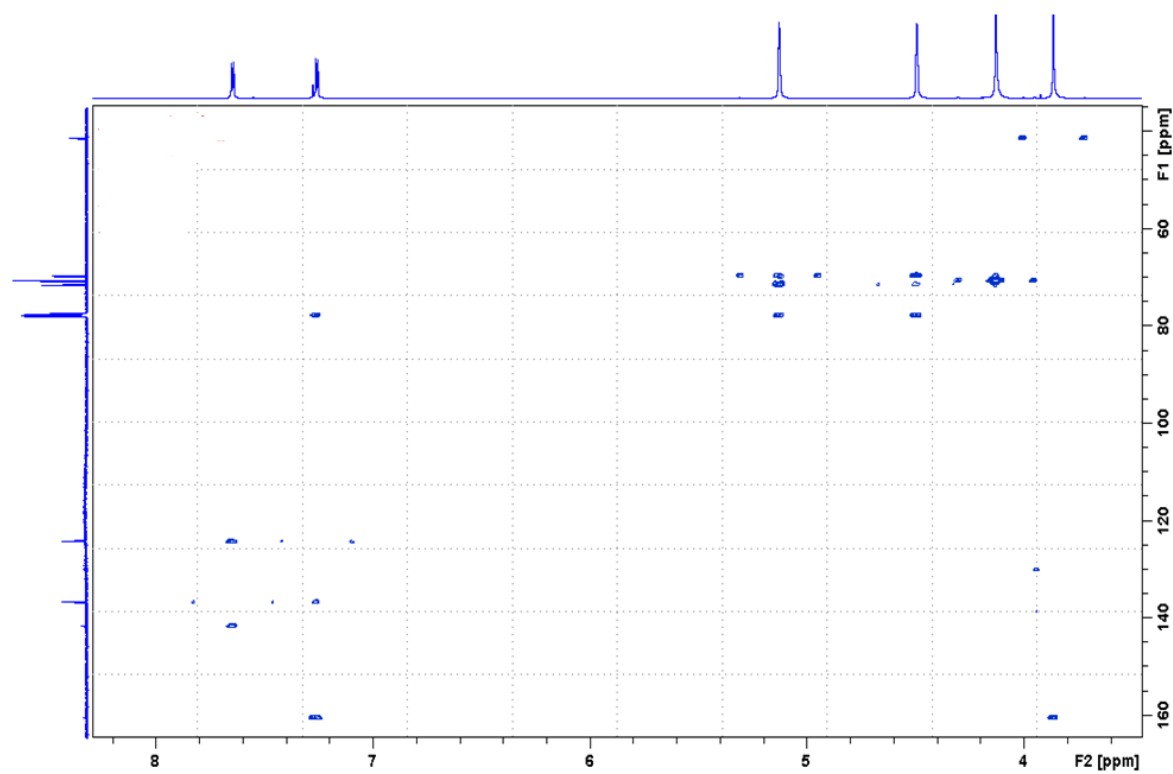


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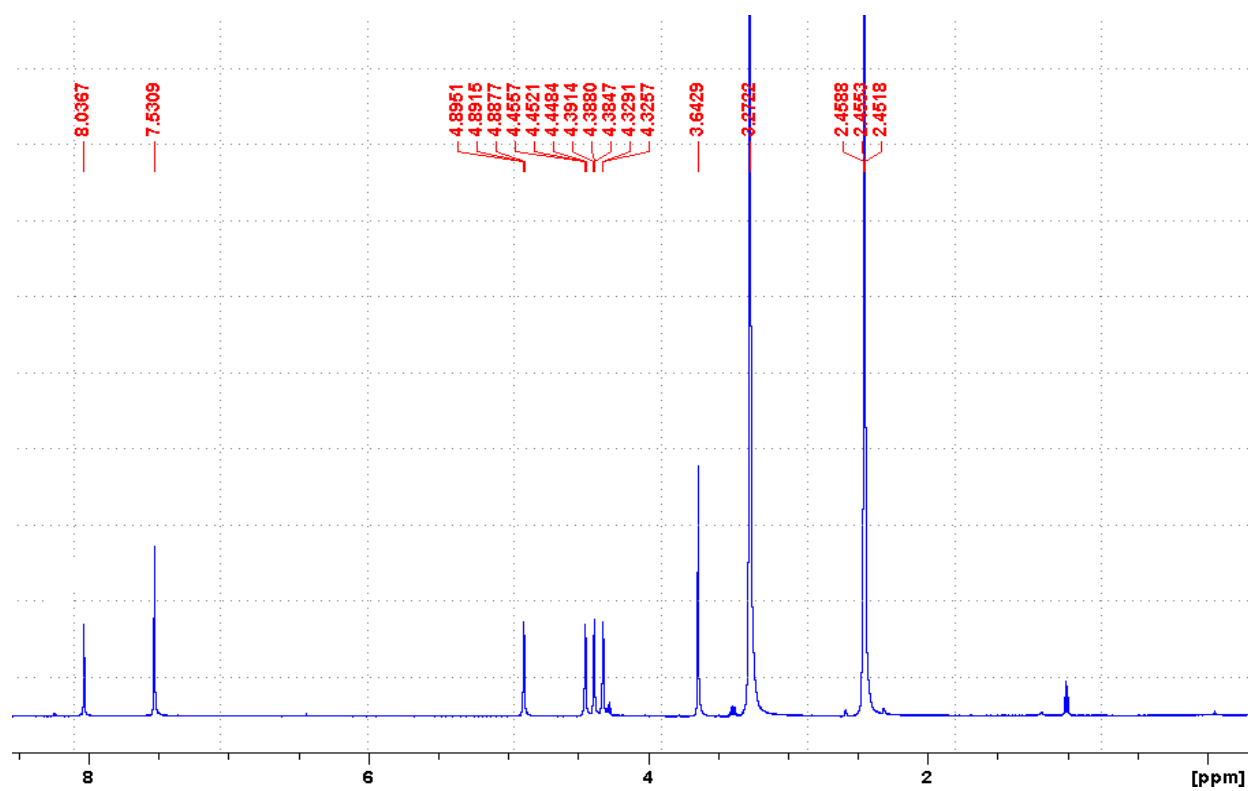




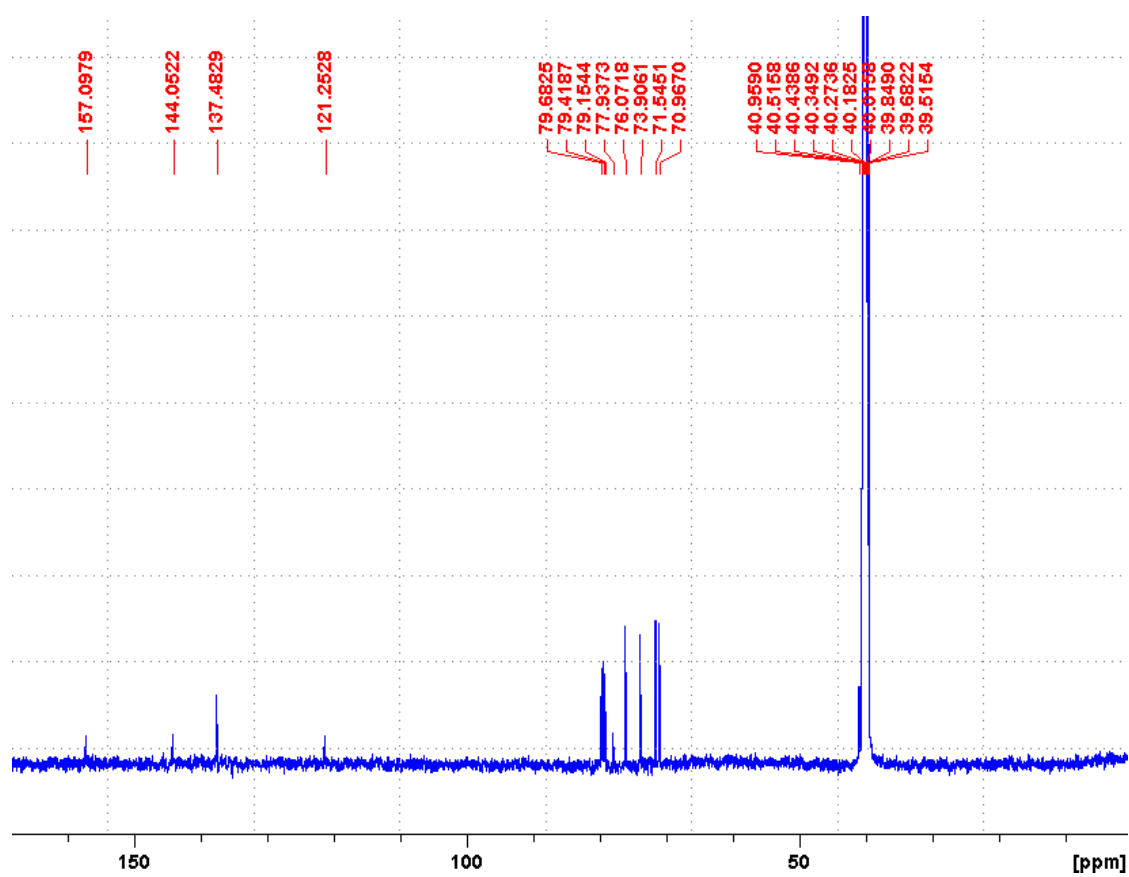
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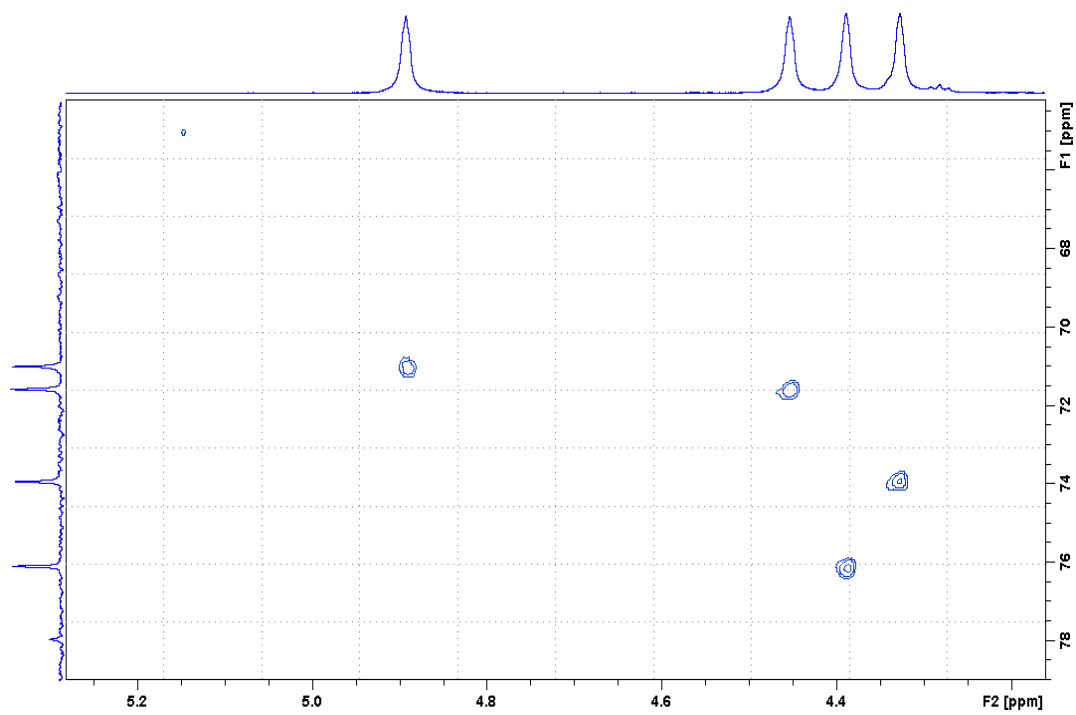
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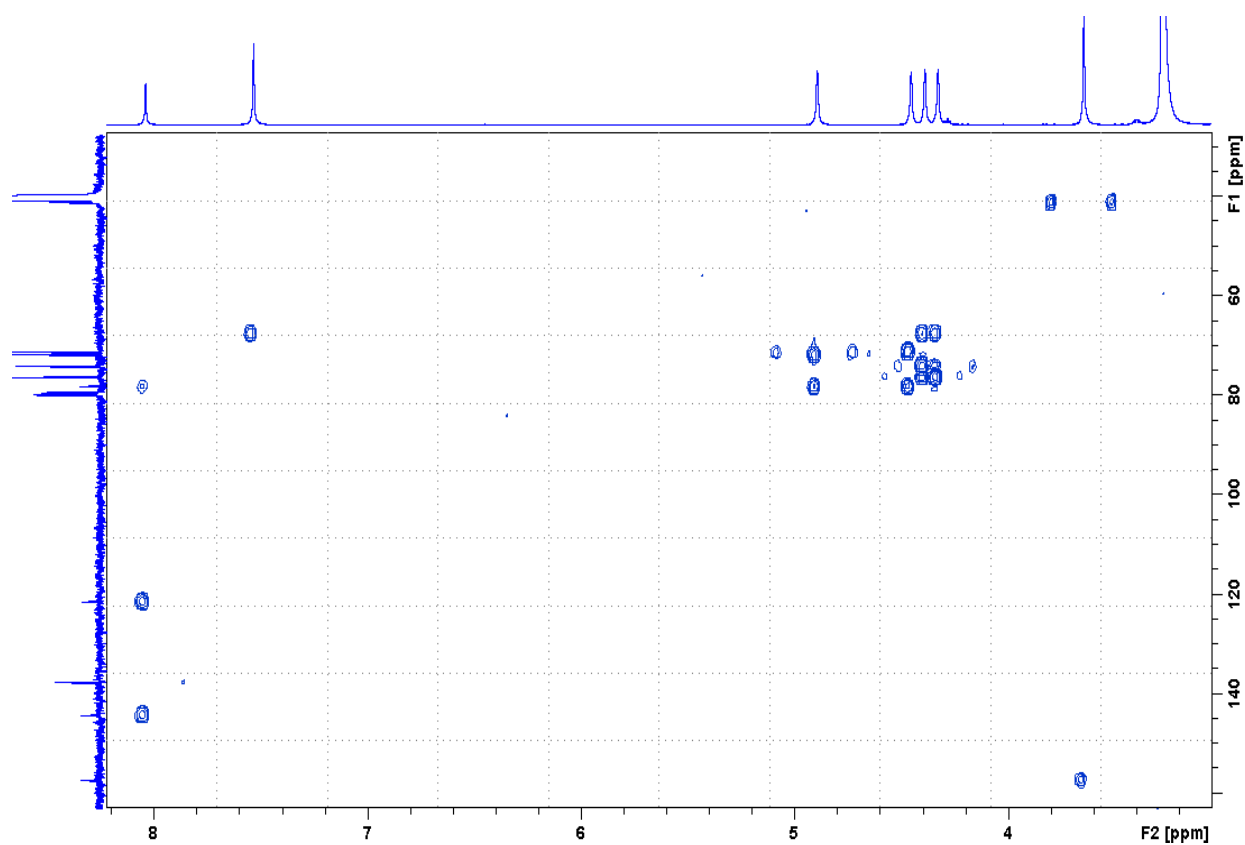


<sup>13</sup>C NMR of **11**

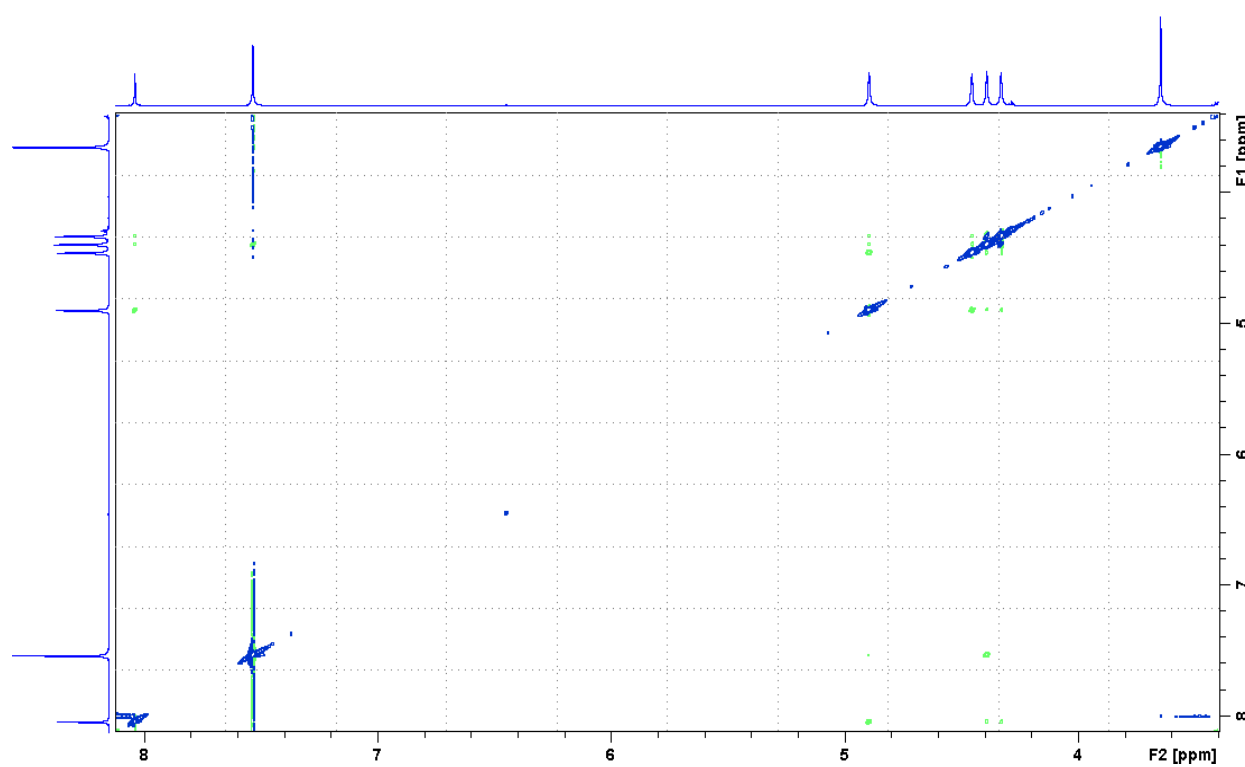


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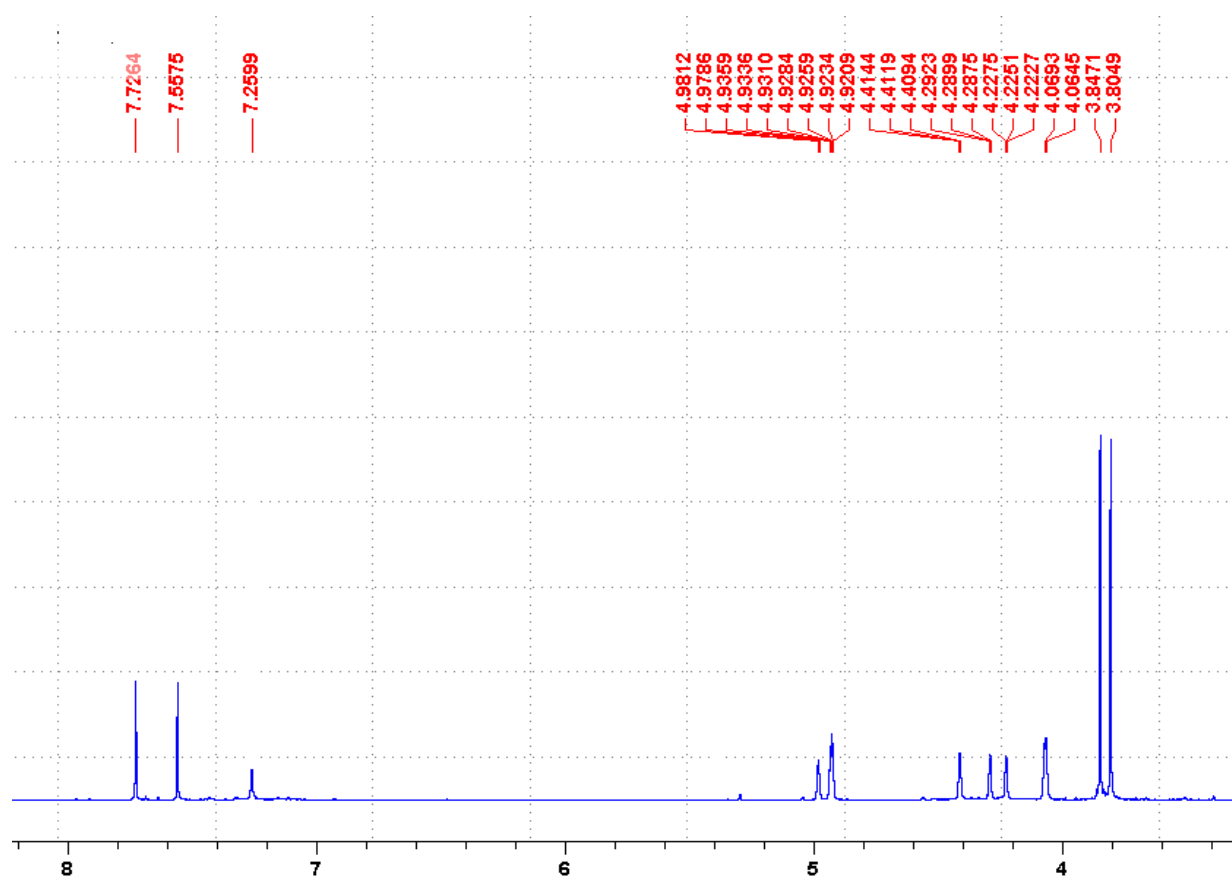




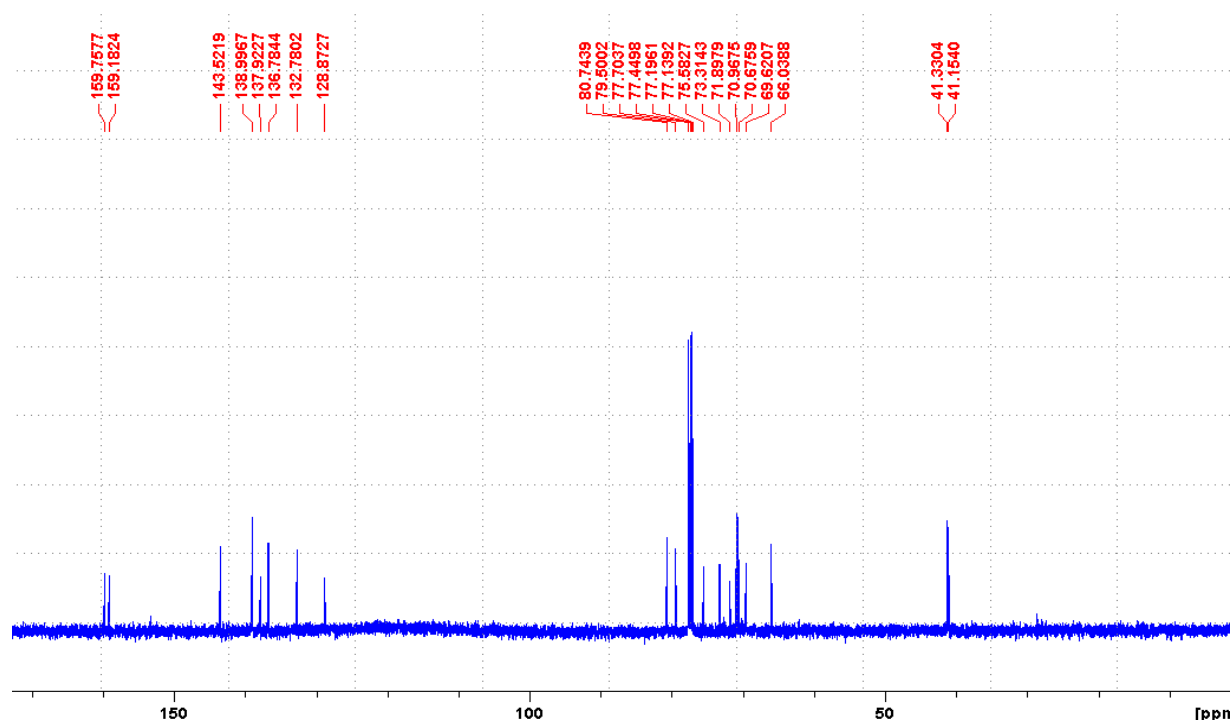
## NOESY of 11



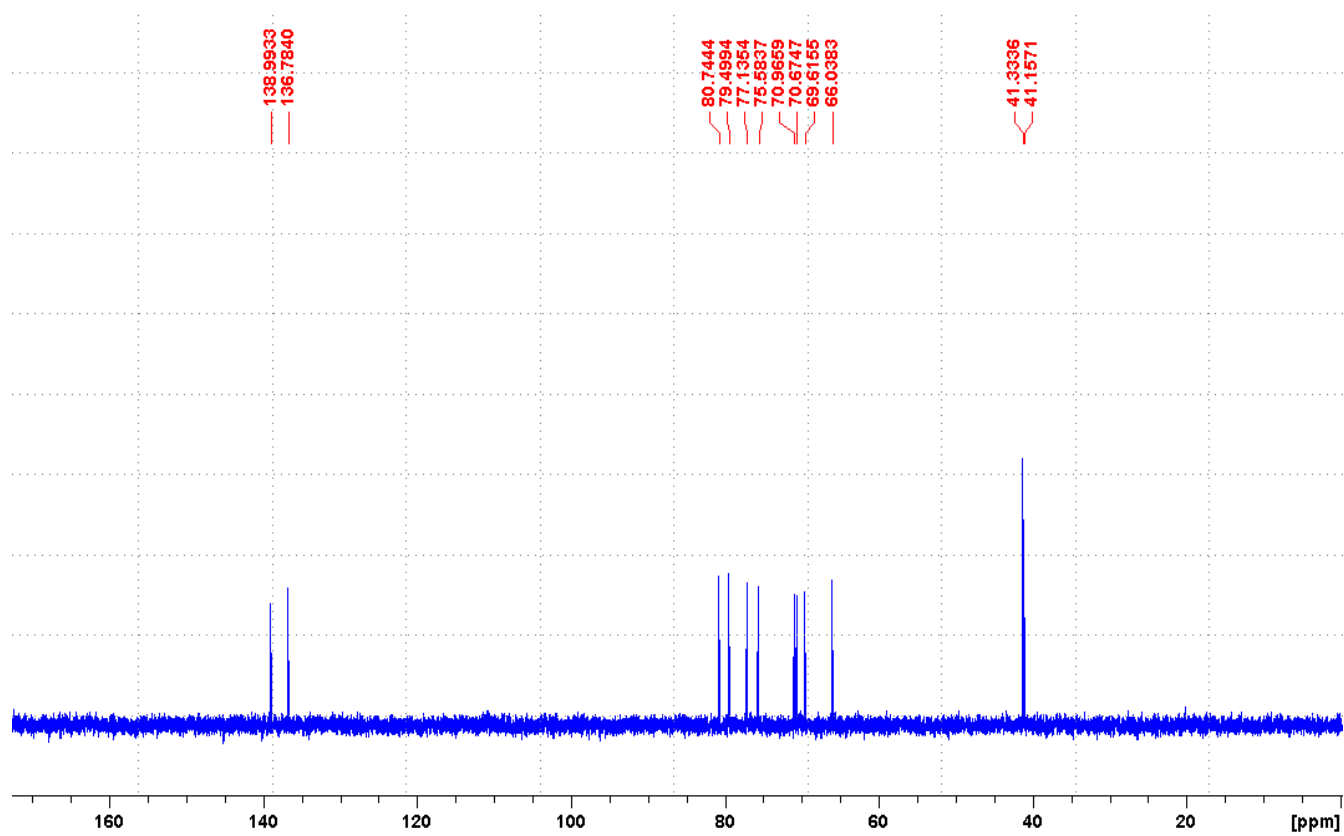
<sup>1</sup>H NMR of 12



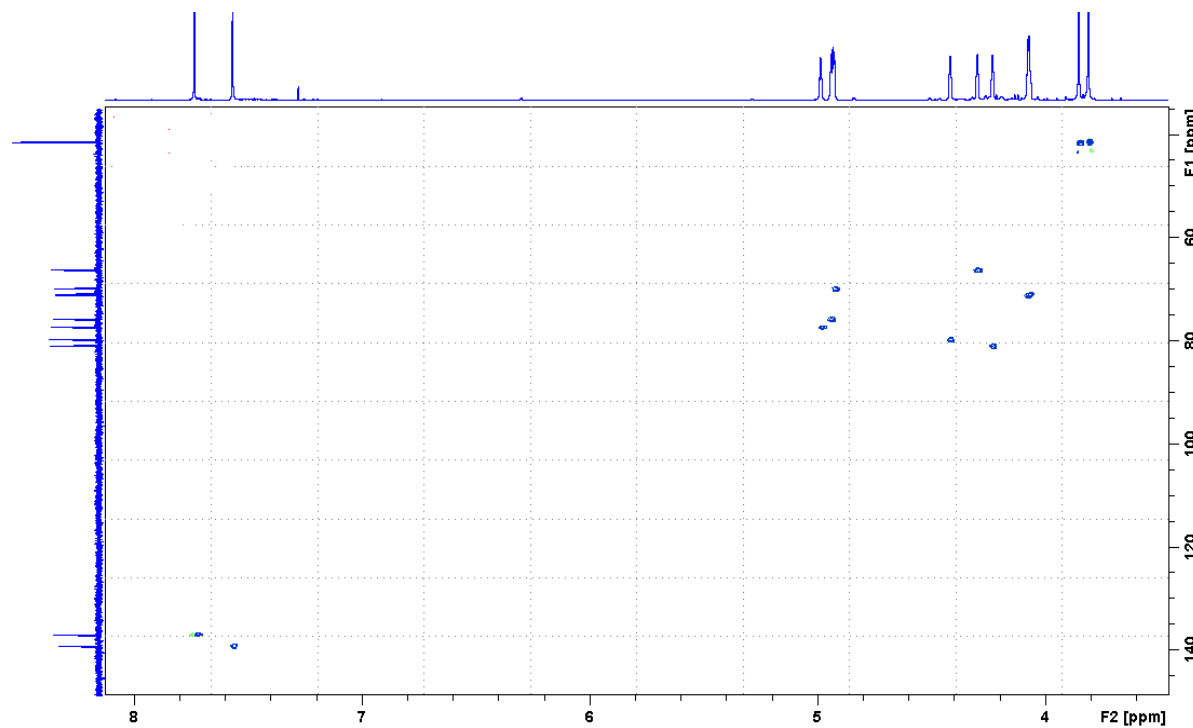
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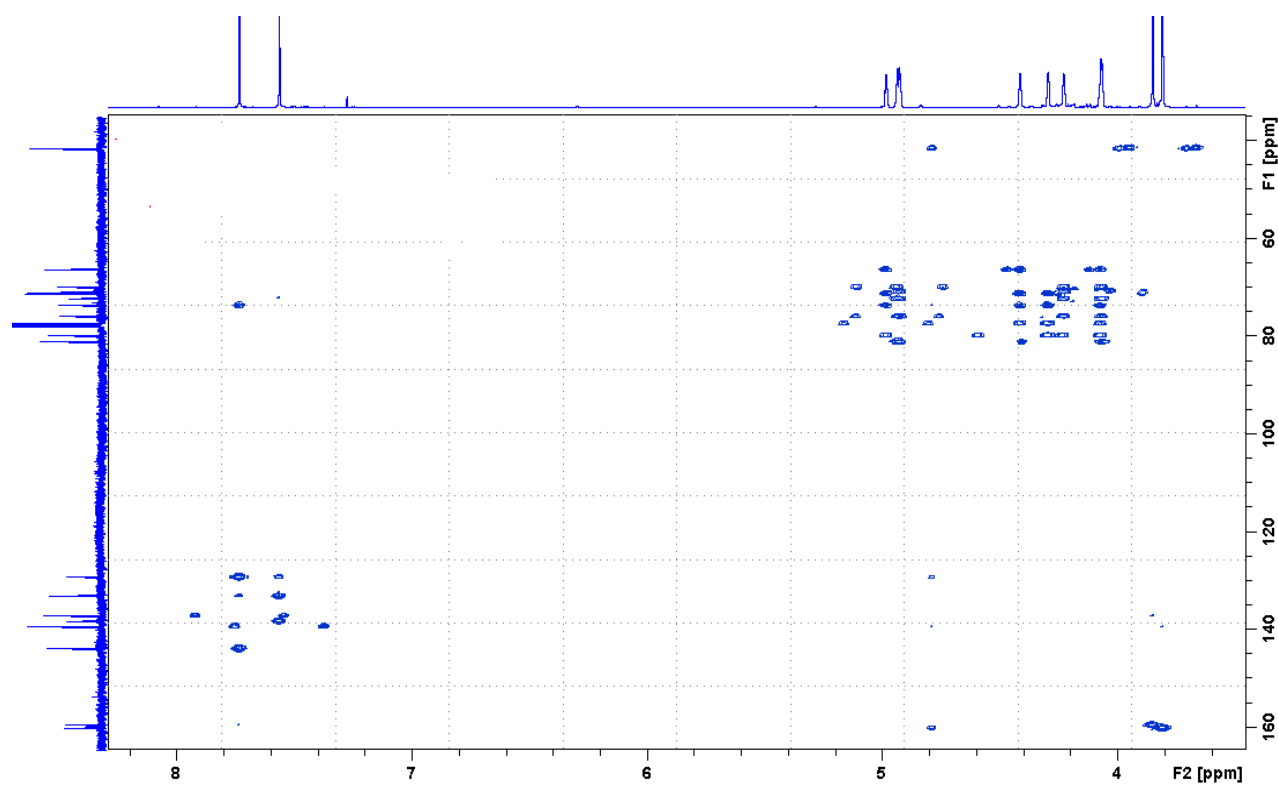
DEPT\_135 of 12



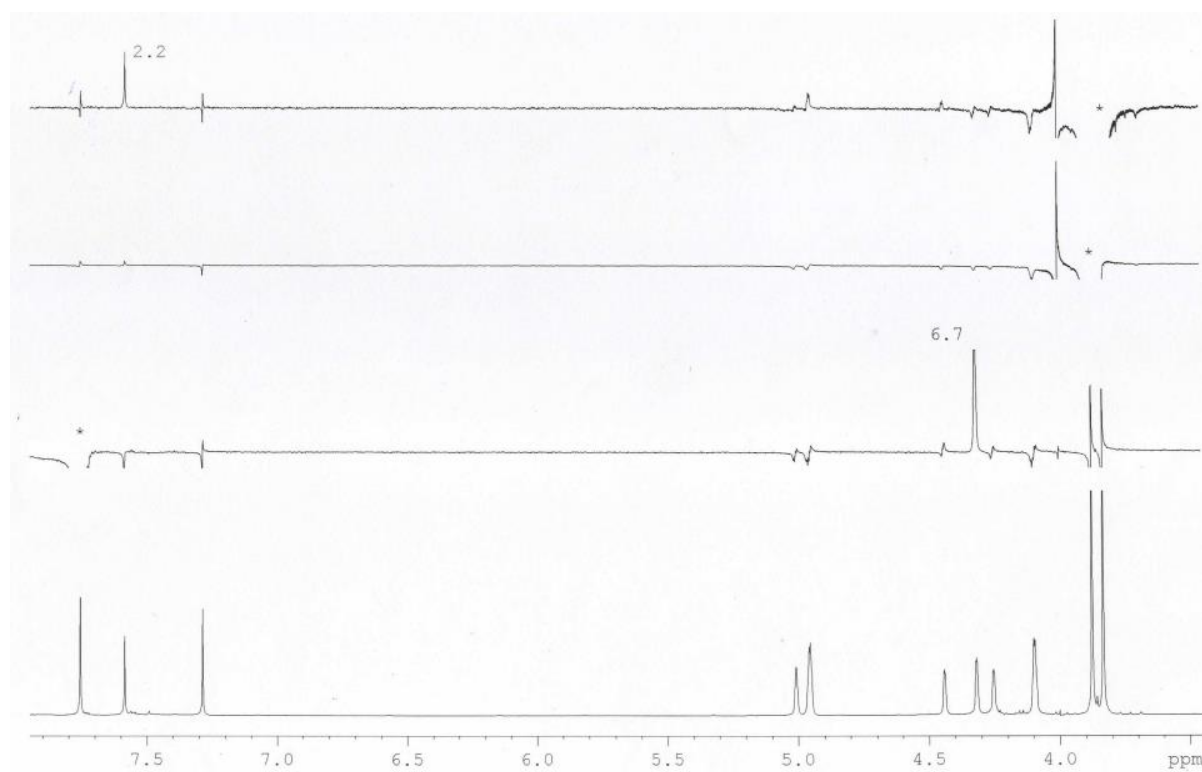
HSQC of 12



HMBC of 12

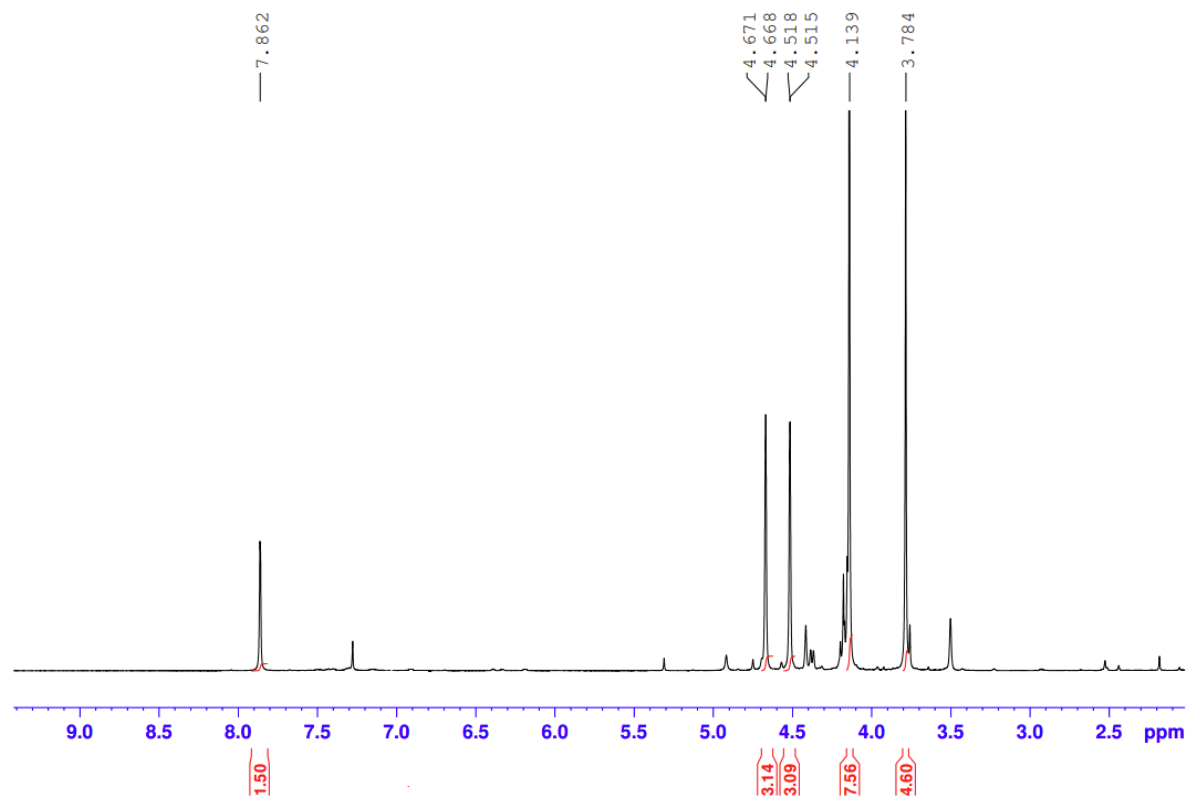


DNOE of 12

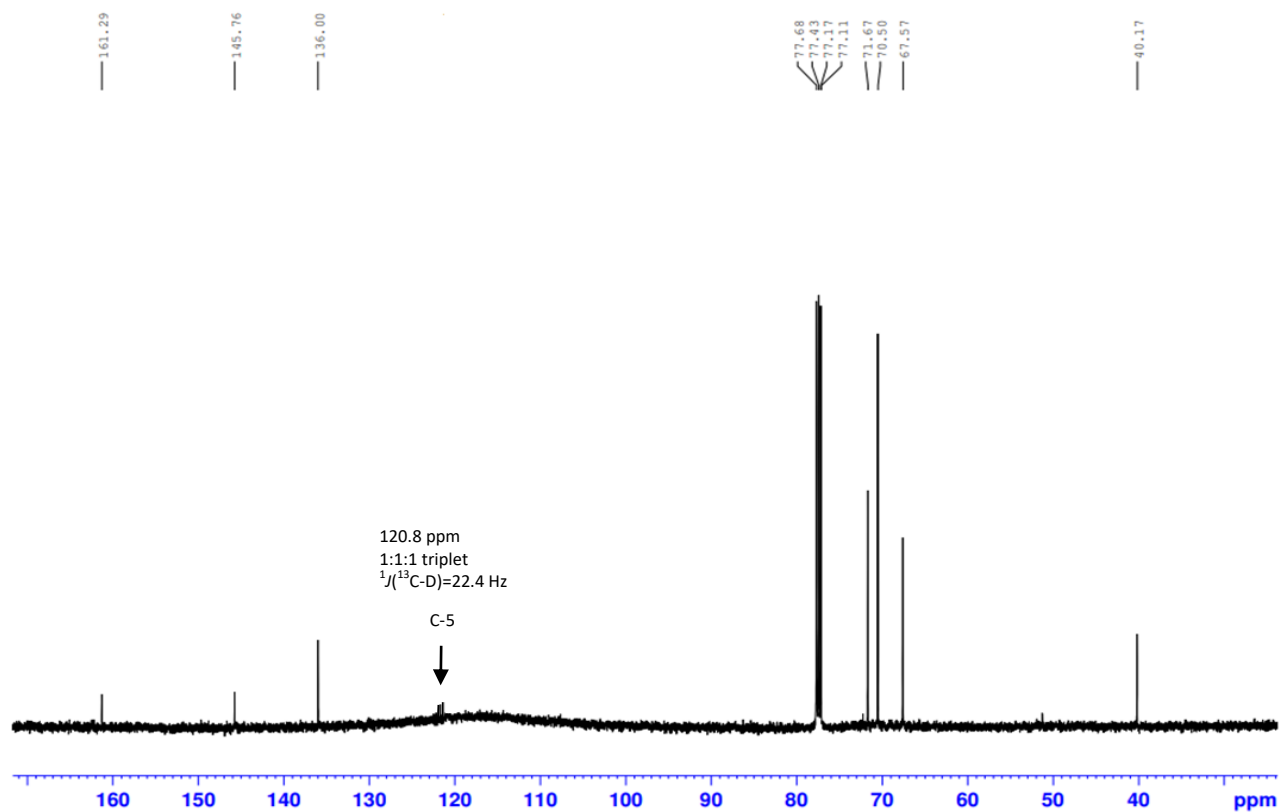


## S.2. Copies of the $^1\text{H}$ - and $^{13}\text{C}$ -NMR spectra of the deuterated products

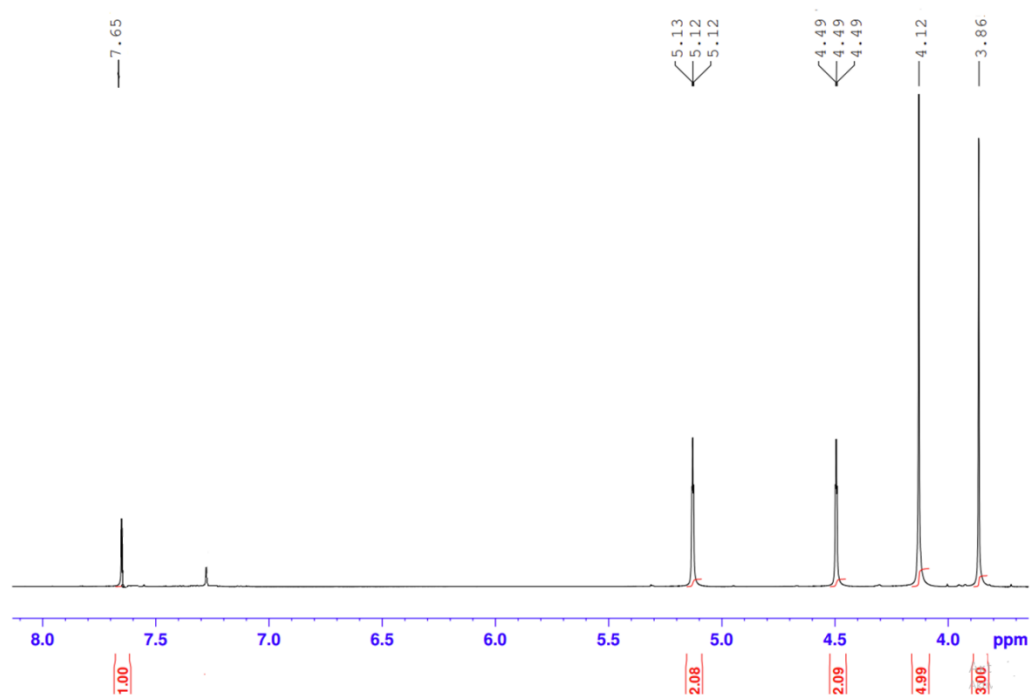
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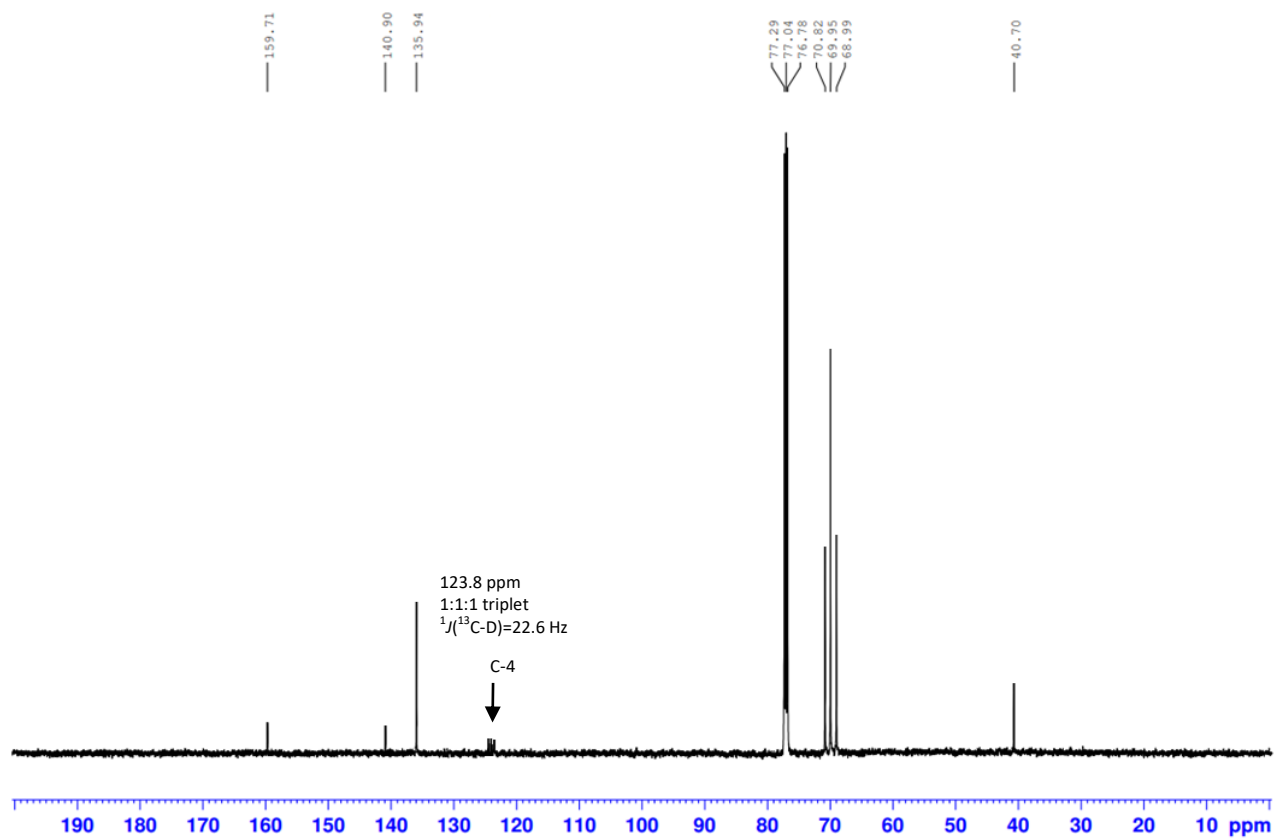
### $^{13}\text{C}$ NMR of 8[D-5]



$^1\text{H}$  NMR of **9[D-4]**

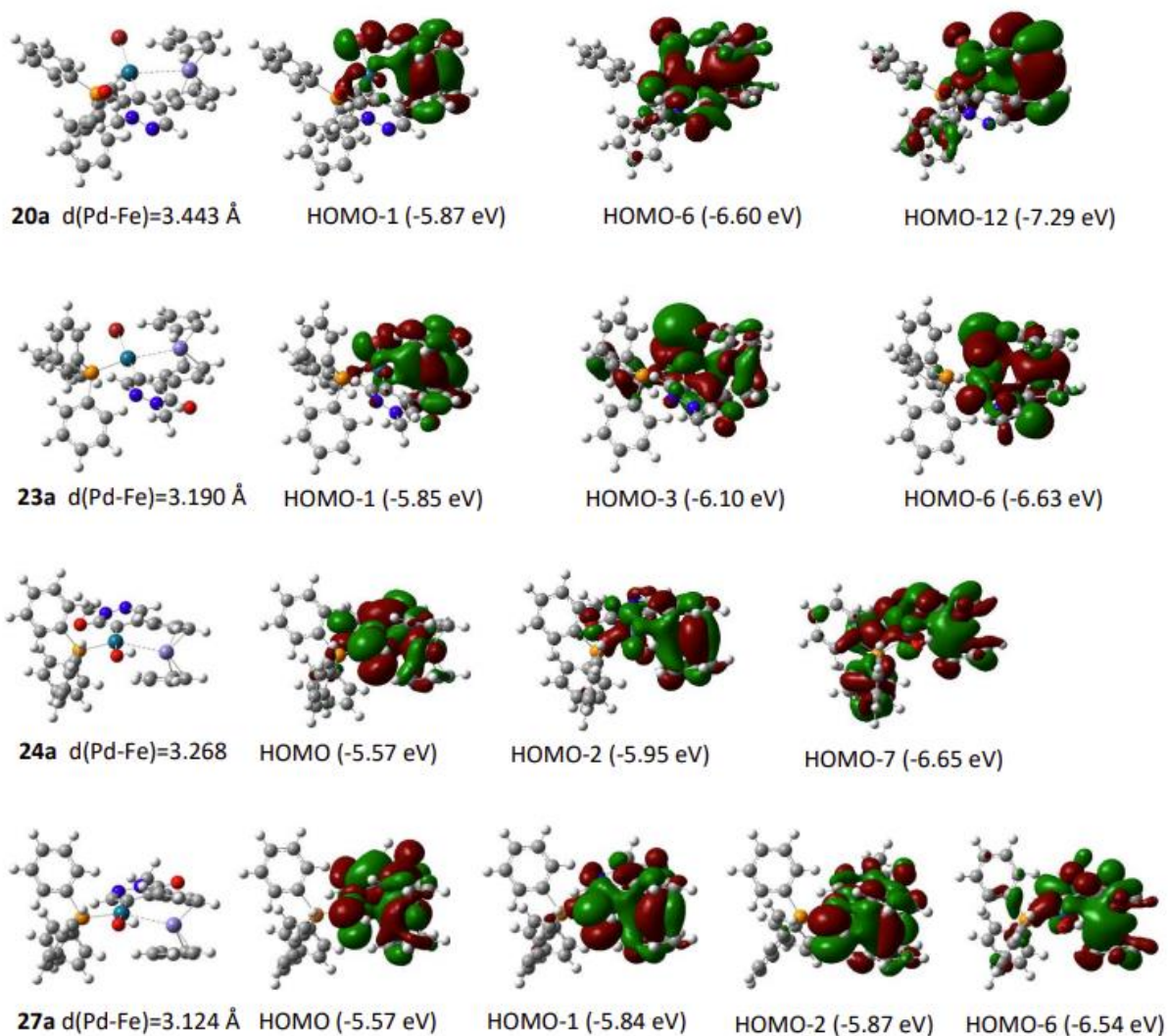


$^{13}\text{C}$  NMR of **9[D-4]**





### S.3. Bonding orbitals contributing to Fe-Pd interaction in compounds 20a, 23a, 24a and 27a



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#### S.4. XYZ coordinates of the structures optimized by B3PW91/DGTZVP method

**1:**

Row	Highlight		Display Tag		Symbol	X	Y	Z
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4	No	Show	4	C		1.3625520	-1.3840760	-1.1574050
5	No	Show	5	C		1.3617600	-1.3833380	1.1567810
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8	No	Show	8	Fe		0.6709120	0.1495450	-0.0007840
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19	No	Show	19	H		1.0710800	-1.5565620	2.1856180
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24	No	Show	24	H		-3.7051470	-1.3037260	1.1490230
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**2**

Row	Highlight		Display Tag		Symbol	X	Y	Z
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13	No	Show	13	C		0.3885000	-1.5595460	1.6757620

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18	No	Show	18	H	-0.5494070	1.7561070	-1.6301210
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21	No	Show	21	H	4.4648470	0.5121310	-1.1730970
22	No	Show	22	O	3.2006030	2.1059180	0.0156190
23	No	Show	23	H	2.6080730	2.5753890	0.6165420
24	No	Show	24	B	2.9553930	0.7466030	0.0089050
25	No	Show	25	B	-2.9539380	0.7486370	-0.0204410
26	No	Show	26	O	-3.1940630	2.1086180	-0.0460810
27	No	Show	27	H	-2.5964990	2.5684820	-0.6494520
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#### 4

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#### 5

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7	No	Show	7	C	-0.5509600	1.2056530	0.0002540
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## 10

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5	No	Show	5	H	3.3497680	1.1507370	-0.0004060
6	No	Show	6	C	0.1713990	-0.0000070	-0.0000290
7	No	Show	7	C	-0.5509600	1.2056530	0.0002540
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10	No	Show	10	H	-0.0096680	2.1484510	0.0004660
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## 12

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27	No	Show	27	C	0.5971660	1.3024540	-0.2004220
28	No	Show	28	C	-1.4575310	2.5605540	0.2394640
29	No	Show	29	N	0.3715730	3.5824530	-0.9989910
30	No	Show	30	O	3.1682010	1.6343580	0.8512340
31	No	Show	31	N	-0.8431210	3.6087180	-0.4375970
32	No	Show	32	C	1.0575740	2.4832680	-0.8701270
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34	No	Show	34	O	-2.5985790	2.7161530	0.6848820
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36	No	Show	36	C	-1.5887320	4.8541880	-0.5697820
37	No	Show	37	H	-2.5136160	4.6821120	-1.1254120
38	No	Show	38	H	-1.8526680	5.2359420	0.4187510
39	No	Show	39	H	-0.9487520	5.5588710	-1.0970810
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41	No	Show	41	H	5.5887140	0.7482840	0.3104490
42	No	Show	42	H	5.1199580	0.1029260	1.8886760
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### 13

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2	No	Show	16	C	4.3746400	0.3592890	0.0476640
3	No	Show	3	C	1.8825460	0.4228380	0.0248100
4	No	Show	32	N	4.2775750	1.7596820	0.0369020
5	No	Show	9	C	2.0012340	1.8473110	0.0104720
6	No	Show	18	N	3.1501840	2.4784900	0.0190660
7	No	Show	1	Pd	0.4360400	-1.0302720	-0.0096960
8	No	Show	2	P	-1.3425840	0.4233640	0.0050970
9	No	Show	33	O	5.4615290	-0.2120680	0.0627410
10	No	Show	19	H	1.1352990	2.5007670	-0.0101140

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11	No	Show	5	C	-1.1438150	1.6682050	-1.3241700
12	No	Show	12	C	-0.6532270	1.2243290	-2.5615300
13	No	Show	13	C	-1.4694060	3.0204090	-1.1594100
14	No	Show	24	C	-0.5076270	2.1172770	-3.6212240
15	No	Show	25	H	-0.3817640	0.1792810	-2.6938460
16	No	Show	26	C	-1.3100510	3.9135930	-2.2201680
17	No	Show	27	H	-1.8334330	3.3868920	-0.2037620
18	No	Show	37	C	-0.8334090	3.4643880	-3.4516810
19	No	Show	38	H	-0.1286330	1.7613040	-4.5755070
20	No	Show	39	H	-1.5561290	4.9628440	-2.0794480
21	No	Show	45	H	-0.7081870	4.1629010	-4.2748490
22	No	Show	6	C	-1.5043890	1.3274010	1.5905470
23	No	Show	14	C	-2.6892380	2.0180370	1.8945430
24	No	Show	15	C	-0.4581180	1.3225230	2.5206200
25	No	Show	28	C	-2.8075670	2.7142670	3.0954770
26	No	Show	29	H	-3.5269100	1.9972150	1.2022080
27	No	Show	30	C	-0.5817370	2.0180620	3.7237890
28	No	Show	31	H	0.4481930	0.7610580	2.3109880
29	No	Show	40	C	-1.7526660	2.7186170	4.0107680
30	No	Show	41	H	-3.7290840	3.2450190	3.3202490
31	No	Show	42	H	0.2359930	2.0023540	4.4392650
32	No	Show	46	H	-1.8497840	3.2565420	4.9502360
33	No	Show	4	C	-3.0206730	-0.2546980	-0.2521940
34	No	Show	11	C	-3.7811660	0.0632970	-1.3823760
35	No	Show	10	C	-3.5527540	-1.1102760	0.7240100
36	No	Show	22	C	-5.0666350	-0.4615930	-1.5301520
37	No	Show	23	H	-3.3827060	0.7228300	-2.1473340
38	No	Show	20	C	-4.8376770	-1.6223510	0.5754940
39	No	Show	21	H	-2.9618250	-1.3848690	1.5927010
40	No	Show	34	C	-5.5969730	-1.3012980	-0.5525230
41	No	Show	36	H	-5.6504460	-0.2099070	-2.4117450
42	No	Show	35	H	-5.2401620	-2.2871490	1.3349180
43	No	Show	44	H	-6.5972640	-1.7102110	-0.6698960
44	No	Show	7	Br	-0.8986940	-3.1222290	-0.1117460
45	No	Show	17	Br	2.9253500	-2.1572790	0.0477730
46	No	Show	43	C	5.5278430	2.5120460	0.0444400
47	No	Show	48	H	6.1048530	2.2670180	0.9388910
48	No	Show	47	H	6.1258770	2.2488120	-0.8307410
49	No	Show	49	H	5.2707900	3.5692470	0.0305140

### 13 (L=NHC)

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	2.2364520	-1.6575960	-0.5280120
2	No	Show	2	C	2.6588330	-2.7922880	-1.2845000

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3	No	Show	3	C	3.1785960	-1.1209230	0.2749980
4	No	Show	4	C	4.5353520	-1.5816170	0.4262980
5	No	Show	5	N	4.7587090	-2.6987060	-0.3944110
6	No	Show	6	H	1.9839850	-3.3044150	-1.9622920
7	No	Show	7	N	3.8721530	-3.2836900	-1.2119910
8	No	Show	8	O	5.4169040	-1.1159940	1.1462280
9	No	Show	9	C	-1.1672740	0.6465960	0.1005430
10	No	Show	10	Pd	0.5369220	-0.5731040	-0.2665220
11	No	Show	11	C	-3.2446510	1.4052020	0.6074170
12	No	Show	12	C	-2.5224520	2.4684890	0.1798370
13	No	Show	13	N	-1.2548000	1.9907040	-0.1153070
14	No	Show	14	N	-2.4097260	0.2994290	0.5435150
15	No	Show	15	C	-0.1612730	2.8397980	-0.5220320
16	No	Show	16	C	0.2391430	2.8364690	-1.8726800
17	No	Show	17	C	0.4395530	3.6667820	0.4491910
18	No	Show	18	C	1.3041710	3.6717840	-2.2264600
19	No	Show	19	C	1.4934770	4.4875190	0.0336290
20	No	Show	20	C	1.9290680	4.4845590	-1.2866330
21	No	Show	21	H	1.6479370	3.6903570	-3.2562340
22	No	Show	22	H	1.9847330	5.1356460	0.7544450
23	No	Show	23	H	2.7572900	5.1222000	-1.5858150
24	No	Show	24	C	-2.8422590	-1.0160070	0.9540490
25	No	Show	25	C	-2.3605900	-1.5377410	2.1699580
26	No	Show	26	C	-3.7882300	-1.6967640	0.1598320
27	No	Show	27	C	-2.8390560	-2.7899340	2.5708500
28	No	Show	28	C	-4.2361330	-2.9399420	0.6172250
29	No	Show	29	C	-3.7661240	-3.4866850	1.8058570
30	No	Show	30	H	-2.4852600	-3.2223990	3.5028660
31	No	Show	31	H	-4.9593130	-3.4950430	0.0265750
32	No	Show	32	H	-4.1242380	-4.4584950	2.1367190
33	No	Show	33	H	-2.7905660	3.5073080	0.0628320
34	No	Show	34	H	-4.2634810	1.3360480	0.9549090
35	No	Show	35	C	-0.4862080	2.0292890	-2.9378380
36	No	Show	36	H	-0.9939720	1.1931560	-2.4507950
37	No	Show	37	C	-0.0419350	3.7398160	1.8922730
38	No	Show	38	H	-0.7299100	2.9072830	2.0671950
39	No	Show	39	C	0.4554220	1.4143720	-3.9785320
40	No	Show	40	H	-0.1058880	0.7263800	-4.6170960
41	No	Show	41	H	0.9079290	2.1703590	-4.6295060
42	No	Show	42	H	1.2543860	0.8397200	-3.5024380
43	No	Show	43	C	-1.5591330	2.8980400	-3.6165560
44	No	Show	44	H	-2.1103340	2.3095380	-4.3577570
45	No	Show	45	H	-2.2819800	3.2883490	-2.8927580
46	No	Show	46	H	-1.1071610	3.7530020	-4.1317950
47	No	Show	47	C	1.0922720	3.6071560	2.9173910

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48	No	Show	48	H	0.6777810	3.5825390	3.9305760
49	No	Show	49	H	1.6689170	2.6907050	2.7703030
50	No	Show	50	H	1.7899410	4.4491460	2.8728910
51	No	Show	51	C	-0.8196640	5.0444000	2.1375790
52	No	Show	52	H	-1.6581080	5.1578210	1.4441730
53	No	Show	53	H	-1.2191090	5.0676430	3.1571030
54	No	Show	54	H	-0.1701730	5.9168660	2.0109300
55	No	Show	55	C	-1.3987030	-0.7923950	3.0832110
56	No	Show	56	H	-1.0272330	0.0867010	2.5504140
57	No	Show	57	C	-4.3563130	-1.1342490	-1.1359610
58	No	Show	58	H	-3.7225320	-0.2996440	-1.4500840
59	No	Show	59	C	-5.7861440	-0.6039180	-0.9302650
60	No	Show	60	H	-6.4659760	-1.4144370	-0.6465460
61	No	Show	61	H	-5.8436390	0.1577180	-0.1469340
62	No	Show	62	H	-6.1642200	-0.1598680	-1.8574190
63	No	Show	63	C	-4.3444510	-2.1585170	-2.2794780
64	No	Show	64	H	-5.0644860	-2.9668210	-2.1122730
65	No	Show	65	H	-4.6232090	-1.6672880	-3.2177110
66	No	Show	66	H	-3.3524690	-2.5961700	-2.4054810
67	No	Show	67	C	-0.1739780	-1.6419470	3.4487490
68	No	Show	68	H	0.3318060	-2.0139800	2.5529900
69	No	Show	69	H	0.5441980	-1.0448210	4.0195740
70	No	Show	70	H	-0.4442110	-2.5058140	4.0648240
71	No	Show	71	C	-2.1221760	-0.2928870	4.3439840
72	No	Show	72	H	-2.9692860	0.3527510	4.0909320
73	No	Show	73	H	-2.5067700	-1.1279430	4.9391420
74	No	Show	74	H	-1.4359090	0.2799500	4.9772250
75	No	Show	75	Br	2.5678430	0.4062270	1.2789970
76	No	Show	76	Br	-0.5910370	-1.8420700	-2.0379130
77	No	Show	77	C	6.0924130	-3.2891000	-0.3593360
78	No	Show	78	H	6.8362560	-2.5496120	-0.6644060
79	No	Show	79	H	6.3299100	-3.6144660	0.6559620
80	No	Show	80	H	6.0900950	-4.1354810	-1.0431230

### 13\*

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	3.9544950	0.5778860	-1.2073680
2	No	Show	2	C	3.5510470	1.5544870	-2.1721850
3	No	Show	3	C	5.1548960	0.7890880	-0.5992500
4	No	Show	4	N	4.2629270	2.6030060	-2.4967960
5	No	Show	5	C	5.9881310	1.9498230	-0.8905160
6	No	Show	6	N	5.4327660	2.7781950	-1.8753380
7	No	Show	7	Pd	2.9575970	-1.1679380	-1.0178160
8	No	Show	8	P	1.4314540	-0.2052370	0.3894150



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9	No	Show	9	C	1.5573610	1.5966330	0.6541350
10	No	Show	10	C	2.6157700	2.0670680	1.4479110
11	No	Show	11	C	0.6979750	2.5170170	0.0437890
12	No	Show	12	C	2.7956660	3.4339200	1.6396800
13	No	Show	13	H	3.3004190	1.3670040	1.9202750
14	No	Show	14	C	0.8874890	3.8871320	0.2324270
15	No	Show	15	H	-0.1347350	2.1728360	-0.5599110
16	No	Show	16	C	1.9330230	4.3485260	1.0305320
17	No	Show	17	H	3.6171340	3.7833400	2.2594200
18	No	Show	18	H	0.2125600	4.5924450	-0.2455690
19	No	Show	19	H	2.0782760	5.4157000	1.1764930
20	No	Show	20	C	1.5313100	-0.9202540	2.0704500
21	No	Show	21	C	0.9405750	-0.2463710	3.1508980
22	No	Show	22	C	2.1590380	-2.1526560	2.2851610
23	No	Show	23	C	0.9748570	-0.8042940	4.4265750
24	No	Show	24	H	0.4661970	0.7191880	3.0028010
25	No	Show	25	C	2.1859770	-2.7082750	3.5650150
26	No	Show	26	H	2.6105610	-2.6853010	1.4521190
27	No	Show	27	C	1.5965060	-2.0376870	4.6357680
28	No	Show	28	H	0.5190930	-0.2730440	5.2583180
29	No	Show	29	H	2.6744860	-3.6664490	3.7199260
30	No	Show	30	H	1.6252960	-2.4700540	5.6326990
31	No	Show	31	O	7.0624340	2.2353180	-0.3681590
32	No	Show	32	H	2.6104220	1.4646720	-2.7080000
33	No	Show	33	H	-2.7069660	-0.9067220	-2.4564600
34	No	Show	34	C	-1.9874480	-1.0341720	-1.6580590
35	No	Show	35	C	-2.0291650	-2.0197050	-0.6282230
36	No	Show	36	C	-0.8692500	-0.1892550	-1.4231520
37	No	Show	37	C	-0.9376600	-1.7874120	0.2505730
38	No	Show	38	H	-2.7906220	-2.7796410	-0.5065360
39	No	Show	39	C	-0.2083730	-0.6446590	-0.2289620
40	No	Show	40	Fe	-2.1457280	-0.1439080	0.1853820
41	No	Show	41	C	-2.7338160	0.2220450	2.1082000
42	No	Show	42	C	-2.2263170	1.4177040	1.5150200
43	No	Show	43	C	-3.8360930	-0.2242110	1.3209630
44	No	Show	44	H	-2.3263700	-0.2858630	2.9738440
45	No	Show	45	C	-3.0031530	1.6997940	0.3534710
46	No	Show	46	C	-4.0192770	0.6902270	0.2298310
47	No	Show	47	H	-4.4103000	-1.1273110	1.4842790
48	No	Show	48	H	-2.8565480	2.5276670	-0.3301960
49	No	Show	49	H	-0.5738900	0.6432190	-2.0489070
50	No	Show	50	H	-0.6963160	-2.3587690	1.1370940
51	No	Show	51	P	-5.2527770	0.6862670	-1.1201890
52	No	Show	52	C	-6.0372360	-0.9749220	-0.9141720
53	No	Show	53	C	-6.9118360	-1.2959410	0.1347490

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54	No	Show	54	C	-5.7584770	-1.9535650	-1.8784810
55	No	Show	55	C	-7.4717270	-2.5699940	0.2282300
56	No	Show	56	H	-7.1660430	-0.5423920	0.8760880
57	No	Show	57	C	-6.3136660	-3.2312870	-1.7841140
58	No	Show	58	H	-5.1138700	-1.7112890	-2.7206010
59	No	Show	59	C	-7.1697830	-3.5427820	-0.7276420
60	No	Show	60	H	-8.1493810	-2.8024100	1.0462580
61	No	Show	61	H	-6.0853000	-3.9772840	-2.5412960
62	No	Show	62	H	-7.6092190	-4.5344500	-0.6552790
63	No	Show	63	C	-6.5598610	1.7847680	-0.4164480
64	No	Show	64	C	-7.6442610	2.0975640	-1.2517060
65	No	Show	65	C	-6.5119490	2.3561900	0.8621050
66	No	Show	66	C	-8.6669410	2.9356060	-0.8111700
67	No	Show	67	H	-7.6914390	1.6787390	-2.2552850
68	No	Show	68	C	-7.5299090	3.2072200	1.2988670
69	No	Show	69	H	-5.6785500	2.1377400	1.5240770
70	No	Show	70	C	-8.6117790	3.4959360	0.4673770
71	No	Show	71	H	-9.5025290	3.1595420	-1.4697730
72	No	Show	72	H	-7.4768530	3.6419650	2.2942960
73	No	Show	73	H	-9.4041380	4.1568620	0.8094790
74	No	Show	74	H	-1.3723990	1.9896570	1.8548600
75	No	Show	75	C	6.1928800	3.9658950	-2.2480980
76	No	Show	76	H	7.1891360	3.6770050	-2.5891820
77	No	Show	77	H	6.3063190	4.6250010	-1.3842200
78	No	Show	78	H	5.6434390	4.4668180	-3.0426880
79	No	Show	79	Br	2.1411150	-3.5043130	-1.1880950
80	No	Show	80	Br	5.8448280	-0.4082740	0.7003780

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Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	-2.2538280	-1.1527350	0.7046250
2	No	Show	2	C	-2.8216600	-1.1727560	2.0178140
3	No	Show	3	C	-3.0984880	-1.4573350	-0.3165740
4	No	Show	4	N	-4.0736890	-1.4464110	2.2767040
5	No	Show	5	C	-4.5054470	-1.7711720	-0.1083290
6	No	Show	6	N	-4.8730220	-1.7285310	1.2423670
7	No	Show	7	Pd	-0.2573190	-0.7673740	0.4612820
8	No	Show	8	P	-0.8127480	1.5030890	0.1008970
9	No	Show	9	C	-2.5772250	1.9620210	-0.0958710
10	No	Show	10	C	-3.3959280	2.0608950	1.0388550

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11	No	Show	11	C	-3.1391050	2.1483150	-1.3638700
12	No	Show	12	C	-4.7517660	2.3491760	0.9041830
13	No	Show	13	H	-2.9784200	1.9156530	2.0314390
14	No	Show	14	C	-4.4989460	2.4320640	-1.4946840
15	No	Show	15	H	-2.5224470	2.0675390	-2.2537360
16	No	Show	16	C	-5.3074860	2.5335370	-0.3636340
17	No	Show	17	H	-5.3750920	2.4204520	1.7917520
18	No	Show	18	H	-4.9258550	2.5649250	-2.4851710
19	No	Show	19	H	-6.3675740	2.7491720	-0.4688780
20	No	Show	20	C	-0.2884460	2.5812070	1.4911590
21	No	Show	21	C	-0.6471600	3.9375080	1.5388810
22	No	Show	22	C	0.4499960	2.0357530	2.5483120
23	No	Show	23	C	-0.2416790	4.7360070	2.6060080
24	No	Show	24	H	-1.2692580	4.3645920	0.7565310
25	No	Show	25	C	0.8519760	2.8357940	3.6196660
26	No	Show	26	H	0.7056440	0.9787330	2.5398800
27	No	Show	27	C	0.5135520	4.1881440	3.6462520
28	No	Show	28	H	-0.5261260	5.7849470	2.6320320
29	No	Show	29	H	1.4238780	2.3963950	4.4326130
30	No	Show	30	H	0.8231570	4.8116210	4.4811320
31	No	Show	31	O	-5.3377770	-2.0498290	-0.9696050
32	No	Show	32	H	-2.2121210	-0.9733590	2.8940280
33	No	Show	33	H	1.4044830	4.3358510	-3.5227970
34	No	Show	34	C	0.9461180	3.4896070	-3.0251190
35	No	Show	35	C	0.8535140	2.1618550	-3.5402420
36	No	Show	36	C	0.3955720	3.4987970	-1.7099550
37	No	Show	37	C	0.2479150	1.3431280	-2.5458030
38	No	Show	38	H	1.2245760	1.8226190	-4.4995730
39	No	Show	39	C	-0.0418880	2.1645180	-1.4001330
40	No	Show	40	Fe	1.9383570	2.1810600	-1.7971180
41	No	Show	41	C	3.5407110	0.9210910	-1.9348370
42	No	Show	42	C	2.9415660	0.8465100	-0.6326850
43	No	Show	43	C	3.9525450	2.2670370	-2.1631430
44	No	Show	44	H	3.6245460	0.1006910	-2.6361270
45	No	Show	45	C	2.9927910	2.1681440	-0.0652930
46	No	Show	46	C	3.6219030	3.0343210	-1.0062720
47	No	Show	47	H	4.4015280	2.6459340	-3.0733770
48	No	Show	48	H	2.6037520	2.4611120	0.9012030
49	No	Show	49	H	3.7727860	4.0999330	-0.8818660
50	No	Show	50	H	0.3708770	4.3500330	-1.0422860
51	No	Show	51	H	0.0603340	0.2789360	-2.6119300
52	No	Show	52	P	2.1904260	-0.6293900	0.1452070
53	No	Show	53	C	2.7818260	-1.9584860	-0.9761100
54	No	Show	54	C	4.1000010	-2.4293190	-0.9303000
55	No	Show	55	C	1.8993260	-2.4814060	-1.9289350

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56	No	Show	56	C	4.5328190	-3.3967850	-1.8362570
57	No	Show	57	H	4.7900940	-2.0516080	-0.1807680
58	No	Show	58	C	2.3369000	-3.4426430	-2.8400230
59	No	Show	59	H	0.8599600	-2.1645180	-1.9409390
60	No	Show	60	C	3.6537970	-3.9007830	-2.7968200
61	No	Show	61	H	5.5557290	-3.7616360	-1.7865380
62	No	Show	62	H	1.6397210	-3.8478380	-3.5687150
63	No	Show	63	H	3.9908080	-4.6587480	-3.4995210
64	No	Show	64	C	3.2061630	-0.7947830	1.6735600
65	No	Show	65	C	4.4621720	-0.1807550	1.7993590
66	No	Show	66	C	2.7159120	-1.5641910	2.7383360
67	No	Show	67	C	5.2121560	-0.3361460	2.9651940
68	No	Show	68	H	4.8598900	0.4240270	0.9894470
69	No	Show	69	C	3.4708060	-1.7188080	3.9012180
70	No	Show	70	H	1.7541690	-2.0631780	2.6452010
71	No	Show	71	C	4.7186640	-1.1056210	4.0197570
72	No	Show	72	H	6.1840200	0.1445950	3.0466060
73	No	Show	73	H	3.0797630	-2.3251410	4.7143520
74	No	Show	74	H	5.3043630	-1.2272940	4.9276280
75	No	Show	75	C	-6.2588400	-2.0466940	1.5623770
76	No	Show	76	H	-6.5006060	-3.0538670	1.2152350
77	No	Show	77	H	-6.3657340	-1.9787610	2.6434160
78	No	Show	78	H	-6.9305250	-1.3449870	1.0625520
79	No	Show	79	Br	-2.5264630	-1.5318860	-2.1257370
80	No	Show	80	Br	-0.0387300	-3.2071850	1.0251950

#### 14

Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	C	-	3.2753450	-0.3656940	-0.1399200
2	No	Show	2	C	-	4.5576880	0.2316860	-0.0758170
3	No	Show	3	C	-	2.1033170	0.3127360	-0.1102310
4	No	Show	4	N	-	4.6653600	1.5300310	0.0252400
5	No	Show	5	C	-	2.2154370	1.7611650	-0.0146980
6	No	Show	6	N	-	3.5390540	2.2470910	0.0598260
7	No	Show	7	Pd	-	0.6070490	-1.0812320	-0.0676610
8	No	Show	8	P	1.	1476500	0.4019010	0.0027650
9	No	Show	9	C	1.	0890610	1.3504950	1.5614980
10	No	Show	10	C	0.	8605740	0.6255750	2.7398230
11	No	Show	11	C	1.	2771020	2.7348330	1.6244960
12	No	Show	12	C	0.	8473610	1.2782180	3.9715730
13	No	Show	13	H	0.	6966890	-0.4492990	2.6952840
14	No	Show	14	C	1.	2612640	3.3824470	2.8594330
15	No	Show	15	H	1.	4048250	3.3121670	0.7146810
16	No	Show	16	C	1.	0510420	2.6578570	4.0335860

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17	No	Show	17	H	0.6725240	0.7078050	4.8800600
18	No	Show	18	H	1.4016450	4.4595650	2.9009880
19	No	Show	19	H	1.0359060	3.1679120	4.9934570
20	No	Show	20	C	1.2785800	1.5179580	-1.4401990
21	No	Show	21	C	2.4175820	2.3226070	-1.5943390
22	No	Show	22	C	0.2983670	1.5181590	-2.4369920
23	No	Show	23	C	2.5508140	3.1412200	-2.7140410
24	No	Show	24	H	3.2114280	2.2992160	-0.8523050
25	No	Show	25	C	0.4431890	2.3247760	-3.5648560
26	No	Show	26	H	-0.5743350	0.8793240	-2.3335620
27	No	Show	27	C	1.5641930	3.1433090	-3.7018470
28	No	Show	28	H	3.4336000	3.7664360	-2.8206300
29	No	Show	29	H	-0.3214690	2.3114940	-4.3371660
30	No	Show	30	H	1.6752280	3.7736620	-4.5804990
31	No	Show	31	C	2.8166580	-0.3603590	-0.0051610
32	No	Show	32	C	3.7220830	-0.1972170	1.0480240
33	No	Show	33	C	3.2032330	-1.0885310	-1.1400090
34	No	Show	34	C	5.0020490	-0.7504280	0.9630670
35	No	Show	35	H	3.4412110	0.3620260	1.9351900
36	No	Show	36	C	4.4800070	-1.6327100	-1.2224470
37	No	Show	37	H	2.5017050	-1.2423770	-1.9552080
38	No	Show	38	C	5.3838590	-1.4658090	-0.1696940
39	No	Show	39	H	5.6980280	-0.6182890	1.7875660
40	No	Show	40	H	4.7659010	-2.1999310	-2.1041880
41	No	Show	41	H	6.3796400	-1.8973040	-0.2325420
42	No	Show	42	Br	0.7386170	-3.1505130	0.1586080
43	No	Show	43	Br	-3.0925610	-2.2930880	-0.2333500
44	No	Show	44	H	-5.4820170	-0.3373890	-0.1014540
45	No	Show	45	O	-1.2865700	2.5693390	0.0020280
46	No	Show	46	C	-3.7080070	3.6922950	0.1748440
47	No	Show	47	H	-3.1739200	4.0581870	1.0541540
48	No	Show	48	H	-3.2942400	4.1886310	-0.7061480
49	No	Show	49	H	-4.7747280	3.8902630	0.2609700

#### 14 (L=NHC)

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	3.2770090	-0.8431560	0.7850370
2	No	Show	2	C	4.6177750	-1.1669770	1.0991320
3	No	Show	3	C	2.4334610	-1.5638580	0.0211800
4	No	Show	4	C	2.9754220	-2.8296080	-0.4803000
5	No	Show	5	N	4.3451600	-3.0387560	-0.1424060
6	No	Show	6	H	5.2622220	-0.5496700	1.7175080
7	No	Show	7	N	5.1280300	-2.2678970	0.6152890
8	No	Show	8	O	2.4017010	-3.6956670	-1.1241050

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9	No	Show	9	C	-1.0895660	0.6597220	-0.0097960
10	No	Show	10	Pd	0.6612010	-0.5228770	-0.0440120
11	No	Show	11	C	-3.2330720	1.3727410	0.1906680
12	No	Show	12	C	-2.5066890	2.4135670	-0.2815590
13	No	Show	13	N	-1.1982760	1.9663400	-0.3872210
14	No	Show	14	N	-2.3590270	0.3065860	0.3438140
15	No	Show	15	C	-0.0974210	2.8233010	-0.7563090
16	No	Show	16	C	0.4681250	2.6952400	-2.0403350
17	No	Show	17	C	0.3437060	3.7826440	0.1783990
18	No	Show	18	C	1.5405600	3.5369760	-2.3539950
19	No	Show	19	C	1.4108490	4.6059820	-0.1976450
20	No	Show	20	C	2.0121270	4.4781160	-1.4446780
21	No	Show	21	H	2.0113600	3.4579250	-3.3291180
22	No	Show	22	H	1.7807120	5.3552740	0.4973860
23	No	Show	23	H	2.8481680	5.1197450	-1.7122600
24	No	Show	24	C	-2.7930180	-0.9736570	0.8530140
25	No	Show	25	C	-2.3940640	-1.3602980	2.1472400
26	No	Show	26	C	-3.6581950	-1.7586890	0.0623810
27	No	Show	27	C	-2.8697610	-2.5829960	2.6325290
28	No	Show	28	C	-4.1089250	-2.9652630	0.6064930
29	No	Show	29	C	-3.7173480	-3.3804120	1.8737440
30	No	Show	30	H	-2.5765680	-2.9127750	3.6255190
31	No	Show	31	H	-4.7691710	-3.5983060	0.0206130
32	No	Show	32	H	-4.0727940	-4.3282510	2.2704160
33	No	Show	33	H	-2.7956480	3.4187170	-0.5475300
34	No	Show	34	H	-4.2806930	1.2956080	0.4358870
35	No	Show	35	C	-0.0954650	1.7477570	-3.0865760
36	No	Show	36	H	-0.5964670	0.9235610	-2.5730290
37	No	Show	37	C	-0.3191440	3.9916500	1.5340540
38	No	Show	38	H	-1.0102280	3.1625000	1.7119220
39	No	Show	39	C	0.9786640	1.1061490	-3.9704810
40	No	Show	40	H	0.5256900	0.3171850	-4.5770950
41	No	Show	41	H	1.4399220	1.8247690	-4.6573830
42	No	Show	42	H	1.7640470	0.6423300	-3.3678330
43	No	Show	43	C	-1.1460610	2.4761720	-3.9426330
44	No	Show	44	H	-1.5790690	1.7874260	-4.6758440
45	No	Show	45	H	-1.9639120	2.8714280	-3.3312720
46	No	Show	46	H	-0.7000190	3.3155650	-4.4878040
47	No	Show	47	C	0.6774830	4.0000340	2.7011870
48	No	Show	48	H	0.1392220	4.0892310	3.6506500
49	No	Show	49	H	1.2672130	3.0803740	2.7381410
50	No	Show	50	H	1.3749010	4.8415630	2.6429970
51	No	Show	51	C	-1.1441220	5.2901710	1.5377430
52	No	Show	52	H	-1.8836270	5.3063780	0.7316560
53	No	Show	53	H	-1.6770560	5.4037910	2.4877980

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54	No	Show	54	H	-0.4990600	6.1653450	1.4074230
55	No	Show	55	C	-1.5287280	-0.4973000	3.0533610
56	No	Show	56	H	-1.1092560	0.3173770	2.4574430
57	No	Show	57	C	-4.1380810	-1.3521980	-1.3243230
58	No	Show	58	H	-3.5223730	-0.5157930	-1.6667920
59	No	Show	59	C	-5.6055090	-0.8899060	-1.2894600
60	No	Show	60	H	-6.2666000	-1.7101470	-0.9896320
61	No	Show	61	H	-5.7716000	-0.0666720	-0.5877300
62	No	Show	62	H	-5.9218080	-0.5529260	-2.2825380
63	No	Show	63	C	-3.9752270	-2.4770480	-2.3571690
64	No	Show	64	H	-4.6666010	-3.3056730	-2.1706880
65	No	Show	65	H	-4.1946430	-2.0922240	-3.3587780
66	No	Show	66	H	-2.9556300	-2.8668360	-2.3564090
67	No	Show	67	C	-0.3427420	-1.2760220	3.6384840
68	No	Show	68	H	0.2351370	-1.7697750	2.8517760
69	No	Show	69	H	0.3256260	-0.5962790	4.1769190
70	No	Show	70	H	-0.6677930	-2.0436880	4.3485590
71	No	Show	71	C	-2.3760390	0.1398530	4.1668720
72	No	Show	72	H	-3.1920000	0.7418540	3.7540080
73	No	Show	73	H	-2.8212760	-0.6240890	4.8130050
74	No	Show	74	H	-1.7574170	0.7905690	4.7948070
75	No	Show	75	Br	2.4661350	0.8055100	1.4747870
76	No	Show	76	Br	-0.3346410	-1.8841640	-1.8065640
77	No	Show	77	C	4.9572790	-4.2666060	-0.6387670
78	No	Show	78	H	4.4639490	-5.1372280	-0.1993800
79	No	Show	79	H	4.8412340	-4.3246320	-1.7227780
80	No	Show	80	H	6.0098350	-4.2433830	-0.3622450

#### 14\*

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	-5.0940680	1.2908180	-0.8245660
2	No	Show	2	C	-5.6556840	2.5525980	-1.1731850
3	No	Show	3	C	-3.8094580	0.9664240	-1.1348000
4	No	Show	4	N	-4.9641960	3.4630330	-1.8018630
5	No	Show	5	C	-3.0185670	1.9848210	-1.8175740
6	No	Show	6	N	-3.6951680	3.1764270	-2.1088720
7	No	Show	7	Pd	-3.1029380	-0.9172670	-0.9868440
8	No	Show	8	P	-1.5845780	-0.2544580	0.5805170
9	No	Show	9	C	-1.6712280	1.4759960	1.1563140
10	No	Show	10	C	-2.7596590	1.8337090	1.9673100
11	No	Show	11	C	-0.7357290	2.4486620	0.7915890
12	No	Show	12	C	-2.8959310	3.1422990	2.4217840
13	No	Show	13	H	-3.5020900	1.0898820	2.2466220
14	No	Show	14	C	-0.8777320	3.7602270	1.2483040

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15	No	Show	15	H	0.1013820	2.1867870	0.1550130
16	No	Show	16	C	-1.9538270	4.1097720	2.0633930
17	No	Show	17	H	-3.7408050	3.4073790	3.0519330
18	No	Show	18	H	-0.1435240	4.5091780	0.9620930
19	No	Show	19	H	-2.0615810	5.1322700	2.4162210
20	No	Show	20	C	-1.7257020	-1.2124700	2.1364620
21	No	Show	21	C	-1.0290060	-0.7688630	3.2722450
22	No	Show	22	C	-2.5012610	-2.3736920	2.2143180
23	No	Show	23	C	-1.1039730	-1.4839320	4.4646410
24	No	Show	24	H	-0.4369580	0.1402920	3.2297570
25	No	Show	25	C	-2.5731390	-3.0862530	3.4129070
26	No	Show	26	H	-3.0306100	-2.7328810	1.3359080
27	No	Show	27	C	-1.8777390	-2.6450010	4.5373200
28	No	Show	28	H	-0.5622880	-1.1310520	5.3386720
29	No	Show	29	H	-3.1772530	-3.9882520	3.4612330
30	No	Show	30	H	-1.9395320	-3.1998990	5.4701110
31	No	Show	31	O	-1.8319230	1.8718300	-2.1466670
32	No	Show	32	H	-6.6841080	2.8086030	-0.9376480
33	No	Show	33	H	2.4504890	-0.6384460	-2.4268640
34	No	Show	34	C	1.7491460	-0.8657250	-1.6342880
35	No	Show	35	C	1.7768800	-2.0084140	-0.7795830
36	No	Show	36	C	0.6775870	-0.0258710	-1.2318250
37	No	Show	37	C	0.7216170	-1.8797210	0.1628340
38	No	Show	38	H	2.5039240	-2.8100770	-0.8112210
39	No	Show	39	C	0.0326020	-0.6461630	-0.1072810
40	No	Show	40	Fe	2.0054250	-0.3010360	0.3229140
41	No	Show	41	C	2.7100120	-0.2969220	2.2440450
42	No	Show	42	C	2.2164810	0.9983960	1.9013070
43	No	Show	43	C	3.7505100	-0.6267840	1.3258900
44	No	Show	44	H	2.3345910	-0.9358350	3.0340810
45	No	Show	45	C	2.9371040	1.4599860	0.7606950
46	No	Show	46	C	3.9069110	0.4604720	0.4020720
47	No	Show	47	H	4.3011800	-1.5584770	1.2968770
48	No	Show	48	H	2.7849660	2.3985830	0.2410100
49	No	Show	49	H	0.3650810	0.8938290	-1.7081650
50	No	Show	50	H	0.4774100	-2.5788870	0.9517310
51	No	Show	51	P	5.0517360	0.6460840	-1.0114580
52	No	Show	52	C	5.8173120	-1.0349370	-1.0977490
53	No	Show	53	C	6.7845460	-1.4988300	-0.1935840
54	No	Show	54	C	5.4198870	-1.8785530	-2.1447620
55	No	Show	55	C	7.3198250	-2.7807750	-0.3211220
56	No	Show	56	H	7.1302310	-0.8520060	0.6090240
57	No	Show	57	C	5.9491000	-3.1643690	-2.2703930
58	No	Show	58	H	4.6997240	-1.5230510	-2.8782280
59	No	Show	59	C	6.8992120	-3.6194590	-1.3558830



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60	No	Show	60	H	8.0700300	-3.1241490	0.3872760
61	No	Show	61	H	5.6264200	-3.8042330	-3.0880050
62	No	Show	62	H	7.3187550	-4.6174750	-1.4548210
63	No	Show	63	C	6.4201480	1.6253360	-0.2522600
64	No	Show	64	C	7.4333840	2.0735720	-1.1145850
65	No	Show	65	C	6.4831730	1.9851680	1.1004600
66	No	Show	66	C	8.4943930	2.8386750	-0.6335440
67	No	Show	67	H	7.3929100	1.8193480	-2.1722140
68	No	Show	68	C	7.5386070	2.7640920	1.5803560
69	No	Show	69	H	5.7064200	1.6561970	1.7853140
70	No	Show	70	C	8.5488510	3.1893370	0.7176420
71	No	Show	71	H	9.2736930	3.1701070	-1.3154750
72	No	Show	72	H	7.5714050	3.0355430	2.6329710
73	No	Show	73	H	9.3704920	3.7942660	1.0928180
74	No	Show	74	H	1.4071010	1.5254550	2.3902690
75	No	Show	75	Br	-6.2400590	0.0541260	0.0823360
76	No	Show	76	C	-2.9541160	4.2190120	-2.8098930
77	No	Show	77	H	-2.0995610	4.5367360	-2.2085710
78	No	Show	78	H	-2.5795010	3.8335830	-3.7605240
79	No	Show	79	H	-3.6374730	5.0499220	-2.9742360
80	No	Show	80	Br	-2.6038300	-3.3253570	-1.2895170

#### 14a\*\*

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	-3.1730250	-1.8393870	0.4625630
2	No	Show	2	C	-4.4344920	-2.2781070	-0.0341580
3	No	Show	3	C	-2.2196470	-1.3495220	-0.3694730
4	No	Show	4	N	-4.7383670	-2.2313350	-1.3017350
5	No	Show	5	C	-2.5605920	-1.2468690	-1.7814720
6	No	Show	6	N	-3.8187290	-1.7316040	-2.1381920
7	No	Show	7	Pd	-0.2778320	-0.8343190	-0.0110090
8	No	Show	8	P	-0.9836040	1.4122300	0.1106230
9	No	Show	9	C	-2.7509170	1.8062200	-0.1969550
10	No	Show	10	C	-3.6966640	1.5811230	0.8140720
11	No	Show	11	C	-3.1793140	2.2848790	-1.4404630
12	No	Show	12	C	-5.0450350	1.8474370	0.5877190
13	No	Show	13	H	-3.3837920	1.1978300	1.7817880
14	No	Show	14	C	-4.5315710	2.5497100	-1.6632230
15	No	Show	15	H	-2.4628100	2.4476360	-2.2395010
16	No	Show	16	C	-5.4665230	2.3348970	-0.6512080
17	No	Show	17	H	-5.7675000	1.6685760	1.3799400
18	No	Show	18	H	-4.8515270	2.9251240	-2.6320920
19	No	Show	19	H	-6.5192590	2.5413790	-0.8268750
20	No	Show	20	C	-0.7083420	2.1654270	1.7618720

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21	No	Show	21	C	-1.1748790	3.4550010	2.0621900
22	No	Show	22	C	-0.0529270	1.4300180	2.7564450
23	No	Show	23	C	-0.9550200	4.0080020	3.3217180
24	No	Show	24	H	-1.7370490	4.0178980	1.3216050
25	No	Show	25	C	0.1624280	1.9837420	4.0200400
26	No	Show	26	H	0.2784860	0.4153750	2.5487000
27	No	Show	27	C	-0.2807290	3.2752680	4.3020670
28	No	Show	28	H	-1.3208240	5.0077170	3.5425110
29	No	Show	29	H	0.6706580	1.3990770	4.7822330
30	No	Show	30	H	-0.1152730	3.7061200	5.2863020
31	No	Show	31	O	-1.8237770	-0.7627900	-2.6563310
32	No	Show	32	H	-5.1977170	-2.6831070	0.6233540
33	No	Show	33	H	1.3787690	5.1228820	-2.4832180
34	No	Show	34	C	0.9313150	4.1644310	-2.2481170
35	No	Show	35	C	0.9790070	2.9924510	-3.0619550
36	No	Show	36	C	0.2524580	3.8400910	-1.0365730
37	No	Show	37	C	0.3318210	1.9371720	-2.3606240
38	No	Show	38	H	1.4651140	2.9065760	-4.0261440
39	No	Show	39	C	-0.1201850	2.4523020	-1.0955540
40	No	Show	40	Fe	1.8835410	2.6534570	-1.2459170
41	No	Show	41	C	3.5847040	1.5412860	-1.4653430
42	No	Show	42	C	2.8583160	1.1403420	-0.2938160
43	No	Show	43	C	3.9132880	2.9228990	-1.3372620
44	No	Show	44	H	3.8070910	0.9085070	-2.3149900
45	No	Show	45	C	2.7456740	2.2966700	0.5541990
46	No	Show	46	C	3.4022700	3.3865280	-0.0879020
47	No	Show	47	H	4.4276020	3.5225410	-2.0786530
48	No	Show	48	H	2.2314540	2.3402270	1.5055930
49	No	Show	49	H	3.4558620	4.4016440	0.2869450
50	No	Show	50	H	0.1065820	4.5075080	-0.1975160
51	No	Show	51	H	0.1884220	0.9179130	-2.6983880
52	No	Show	52	P	2.1512120	-0.5116150	0.0397960
53	No	Show	53	C	2.9355550	-1.4957720	-1.2980300
54	No	Show	54	C	4.2495460	-1.9670990	-1.1941510
55	No	Show	55	C	2.2098500	-1.7341160	-2.4722600
56	No	Show	56	C	4.8359030	-2.6537700	-2.2573090
57	No	Show	57	H	4.8162340	-1.8124310	-0.2800870
58	No	Show	58	C	2.8031430	-2.4110120	-3.5374140
59	No	Show	59	H	1.1710840	-1.4231250	-2.5471830
60	No	Show	60	C	4.1165610	-2.8707870	-3.4334800
61	No	Show	61	H	5.8537850	-3.0240000	-2.1627200
62	No	Show	62	H	2.2277630	-2.5963750	-4.4407340
63	No	Show	63	H	4.5735580	-3.4088420	-4.2603500
64	No	Show	64	C	3.0248070	-0.9921710	1.5862360
65	No	Show	65	C	4.2159320	-0.3700250	1.9904690

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66	No	Show	66	C	2.4824390	-2.0102030	2.3838480
67	No	Show	67	C	4.8531980	-0.7609970	3.1681330
68	No	Show	68	H	4.6505590	0.4240780	1.3901450
69	No	Show	69	C	3.1248050	-2.3988720	3.5596460
70	No	Show	70	H	1.5690280	-2.5111180	2.0712330
71	No	Show	71	C	4.3089520	-1.7759960	3.9564190
72	No	Show	72	H	5.7759050	-0.2700720	3.4680310
73	No	Show	73	H	2.6953490	-3.1934290	4.1646130
74	No	Show	74	H	4.8057860	-2.0799140	4.8745180
75	No	Show	75	Br	-2.8928260	-1.9920800	2.3466460
76	No	Show	76	C	-4.1914990	-1.6848230	-3.5458470
77	No	Show	77	H	-3.4467130	-2.2141180	-4.1438620
78	No	Show	78	H	-5.1675560	-2.1572530	-3.6405650
79	No	Show	79	H	-4.2327290	-0.6482250	-3.8893170
80	No	Show	80	Br	0.0972250	-3.3214160	-0.0821170

### 15a

Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	H	-	3.0348480	-0.2492140	1.7930850
2	No	Show	2	C	-	2.5032870	-0.6786710	0.9512510
3	No	Show	3	C	-	2.8107860	-0.4707150	-0.4321790
4	No	Show	4	C	-	1.3299600	-1.4964890	1.0237800
5	No	Show	5	C	-	1.8266140	-1.1629860	-1.2090150
6	No	Show	6	H	-	3.6204340	0.1373630	-0.8204720
7	No	Show	7	C	-	0.9109960	-1.7957320	-0.3102040
8	No	Show	8	Fe	-	0.9344590	0.2132730	-0.0031690
9	No	Show	9	C	0	3.863140	1.2616090	-1.1512770
10	No	Show	10	C	1	0.818920	0.7224250	-0.0205840
11	No	Show	11	C	-	0.6905710	2.1007110	-0.7126760
12	No	Show	12	H	0	6.064330	1.0090840	-2.1829510
13	No	Show	13	C	0	4.076930	1.2512700	1.1283280
14	No	Show	14	C	-	0.6763930	2.0944120	0.7192830
15	No	Show	15	H	-	1.4145030	2.6088950	-1.3422050
16	No	Show	16	H	0	6.520480	0.9833000	2.1504080
17	No	Show	17	H	-	1.3882570	2.5968460	1.3669480
18	No	Show	18	H	-	0.7905660	-1.7623090	1.9246290
19	No	Show	19	H	-	1.7484120	-1.1575750	-2.2900250
20	No	Show	20	H	0	0.093260	-2.2904410	-0.5963420
21	No	Show	21	O	3	6.246170	0.4954620	-0.2250630
22	No	Show	22	H	4	1.106470	0.3652550	0.5998930
23	No	Show	23	O	2	4.623330	-0.9646100	1.3209180
24	No	Show	24	H	2	4.301430	-1.9035270	1.0975150
25	No	Show	25	O	2	2.547560	-1.2981340	-1.0940310
26	No	Show	26	H	3	1.268660	-1.2693030	-1.5109080
27	No	Show	27	B	2	3.720200	-0.2860470	-0.0084030

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**15b**

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	O	2.0558620	0.0684320	1.4042690
2	No	Show	2	H	2.5942000	-0.7303630	1.4827260
3	No	Show	3	O	2.0996590	-1.2461440	-0.6042380
4	No	Show	4	H	2.3732920	-0.9763290	-1.4900460
5	No	Show	5	O	2.0432520	1.2018730	-0.7479710
6	No	Show	6	H	2.7923630	1.5046670	-0.2171070
7	No	Show	7	B	1.5578320	0.0129100	0.0020590
8	No	Show	8	C	-0.0894850	0.0081790	-0.0221540
9	No	Show	9	C	-0.8406990	1.1966740	-0.0085370
10	No	Show	10	C	-0.8261170	-1.1896630	-0.0250780
11	No	Show	11	C	-2.2395870	1.1982790	0.0130320
12	No	Show	12	H	-0.3011850	2.1424930	-0.0296200
13	No	Show	13	C	-2.2245150	-1.2093790	-0.0027650
14	No	Show	14	H	-0.2744540	-2.1283530	-0.0601400
15	No	Show	15	C	-2.9436970	-0.0099500	0.0190040
16	No	Show	16	H	-2.7862170	2.1424980	0.0207780
17	No	Show	17	H	-2.7592190	-2.1604400	-0.0074820
18	No	Show	18	H	-4.0335170	-0.0168510	0.0331010

**20**

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	14	H	3.9358130	1.0862420	-2.0953260
2	No	Show	10	C	4.0337290	0.0868870	-1.6892490
3	No	Show	13	C	3.0007570	-0.8989940	-1.6298350
4	No	Show	9	C	5.2043940	-0.4714000	-1.0957430
5	No	Show	15	C	3.5278910	-2.0578180	-0.9749040
6	No	Show	12	H	6.1517610	0.0364160	-0.9597410
7	No	Show	11	C	4.8902860	-1.7951990	-0.6554080
8	No	Show	8	Fe	3.6906240	-0.4151990	0.2652590
9	No	Show	7	C	2.6287160	1.0385490	1.2297990
10	No	Show	5	C	4.0353100	1.2044890	1.4544650
11	No	Show	4	C	2.2686920	-0.2569200	1.7444640
12	No	Show	3	C	4.5343460	0.0216990	2.0757220
13	No	Show	2	C	3.4422130	-0.8785970	2.2540850
14	No	Show	6	H	5.5695250	-0.1731060	2.3283750
15	No	Show	1	H	3.4959750	-1.8736380	2.6780150
16	No	Show	16	H	5.5581700	-2.4630350	-0.1249440
17	No	Show	17	H	2.0263500	-0.8314370	-2.1136260
18	No	Show	18	H	2.9634400	-2.9543760	-0.7532790
19	No	Show	19	H	1.2734490	-0.6844760	1.7665540
20	No	Show	20	H	4.6352050	2.0477440	1.1338190
21	No	Show	21	C	1.7663460	1.9592070	0.4706950
22	No	Show	22	C	2.0542080	3.3620950	0.4840540

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23	No	Show	23	C	0.7218160	1.5175330	-0.3069880
24	No	Show	24	N	1.4130260	4.2474970	-0.2290760
25	No	Show	25	C	0.0339530	2.4648360	-1.1615780
26	No	Show	26	N	0.4391970	3.7978870	-1.0273460
27	No	Show	27	Pd	0.3466260	-0.4580090	-0.5574340
28	No	Show	28	P	-1.8245260	-0.1798460	0.1968070
29	No	Show	29	C	-3.0235900	-0.7703790	-1.0474270
30	No	Show	30	C	-4.0592280	-1.6499000	-0.7112650
31	No	Show	31	C	-2.8811380	-0.3307230	-2.3713670
32	No	Show	32	C	-4.9565560	-2.0749000	-1.6913690
33	No	Show	33	H	-4.1639360	-2.0160450	0.3057900
34	No	Show	34	C	-3.7868420	-0.7543270	-3.3414390
35	No	Show	35	H	-2.0716100	0.3475910	-2.6286270
36	No	Show	36	C	-4.8242350	-1.6266410	-3.0054790
37	No	Show	37	H	-5.7544470	-2.7636680	-1.4256810
38	No	Show	38	H	-3.6731120	-0.4096140	-4.3660120
39	No	Show	39	H	-5.5222420	-1.9634160	-3.7679360
40	No	Show	40	C	-2.3851480	1.4978600	0.6768160
41	No	Show	41	C	-3.4729150	2.1239970	0.0600400
42	No	Show	42	C	-1.7149340	2.1557460	1.7193120
43	No	Show	43	C	-3.8898500	3.3864080	0.4858020
44	No	Show	44	H	-3.9968740	1.6318360	-0.7533130
45	No	Show	45	C	-2.1337200	3.4150410	2.1421530
46	No	Show	46	H	-0.8694200	1.6811110	2.2107460
47	No	Show	47	C	-3.2234760	4.0344050	1.5253610
48	No	Show	48	H	-4.7383300	3.8617030	0.0000220
49	No	Show	49	H	-1.6061270	3.9131860	2.9513890
50	No	Show	50	H	-3.5494570	5.0180080	1.8541690
51	No	Show	51	C	-2.1594390	-1.1299730	1.7378420
52	No	Show	52	C	-3.1716970	-0.7047730	2.6147860
53	No	Show	53	C	-1.4394810	-2.2924250	2.0426360
54	No	Show	54	C	-3.4543100	-1.4295970	3.7711670
55	No	Show	55	H	-3.7430410	0.1931370	2.3990680
56	No	Show	56	C	-1.7258120	-3.0131090	3.2027090
57	No	Show	57	H	-0.6764830	-2.6507520	1.3559870
58	No	Show	58	C	-2.7295160	-2.5843320	4.0706110
59	No	Show	59	H	-4.2412570	-1.0878310	4.4387560
60	No	Show	60	H	-1.1601950	-3.9148470	3.4227660
61	No	Show	61	H	-2.9474980	-3.1459840	4.9755920
62	No	Show	62	Br	-0.0148510	-2.8895230	-1.1623800
63	No	Show	63	H	2.8371640	3.7676730	1.1196620
64	No	Show	64	O	-0.8483670	2.1905990	-1.9900640
65	No	Show	65	C	-0.2327140	4.7971950	-1.8486700
66	No	Show	66	H	0.1577970	5.7713080	-1.5597530
67	No	Show	67	H	-0.0403450	4.6063550	-2.9074300

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68	No	Show	68	H	-1.3105520	4.7463960	-1.6839310
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**21a**

Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	H	3.2598920		-0.0198710	-2.5181720
2	No	Show	2	C	2.4732740		-0.5056240	-1.9540090
3	No	Show	3	C	2.5738170		-1.7583620	-1.2780880
4	No	Show	4	C	1.1776840		0.0318310	-1.7126940
5	No	Show	5	C	1.3342620		-2.0036490	-0.6237250
6	No	Show	6	H	3.4510740		-2.3915630	-1.2310380
7	No	Show	7	C	0.4464200		-0.8979180	-0.8897250
8	No	Show	8	Fe	2.1502050		-0.2702630	0.0546390
9	No	Show	9	C	3.6883920		-0.3014750	1.3948520
10	No	Show	10	C	2.4412960		-0.4989310	2.0638500
11	No	Show	11	C	3.6350780		0.9594900	0.7248500
12	No	Show	12	H	4.5144290		-1.0017210	1.3680470
13	No	Show	13	C	1.6193460		0.6400720	1.8067370
14	No	Show	14	H	2.1555090		-1.3745890	2.6338380
15	No	Show	15	C	2.3557810		1.5410930	0.9794930
16	No	Show	16	H	4.4125160		1.3798560	0.0987090
17	No	Show	17	H	0.5973970		0.7767420	2.1377220
18	No	Show	18	H	1.9901400		2.4787070	0.5814030
19	No	Show	19	H	0.8102520		0.9775870	-2.0831380
20	No	Show	20	H	1.1228630		-2.8556330	0.0104150
21	No	Show	21	C	-0.9533940		-0.8422250	-0.4405550
22	No	Show	22	C	-1.6029540		-2.1056060	-0.2051160
23	No	Show	23	C	-1.7466650		0.2637170	-0.2405820
24	No	Show	24	N	-2.8334940		-2.2630090	0.1910640
25	No	Show	25	C	-3.1315410		0.1523630	0.2111170
26	No	Show	26	N	-3.5615050		-1.1646400	0.3991230
27	No	Show	27	H	-1.0664440		-3.0305910	-0.3858670
28	No	Show	28	O	-3.8976440		1.0869540	0.4305060
29	No	Show	29	C	-4.9348820		-1.3640990	0.8471990
30	No	Show	30	H	-5.0976640		-2.4374890	0.9218650
31	No	Show	31	H	-5.0854280		-0.8824400	1.8158210
32	No	Show	32	H	-5.6287570		-0.9163390	0.1325520
33	No	Show	33	Br	-1.1900130		2.0502300	-0.4737080

**21b**

Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	-0.0752350		-0.7498680	0.0706170
2	No	Show	2	C	0.4983460		-2.0610600	0.1613050
3	No	Show	3	C	0.8080930		0.2950810	-0.0063400
4	No	Show	4	N	1.7777120		-2.3137390	0.1803430
5	No	Show	5	C	2.2534690		0.0764260	0.0158080

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6	No	Show	6	N	2.6122300	-1.2740050	0.1120770
7	No	Show	7	H	-0.1481330	-2.9305050	0.2367130
8	No	Show	8	O	3.1187760	0.9437540	-0.0473930
9	No	Show	9	C	4.0384480	-1.5818720	0.1331200
10	No	Show	10	H	4.1347960	-2.6625670	0.2152180
11	No	Show	11	H	4.5110030	-1.2194880	-0.7823510
12	No	Show	12	H	4.5135190	-1.0849960	0.9815940
13	No	Show	13	Br	0.2850170	2.0933310	-0.2046600
14	No	Show	14	C	-1.5545700	-0.6380380	0.0609120
15	No	Show	15	C	-2.2313290	0.1213550	1.0247330
16	No	Show	16	C	-2.2972530	-1.3442370	-0.8955510
17	No	Show	17	C	-3.6236880	0.1766860	1.0262570
18	No	Show	18	H	-1.6671290	0.6587080	1.7813430
19	No	Show	19	C	-3.6900790	-1.2775560	-0.8994420
20	No	Show	20	H	-1.7824660	-1.9308500	-1.6527860
21	No	Show	21	C	-4.3568980	-0.5182790	0.0626580
22	No	Show	22	H	-4.1369880	0.7634230	1.7834900
23	No	Show	23	H	-4.2531700	-1.8185020	-1.6553830
24	No	Show	24	H	-5.4426500	-0.4694680	0.0630050

## 22a

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	H	2.9450520	-0.1884990	-2.6204010
2	No	Show	2	C	2.1078200	-0.5629680	-2.0441280
3	No	Show	3	C	1.9917780	-1.8636770	-1.4694660
4	No	Show	4	C	0.9550740	0.1870300	-1.6838380
5	No	Show	5	C	0.7623290	-1.9283230	-0.7612230
6	No	Show	6	H	2.7281830	-2.6557680	-1.5275640
7	No	Show	7	C	0.0905480	-0.6572620	-0.8891980
8	No	Show	8	Fe	1.9324840	-0.4365730	-0.0084310
9	No	Show	9	C	2.2184170	-0.8664840	1.9668630
10	No	Show	10	C	1.6856970	0.4503070	1.8170470
11	No	Show	11	C	3.4569130	-0.9219520	1.2564930
12	No	Show	12	H	1.7464970	-1.6888460	2.4903240
13	No	Show	13	C	2.5909220	1.2080390	1.0136300
14	No	Show	14	H	0.7362280	0.7994020	2.2039130
15	No	Show	15	C	3.6865150	0.3591700	0.6668200
16	No	Show	16	H	4.0897420	-1.7943620	1.1485510
17	No	Show	17	H	2.4505070	2.2315940	0.6902850
18	No	Show	18	H	4.5243750	0.6269920	0.0346430
19	No	Show	19	H	0.7665380	1.2098760	-1.9729060
20	No	Show	20	H	0.3907960	-2.7765570	-0.2085880
21	No	Show	21	C	-1.2358360	-0.3347350	-0.3503110
22	No	Show	22	C	-2.1495160	-1.4703420	-0.0820200
23	No	Show	23	C	-1.7615450	0.9114700	-0.0912340

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24	No	Show	24	N	-3.4331880	-1.1398510	0.3577950
25	No	Show	25	C	-3.0944840	1.0812690	0.3745620
26	No	Show	26	N	-3.9076800	0.0859820	0.5899020
27	No	Show	27	O	-1.8697180	-2.6609620	-0.2219230
28	No	Show	28	H	-3.4921610	2.0710220	0.5727680
29	No	Show	29	C	-4.3566110	-2.2429920	0.6023840
30	No	Show	30	H	-4.4676100	-2.8420050	-0.3036270
31	No	Show	31	H	-3.9689440	-2.8894650	1.3928090
32	No	Show	32	H	-5.3089110	-1.8061460	0.8961650
33	No	Show	33	Br	-0.8208340	2.5607750	-0.2683990

## 22b

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	0.3270580	-0.3433880	0.0273540
2	No	Show	2	C	1.3062140	-1.4411560	0.0597540
3	No	Show	3	C	0.8260070	0.9307890	-0.0193650
4	No	Show	4	N	2.6485610	-1.0450760	0.1151370
5	No	Show	5	C	2.2301620	1.1709690	0.0153010
6	No	Show	6	N	3.1061390	0.2076880	0.0866060
7	No	Show	7	O	1.0272550	-2.6379520	0.0464710
8	No	Show	8	H	2.6302430	2.1789420	-0.0175290
9	No	Show	9	C	3.6542330	-2.1002300	0.1823580
10	No	Show	10	H	3.4558450	-2.7446490	1.0409570
11	No	Show	11	H	3.6152900	-2.7135990	-0.7207310
12	No	Show	12	H	4.6249650	-1.6177450	0.2764660
13	No	Show	13	Br	-0.2672690	2.4787450	-0.1862680
14	No	Show	14	C	-1.1065050	-0.7071200	0.0413370
15	No	Show	15	C	-1.6202100	-1.6040790	-0.9059510
16	No	Show	16	C	-1.9647110	-0.1820380	1.0174040
17	No	Show	17	C	-2.9723740	-1.9386090	-0.8964980
18	No	Show	18	H	-0.9596760	-2.0403390	-1.6482740
19	No	Show	19	C	-3.3133350	-0.5325500	1.0354800
20	No	Show	20	H	-1.5732150	0.4896170	1.7762330
21	No	Show	21	C	-3.8230200	-1.4053550	0.0733820
22	No	Show	22	H	-3.3603260	-2.6263020	-1.6433720
23	No	Show	23	H	-3.9648700	-0.1246310	1.8038570
24	No	Show	24	H	-4.8758980	-1.6754340	0.0844680

## 23a

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	H	-3.0246530	-2.4552380	-2.6414990
2	No	Show	2	C	-3.1993270	-1.4871310	-2.1894760
3	No	Show	3	C	-4.4653460	-0.9086160	-1.8803850
4	No	Show	4	C	-2.1912150	-0.5659620	-1.7895280
5	No	Show	5	C	-4.2454400	0.3653380	-1.2787420



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6	No	Show	6	H	-5.4312360	-1.3722090	-2.0397950
7	No	Show	7	C	-2.8356110	0.5810210	-1.1908050
8	No	Show	8	Fe	-3.3651670	-1.1168550	-0.1722580
9	No	Show	9	C	-4.6896960	-1.3420670	1.3603350
10	No	Show	10	C	-3.5003780	-0.7223130	1.8416030
11	No	Show	11	C	-4.3371950	-2.6188300	0.8209160
12	No	Show	12	H	-5.6790310	-0.9008530	1.3576680
13	No	Show	13	C	-2.4123940	-1.6192960	1.6112950
14	No	Show	14	H	-3.4279590	0.2654400	2.2800810
15	No	Show	15	C	-2.9316100	-2.7857770	0.9574560
16	No	Show	16	H	-5.0134920	-3.3127570	0.3366680
17	No	Show	17	H	-1.3932070	-1.5000100	1.9670540
18	No	Show	18	H	-2.3354340	-3.6202580	0.6127200
19	No	Show	19	H	-1.1335490	-0.6764190	-2.0126090
20	No	Show	20	H	-4.9982700	1.0415130	-0.8990610
21	No	Show	21	C	-2.1419120	1.6266540	-0.4303900
22	No	Show	22	C	-2.7898090	2.9240080	-0.2615120
23	No	Show	23	C	-0.9450640	1.3652270	0.2035250
24	No	Show	24	N	-2.0844850	3.8201900	0.5454160
25	No	Show	25	C	-0.4020000	2.3881270	1.0305700
26	No	Show	26	N	-0.9453930	3.5701790	1.1982490
27	No	Show	27	Pd	-0.2348750	-0.5549600	0.0761230
28	No	Show	28	P	1.9903140	0.1401360	-0.0222140
29	No	Show	29	O	-3.8712330	3.2676790	-0.7523790
30	No	Show	30	H	0.5069540	2.2403760	1.6044310
31	No	Show	31	C	2.5572760	0.4961230	1.6832890
32	No	Show	32	C	2.3753470	-0.5217510	2.6351300
33	No	Show	33	C	3.1001080	1.7228230	2.0849880
34	No	Show	34	C	2.7584900	-0.3189660	3.9584850
35	No	Show	35	H	1.9346580	-1.4710330	2.3344420
36	No	Show	36	C	3.4699200	1.9238980	3.4168270
37	No	Show	37	H	3.2243010	2.5310820	1.3701900
38	No	Show	38	C	3.3060330	0.9045020	4.3533480
39	No	Show	39	H	2.6193010	-1.1158580	4.6843970
40	No	Show	40	H	3.8825350	2.8830830	3.7186530
41	No	Show	41	H	3.5954050	1.0638570	5.3888620
42	No	Show	42	C	2.4041630	1.5952180	-1.0665050
43	No	Show	43	C	3.7367550	2.0325580	-1.1535320
44	No	Show	44	C	1.4355420	2.2068390	-1.8679970
45	No	Show	45	C	4.0786050	3.0878600	-1.9945760
46	No	Show	46	H	4.5145660	1.5362490	-0.5789310
47	No	Show	47	C	1.7824230	3.2579010	-2.7191440
48	No	Show	48	H	0.4080000	1.8589500	-1.8326150
49	No	Show	49	C	3.1004230	3.7058360	-2.7780430
50	No	Show	50	H	5.1125790	3.4188950	-2.0487410

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51	No	Show	51	H	1.0176120	3.7220750	-3.3362030
52	No	Show	52	H	3.3697490	4.5253160	-3.4394710
53	No	Show	53	C	3.2072360	-1.0659930	-0.6795090
54	No	Show	54	C	4.3533800	-1.4372710	0.0290700
55	No	Show	55	C	3.0072360	-1.5598350	-1.9757980
56	No	Show	56	C	5.2890530	-2.2953880	-0.5534690
57	No	Show	57	H	4.5241020	-1.0661180	1.0353140
58	No	Show	58	C	3.9445960	-2.4085310	-2.5547480
59	No	Show	59	H	2.1103210	-1.2934570	-2.5289550
60	No	Show	60	C	5.0888220	-2.7805490	-1.8439080
61	No	Show	61	H	6.1742820	-2.5831080	0.0081320
62	No	Show	62	H	3.7762790	-2.7909210	-3.5580330
63	No	Show	63	H	5.8168340	-3.4503670	-2.2943450
64	No	Show	64	Br	0.4989360	-2.9885300	0.0588970
65	No	Show	65	C	-2.6676670	5.1405970	0.7502560
66	No	Show	66	H	-2.8258420	5.6307790	-0.2125810
67	No	Show	67	H	-3.6363540	5.0519900	1.2481610
68	No	Show	68	H	-1.9727650	5.7103460	1.3641640

### 23b

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	-3.0287820	0.2211460	-0.2369800
2	No	Show	2	C	-4.1146760	1.1916830	-0.1970980
3	No	Show	3	C	-1.7514710	0.6089970	-0.5764470
4	No	Show	4	N	-3.7501220	2.4645980	-0.6473140
5	No	Show	5	C	-1.5643620	1.9633110	-0.9820460
6	No	Show	6	N	-2.5300670	2.8464220	-1.0389240
7	No	Show	7	Pd	-0.4008720	-0.9271760	-0.5102620
8	No	Show	8	P	1.3754200	0.4139620	0.1447970
9	No	Show	9	O	-5.2712590	0.9814050	0.1811380
10	No	Show	10	H	-0.5996900	2.3471580	-1.2989950
11	No	Show	11	C	0.8453340	1.8630470	1.1407310
12	No	Show	12	C	-0.1452990	1.6617510	2.1140060
13	No	Show	13	C	1.4011190	3.1383120	0.9867480
14	No	Show	14	C	-0.5548370	2.7124980	2.9320970
15	No	Show	15	H	-0.6063600	0.6827440	2.2251080
16	No	Show	16	C	0.9779730	4.1923390	1.7980280
17	No	Show	17	H	2.1524090	3.3232830	0.2249500
18	No	Show	18	C	0.0054550	3.9816430	2.7748150
19	No	Show	19	H	-1.3221730	2.5412750	3.6825080
20	No	Show	20	H	1.4081300	5.1808980	1.6598200
21	No	Show	21	H	-0.3231360	4.8048560	3.4038400
22	No	Show	22	C	2.3043150	1.0623170	-1.2912370
23	No	Show	23	C	3.5793660	1.6293220	-1.1362200
24	No	Show	24	C	1.7369050	0.9914160	-2.5691040

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25	No	Show	25	C	4.2592750	2.1381940	-2.2407720
26	No	Show	26	H	4.0501740	1.6568960	-0.1568960
27	No	Show	27	C	2.4192710	1.5042460	-3.6724450
28	No	Show	28	H	0.7699010	0.5127650	-2.7029370
29	No	Show	29	C	3.6782220	2.0814920	-3.5095740
30	No	Show	30	H	5.2474830	2.5718140	-2.1107900
31	No	Show	31	H	1.9710130	1.4382890	-4.6601690
32	No	Show	32	H	4.2127420	2.4742710	-4.3706480
33	No	Show	33	C	2.6653530	-0.3667210	1.1881700
34	No	Show	34	C	2.7501520	-0.1130530	2.5630600
35	No	Show	35	C	3.5822210	-1.2477880	0.5935380
36	No	Show	36	C	3.7386290	-0.7290090	3.3316800
37	No	Show	37	H	2.0587450	0.5725610	3.0427310
38	No	Show	38	C	4.5715380	-1.8515300	1.3647270
39	No	Show	39	H	3.5190460	-1.4713970	-0.4660990
40	No	Show	40	C	4.6515050	-1.5975360	2.7352890
41	No	Show	41	H	3.7944100	-0.5223140	4.3973520
42	No	Show	42	H	5.2739470	-2.5328510	0.8921160
43	No	Show	43	H	5.4216120	-2.0759580	3.3350990
44	No	Show	44	Br	1.0145940	-2.9882530	-0.8309030
45	No	Show	45	C	-4.7903450	3.4850380	-0.6919860
46	No	Show	46	H	-5.6346760	3.1285400	-1.2855700
47	No	Show	47	H	-5.1515110	3.6998630	0.3167930
48	No	Show	48	H	-4.3525990	4.3759270	-1.1381600
49	No	Show	49	C	-3.2581140	-1.1954930	0.0886300
50	No	Show	50	C	-4.0882180	-1.6352160	1.1295090
51	No	Show	51	C	-2.5249580	-2.1565730	-0.6452660
52	No	Show	52	C	-4.1449590	-2.9901270	1.4474620
53	No	Show	53	H	-4.6800900	-0.9122870	1.6798920
54	No	Show	54	C	-2.5714570	-3.5135890	-0.3062730
55	No	Show	55	H	-2.0760310	-1.8691810	-1.6086080
56	No	Show	56	C	-3.3810270	-3.9301010	0.7454230
57	No	Show	57	H	-4.7881300	-3.3194220	2.2600540
58	No	Show	58	H	-1.9760850	-4.2247750	-0.8699210
59	No	Show	59	H	-3.4284540	-4.9819170	1.0140340

#### 24a

Row	Highlight		Display Tag	Symbol	X	Y	Z
1	No	Show	1	H	-3.8680350	-1.9758070	-2.6118940
2	No	Show	2	C	-3.8566370	-1.0533000	-2.0448820
3	No	Show	3	C	-4.9816730	-0.4235920	-1.4368880
4	No	Show	4	C	-2.7124260	-0.2318600	-1.7981920
5	No	Show	5	C	-4.5336680	0.7672610	-0.7859640
6	No	Show	6	H	-5.9947160	-0.8065840	-1.4300760
7	No	Show	7	C	-3.1264680	0.8947860	-0.9997230

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8	No	Show	8	Fe	-3.5876070	-0.8729180	-0.0248000
9	No	Show	9	C	-4.1527890	-0.8220700	1.9344670
10	No	Show	10	C	-2.7324650	-0.9140710	1.8460640
11	No	Show	11	C	-4.7093750	-1.9620920	1.2773300
12	No	Show	12	H	-4.7114550	-0.0079620	2.3798930
13	No	Show	13	C	-2.4067680	-2.1171390	1.1448720
14	No	Show	14	H	-2.0293170	-0.1731570	2.2062350
15	No	Show	15	C	-3.6291190	-2.7571670	0.7851610
16	No	Show	16	H	-5.7646800	-2.1661000	1.1426610
17	No	Show	17	H	-1.4148790	-2.4619640	0.8695560
18	No	Show	18	H	-3.7213190	-3.6739420	0.2158780
19	No	Show	19	H	-1.7554330	-0.3287440	-2.3203340
20	No	Show	20	H	-5.1488130	1.4236820	-0.1827880
21	No	Show	21	C	-2.1951660	1.9223070	-0.5131720
22	No	Show	22	C	-2.6648820	3.2472280	-0.2605040
23	No	Show	23	C	-0.8619050	1.6090930	-0.3264810
24	No	Show	24	N	-1.8968150	4.2200230	0.1477090
25	No	Show	25	C	0.0185610	2.7007530	0.0464270
26	No	Show	26	N	-0.5980680	3.9338290	0.3023410
27	No	Show	27	Pd	-0.4144910	-0.3685090	-0.6245140
28	No	Show	28	P	1.8297390	-0.2967530	-0.0193000
29	No	Show	29	C	2.1726990	0.4061160	1.6352940
30	No	Show	30	C	1.3168640	0.0468980	2.6838110
31	No	Show	31	C	3.2630910	1.2414210	1.8984210
32	No	Show	32	C	1.5551990	0.5033480	3.9802660
33	No	Show	33	H	0.4638020	-0.5992170	2.4890410
34	No	Show	34	C	3.4993520	1.6972590	3.1944480
35	No	Show	35	H	3.9126800	1.5621790	1.0900850
36	No	Show	36	C	2.6498180	1.3291420	4.2392860
37	No	Show	37	H	0.8842550	0.2135980	4.7852010
38	No	Show	38	H	4.3461770	2.3518390	3.3856110
39	No	Show	39	H	2.8359900	1.6893300	5.2479650
40	No	Show	40	C	2.9435630	0.4702010	-1.2555300
41	No	Show	41	C	4.3213870	0.2095710	-1.2248210
42	No	Show	42	C	2.4218090	1.2727910	-2.2750320
43	No	Show	43	C	5.1647320	0.7678540	-2.1846950
44	No	Show	44	H	4.7376010	-0.4426980	-0.4614360
45	No	Show	45	C	3.2647790	1.8183570	-3.2418950
46	No	Show	46	H	1.3542490	1.4678970	-2.3085430
47	No	Show	47	C	4.6377100	1.5728190	-3.1957610
48	No	Show	48	H	6.2315980	0.5619750	-2.1483540
49	No	Show	49	H	2.8472300	2.4370180	-4.0322940
50	No	Show	50	H	5.2941510	1.9999790	-3.9499160
51	No	Show	51	C	2.5440190	-1.9850930	0.0986990
52	No	Show	52	C	3.0436370	-2.5131200	1.2952990

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53	No	Show	53	C	2.6053520	-2.7623350	-1.0689020
54	No	Show	54	C	3.6100230	-3.7890740	1.3230090
55	No	Show	55	H	3.0107890	-1.9307780	2.2107750
56	No	Show	56	C	3.1795600	-4.0298520	-1.0386970
57	No	Show	57	H	2.1972050	-2.3773610	-1.9967520

## 24b

Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	C	-3.1128140	0.5653830	-0.1137410	
2	No	Show	2	C	-3.9893230	1.6467460	0.2032210	
3	No	Show	3	C	-1.8077450	0.8179700	-0.4747160	
4	No	Show	4	N	-3.6264160	2.9000750	0.1496900	
5	No	Show	5	C	-1.4025250	2.2067370	-0.6072480	
6	No	Show	6	N	-2.3687940	3.1531250	-0.2395760	
7	No	Show	7	Pd	-0.7046190	-0.8410330	-0.8940980	
8	No	Show	8	P	1.2728370	-0.1415910	0.0532060	
9	No	Show	9	C	1.1418690	1.1938670	1.2956400	
10	No	Show	10	C	0.1143870	1.1194080	2.2457430	
11	No	Show	11	C	2.0481790	2.2581450	1.3447530	
12	No	Show	12	C	0.0056430	2.0879550	3.2422920	
13	No	Show	13	H	-0.6050200	0.3048230	2.2032380	
14	No	Show	14	C	1.9333000	3.2291480	2.3400330	
15	No	Show	15	H	2.8327950	2.3414590	0.5984760	
16	No	Show	16	C	0.9160550	3.1456240	3.2914790	
17	No	Show	17	H	-0.7951260	2.0204120	3.9743790	
18	No	Show	18	H	2.6379940	4.0565350	2.3658430	
19	No	Show	19	H	0.8281620	3.9053150	4.0642050	
20	No	Show	20	C	2.5040270	0.3939770	-1.1879450	
21	No	Show	21	C	3.8744830	0.1687840	-0.9925820	
22	No	Show	22	C	2.0697510	1.0459450	-2.3488280	
23	No	Show	23	C	4.7973190	0.5955940	-1.9469740	
24	No	Show	24	H	4.2256130	-0.3444280	-0.1017540	
25	No	Show	25	C	2.9971480	1.4699290	-3.2989740	
26	No	Show	26	H	1.0117250	1.2431740	-2.4876400	
27	No	Show	27	C	4.3603480	1.2448030	-3.1024930	
28	No	Show	28	H	5.8573560	0.4144130	-1.7878640	
29	No	Show	29	H	2.6508220	1.9759080	-4.1964300	
30	No	Show	30	H	5.0805570	1.5714090	-3.8486490	
31	No	Show	31	C	2.1301700	-1.4884080	0.9662800	
32	No	Show	32	C	2.4700300	-1.3692970	2.3203880	
33	No	Show	33	C	2.4826690	-2.6557870	0.2675040	
34	No	Show	34	C	3.1499590	-2.4023420	2.9692870	
35	No	Show	35	H	2.2176420	-0.4708750	2.8750640	
36	No	Show	36	C	3.1678600	-3.6778090	0.9209830	
37	No	Show	37	H	2.1896600	-2.7567700	-0.7751520	

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38	No	Show	38	C	3.5013130	-3.5573420	2.2724640
39	No	Show	39	H	3.4080360	-2.2963990	4.0200780
40	No	Show	40	H	3.4379140	-4.5760280	0.3708560
41	No	Show	41	H	4.0332970	-4.3593660	2.7784360
42	No	Show	42	O	0.1537270	-2.5597220	-1.5787180
43	No	Show	43	H	-0.0748230	-3.2658510	-0.9531040
44	No	Show	44	C	-3.5616020	-0.8446220	-0.0816420
45	No	Show	45	C	-4.3308250	-1.3804050	0.9602150
46	No	Show	46	C	-3.1356850	-1.7051330	-1.1138330
47	No	Show	47	C	-4.6432670	-2.7389050	0.9802780
48	No	Show	48	H	-4.6582800	-0.7386390	1.7745880
49	No	Show	49	C	-3.4309650	-3.0701620	-1.0807390
50	No	Show	50	H	-2.6798820	-1.2819750	-2.0166190
51	No	Show	51	C	-4.1872970	-3.5894070	-0.0318480
52	No	Show	52	H	-5.2342370	-3.1415340	1.7992090
53	No	Show	53	H	-3.0782630	-3.7130310	-1.8820240
54	No	Show	54	H	-4.4277120	-4.6488160	-0.0025640
55	No	Show	55	O	-0.3033810	2.6069880	-1.0159100
56	No	Show	56	H	-5.0231170	1.4785090	0.4959520
57	No	Show	57	C	-2.0001190	4.5606550	-0.3245420

## 25a

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	H	1.0173060	-3.0861800	-3.3227310
2	No	Show	2	C	0.7458230	-3.1200190	-2.2747850
3	No	Show	3	C	0.1955820	-4.2413070	-1.5831520
4	No	Show	4	C	0.9251530	-2.0654640	-1.3324090
5	No	Show	5	C	0.0464180	-3.8816330	-0.2115680
6	No	Show	6	H	-0.0294950	-5.2094590	-2.0136870
7	No	Show	7	C	0.4842680	-2.5227250	-0.0463290
8	No	Show	8	Fe	1.9933650	-3.7220810	-0.7757070
9	No	Show	9	C	3.0722840	-5.0032230	0.3931310
10	No	Show	10	C	3.5688550	-3.6703010	0.5266570
11	No	Show	11	C	3.1719940	-5.3747670	-0.9828530
12	No	Show	12	H	2.6636030	-5.6142520	1.1887140
13	No	Show	13	C	3.9746320	-3.2174660	-0.7665920
14	No	Show	14	H	3.5853830	-3.0929780	1.4426810
15	No	Show	15	C	3.7287420	-4.2713740	-1.6994130
16	No	Show	16	H	2.8440870	-6.3126940	-1.4139500
17	No	Show	17	H	4.3664230	-2.2372750	-1.0086470
18	No	Show	18	H	3.8969390	-4.2263160	-2.7683830
19	No	Show	19	H	1.3585380	-1.0966970	-1.5483680
20	No	Show	20	H	-0.3409750	-4.5220730	0.5712970
21	No	Show	21	C	0.4524650	-1.7632190	1.2174300
22	No	Show	22	C	0.6821930	-2.4759790	2.4420880

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23	No	Show	23	C	0.1786700	-0.4189340	1.3078320
24	No	Show	24	N	0.6621790	-1.9387220	3.6290030
25	No	Show	25	C	0.1824710	0.2210840	2.6112930
26	No	Show	26	N	0.4183170	-0.6223790	3.6971000
27	No	Show	27	Pd	-0.4467030	0.7038250	-0.2292220
28	No	Show	28	P	1.4971770	1.9844640	-0.1572750
29	No	Show	29	C	2.8254670	1.6457260	1.0546030
30	No	Show	30	C	3.3771290	0.3581230	1.1375670
31	No	Show	31	C	3.3052170	2.6499800	1.9038710
32	No	Show	32	C	4.4098470	0.0920160	2.0353440
33	No	Show	33	H	3.0001660	-0.4420330	0.5056390
34	No	Show	34	C	4.3317350	2.3762960	2.8081490
35	No	Show	35	H	2.8724950	3.6449710	1.8712070
36	No	Show	36	C	4.8901210	1.1003020	2.8729490
37	No	Show	37	H	4.8359670	-0.9063560	2.0862710
38	No	Show	38	H	4.6914250	3.1646360	3.4644190
39	No	Show	39	H	5.6910080	0.8888400	3.5769170
40	No	Show	40	C	1.0195970	3.7312500	0.1011900
41	No	Show	41	C	1.7569010	4.7752880	-0.4778920
42	No	Show	42	C	-0.0907580	4.0267080	0.9019830
43	No	Show	43	C	1.3867240	6.1003000	-0.2544460
44	No	Show	44	H	2.6167590	4.5583580	-1.1061090
45	No	Show	45	C	-0.4552860	5.3549370	1.1201520
46	No	Show	46	H	-0.6508360	3.2215680	1.3672590
47	No	Show	47	C	0.2781670	6.3916550	0.5433000
48	No	Show	48	H	1.9617850	6.9034430	-0.7084200
49	No	Show	49	H	-1.3215730	5.5753330	1.7381270
50	No	Show	50	H	-0.0143760	7.4254190	0.7102020
51	No	Show	51	C	2.3450830	2.0062000	-1.7891730
52	No	Show	52	C	3.6670110	1.5811820	-1.9703140
53	No	Show	53	C	1.6151040	2.4628860	-2.9002800
54	No	Show	54	C	4.2457750	1.6002090	-3.2413210
55	No	Show	55	H	4.2587020	1.2519130	-1.1216350
56	No	Show	56	C	2.1993620	2.4839720	-4.1642940
57	No	Show	57	H	0.5978560	2.8210270	-2.7666160
58	No	Show	58	C	3.5145850	2.0469690	-4.3407300
59	No	Show	59	H	5.2749350	1.2727800	-3.3660920
60	No	Show	60	H	1.6247970	2.8452400	-5.0134710
61	No	Show	61	H	3.9680830	2.0629390	-5.3284960
62	No	Show	62	O	-0.0075590	1.4298540	2.8185560
63	No	Show	63	H	0.9024300	-3.5400210	2.4257220
64	No	Show	64	C	0.4116320	-0.0352640	5.0303630
65	No	Show	65	H	1.1902760	0.7270930	5.1079760
66	No	Show	66	H	-0.5515240	0.4424600	5.2239300
67	No	Show	67	H	0.5904920	-0.8401910	5.7411520

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68	No	Show	68	H	-6.1306960	-3.0199820	-0.1542300
69	No	Show	69	C	-6.1660850	-1.9372950	-0.1465810
70	No	Show	70	C	-6.3408670	-1.1103860	1.0060060
71	No	Show	71	C	-5.9915930	-1.0826790	-1.2791970
72	No	Show	72	C	-6.2699240	0.2537230	0.5860700
73	No	Show	73	H	-6.4584090	-1.4586420	2.0250550
74	No	Show	74	C	-6.0555940	0.2708150	-0.8236500
75	No	Show	75	Fe	-4.5427670	-0.7320840	0.1270100
76	No	Show	76	C	-3.0485960	0.3279950	1.0082150
77	No	Show	77	C	-2.7528960	0.1749150	-0.4092760
78	No	Show	78	C	-3.1722100	-0.9582780	1.6106800
79	No	Show	79	H	-3.1984250	1.2809870	1.4994490
80	No	Show	80	C	-2.7254890	-1.2618800	-0.6345330
81	No	Show	81	C	-2.9709450	-1.9423560	0.5929590
82	No	Show	82	H	-3.4126450	-1.1568240	2.6485440
83	No	Show	83	H	-2.5701580	-1.7319990	-1.5982280
84	No	Show	84	H	-3.0360310	-3.0157510	0.7250030
85	No	Show	85	H	-5.8140840	-1.4127330	-2.2961340
86	No	Show	86	H	-6.3127430	1.1247830	1.2277400
87	No	Show	87	H	-5.8866100	1.1653740	-1.4096900
88	No	Show	88	O	-3.2202900	0.8592410	-2.8738690
89	No	Show	89	H	-4.0633750	0.3999270	-2.7750970
90	No	Show	90	O	-3.4978720	2.4860990	-1.0258520
91	No	Show	91	H	-3.4436620	3.1996330	-1.6773070
92	No	Show	92	B	-2.7910290	1.3539100	-1.5672950
93	No	Show	93	O	-1.3211190	1.7747150	-1.8722080
94	No	Show	94	H	-1.1249310	1.3021170	-2.6980290

## 25b

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	2.3659240	-1.3937230	-0.2198780
2	No	Show	2	C	3.0015140	-2.3543870	-1.0796460
3	No	Show	3	C	1.3561470	-0.6332360	-0.7639580
4	No	Show	4	N	2.7075950	-2.5422760	-2.3352150
5	No	Show	5	C	0.9778290	-0.8420270	-2.1539320
6	No	Show	6	N	1.7341580	-1.7831390	-2.8517530
7	No	Show	7	Pd	0.3868400	0.8837490	0.1202870
8	No	Show	8	P	-1.5901960	-0.3920390	0.1882850
9	No	Show	9	C	-1.6275380	-2.0993570	-0.4693920
10	No	Show	10	C	-0.7393770	-3.0588040	0.0414340
11	No	Show	11	C	-2.5063470	-2.4644930	-1.4963610
12	No	Show	12	C	-0.7491310	-4.3633330	-0.4482970
13	No	Show	13	H	-0.0331570	-2.7937470	0.8232170
14	No	Show	14	C	-2.5092350	-3.7702910	-1.9885640
15	No	Show	15	H	-3.1819590	-1.7300300	-1.9234900



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16	No	Show	16	C	-1.6354910	-4.7228920	-1.4652170
17	No	Show	17	H	-0.0554930	-5.0942730	-0.0410950
18	No	Show	18	H	-3.1957030	-4.0389090	-2.7874720
19	No	Show	19	H	-1.6387420	-5.7387200	-1.8521930
20	No	Show	20	C	-2.9094430	0.5166080	-0.6906430
21	No	Show	21	C	-4.2542870	0.3629070	-0.3184260
22	No	Show	22	C	-2.5725030	1.3663720	-1.7501630
23	No	Show	23	C	-5.2516300	1.0475920	-1.0091540
24	No	Show	24	H	-4.5245110	-0.2859290	0.5107510
25	No	Show	25	C	-3.5769580	2.0514680	-2.4343540
26	No	Show	26	H	-1.5347340	1.4854160	-2.0420040
27	No	Show	27	C	-4.9131860	1.8935790	-2.0685320
28	No	Show	28	H	-6.2912960	0.9249000	-0.7160800
29	No	Show	29	H	-3.3059490	2.7155070	-3.2505730
30	No	Show	30	H	-5.6921170	2.4329720	-2.6020650
31	No	Show	31	C	-2.2370020	-0.5231410	1.9045560
32	No	Show	32	C	-2.4866280	-1.7417540	2.5474600
33	No	Show	33	C	-2.4867150	0.6774320	2.5915490
34	No	Show	34	C	-2.9671560	-1.7607360	3.8588650
35	No	Show	35	H	-2.3264350	-2.6813910	2.0276310
36	No	Show	36	C	-2.9715750	0.6518220	3.8965960
37	No	Show	37	H	-2.3188250	1.6273030	2.0907210
38	No	Show	38	C	-3.2076600	-0.5671970	4.5375420
39	No	Show	39	H	-3.1600850	-2.7141380	4.3442890
40	No	Show	40	H	-3.1681590	1.5877780	4.4135540
41	No	Show	41	H	-3.5839480	-0.5846880	5.5572220
42	No	Show	42	O	0.0548110	-0.2580570	-2.7410840
43	No	Show	43	H	3.7745480	-3.0146600	-0.6962290
44	No	Show	44	C	1.4091950	-2.0132880	-4.2531910
45	No	Show	45	H	0.3885870	-2.3926070	-4.3439080
46	No	Show	46	H	1.4736610	-1.0749400	-4.8080190
47	No	Show	47	H	2.1233760	-2.7390930	-4.6381320
48	No	Show	48	O	0.6095180	4.6749850	1.1096700
49	No	Show	49	H	1.1068150	5.3910740	0.6942550
50	No	Show	50	O	-0.4741410	4.1154440	-1.0318890
51	No	Show	51	H	-1.2388130	4.6072190	-0.7013370
52	No	Show	52	B	0.2827720	3.6670710	0.1055840
53	No	Show	53	O	-0.5532810	2.6477320	0.9341570
54	No	Show	54	H	-0.2985030	2.8147460	1.8558550
55	No	Show	55	C	2.8441450	-1.3098980	1.1839840
56	No	Show	56	C	1.9690050	-1.0666210	2.2539930
57	No	Show	57	C	4.2057160	-1.4955640	1.4794680
58	No	Show	58	C	2.4336340	-1.0121250	3.5668200
59	No	Show	59	H	0.9088280	-0.9242440	2.0631110
60	No	Show	60	C	4.6737280	-1.4354740	2.7907660

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61	No	Show	61	H	4.9163890	-1.6547700	0.6727540
62	No	Show	62	C	3.7888790	-1.1958110	3.8432520
63	No	Show	63	H	1.7310850	-0.8269820	4.3754710
64	No	Show	64	H	5.7342110	-1.5694190	2.9892690
65	No	Show	65	H	4.1522780	-1.1499860	4.8665990
66	No	Show	66	C	1.6051270	2.8407180	-0.4420240
67	No	Show	67	C	2.5564770	2.3258030	0.4745260
68	No	Show	68	C	1.9287930	2.7405430	-1.8192020
69	No	Show	69	C	3.7872730	1.8020200	0.0467860
70	No	Show	70	H	2.3806300	2.4450810	1.5429230
71	No	Show	71	C	3.1450100	2.2214110	-2.2451840
72	No	Show	72	H	1.2088840	3.1160790	-2.5409800
73	No	Show	73	C	4.0837020	1.7586200	-1.3099500
74	No	Show	74	H	4.5081580	1.4478790	0.7788680
75	No	Show	75	H	3.3761570	2.1793630	-3.3075130
76	No	Show	76	H	5.0403260	1.3665840	-1.6480490

## 26a

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	H	2.1357240	-1.5644780	-3.7419360
2	No	Show	2	C	2.1368170	-1.9289550	-2.7216590
3	No	Show	3	C	2.6493430	-3.1856340	-2.2760690
4	No	Show	4	C	1.6850590	-1.2124010	-1.5761090
5	No	Show	5	C	2.5267250	-3.2387420	-0.8578740
6	No	Show	6	H	3.1031720	-3.9464680	-2.8998460
7	No	Show	7	C	1.9063460	-2.0201590	-0.4092930
8	No	Show	8	Fe	3.6687720	-1.6457290	-1.4072750
9	No	Show	9	C	5.5028480	-1.9461920	-0.5685570
10	No	Show	10	C	4.9356030	-0.7216810	-0.1029610
11	No	Show	11	C	5.6107050	-1.8662940	-1.9910130
12	No	Show	12	H	5.7398650	-2.8025340	0.0493350
13	No	Show	13	C	4.6878180	0.1158550	-1.2348900
14	No	Show	14	H	4.6862340	-0.5050170	0.9277440
15	No	Show	15	C	5.1049620	-0.5943340	-2.4037830
16	No	Show	16	H	5.9673600	-2.6509080	-2.6473360
17	No	Show	17	H	4.2278090	1.0967640	-1.2210320
18	No	Show	18	H	5.0145860	-0.2462060	-3.4256360
19	No	Show	19	H	1.2840910	-0.2078830	-1.5778500
20	No	Show	20	H	2.8702720	-4.0328360	-0.2112260
21	No	Show	21	C	1.5293870	-1.6815050	0.9705820
22	No	Show	22	C	2.3184800	-2.2766120	2.0553720
23	No	Show	23	C	0.4423970	-0.8970620	1.3017950
24	No	Show	24	N	1.8892140	-1.9708240	3.3481970
25	No	Show	25	C	0.1575030	-0.6930720	2.6874210
26	No	Show	26	N	0.8382350	-1.2112380	3.6772860

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27	No	Show	27	Pd	-0.8962720	-0.0232200	0.0642470
28	No	Show	28	P	-0.0082810	2.2541270	0.3049560
29	No	Show	29	C	1.0033890	2.6261820	1.7871280
30	No	Show	30	C	2.2183600	1.9399990	1.9441480
31	No	Show	31	C	0.5992000	3.5327990	2.7740990
32	No	Show	32	C	3.0181670	2.1727860	3.0600360
33	No	Show	33	H	2.5405070	1.2234900	1.1929340
34	No	Show	34	C	1.3983620	3.7529910	3.8979050
35	No	Show	35	H	-0.3362720	4.0753640	2.6715100
36	No	Show	36	C	2.6090670	3.0773430	4.0422320
37	No	Show	37	H	3.9579270	1.6375400	3.1673720
38	No	Show	38	H	1.0720750	4.4583020	4.6581040
39	No	Show	39	H	3.2302090	3.2505610	4.9172320
40	No	Show	40	C	-1.3829100	3.4751340	0.4026420
41	No	Show	41	C	-1.3146900	4.7602000	-0.1576250
42	No	Show	42	C	-2.5502290	3.0928400	1.0851430
43	No	Show	43	C	-2.3891800	5.6428070	-0.0326400
44	No	Show	44	H	-0.4255100	5.0711310	-0.6993030
45	No	Show	45	C	-3.6160860	3.9814000	1.2199970
46	No	Show	46	H	-2.6233870	2.0914960	1.5035280
47	No	Show	47	C	-3.5380340	5.2578670	0.6595620
48	No	Show	48	H	-2.3262340	6.6319540	-0.4787810
49	No	Show	49	H	-4.5120130	3.6717010	1.7516970
50	No	Show	50	H	-4.3733700	5.9466690	0.7542330
51	No	Show	51	C	1.0195400	2.8838080	-1.0830630
52	No	Show	52	C	2.0679430	3.7974520	-0.9027320
53	No	Show	53	C	0.7190320	2.4421520	-2.3794730
54	No	Show	54	C	2.7965010	4.2596520	-1.9990590
55	No	Show	55	H	2.3219260	4.1451030	0.0949210
56	No	Show	56	C	1.4404570	2.9141910	-3.4751950
57	No	Show	57	H	-0.0805280	1.7223710	-2.5373710
58	No	Show	58	C	2.4829160	3.8223680	-3.2869710
59	No	Show	59	H	3.6115500	4.9622580	-1.8446850
60	No	Show	60	H	1.1933960	2.5628880	-4.4735540
61	No	Show	61	H	3.0535300	4.1827020	-4.1390430
62	No	Show	62	H	-5.8678170	-3.5596420	-1.3676280
63	No	Show	63	C	-5.5638880	-2.9044930	-0.5605250
64	No	Show	64	C	-5.3491540	-3.2876540	0.7986760
65	No	Show	65	C	-5.2653350	-1.5132530	-0.6808340
66	No	Show	66	C	-4.9110300	-2.1354150	1.5210780
67	No	Show	67	H	-5.4579830	-4.2868320	1.2022780
68	No	Show	68	C	-4.8635830	-1.0374900	0.6107210
69	No	Show	69	Fe	-3.6267050	-2.5598990	-0.0101540
70	No	Show	70	C	-1.8311000	-2.9735010	0.8759100
71	No	Show	71	C	-1.6295040	-1.9414240	-0.0939460

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72	No	Show	72	C	-2.3655430	-4.1333070	0.2337660
73	No	Show	73	H	-1.6384810	-2.8856070	1.9383130
74	No	Show	74	C	-2.0694550	-2.4884220	-1.3520420
75	No	Show	75	C	-2.5172360	-3.8308530	-1.1521830
76	No	Show	76	H	-2.6469950	-5.0610990	0.7185020
77	No	Show	77	H	-2.0571550	-1.9829820	-2.3115560
78	No	Show	78	H	-2.9284100	-4.4877720	-1.9100820
79	No	Show	79	H	-5.3402790	-0.9295550	-1.5913490
80	No	Show	80	H	-4.6260120	-2.1095460	2.5657440
81	No	Show	81	H	-4.5540680	-0.0280070	0.8514070
82	No	Show	82	O	-4.0450990	0.6533290	-3.2401740
83	No	Show	83	H	-4.3279130	1.2713450	-3.9285390
84	No	Show	84	O	-2.8684430	2.5897490	-2.5429010
85	No	Show	85	H	-2.3938190	2.9712560	-1.7878750
86	No	Show	86	B	-3.2216970	1.2842140	-2.3426340
87	No	Show	87	O	-2.7653200	0.5725540	-1.2471220
88	No	Show	88	H	-3.1819730	-0.3169000	-1.1701700
89	No	Show	89	H	-0.6856830	-0.0861600	3.0044960
90	No	Show	90	O	3.3040520	-3.0135240	1.9220750
91	No	Show	91	C	2.6268660	-2.5602810	4.4577030
92	No	Show	92	H	2.1733650	-2.1944510	5.3772310
93	No	Show	93	H	2.5737130	-3.6508270	4.4111780
94	No	Show	94	H	3.6794050	-2.2727110	4.4057220

## 26b

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	2.5043540	-0.7719030	-0.0155690
2	No	Show	2	C	3.4681450	-1.5839980	-0.7709820
3	No	Show	3	C	1.4441170	-0.2227260	-0.7026290
4	No	Show	4	N	3.2216190	-1.6821540	-2.1428400
5	No	Show	5	C	1.3433200	-0.4385950	-2.1090310
6	No	Show	6	N	2.2026850	-1.1330090	-2.8079230
7	No	Show	7	Pd	0.0751260	1.0136240	0.0940580
8	No	Show	8	P	-1.5603800	-0.6995650	0.0115650
9	No	Show	9	C	-1.1130550	-2.3206230	-0.7107890
10	No	Show	10	C	-0.0970300	-3.0838310	-0.1114990
11	No	Show	11	C	-1.7141570	-2.7935840	-1.8846710
12	No	Show	12	C	0.2847340	-4.3062130	-0.6585170
13	No	Show	13	H	0.4075560	-2.7278930	0.7823140
14	No	Show	14	C	-1.3209370	-4.0143310	-2.4354430
15	No	Show	15	H	-2.4867480	-2.2118120	-2.3782920
16	No	Show	16	C	-0.3267140	-4.7753060	-1.8230020
17	No	Show	17	H	1.0706470	-4.8838890	-0.1792480
18	No	Show	18	H	-1.7945060	-4.3659260	-3.3483980
19	No	Show	19	H	-0.0222750	-5.7254050	-2.2543830

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20	No	Show	20	C	-3.0205020	-0.1349340	-0.9337890
21	No	Show	21	C	-4.2460140	-0.8086160	-0.8020010
22	No	Show	22	C	-2.9243930	0.9627460	-1.7951770
23	No	Show	23	C	-5.3515310	-0.4012280	-1.5434930
24	No	Show	24	H	-4.3382630	-1.6479310	-0.1170450
25	No	Show	25	C	-4.0372410	1.3678010	-2.5351970
26	No	Show	26	H	-2.0063200	1.5388940	-1.8662010
27	No	Show	27	C	-5.2468570	0.6860910	-2.4159710
28	No	Show	28	H	-6.2964500	-0.9276860	-1.4354990
29	No	Show	29	H	-3.9524910	2.2297980	-3.1911520
30	No	Show	30	H	-6.1126430	1.0069250	-2.9899640
31	No	Show	31	C	-2.2646400	-1.0610640	1.6690150
32	No	Show	32	C	-2.2929410	-2.3374680	2.2429760
33	No	Show	33	C	-2.8131940	0.0236080	2.3739250
34	No	Show	34	C	-2.8519350	-2.5250030	3.5090450
35	No	Show	35	H	-1.8956970	-3.1931270	1.7055750
36	No	Show	36	C	-3.3751330	-0.1719100	3.6329460
37	No	Show	37	H	-2.8126470	1.0132250	1.9235350
38	No	Show	38	C	-3.3912190	-1.4456350	4.2070540
39	No	Show	39	H	-2.8694370	-3.5210340	3.9440140
40	No	Show	40	H	-3.8030410	0.6731260	4.1663250
41	No	Show	41	H	-3.8272870	-1.5954690	5.1913800
42	No	Show	42	O	-0.7423530	4.7765500	0.9800580
43	No	Show	43	H	-0.3990220	5.5839850	0.5766470
44	No	Show	44	O	-1.6257680	3.9327300	-1.1572790
45	No	Show	45	H	-2.4714350	4.2695720	-0.8289310
46	No	Show	46	B	-0.7780870	3.7073060	-0.0107600
47	No	Show	47	O	-1.3201610	2.5103130	0.8219690
48	No	Show	48	H	-1.1565270	2.7579700	1.7462050
49	No	Show	49	C	2.7529590	-0.5815850	1.4348260
50	No	Show	50	C	1.6979730	-0.5389460	2.3616670
51	No	Show	51	C	4.0601020	-0.4063690	1.9243260
52	No	Show	52	C	1.9304920	-0.3142690	3.7179600
53	No	Show	53	H	0.6757750	-0.7018240	2.0314220
54	No	Show	54	C	4.2918000	-0.1680170	3.2770880
55	No	Show	55	H	4.8980820	-0.4617190	1.2397360
56	No	Show	56	C	3.2306210	-0.1208780	4.1832340
57	No	Show	57	H	1.0914130	-0.2955210	4.4089460
58	No	Show	58	H	5.3116350	-0.0256740	3.6262830
59	No	Show	59	H	3.4163840	0.0572020	5.2394650
60	No	Show	60	C	0.7112270	3.2554690	-0.5499580
61	No	Show	61	C	1.7208240	2.8786660	0.3734830
62	No	Show	62	C	1.0892800	3.3295940	-1.9130020
63	No	Show	63	C	3.0465840	2.6371700	-0.0392480
64	No	Show	64	H	1.5088800	2.9165490	1.4421950

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65	No	Show	65	C	2.3965730	3.0955780	-2.3192170
66	No	Show	66	H	0.3320390	3.6159720	-2.6385890
67	No	Show	67	C	3.3834690	2.7517930	-1.3794480
68	No	Show	68	H	3.8007240	2.3752640	0.6978360
69	No	Show	69	H	2.6637140	3.1830320	-3.3703390
70	No	Show	70	H	4.4068370	2.5780610	-1.7031920
71	No	Show	71	O	4.4477920	-2.1739270	-0.3026120
72	No	Show	72	H	0.5337550	-0.0096670	-2.6913710
73	No	Show	73	C	4.1573670	-2.4691710	-2.9363350
74	No	Show	74	H	3.8200550	-2.4257030	-3.9701860
75	No	Show	75	H	5.1658600	-2.0602720	-2.8420490
76	No	Show	76	H	4.1768660	-3.5018300	-2.5805840

## 27a

Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	H	-	3.0665750	-2.6707790	-2.5786160
2	No	Show	2	C	-	3.2680120	-1.7521840	-2.0416040
3	No	Show	3	C	-	4.5272580	-1.3391820	-1.5187700
4	No	Show	4	C	-	2.3255500	-0.7082660	-1.7766470
5	No	Show	5	C	-	4.3672200	-0.0617540	-0.9006180
6	No	Show	6	H	-	5.4443670	-1.9144600	-1.5510370
7	No	Show	7	C	-	3.0052910	0.3337450	-1.0402120
8	No	Show	8	Fe	-	3.1566650	-1.4686410	-0.0165940
9	No	Show	9	C	-	3.9662820	-1.5118900	1.8524840
10	No	Show	10	C	-	2.5711350	-1.2350150	1.9461120
11	No	Show	11	C	-	4.1220940	-2.7766550	1.2051930
12	No	Show	12	H	-	4.7676640	-0.8551460	2.1676220
13	No	Show	13	C	-	1.8618440	-2.3350920	1.3709900
14	No	Show	14	H	-	2.1315750	-0.3278430	2.3422750
15	No	Show	15	C	-	2.8212890	-3.2797970	0.8997590
16	No	Show	16	H	-	5.0631990	-3.2507260	0.9550130
17	No	Show	17	H	-	0.7891010	-2.4492120	1.2695860
18	No	Show	18	H	-	2.5983680	-4.2083930	0.3889890
19	No	Show	19	H	-	1.3616410	-0.6080400	-2.2838140
20	No	Show	20	H	-	5.1252620	0.5062430	-0.3803030
21	No	Show	21	C	-	2.2984090	1.4878560	-0.4784250
22	No	Show	22	C	-	3.0408030	2.7110820	-0.2160670
23	No	Show	23	C	-	0.9513810	1.3811300	-0.1751990
24	No	Show	24	N	-	2.2555900	3.7602870	0.2649600
25	No	Show	25	C	-	0.3356690	2.5604530	0.3400300
26	No	Show	26	N	-	0.9483030	3.7035020	0.5411090
27	No	Show	27	Pd	-	0.2125710	-0.5266590	-0.4660730
28	No	Show	28	P	-	2.0257880	-0.0873810	-0.0280470
29	No	Show	29	O	-	4.2572680	2.8793050	-0.3751340
30	No	Show	30	H	-	0.7160370	2.5902750	0.6049550

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31	No	Show	31	C	2.3270980	0.8324310	1.5304520
32	No	Show	32	C	1.5592070	0.4838950	2.6513280
33	No	Show	33	C	3.2896000	1.8426780	1.6497600
34	No	Show	34	C	1.7621390	1.1218040	3.8731760
35	No	Show	35	H	0.7951960	-0.2849910	2.5626790
36	No	Show	36	C	3.4825570	2.4887580	2.8721580
37	No	Show	37	H	3.8829550	2.1384050	0.7891250
38	No	Show	38	C	2.7237880	2.1282000	3.9855170
39	No	Show	39	H	1.1613680	0.8408020	4.7342970
40	No	Show	40	H	4.2255870	3.2782850	2.9503840
41	No	Show	41	H	2.8743740	2.6348720	4.9352460
42	No	Show	42	C	2.8508370	0.8792930	-1.3516820
43	No	Show	43	C	4.2404670	0.8121080	-1.5376840
44	No	Show	44	C	2.0882650	1.6993310	-2.1927090
45	No	Show	45	C	4.8536240	1.5659640	-2.5371460
46	No	Show	46	H	4.8431200	0.1608460	-0.9100240
47	No	Show	47	C	2.7053520	2.4559430	-3.1889770
48	No	Show	48	H	1.0088030	1.7378630	-2.0724790
49	No	Show	49	C	4.0880350	2.3920820	-3.3624200
50	No	Show	50	H	5.9301920	1.5026920	-2.6742440
51	No	Show	51	H	2.1015470	3.0884520	-3.8344980
52	No	Show	52	H	4.5674130	2.9766600	-4.1435840
53	No	Show	53	C	3.0839370	-1.5697750	0.1281260
54	No	Show	54	C	3.8264330	-1.8405470	1.2845140
55	No	Show	55	C	3.1523750	-2.4543030	-0.9595590
56	No	Show	56	C	4.6391980	-2.9735810	1.3482350
57	No	Show	57	H	3.7846680	-1.1678350	2.1361750
58	No	Show	58	C	3.9725760	-3.5776090	-0.8921950
59	No	Show	59	H	2.5495320	-2.2738920	-1.8422700
60	No	Show	60	C	4.7162440	-3.8417390	0.2596300
61	No	Show	61	H	5.2150600	-3.1712070	2.2489320
62	No	Show	62	H	4.0187250	-4.2572250	-1.7393050
63	No	Show	63	H	5.3511990	-4.7230040	0.3095290
64	No	Show	64	O	0.3793090	-2.4623900	-0.8360410
65	No	Show	65	H	-0.4313300	-2.9002340	-1.1427040
66	No	Show	66	C	-2.9153940	5.0325560	0.5264370
67	No	Show	67	H	-3.4321130	5.3758700	-0.3722750
68	No	Show	68	H	-3.6579780	4.9180960	1.3202930
69	No	Show	69	H	-2.1455720	5.7419540	0.8245750

## 27b

Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	C	3.0207100		0.2027680	0.1812630
2	No	Show	2	C	4.0847230		1.1713090	-0.0259410
3	No	Show	3	C	1.7436390		0.6007240	0.5172830

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4	No	Show	4	N	3.7099800	2.4860250	0.2720540
5	No	Show	5	C	1.5500040	1.9943150	0.7561160
6	No	Show	6	N	2.4973180	2.8953910	0.6633280
7	No	Show	7	Pd	0.4634860	-0.9878370	0.6501200
8	No	Show	8	P	-1.4800100	0.0433820	-0.0502850
9	No	Show	9	O	5.2328630	0.9326560	-0.4178470
10	No	Show	10	H	0.5881500	2.3991560	1.0567810
11	No	Show	11	C	-1.2733090	1.6468560	-0.9110270
12	No	Show	12	C	-0.3337060	1.7197810	-1.9510780
13	No	Show	13	C	-2.0180190	2.7853430	-0.5814750
14	No	Show	14	C	-0.1597000	2.9047350	-2.6616560
15	No	Show	15	H	0.2685370	0.8488580	-2.2002290
16	No	Show	16	C	-1.8307890	3.9760400	-1.2869010
17	No	Show	17	H	-2.7414260	2.7512100	0.2281150
18	No	Show	18	C	-0.9068480	4.0371980	-2.3292450
19	No	Show	19	H	0.5710430	2.9478010	-3.4650210
20	No	Show	20	H	-2.4086780	4.8561640	-1.0167040
21	No	Show	21	H	-0.7611520	4.9658070	-2.8750020
22	No	Show	22	C	-2.5686500	0.3828080	1.3806590
23	No	Show	23	C	-3.9611990	0.4613650	1.2395480
24	No	Show	24	C	-1.9934310	0.5878090	2.6408850
25	No	Show	25	C	-4.7616300	0.7562700	2.3425120
26	No	Show	26	H	-4.4225810	0.2827220	0.2718970
27	No	Show	27	C	-2.7958530	0.8892050	3.7404590
28	No	Show	28	H	-0.9169310	0.4949260	2.7634950
29	No	Show	29	C	-4.1807190	0.9744880	3.5930210
30	No	Show	30	H	-5.8409640	0.8092770	2.2247800
31	No	Show	31	H	-2.3391040	1.0425830	4.7146240
32	No	Show	32	H	-4.8072570	1.1993600	4.4523850
33	No	Show	33	C	-2.5333130	-0.9232530	-1.2023460
34	No	Show	34	C	-2.9995020	-0.3846350	-2.4094900
35	No	Show	35	C	-2.9154190	-2.2220810	-0.8283940
36	No	Show	36	C	-3.8358250	-1.1374120	-3.2361070
37	No	Show	37	H	-2.7226960	0.6213430	-2.7096190
38	No	Show	38	C	-3.7573270	-2.9613510	-1.6569330
39	No	Show	39	H	-2.5161850	-2.6381420	0.0957940
40	No	Show	40	C	-4.2177900	-2.4251800	-2.8617480
41	No	Show	41	H	-4.1897460	-0.7107570	-4.1713060
42	No	Show	42	H	-4.0500110	-3.9657880	-1.3607220
43	No	Show	43	H	-4.8708520	-3.0086920	-3.5061530
44	No	Show	44	O	-0.6428350	-2.6733510	1.0437660
45	No	Show	45	H	-0.2901460	-3.3707400	0.4682430
46	No	Show	46	C	3.2701410	-1.2446650	0.0404970
47	No	Show	47	C	4.0359830	-1.8092990	-0.9910010
48	No	Show	48	C	2.6364140	-2.1100410	0.9609220



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49	No	Show	49	C	4.1242810	-3.1928910	-1.1173410
50	No	Show	50	H	4.5554720	-1.1566820	-1.6841550
51	No	Show	51	C	2.7172300	-3.5007870	0.8187610
52	No	Show	52	H	2.2251550	-1.6974730	1.8913040
53	No	Show	53	C	3.4584760	-4.0438710	-0.2257220
54	No	Show	54	H	4.7172680	-3.6175700	-1.9238020
55	No	Show	55	H	2.2167280	-4.1413880	1.5393300
56	No	Show	56	H	3.5354050	-5.1219050	-0.3405220
57	No	Show	57	C	4.7292330	3.5200930	0.1467340
58	No	Show	58	H	5.5937840	3.2687950	0.7650710
59	No	Show	59	H	5.0655880	3.5950210	-0.8903350
60	No	Show	60	H	4.2822720	4.4576800	0.4719380

### 33a

Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	H	-4.4710700	-2.0021310	-1.5432820	
2	No	Show	2	C	-4.2513680	-0.9715160	-1.2941730	
3	No	Show	3	C	-5.1655520	-0.0176380	-0.7519950	
4	No	Show	4	C	-2.9897130	-0.3231640	-1.4477480	
5	No	Show	5	C	-4.4646170	1.2110160	-0.5578680	
6	No	Show	6	H	-6.2015740	-0.2060070	-0.4984840	
7	No	Show	7	C	-3.1105610	1.0340090	-0.9911380	
8	No	Show	8	Fe	-3.6050900	-0.2984060	0.5143900	
9	No	Show	9	C	-3.8277190	0.2808650	2.4547120	
10	No	Show	10	C	-2.4472540	0.0565880	2.1666320	
11	No	Show	11	C	-4.5294310	-0.9395870	2.2108140	
12	No	Show	12	H	-4.2705920	1.2203420	2.7624320	
13	No	Show	13	C	-2.2918020	-1.2998750	1.7475730	
14	No	Show	14	H	-1.6580320	0.7947270	2.2258840	
15	No	Show	15	C	-3.5796840	-1.9125390	1.7706740	
16	No	Show	16	H	-5.5983190	-1.0913960	2.2996760	
17	No	Show	17	H	-1.3717340	-1.7744610	1.4291440	
18	No	Show	18	H	-3.8029910	-2.9297390	1.4727370	
19	No	Show	19	H	-2.1119730	-0.7771080	-1.9122260	
20	No	Show	20	H	-4.8810740	2.1104170	-0.1203840	
21	No	Show	21	C	-0.7060480	1.6885200	-1.1155110	
22	No	Show	22	C	0.2579660	2.6841120	-1.5438280	
23	No	Show	23	C	-2.0419430	2.0355770	-1.1193460	
24	No	Show	24	N	-0.2476980	3.9752180	-1.7330090	
25	No	Show	25	C	-2.3981090	3.3980680	-1.3818520	
26	No	Show	26	N	-1.5344220	4.3368730	-1.6564390	
27	No	Show	27	Pd	-0.2267860	-0.2424170	-0.7582450	
28	No	Show	28	P	1.6954030	0.1899350	0.4568260	
29	No	Show	29	O	1.4611140	2.4849080	-1.7672100	
30	No	Show	30	H	-3.4357300	3.7226190	-1.3708870	

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31	No	Show	31	C	2.0475200	1.8827770	1.0598460
32	No	Show	32	C	1.0094120	2.6580600	1.5915550
33	No	Show	33	C	3.3484050	2.3984050	1.0478170
34	No	Show	34	C	1.2691920	3.9236980	2.1159360
35	No	Show	35	H	-0.0095510	2.2792060	1.5877460
36	No	Show	36	C	3.6055540	3.6656410	1.5706330
37	No	Show	37	H	4.1624380	1.8222290	0.6187070
38	No	Show	38	C	2.5699220	4.4305870	2.1083820
39	No	Show	39	H	0.4525190	4.5136530	2.5242260
40	No	Show	40	H	4.6196900	4.0567120	1.5510600
41	No	Show	41	H	2.7738500	5.4185310	2.5136350
42	No	Show	42	C	3.1757050	-0.3371830	-0.4826660
43	No	Show	43	C	4.2573230	-0.9691010	0.1478630
44	No	Show	44	C	3.2370530	-0.0788350	-1.8595390
45	No	Show	45	C	5.3841060	-1.3339570	-0.5881680
46	No	Show	46	H	4.2250180	-1.1784750	1.2131430
47	No	Show	47	C	4.3674970	-0.4446440	-2.5889060
48	No	Show	48	H	2.4130200	0.4305730	-2.3488350
49	No	Show	49	C	5.4415720	-1.0731500	-1.9577380
50	No	Show	50	H	6.2143890	-1.8268410	-0.0889090
51	No	Show	51	H	4.4055070	-0.2371770	-3.6552170
52	No	Show	52	H	6.3190420	-1.3620970	-2.5311160
53	No	Show	53	C	1.7230920	-0.8122090	1.9999330
54	No	Show	54	C	1.6988970	-0.2040920	3.2643800
55	No	Show	55	C	1.7690380	-2.2151810	1.9193260
56	No	Show	56	C	1.7126340	-0.9795400	4.4244640
57	No	Show	57	H	1.6857890	0.8769830	3.3562300
58	No	Show	58	C	1.7944280	-2.9807610	3.0839500
59	No	Show	59	H	1.7548710	-2.6997290	0.9486700
60	No	Show	60	C	1.7615130	-2.3699860	4.3385600
61	No	Show	61	H	1.6927440	-0.4907500	5.3952720
62	No	Show	62	H	1.8342650	-4.0643360	3.0049550
63	No	Show	63	H	1.7765190	-2.9735340	5.2428700
64	No	Show	64	O	0.1581150	-2.2684140	-0.5102830
65	No	Show	65	C	0.6937980	5.0229660	-2.1078970
66	No	Show	66	H	1.5130190	5.0570730	-1.3868030
67	No	Show	67	H	1.1165750	4.8160910	-3.0944630
68	No	Show	68	H	0.1462910	5.9638520	-2.1187970
69	No	Show	69	C	0.4265310	-2.8849290	-1.6906430
70	No	Show	70	H	1.2230210	-2.4022620	-2.2793590
71	No	Show	71	O	-0.7177060	-2.7891470	-2.5905660
72	No	Show	72	H	-1.4700540	-3.1187910	-2.0729110
73	No	Show	73	N	0.8564140	-4.2564620	-1.4601960
74	No	Show	74	C	-0.0965880	-5.0610090	-0.7135910
75	No	Show	75	H	-0.9833820	-5.3606990	-1.3046850

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76	No	Show	76	H	0.3913710	-5.9820290	-0.3760230
77	No	Show	77	H	-0.4289750	-4.5040490	0.1646360
78	No	Show	78	C	1.2966240	-4.9205920	-2.6761950
79	No	Show	79	H	1.7684520	-5.8749400	-2.4174590
80	No	Show	80	H	0.4782240	-5.1185110	-3.3888280
81	No	Show	81	H	2.0452870	-4.3038300	-3.1831290

### 33b

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	1.4545010	1.4764690	-0.7823170
2	No	Show	2	C	2.5473790	0.8220410	-1.4831620
3	No	Show	3	C	1.6531540	2.7580950	-0.3213720
4	No	Show	4	N	3.7481630	1.5413250	-1.5212530
5	No	Show	5	C	2.9409040	3.3630890	-0.4616530
6	No	Show	6	N	3.9546650	2.7720970	-1.0340750
7	No	Show	7	Pd	-0.4067420	0.7100340	-0.6476320
8	No	Show	8	P	0.2743090	-1.2585940	0.3573410
9	No	Show	9	O	2.4942670	-0.2825790	-2.0409890
10	No	Show	10	H	3.1354680	4.3727150	-0.1074160
11	No	Show	11	C	2.0336720	-1.4397060	0.8152880
12	No	Show	12	C	2.6176760	-0.4666200	1.6392990
13	No	Show	13	C	2.7965030	-2.5359290	0.3998870
14	No	Show	14	C	3.9434770	-0.5948860	2.0472870
15	No	Show	15	H	2.0333340	0.3894310	1.9680170
16	No	Show	16	C	4.1253100	-2.6597300	0.8081640
17	No	Show	17	H	2.3604050	-3.2897260	-0.2485080
18	No	Show	18	C	4.7012410	-1.6924880	1.6315130
19	No	Show	19	H	4.3859170	0.1644320	2.6870670
20	No	Show	20	H	4.7101400	-3.5142780	0.4774280
21	No	Show	21	H	5.7368040	-1.7906480	1.9475020
22	No	Show	22	C	-0.1310870	-2.6597610	-0.7398830
23	No	Show	23	C	-0.7782310	-3.8012650	-0.2504910
24	No	Show	24	C	0.2120800	-2.5799290	-2.0969760
25	No	Show	25	C	-1.0700420	-4.8598100	-1.1111130
26	No	Show	26	H	-1.0623760	-3.8662820	0.7958030
27	No	Show	27	C	-0.0770960	-3.6447170	-2.9479370
28	No	Show	28	H	0.7227430	-1.6967610	-2.4716990
29	No	Show	29	C	-0.7199520	-4.7839950	-2.4592150
30	No	Show	30	H	-1.5772530	-5.7405090	-0.7255330
31	No	Show	31	H	0.1944570	-3.5791830	-3.9984530
32	No	Show	32	H	-0.9528710	-5.6082090	-3.1289000
33	No	Show	33	C	-0.6102330	-1.5842900	1.9307550
34	No	Show	34	C	0.0526740	-2.1432610	3.0350770
35	No	Show	35	C	-1.9831770	-1.3090630	2.0133250
36	No	Show	36	C	-0.6511790	-2.4174080	4.2077330

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37	No	Show	37	H	1.1124020	-2.3735120	2.9866490
38	No	Show	38	C	-2.6770300	-1.5865240	3.1902920
39	No	Show	39	H	-2.4999320	-0.8795980	1.1579390
40	No	Show	40	C	-2.0162320	-2.1376720	4.2890470
41	No	Show	41	H	-0.1287100	-2.8512360	5.0567730
42	No	Show	42	H	-3.7390020	-1.3614920	3.2403180
43	No	Show	43	H	-2.5612390	-2.3496660	5.2058500
44	No	Show	44	O	-2.3116500	-0.0757440	-0.8225010
45	No	Show	45	C	4.8861730	0.9190950	-2.1873760
46	No	Show	46	H	5.0832080	-0.0583350	-1.7428610
47	No	Show	47	H	4.6687770	0.7736580	-3.2484800
48	No	Show	48	H	5.7400020	1.5822600	-2.0608650
49	No	Show	49	C	-3.3911060	0.7493700	-0.7613280
50	No	Show	50	H	-3.2358170	1.6644170	-1.3962180
51	No	Show	51	O	-3.6911130	1.2075550	0.5669460
52	No	Show	52	H	-2.9235050	1.7245560	0.8543710
53	No	Show	53	N	-4.5918010	0.0523400	-1.2007610
54	No	Show	54	C	-5.7444670	0.9386620	-1.2546320
55	No	Show	55	H	-5.6345600	1.7463770	-2.0058800
56	No	Show	56	H	-6.6328950	0.3566390	-1.5204030
57	No	Show	57	H	-5.9098250	1.3945190	-0.2777210
58	No	Show	58	C	-4.3887820	-0.6280230	-2.4708490
59	No	Show	59	H	-5.2875270	-1.2060220	-2.7105000
60	No	Show	60	H	-4.2008070	0.0689350	-3.3116290
61	No	Show	61	H	-3.5414330	-1.3081390	-2.3904210
62	No	Show	62	C	0.5144080	3.4946770	0.2670580
63	No	Show	63	C	0.6112170	4.2320950	1.4548870
64	No	Show	64	C	-0.7365100	3.4290720	-0.3819750
65	No	Show	65	C	-0.5102980	4.8613640	1.9926160
66	No	Show	66	H	1.5642620	4.2875100	1.9762450
67	No	Show	67	C	-1.8601680	4.0604560	0.1587090
68	No	Show	68	H	-0.7935990	3.0087060	-1.3912160
69	No	Show	69	C	-1.7494940	4.7724180	1.3530690
70	No	Show	70	H	-0.4191250	5.4188220	2.9215950
71	No	Show	71	H	-2.8117080	4.0099190	-0.3632550
72	No	Show	72	H	-2.6211530	5.2628870	1.7779740

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Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	H	3.9764630	-1.1583410	-1.2385640
2	No	Show	2	C	3.2100950	-1.9176100	-1.1517360
3	No	Show	3	C	3.4135490	-3.2873210	-0.8212350
4	No	Show	4	C	1.8056970	-1.7229340	-1.3508210
5	No	Show	5	C	2.1398530	-3.9380520	-0.7759970
6	No	Show	6	H	4.3664930	-3.7480370	-0.5918190

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7	No	Show	7	C	1.1351000	-2.9773060	-1.0931280
8	No	Show	8	Fe	2.2259890	-2.4037530	0.5739110
9	No	Show	9	C	2.1583080	-3.4259350	2.3323440
10	No	Show	10	C	1.0756400	-2.4995750	2.2796500
11	No	Show	11	C	3.3778270	-2.6860190	2.2262600
12	No	Show	12	H	2.0709300	-4.5038620	2.3939670
13	No	Show	13	C	1.6307070	-1.1884260	2.1579720
14	No	Show	14	H	0.0215150	-2.7486770	2.2869970
15	No	Show	15	C	3.0526430	-1.3025120	2.1024400
16	No	Show	16	H	4.3750300	-3.1076720	2.1931870
17	No	Show	17	H	1.0843210	-0.2550990	2.1223040
18	No	Show	18	H	3.7438050	-0.4841790	1.9397750
19	No	Show	19	H	1.3678880	-0.8653500	-1.8766560
20	No	Show	20	H	1.9680480	-4.9669080	-0.4836440
21	No	Show	21	C	-1.0754210	-1.9625900	-0.8345760
22	No	Show	22	C	-2.5132210	-2.0899340	-0.9666230
23	No	Show	23	C	-0.3296340	-3.0915390	-1.1097840
24	No	Show	24	N	-3.0005300	-3.3825990	-1.2272660
25	No	Show	25	C	-0.9672910	-4.3314160	-1.4189150
26	No	Show	26	N	-2.2642180	-4.4770810	-1.4602340
27	No	Show	27	Pd	0.0946380	-0.2842380	-0.2766000
28	No	Show	28	P	-1.5622010	1.2601270	0.1685960
29	No	Show	29	O	-3.3374600	-1.1662190	-0.8803560
30	No	Show	30	H	-0.3975650	-5.2323910	-1.6344830
31	No	Show	31	C	-2.8592130	0.6735890	1.3219140
32	No	Show	32	C	-2.4558460	-0.0676450	2.4392530
33	No	Show	33	C	-4.2154700	0.9683010	1.1499400
34	No	Show	34	C	-3.3915250	-0.4913450	3.3826420
35	No	Show	35	H	-1.4065920	-0.3199080	2.5741130
36	No	Show	36	C	-5.1501040	0.5413160	2.0922150
37	No	Show	37	H	-4.5495210	1.5055330	0.2678730
38	No	Show	38	C	-4.7423720	-0.1850020	3.2122360
39	No	Show	39	H	-3.0643400	-1.0649210	4.2463430
40	No	Show	40	H	-6.2029230	0.7683940	1.9436100
41	No	Show	41	H	-5.4743690	-0.5185290	3.9435750
42	No	Show	42	C	-2.3860390	1.9422770	-1.3221880
43	No	Show	43	C	-3.0375850	3.1838190	-1.2816570
44	No	Show	44	C	-2.3373750	1.2339930	-2.5280530
45	No	Show	45	C	-3.6461190	3.6974160	-2.4264420
46	No	Show	46	H	-3.0611580	3.7593390	-0.3598630
47	No	Show	47	C	-2.9386690	1.7540740	-3.6731070
48	No	Show	48	H	-1.8335160	0.2733190	-2.5629840
49	No	Show	49	C	-3.5965330	2.9836980	-3.6249760
50	No	Show	50	H	-4.1504870	4.6595160	-2.3821380
51	No	Show	51	H	-2.8932870	1.1952150	-4.6044130

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52	No	Show	52	H	-4.0642480	3.3879950	-4.5193890
53	No	Show	53	C	-0.9790860	2.8097890	0.9919160
54	No	Show	54	C	-1.5000480	3.2642100	2.2082710
55	No	Show	55	C	0.0055730	3.5748540	0.3489910
56	No	Show	56	C	-1.0392010	4.4570250	2.7745590
57	No	Show	57	H	-2.2684550	2.6950610	2.7225490
58	No	Show	58	C	0.4531770	4.7680360	0.9063610
59	No	Show	59	H	0.4287760	3.2333410	-0.5919670
60	No	Show	60	C	-0.0652950	5.2124300	2.1265660
61	No	Show	61	H	-1.4489550	4.7913310	3.7245480
62	No	Show	62	H	1.2156840	5.3476840	0.3923800
63	No	Show	63	H	0.2920610	6.1395170	2.5678300
64	No	Show	64	O	4.6037390	1.3023920	0.5603000
65	No	Show	65	C	-4.4439220	-3.5560940	-1.3188300
66	No	Show	66	H	-4.9213410	-3.1743000	-0.4139510
67	No	Show	67	H	-4.8403420	-2.9962100	-2.1701790
68	No	Show	68	H	-4.6383890	-4.6205760	-1.4400200
69	No	Show	69	C	4.3926610	2.0267820	-0.4075970
70	No	Show	70	H	1.0814880	0.9669660	0.0819820
71	No	Show	71	O	3.1856230	2.1174200	-1.0132560
72	No	Show	72	H	2.5500500	1.5525620	-0.5106290
73	No	Show	73	N	5.3337540	2.8180700	-0.9976940
74	No	Show	74	C	6.6805070	2.8355900	-0.4623980
75	No	Show	75	H	7.4007070	2.4996490	-1.2189060
76	No	Show	76	H	6.9558610	3.8507400	-0.1508090
77	No	Show	77	H	6.7305720	2.1720140	0.3991710
78	No	Show	78	C	5.0784770	3.6658860	-2.1468480
79	No	Show	79	H	5.2735920	4.7167480	-1.8980350
80	No	Show	80	H	5.7344780	3.3853930	-2.9804990
81	No	Show	81	H	4.0443790	3.5668190	-2.4671250

### 34b+32

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	0.5600290	2.0351690	-0.6786840
2	No	Show	2	C	1.3670550	1.9290190	-1.8791670
3	No	Show	3	C	0.3942770	3.2901170	-0.1379950
4	No	Show	4	N	1.9965230	3.1144200	-2.2903080
5	No	Show	5	C	1.0772760	4.4154370	-0.6898570
6	No	Show	6	N	1.8621440	4.3259960	-1.7300600
7	No	Show	7	Pd	-0.5093630	0.5681510	0.3648060
8	No	Show	8	P	0.9424930	-1.1870660	0.2766310
9	No	Show	9	O	1.5337570	0.9074910	-2.5641660
10	No	Show	10	H	0.9712330	5.4170140	-0.2790030
11	No	Show	11	C	2.6773910	-0.7859340	-0.1581240
12	No	Show	12	C	3.3013300	0.2487480	0.5514710

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13	No	Show	13	C	3.4032490	-1.4945260	-1.1204970
14	No	Show	14	C	4.6362710	0.5625280	0.3076680
15	No	Show	15	H	2.7396600	0.8154220	1.2908550
16	No	Show	16	C	4.7396700	-1.1754310	-1.3651160
17	No	Show	17	H	2.9285860	-2.2885610	-1.6896040
18	No	Show	18	C	5.3595410	-0.1498090	-0.6522210
19	No	Show	19	H	5.1098970	1.3686660	0.8622930
20	No	Show	20	H	5.2933880	-1.7282790	-2.1199160
21	No	Show	21	H	6.4000520	0.0985880	-0.8461960
22	No	Show	22	C	0.3898370	-2.4457440	-0.9298490
23	No	Show	23	C	0.0907160	-3.7599060	-0.5511890
24	No	Show	24	C	0.2143430	-2.0467710	-2.2646380
25	No	Show	25	C	-0.3670550	-4.6737380	-1.5019570
26	No	Show	26	H	0.2076360	-4.0749360	0.4818610
27	No	Show	27	C	-0.2342440	-2.9692280	-3.2079520
28	No	Show	28	H	0.4473130	-1.0233390	-2.5557140
29	No	Show	29	C	-0.5273250	-4.2820310	-2.8307610
30	No	Show	30	H	-0.5989400	-5.6919760	-1.1996570
31	No	Show	31	H	-0.3602220	-2.6566890	-4.2415500
32	No	Show	32	H	-0.8826030	-4.9960580	-3.5698110
33	No	Show	33	C	1.1785600	-2.0893990	1.8674050
34	No	Show	34	C	2.2924720	-2.9309600	2.0251610
35	No	Show	35	C	0.2766060	-1.9558190	2.9288770
36	No	Show	36	C	2.4845390	-3.6354520	3.2117030
37	No	Show	37	H	3.0166020	-3.0345360	1.2219390
38	No	Show	38	C	0.4733510	-2.6594830	4.1185370
39	No	Show	39	H	-0.5798950	-1.2965130	2.8172980
40	No	Show	40	C	1.5747760	-3.5016770	4.2629070
41	No	Show	41	H	3.3502580	-4.2846090	3.3164210
42	No	Show	42	H	-0.2358040	-2.5418260	4.9339680
43	No	Show	43	H	1.7294050	-4.0463670	5.1910190
44	No	Show	44	O	-3.9849760	0.7577460	-0.4078100
45	No	Show	45	C	2.8422750	3.0558750	-3.4751090
46	No	Show	46	H	3.5943320	2.2735930	-3.3540180
47	No	Show	47	H	2.2425780	2.8153890	-4.3570850
48	No	Show	48	H	3.3119490	4.0313940	-3.5902490
49	No	Show	49	C	-4.3077800	-0.4236870	-0.5242940
50	No	Show	50	H	-1.4060090	-0.5245200	1.2114580
51	No	Show	51	O	-3.5636980	-1.4381580	-0.0372170
52	No	Show	52	H	-2.7507400	-1.0322760	0.3557790
53	No	Show	53	N	-5.4432550	-0.8500910	-1.1453260
54	No	Show	54	C	-6.3520990	0.1260710	-1.7118240
55	No	Show	55	H	-6.4578130	-0.0291310	-2.7927420
56	No	Show	56	H	-7.3445190	0.0396940	-1.2520370
57	No	Show	57	H	-5.9594310	1.1253710	-1.5319170

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58	No	Show	58	C	-5.8080820	-2.2462940	-1.2921650
59	No	Show	59	H	-6.7605760	-2.4495010	-0.7862570
60	No	Show	60	H	-5.9239510	-2.4982580	-2.3537280
61	No	Show	61	H	-5.0385410	-2.8833370	-0.8633360
62	No	Show	62	C	-0.5227390	3.3954540	1.0179950
63	No	Show	63	C	-0.2439000	4.1586620	2.1590180
64	No	Show	64	C	-1.7030120	2.6166170	0.9965230
65	No	Show	65	C	-1.1049070	4.1269130	3.2556000
66	No	Show	66	H	0.6656380	4.7528360	2.2031100
67	No	Show	67	C	-2.5556180	2.5787950	2.1058550
68	No	Show	68	H	-2.0655150	2.1805300	0.0553660
69	No	Show	69	C	-2.2554930	3.3317170	3.2391650
70	No	Show	70	H	-0.8707460	4.7192240	4.1370380
71	No	Show	71	H	-3.4596530	1.9805210	2.0468280
72	No	Show	72	H	-2.9166890	3.3131990	4.1015620

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Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	H		3.6452530	1.3343570	1.3565850
2	No	Show	2	C		2.8380590	2.0347070	1.1851590
3	No	Show	3	C		2.9658600	3.4083200	0.8338570
4	No	Show	4	C		1.4408840	1.7452190	1.3004150
5	No	Show	5	C		1.6583220	3.9699210	0.7013410
6	No	Show	6	H		3.8977460	3.9305700	0.6543780
7	No	Show	7	C		0.7045300	2.9469820	0.9660870
8	No	Show	8	Fe		1.9344850	2.4129030	-0.6142620
9	No	Show	9	C		2.0282480	3.4550630	-2.3580300
10	No	Show	10	C		0.9113170	2.5705310	-2.3980260
11	No	Show	11	C		3.2092030	2.6670230	-2.1818630
12	No	Show	12	H		1.9838770	4.5362830	-2.4028420
13	No	Show	13	C		1.4055160	1.2377150	-2.2597570
14	No	Show	14	H		-0.1295510	2.8596540	-2.4768380
15	No	Show	15	C		2.8269560	1.2967690	-2.1034710
16	No	Show	16	H		4.2167170	3.0495040	-2.0725660
17	No	Show	17	H		0.8246640	0.3247340	-2.3148600
18	No	Show	18	H		3.4819810	0.4502430	-1.9311320
19	No	Show	19	H		1.0307170	0.8714540	1.8152490
20	No	Show	20	H		1.4133960	4.9806400	0.4062360
21	No	Show	21	C		-0.7531540	2.9468750	0.8106220
22	No	Show	22	C		-1.4865750	4.1884430	0.9970680
23	No	Show	23	C		-1.3846790	1.7709790	0.4437000
24	No	Show	24	N		-2.8691980	4.0526240	0.8600760
25	No	Show	25	C		-2.8049990	1.8508480	0.3324910
26	No	Show	26	N		-3.5247560	2.9306980	0.5372880
27	No	Show	27	Pd		-0.0044830	0.1918220	0.0334510



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28	No	Show	28	P	-1.4385180	-1.6049930	-0.0994860
29	No	Show	29	O	-1.0006880	5.3010470	1.2455890
30	No	Show	30	H	-3.4061900	0.9878500	0.0612600
31	No	Show	31	C	-2.9247520	-1.3036890	-1.1335270
32	No	Show	32	C	-2.7574390	-0.6101770	-2.3410860
33	No	Show	33	C	-4.2045490	-1.7425000	-0.7708750
34	No	Show	34	C	-3.8457470	-0.3755980	-3.1788230
35	No	Show	35	H	-1.7736560	-0.2396000	-2.6192020
36	No	Show	36	C	-5.2956400	-1.4958130	-1.6062040
37	No	Show	37	H	-4.3567100	-2.2682100	0.1675760
38	No	Show	38	C	-5.1188590	-0.8167650	-2.8117070
39	No	Show	39	H	-3.7017740	0.1651770	-4.1105520
40	No	Show	40	H	-6.2857530	-1.8320750	-1.3091150
41	No	Show	41	H	-5.9708950	-0.6221880	-3.4578760
42	No	Show	42	C	-2.0958720	-2.1096790	1.5417700
43	No	Show	43	C	-2.4506310	-3.4381370	1.8188540
44	No	Show	44	C	-2.2579710	-1.1373220	2.5380760
45	No	Show	45	C	-2.9678460	-3.7828630	3.0676740
46	No	Show	46	H	-2.3167670	-4.2082550	1.0639270
47	No	Show	47	C	-2.7821170	-1.4842590	3.7826580
48	No	Show	48	H	-1.9688830	-0.1086460	2.3384840
49	No	Show	49	C	-3.1373260	-2.8069070	4.0508760
50	No	Show	50	H	-3.2350710	-4.8166780	3.2718930
51	No	Show	51	H	-2.9042090	-0.7195210	4.5453540
52	No	Show	52	H	-3.5378340	-3.0777390	5.0245360
53	No	Show	53	C	-0.7796130	-3.1849330	-0.7781990
54	No	Show	54	C	-1.4268650	-3.8834700	-1.8037180
55	No	Show	55	C	0.3955750	-3.7167460	-0.2279740
56	No	Show	56	C	-0.9050010	-5.0913400	-2.2747060
57	No	Show	57	H	-2.3388840	-3.4918150	-2.2440850
58	No	Show	58	C	0.9044920	-4.9278180	-0.6877770
59	No	Show	59	H	0.9186810	-3.1780980	0.5575510
60	No	Show	60	C	0.2581780	-5.6175960	-1.7172390
61	No	Show	61	H	-1.4132690	-5.6169670	-3.0791780
62	No	Show	62	H	1.8157690	-5.3273420	-0.2504180
63	No	Show	63	H	0.6648540	-6.5563920	-2.0846050
64	No	Show	64	O	4.5766930	-1.3885620	-0.9259370
65	No	Show	65	C	-3.6856110	5.2437580	1.0500010
66	No	Show	66	H	-3.4873110	5.6800590	2.0314700
67	No	Show	67	H	-3.4430470	5.9938790	0.2927500
68	No	Show	68	H	-4.7275010	4.9400160	0.9656860
69	No	Show	69	C	4.5061780	-1.7361670	0.2482650
70	No	Show	70	H	1.1337950	-0.9537750	-0.2291420
71	No	Show	71	O	3.3793060	-1.6050980	0.9897690
72	No	Show	72	H	2.6776110	-1.2302490	0.4043250

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73	No	Show	73	N	5.5346470	-2.2867690	0.9545380
74	No	Show	74	C	6.8119160	-2.4909200	0.3000960
75	No	Show	75	H	7.6020030	-1.9305200	0.8151400
76	No	Show	76	H	7.0818630	-3.5542340	0.3082140
77	No	Show	77	H	6.7430910	-2.1478400	-0.7307760
78	No	Show	78	C	5.4422250	-2.6895080	2.3452720
79	No	Show	79	H	5.6441350	-3.7633170	2.4471590
80	No	Show	80	H	6.1792120	-2.1455510	2.9493710
81	No	Show	81	H	4.4487360	-2.4804320	2.7339140

### 35b+32

Row	Highlight		Display Tag	Symbol	X	Y	Z
1	No	Show	1	C	-1.7034580	2.8554230	-0.1791510
2	No	Show	2	C	-2.8143200	3.7549310	0.0865310
3	No	Show	3	C	-1.8924740	1.5064790	-0.4049770
4	No	Show	4	N	-4.0646540	3.1338710	0.0009280
5	No	Show	5	C	-3.2480170	1.0624190	-0.4271240
6	No	Show	6	N	-4.2921530	1.8377440	-0.2469390
7	No	Show	7	Pd	0.0082030	0.5562760	-0.4783310
8	No	Show	8	P	-0.5829840	-1.6071910	-0.0083830
9	No	Show	9	O	-2.7456030	4.9585050	0.3674490
10	No	Show	10	H	-3.5075010	0.0244590	-0.6135610
11	No	Show	11	C	-2.0238180	-2.1648620	-0.9954630
12	No	Show	12	C	-2.0321890	-1.8686050	-2.3669410
13	No	Show	13	C	-3.0995750	-2.8673930	-0.4391590
14	No	Show	14	C	-3.0907440	-2.2856390	-3.1707620
15	No	Show	15	H	-1.2131900	-1.3003320	-2.8026840
16	No	Show	16	C	-4.1643350	-3.2741120	-1.2459520
17	No	Show	17	H	-3.1164650	-3.0892940	0.6242190
18	No	Show	18	C	-4.1604680	-2.9885810	-2.6111110
19	No	Show	19	H	-3.0869550	-2.0494610	-4.2316340
20	No	Show	20	H	-4.9993220	-3.8103800	-0.8023790
21	No	Show	21	H	-4.9925860	-3.3025860	-3.2358700
22	No	Show	22	C	-1.0650320	-1.8456170	1.7467020
23	No	Show	23	C	-0.9192820	-3.0853070	2.3860480
24	No	Show	24	C	-1.6020200	-0.7655960	2.4603080
25	No	Show	25	C	-1.3173270	-3.2421490	3.7135130
26	No	Show	26	H	-0.4892150	-3.9280700	1.8516920
27	No	Show	27	C	-2.0035410	-0.9277510	3.7856800
28	No	Show	28	H	-1.7001990	0.2039050	1.9785130
29	No	Show	29	C	-1.8621830	-2.1653390	4.4148330
30	No	Show	30	H	-1.1968030	-4.2067160	4.2001610
31	No	Show	31	H	-2.4186830	-0.0822800	4.3278910
32	No	Show	32	H	-2.1683200	-2.2888120	5.4505690
33	No	Show	33	C	0.6556390	-2.9374420	-0.2865390

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34	No	Show	34	C	0.3460380	-4.1043940	-0.9950520
35	No	Show	35	C	1.9370270	-2.7907460	0.2627830
36	No	Show	36	C	1.3056460	-5.1070080	-1.1553640
37	No	Show	37	H	-0.6416190	-4.2390560	-1.4260420
38	No	Show	38	C	2.8867660	-3.7974920	0.1128250
39	No	Show	39	H	2.1978800	-1.8842420	0.8017540
40	No	Show	40	C	2.5754000	-4.9577220	-0.6010060
41	No	Show	41	H	1.0547990	-6.0038810	-1.7160990
42	No	Show	42	H	3.8763030	-3.6681020	0.5430220
43	No	Show	43	H	3.3221580	-5.7373450	-0.7284840
44	No	Show	44	O	4.7196080	1.1762920	-1.5585280
45	No	Show	45	C	-5.2426800	3.9633630	0.2184740
46	No	Show	46	H	-5.1995720	4.4253400	1.2073510
47	No	Show	47	H	-5.2820600	4.7626000	-0.5257540
48	No	Show	48	H	-6.1144370	3.3173710	0.1322230
49	No	Show	49	C	4.9640340	0.7714330	-0.4267790
50	No	Show	50	H	1.5280060	-0.0388920	-0.5277600
51	No	Show	51	O	4.0046370	0.3205280	0.4170190
52	No	Show	52	H	3.1432970	0.3914860	-0.0561820
53	No	Show	53	N	6.2118540	0.7147960	0.1211680
54	No	Show	54	C	7.3500730	1.1396810	-0.6692450
55	No	Show	55	H	7.8655430	1.9776310	-0.1834190
56	No	Show	56	H	8.0652860	0.3160960	-0.7867850
57	No	Show	57	H	7.0037060	1.4544860	-1.6521850
58	No	Show	58	C	6.4895940	0.2490140	1.4661350
59	No	Show	59	H	7.1464540	-0.6299180	1.4405760
60	No	Show	60	H	6.9935110	1.0343280	2.0435270
61	No	Show	61	H	5.5651460	-0.0165900	1.9729540
62	No	Show	62	C	-0.3105440	3.3374180	-0.1690700
63	No	Show	63	C	0.1880790	4.2571490	0.7644170
64	No	Show	64	C	0.5918790	2.7641230	-1.1035510
65	No	Show	65	C	1.5488300	4.5554220	0.7899600
66	No	Show	66	H	-0.4959810	4.7310370	1.4589050
67	No	Show	67	C	1.9636020	3.0664570	-1.0619020
68	No	Show	68	H	0.1871810	2.2666930	-1.9952200
69	No	Show	69	C	2.4426370	3.9538240	-0.1043730
70	No	Show	70	H	1.9211770	5.2677600	1.5224250
71	No	Show	71	H	2.6440270	2.6162690	-1.7784740
72	No	Show	72	H	3.5019850	4.1899160	-0.0660080

### 36a

Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	H	-	2.9967190	-3.3354530	-1.5844560
2	No	Show	2	C	-	3.2751180	-2.3441130	-1.2510230
3	No	Show	3	C	-	4.5343340	-1.9545590	-0.7078640

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4	No	Show	4	C	-2.4646400	-1.1708900	-1.3476710
5	No	Show	5	C	-4.5012240	-0.5532890	-0.4392660
6	No	Show	6	H	-5.3647690	-2.6182930	-0.5000350
7	No	Show	7	C	-3.2216920	-0.0575940	-0.8268640
8	No	Show	8	Fe	-3.0420500	-1.5420560	0.6153690
9	No	Show	9	C	-3.6360720	-1.1823340	2.5298250
10	No	Show	10	C	-2.2837700	-0.7617900	2.3591550
11	No	Show	11	C	-3.7017480	-2.5788310	2.2362300
12	No	Show	12	H	-4.4742030	-0.5452170	2.7838700
13	No	Show	13	C	-1.5096600	-1.8986500	1.9686030
14	No	Show	14	H	-1.9208010	0.2525140	2.4679480
15	No	Show	15	C	-2.3892330	-3.0181240	1.8828670
16	No	Show	16	H	-4.5975220	-3.1877200	2.2384230
17	No	Show	17	H	-0.4513170	-1.9258320	1.7424200
18	No	Show	18	H	-2.1124470	-4.0223570	1.5859530
19	No	Show	19	H	-1.5495000	-1.1206700	-1.9446760
20	No	Show	20	H	-5.2877030	0.0417190	0.0026010
21	No	Show	21	C	-2.6707590	1.2952670	-0.7770430
22	No	Show	22	C	-3.5808620	2.4300560	-0.8841480
23	No	Show	23	C	-1.3051120	1.4886340	-0.6989760
24	No	Show	24	N	-2.9426430	3.6575950	-1.0611390
25	No	Show	25	C	-0.8437880	2.8233560	-0.9010080
26	No	Show	26	N	-1.6209410	3.8605500	-1.0995320
27	No	Show	27	Pd	-0.2273010	-0.2306410	-0.4077870
28	No	Show	28	P	1.8031100	0.7154920	0.2288160
29	No	Show	29	O	-4.8158710	2.3812150	-0.8361080
30	No	Show	30	H	0.2119390	3.0687180	-0.9328500
31	No	Show	31	C	1.7329270	2.3852270	0.9878800
32	No	Show	32	C	0.7197640	2.6485340	1.9215500
33	No	Show	33	C	2.6676320	3.3858960	0.6964750
34	No	Show	34	C	0.6533440	3.8822560	2.5649040
35	No	Show	35	H	-0.0277300	1.8886340	2.1358570
36	No	Show	36	C	2.5920410	4.6256190	1.3336750
37	No	Show	37	H	3.4519970	3.2081350	-0.0335260
38	No	Show	38	C	1.5895110	4.8752560	2.2705750
39	No	Show	39	H	-0.1390940	4.0727290	3.2838330
40	No	Show	40	H	3.3185390	5.3973220	1.0924840
41	No	Show	41	H	1.5308360	5.8430570	2.7616920
42	No	Show	42	C	2.9046320	0.8822010	-1.2230590
43	No	Show	43	C	4.3016530	0.8784330	-1.0985390
44	No	Show	44	C	2.3301350	1.0519040	-2.4897580
45	No	Show	45	C	5.1061140	1.0522710	-2.2238580
46	No	Show	46	H	4.7623620	0.7328700	-0.1253090
47	No	Show	47	C	3.1376910	1.2318220	-3.6122400
48	No	Show	48	H	1.2480270	1.0339330	-2.5972930

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49	No	Show	49	C	4.5266050	1.2321470	-3.4811610
50	No	Show	50	H	6.1878270	1.0429130	-2.1172500
51	No	Show	51	H	2.6797090	1.3605750	-4.5893680
52	No	Show	52	H	5.1566900	1.3631220	-4.3571570
53	No	Show	53	C	2.7748830	-0.2398250	1.4586740
54	No	Show	54	C	2.9651390	0.2462000	2.7606470
55	No	Show	55	C	3.3520390	-1.4676270	1.0935510
56	No	Show	56	C	3.7179690	-0.4797550	3.6837960
57	No	Show	57	H	2.5423050	1.1982400	3.0646910
58	No	Show	58	C	4.1155370	-2.1773140	2.0188240
59	No	Show	59	H	3.1961730	-1.8865750	0.1034970
60	No	Show	60	C	4.2984670	-1.6922320	3.3148280
61	No	Show	61	H	3.8553510	-0.0879380	4.6884400
62	No	Show	62	H	4.5610400	-3.1226800	1.7204440
63	No	Show	63	H	4.8907830	-2.2550270	4.0322480
64	No	Show	64	O	0.8189350	-2.0335930	-0.2246360
65	No	Show	65	C	-3.7820200	4.8353740	-1.2380160
66	No	Show	66	H	-4.4796810	4.6748200	-2.0627630
67	No	Show	67	H	-4.3654570	5.0230710	-0.3331190
68	No	Show	68	H	-3.1223840	5.6754060	-1.4476960
69	No	Show	69	C	1.0438370	-2.6984980	-1.3901380
70	No	Show	70	H	1.3140970	-2.0436970	-2.2368930
71	No	Show	71	O	-0.1654250	-3.3652530	-1.8348660
72	No	Show	72	H	-0.6678260	-3.4898210	-1.0134830
73	No	Show	73	N	2.1585270	-3.6312280	-1.2370460
74	No	Show	74	C	1.9259180	-4.6296650	-0.2020470
75	No	Show	75	H	1.1500880	-5.3648400	-0.4785050
76	No	Show	76	H	2.8547560	-5.1793770	-0.0149990
77	No	Show	77	H	1.6288810	-4.1292260	0.7219080
78	No	Show	78	C	2.5304650	-4.2508810	-2.5007980
79	No	Show	79	H	3.4535870	-4.8247510	-2.3646360
80	No	Show	80	H	1.7549190	-4.9254150	-2.8986980
81	No	Show	81	H	2.7264000	-3.4765700	-3.2498680

### 36b

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	3.1583980	0.5608990	-0.2523500
2	No	Show	2	C	4.5056890	0.0431400	-0.4321420
3	No	Show	3	C	2.0620170	-0.1497920	-0.6545930
4	No	Show	4	N	4.5486800	-1.1595460	-1.1457470
5	No	Show	5	C	2.2995540	-1.3809980	-1.3409770
6	No	Show	6	N	3.4947810	-1.8486460	-1.6018020
7	No	Show	7	Pd	0.3446360	0.8212430	-0.1882020
8	No	Show	8	P	-0.9724470	-1.0214370	0.2369980
9	No	Show	9	O	5.5487200	0.5590010	-0.0200180

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10	No	Show	10	H	1.4926850	-1.9980340	-1.7254000
11	No	Show	11	C	-0.0395760	-2.5388590	0.6667030
12	No	Show	12	C	1.0610930	-2.4154320	1.5280510
13	No	Show	13	C	-0.3983640	-3.8050070	0.1892420
14	No	Show	14	C	1.7739540	-3.5444190	1.9257300
15	No	Show	15	H	1.3672590	-1.4322350	1.8794840
16	No	Show	16	C	0.3255830	-4.9322340	0.5808790
17	No	Show	17	H	-1.2353090	-3.9183230	-0.4937260
18	No	Show	18	C	1.4075690	-4.8058110	1.4520000
19	No	Show	19	H	2.6245840	-3.4356830	2.5933080
20	No	Show	20	H	0.0430850	-5.9099430	0.1991900
21	No	Show	21	H	1.9714490	-5.6853950	1.7514820
22	No	Show	22	C	-1.9659810	-1.4447240	-1.2386570
23	No	Show	23	C	-3.1910400	-2.1189970	-1.1308190
24	No	Show	24	C	-1.4719670	-1.1196020	-2.5090930
25	No	Show	25	C	-3.9017430	-2.4682090	-2.2781650
26	No	Show	26	H	-3.5948270	-2.3647490	-0.1524380
27	No	Show	27	C	-2.1827940	-1.4758490	-3.6546070
28	No	Show	28	H	-0.5327220	-0.5789200	-2.6018600
29	No	Show	29	C	-3.3985150	-2.1507120	-3.5409370
30	No	Show	30	H	-4.8529150	-2.9855470	-2.1832700
31	No	Show	31	H	-1.7901070	-1.2161230	-4.6340670
32	No	Show	32	H	-3.9571900	-2.4207940	-4.4333180
33	No	Show	33	C	-2.1760570	-0.8501570	1.6093040
34	No	Show	34	C	-2.0278300	-1.5912840	2.7907360
35	No	Show	35	C	-3.2661790	0.0256080	1.4782250
36	No	Show	36	C	-2.9570110	-1.4664320	3.8235600
37	No	Show	37	H	-1.1992410	-2.2810220	2.9130360
38	No	Show	38	C	-4.1962890	0.1319830	2.5101170
39	No	Show	39	H	-3.3848640	0.6455890	0.5942490
40	No	Show	40	C	-4.0460390	-0.6070780	3.6846720
41	No	Show	41	H	-2.8285650	-2.0491120	4.7321830
42	No	Show	42	H	-5.0373810	0.8104230	2.3938860
43	No	Show	43	H	-4.7728030	-0.5121670	4.4878210
44	No	Show	44	O	-1.3837550	1.9199750	0.1518680
45	No	Show	45	C	5.8611790	-1.7282340	-1.4254880
46	No	Show	46	H	6.4840630	-0.9914850	-1.9371300
47	No	Show	47	H	6.3596530	-2.0033680	-0.4926550
48	No	Show	48	H	5.7088750	-2.6064370	-2.0501450
49	No	Show	49	C	-2.0071490	2.3658050	-0.9745050
50	No	Show	50	H	-2.0162120	1.6379780	-1.8049460
51	No	Show	51	O	-1.3061630	3.5076770	-1.5246170
52	No	Show	52	H	-0.8776430	3.8974610	-0.7462680
53	No	Show	53	N	-3.4094000	2.6631870	-0.6912380
54	No	Show	54	C	-3.5757410	3.6681180	0.3508680

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55	No	Show	55	H	-3.2698720	4.6781720	0.0277230
56	No	Show	56	H	-4.6308570	3.7159110	0.6421290
57	No	Show	57	H	-2.9872050	3.3820330	1.2251690
58	No	Show	58	C	-4.1494230	3.0119580	-1.8952360
59	No	Show	59	H	-5.2162590	3.0840120	-1.6566180
60	No	Show	60	H	-3.8266430	3.9668340	-2.3416600
61	No	Show	61	H	-4.0280740	2.2249610	-2.6472510
62	No	Show	62	C	2.9624170	1.8691850	0.3714120
63	No	Show	63	C	3.5450260	2.2066400	1.6056120
64	No	Show	64	C	2.1624150	2.8192040	-0.2927100
65	No	Show	65	C	3.3227570	3.4620680	2.1610370
66	No	Show	66	H	4.1728190	1.4885500	2.1105040
67	No	Show	67	C	1.9576140	4.0872840	0.2670440
68	No	Show	68	H	1.7720890	2.6053850	-1.2854430
69	No	Show	69	C	2.5350750	4.4076940	1.4911050
70	No	Show	70	H	3.7752500	3.7139020	3.1114140
71	No	Show	71	H	1.3744040	4.8189830	-0.2739360
72	No	Show	72	H	2.3852220	5.3907770	1.9183880

### 37

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	3.2492550	-0.3952300	-0.0244980
2	No	Show	2	C	4.5658590	0.2027920	0.0159230
3	No	Show	3	C	2.0777180	0.2838660	-0.0302780
4	No	Show	4	N	4.4765740	1.6051470	0.0518940
5	No	Show	5	C	2.2071920	1.7062320	0.0036250
6	No	Show	6	N	3.3563980	2.3379320	0.0441540
7	No	Show	7	Pd	0.5026560	-1.1234560	-0.0896330
8	No	Show	8	P	-1.5928150	-0.0399020	-0.0063640
9	No	Show	9	O	5.6573430	-0.3636230	0.0221220
10	No	Show	10	H	1.3378090	2.3583750	-0.0089460
11	No	Show	11	C	-1.6000050	1.5346210	-0.9468040
12	No	Show	12	C	-0.9330130	1.5610370	-2.1808110
13	No	Show	13	C	-2.2273360	2.6987550	-0.4842290
14	No	Show	14	C	-0.9130440	2.7244470	-2.9479050
15	No	Show	15	H	-0.4157480	0.6709190	-2.5328290
16	No	Show	16	C	-2.1952130	3.8663520	-1.2490920
17	No	Show	17	H	-2.7354190	2.7003040	0.4763680
18	No	Show	18	C	-1.5430110	3.8806380	-2.4823490
19	No	Show	19	H	-0.3915220	2.7322530	-3.9014620
20	No	Show	20	H	-2.6785620	4.7661180	-0.8768300
21	No	Show	21	H	-1.5159750	4.7919970	-3.0741350
22	No	Show	22	C	-2.1194530	0.4286810	1.6878600
23	No	Show	23	C	-3.4642930	0.4587000	2.0826960
24	No	Show	24	C	-1.1260670	0.7698910	2.6176260

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25	No	Show	25	C	-3.8080170	0.8330170	3.3822940
26	No	Show	26	H	-4.2456330	0.1842270	1.3786860
27	No	Show	27	C	-1.4734240	1.1535920	3.9120870
28	No	Show	28	H	-0.0786290	0.7246490	2.3271630
29	No	Show	29	C	-2.8149500	1.1847250	4.2976850
30	No	Show	30	H	-4.8538900	0.8482490	3.6786700
31	No	Show	31	H	-0.6941610	1.4165930	4.6227100
32	No	Show	32	H	-3.0846010	1.4743980	5.3101050
33	No	Show	33	C	-3.0340310	-0.9672270	-0.6687980
34	No	Show	34	C	-3.9430120	-0.4268490	-1.5872630
35	No	Show	35	C	-3.2018600	-2.2952770	-0.2454360
36	No	Show	36	C	-5.0047080	-1.1985720	-2.0645690
37	No	Show	37	H	-3.8260710	0.5966750	-1.9326430
38	No	Show	38	C	-4.2687210	-3.0587220	-0.7128420
39	No	Show	39	H	-2.4947990	-2.7332630	0.4570310
40	No	Show	40	C	-5.1726220	-2.5121500	-1.6275030
41	No	Show	41	H	-5.7019880	-0.7682990	-2.7791430
42	No	Show	42	H	-4.3890540	-4.0836860	-0.3715300
43	No	Show	43	H	-5.9995300	-3.1104480	-2.0012390
44	No	Show	44	Br	3.1538580	-2.3208720	-0.0796500
45	No	Show	45	C	5.7326980	2.3449540	0.0964290
46	No	Show	46	H	6.3030950	2.0604720	0.9835770
47	No	Show	47	H	6.3355470	2.1119920	-0.7843170
48	No	Show	48	H	5.4849620	3.4042730	0.1226790

### 37 (L=NHC)

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	-2.6104110	-0.0412760	-0.8583540
2	No	Show	2	C	-3.1604330	-0.0423210	-2.1848910
3	No	Show	3	C	-3.5478320	-0.0486320	0.1286980
4	No	Show	4	C	-4.9832880	-0.0559730	-0.0928150
5	No	Show	5	N	-5.3029800	-0.0553420	-1.4577490
6	No	Show	6	H	-2.5127190	-0.0373540	-3.0587630
7	No	Show	7	N	-4.4369510	-0.0489740	-2.4787180
8	No	Show	8	O	-5.8761490	-0.0623760	0.7550720
9	No	Show	9	C	1.4967710	0.0210590	-0.0087350
10	No	Show	10	Pd	-0.5864660	-0.0205590	-0.4299490
11	No	Show	11	C	3.6303280	0.7361530	0.3484690
12	No	Show	12	C	3.6539170	-0.6212580	0.3459500
13	No	Show	13	N	2.3486950	-1.0363620	0.1286670
14	No	Show	14	N	2.3113640	1.1066290	0.1324940
15	No	Show	15	C	1.9480030	-2.4176390	0.0504260
16	No	Show	16	C	1.9073050	-3.0381410	-1.2119180
17	No	Show	17	C	1.6349350	-3.0977660	1.2418930
18	No	Show	18	C	1.5323050	-4.3849730	-1.2569910



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19	No	Show	19	C	1.2723050	-4.4449800	1.1389250
20	No	Show	20	C	1.2193260	-5.0834680	-0.0956130
21	No	Show	21	H	1.4820500	-4.8950210	-2.2155020
22	No	Show	22	H	1.0203050	-5.0011590	2.0381040
23	No	Show	23	H	0.9283870	-6.1294220	-0.1532410
24	No	Show	24	C	1.8628570	2.4735240	0.0588420
25	No	Show	25	C	1.5212170	3.1367440	1.2519550
26	No	Show	26	C	1.8042280	3.0974990	-1.2009880
27	No	Show	27	C	1.1074180	4.4693710	1.1528730
28	No	Show	28	C	1.3775790	4.4290090	-1.2423630
29	No	Show	29	C	1.0334850	5.1101080	-0.0794520
30	No	Show	30	H	0.8313320	5.0117270	2.0534080
31	No	Show	31	H	1.3112560	4.9402960	-2.1991790
32	No	Show	32	H	0.7025710	6.1442740	-0.1340420
33	No	Show	33	H	4.4687720	-1.3179980	0.4754560
34	No	Show	34	H	4.4202140	1.4605980	0.4806100
35	No	Show	35	C	2.2458770	-2.3069820	-2.5010910
36	No	Show	36	H	2.5281650	-1.2820120	-2.2455350
37	No	Show	37	C	1.6817320	-2.4303630	2.6070450
38	No	Show	38	H	1.9058630	-1.3701330	2.4593200
39	No	Show	39	C	1.0261410	-2.2214430	-3.4296750
40	No	Show	40	H	1.2686990	-1.6409380	-4.3261440
41	No	Show	41	H	0.6967810	-3.2136150	-3.7554220
42	No	Show	42	H	0.1828400	-1.7374840	-2.9269460
43	No	Show	43	C	3.4465420	-2.9452370	-3.2150380
44	No	Show	44	H	3.7164740	-2.3610340	-4.1012860
45	No	Show	45	H	4.3227150	-2.9920340	-2.5606160
46	No	Show	46	H	3.2249940	-3.9645440	-3.5476010
47	No	Show	47	C	0.3258980	-2.5077640	3.3230580
48	No	Show	48	H	0.3653770	-1.9511870	4.2654280
49	No	Show	49	H	-0.4732860	-2.0820720	2.7105300
50	No	Show	50	H	0.0530540	-3.5403330	3.5641110
51	No	Show	51	C	2.8032800	-3.0195710	3.4764430
52	No	Show	52	H	3.7798740	-2.9306360	2.9896740
53	No	Show	53	H	2.8553220	-2.4963820	4.4371690
54	No	Show	54	H	2.6319670	-4.0808130	3.6850330
55	No	Show	55	C	1.5925490	2.4670730	2.6147420
56	No	Show	56	H	1.8529580	1.4157140	2.4632120
57	No	Show	57	C	2.1736470	2.3840440	-2.4916040
58	No	Show	58	H	2.5232350	1.3799040	-2.2360520
59	No	Show	59	C	3.3231970	3.0919220	-3.2237350
60	No	Show	60	H	3.0330270	4.0903970	-3.5663340
61	No	Show	61	H	4.2001680	3.2032240	-2.5782480
62	No	Show	62	H	3.6225920	2.5160540	-4.1059030
63	No	Show	63	C	0.9494600	2.2185450	-3.4035750

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64	No	Show	64	H	0.5497660	3.1875530	-3.7202140
65	No	Show	65	H	1.2172550	1.6576630	-4.3053890
66	No	Show	66	H	0.1476920	1.6782220	-2.8901310
67	No	Show	67	C	0.2362480	2.4950040	3.3334580
68	No	Show	68	H	-0.5487500	2.0437690	2.7208860
69	No	Show	69	H	0.2969680	1.9369040	4.2738060
70	No	Show	70	H	-0.0720430	3.5165370	3.5787850
71	No	Show	71	C	2.6946140	3.0922590	3.4840970
72	No	Show	72	H	3.6727600	3.0392720	2.9951920
73	No	Show	73	H	2.4865730	4.1461740	3.6964610
74	No	Show	74	H	2.7668480	2.5680520	4.4429620
75	No	Show	75	Br	-3.0174010	-0.0499140	1.9694190
76	No	Show	76	C	-6.7173590	-0.0626560	-1.8080900
77	No	Show	77	H	-7.2021450	-0.9500410	-1.3942490
78	No	Show	78	H	-7.2119210	0.8181910	-1.3918460
79	No	Show	79	H	-6.7822660	-0.0615300	-2.8946300

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Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	-2.2450480	-1.4159430	0.8427980
2	No	Show	2	C	-2.8059150	-1.4079910	2.1641580
3	No	Show	3	C	-3.0743100	-1.9106210	-0.1182570
4	No	Show	4	N	-4.0009410	-1.8385670	2.4845370
5	No	Show	5	C	-4.4146850	-2.4130080	0.1399780
6	No	Show	6	N	-4.7640400	-2.3211040	1.4954660
7	No	Show	7	Pd	-0.2686710	-0.8158530	0.4704220
8	No	Show	8	P	-0.8025330	1.5061780	0.0166420
9	No	Show	9	C	-2.4189750	1.9315240	-0.7411700
10	No	Show	10	C	-3.5884420	1.6660090	-0.0121030
11	No	Show	11	C	-2.5298340	2.4618610	-2.0325340
12	No	Show	12	C	-4.8390810	1.9369020	-0.5611020
13	No	Show	13	H	-3.5245250	1.2489400	0.9894610
14	No	Show	14	C	-3.7854310	2.7256090	-2.5823480
15	No	Show	15	H	-1.6381530	2.6767480	-2.6140890
16	No	Show	16	C	-4.9425940	2.4649190	-1.8498790
17	No	Show	17	H	-5.7356260	1.7243860	0.0155340
18	No	Show	18	H	-3.8557190	3.1356150	-3.5869020
19	No	Show	19	H	-5.9199920	2.6657570	-2.2809350
20	No	Show	20	C	-0.8023200	2.5483880	1.5320920
21	No	Show	21	C	-1.3072620	3.8571530	1.5347030
22	No	Show	22	C	-0.3088190	2.0094350	2.7266890
23	No	Show	23	C	-1.2901400	4.6180100	2.7024460
24	No	Show	24	H	-1.7323430	4.2758740	0.6257750
25	No	Show	25	C	-0.2925470	2.7707940	3.8967340
26	No	Show	26	H	0.0477050	0.9805970	2.7399080

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27	No	Show	27	C	-0.7785950	4.0781420	3.8851230
28	No	Show	28	H	-1.6856410	5.6307570	2.6918520
29	No	Show	29	H	0.0890760	2.3372850	4.8178210
30	No	Show	30	H	-0.7728830	4.6705280	4.7966290
31	No	Show	31	O	-5.2134950	-2.8798490	-0.6719980
32	No	Show	32	H	-2.2371070	-1.0276440	3.0092940
33	No	Show	33	H	2.4622400	4.6366650	-2.3767160
34	No	Show	34	C	1.8454830	3.7717320	-2.1630700
35	No	Show	35	C	1.8223930	2.5532120	-2.9064770
36	No	Show	36	C	0.9634640	3.6316120	-1.0504330
37	No	Show	37	C	0.9326480	1.6543960	-2.2505120
38	No	Show	38	H	2.4170480	2.3292070	-3.7837870
39	No	Show	39	C	0.3865800	2.3168910	-1.0960510
40	No	Show	40	Fe	2.4177050	2.2057760	-0.9773780
41	No	Show	41	C	4.0201020	0.9433090	-1.0007220
42	No	Show	42	C	3.0981580	0.5757240	0.0365290
43	No	Show	43	C	4.4522230	2.2818500	-0.7608200
44	No	Show	44	H	4.2951760	0.3252160	-1.8458360
45	No	Show	45	C	2.9692770	1.7093870	0.9129780
46	No	Show	46	C	3.8095560	2.7511420	0.4242520
47	No	Show	47	H	5.1176290	2.8552830	-1.3950450
48	No	Show	48	H	2.3214230	1.7735090	1.7777960
49	No	Show	49	H	3.8999710	3.7432010	0.8500420
50	No	Show	50	H	0.7981680	4.3671120	-0.2735230
51	No	Show	51	H	0.7227160	0.6330990	-2.5443070
52	No	Show	52	P	2.1430820	-0.9608370	0.2331180
53	No	Show	53	C	2.6684310	-1.9821090	-1.2035940
54	No	Show	54	C	3.9789780	-2.4633350	-1.3387480
55	No	Show	55	C	1.7169180	-2.3113350	-2.1767530
56	No	Show	56	C	4.3340280	-3.2397480	-2.4402420
57	No	Show	57	H	4.7211340	-2.2431380	-0.5751480
58	No	Show	58	C	2.0739440	-3.0884530	-3.2803770
59	No	Show	59	H	0.6868950	-1.9794100	-2.0599160
60	No	Show	60	C	3.3827600	-3.5500720	-3.4157080
61	No	Show	61	H	5.3517920	-3.6107490	-2.5334440
62	No	Show	62	H	1.3235760	-3.3426300	-4.0245330
63	No	Show	63	H	3.6598030	-4.1614440	-4.2708910
64	No	Show	64	C	2.9880540	-1.7899530	1.6437530
65	No	Show	65	C	4.1897820	-1.3306560	2.1970840
66	No	Show	66	C	2.3819290	-2.9333080	2.1855860
67	No	Show	67	C	4.7772190	-2.0057360	3.2687500
68	No	Show	68	H	4.6694840	-0.4422710	1.7954610
69	No	Show	69	C	2.9748430	-3.6118730	3.2484490
70	No	Show	70	H	1.4406220	-3.2928540	1.7732820
71	No	Show	71	C	4.1738420	-3.1478890	3.7949970

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72	No	Show	72	H	5.7088370	-1.6370140	3.6912430
73	No	Show	73	H	2.4958590	-4.4986350	3.6557490
74	No	Show	74	H	4.6319580	-3.6723820	4.6296930
75	No	Show	75	C	-6.0860990	-2.8022360	1.8744490
76	No	Show	76	H	-6.1864070	-3.8613190	1.6249890
77	No	Show	77	H	-6.1914910	-2.6500020	2.9471510
78	No	Show	78	H	-6.8575200	-2.2530230	1.3294900
79	No	Show	79	Br	-2.5329620	-2.0086930	-1.9496580

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Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	-2.3418280	0.1461110	-0.2175150	
2	No	Show	2	C	-2.4610020	1.5964920	-0.2016670	
3	No	Show	3	C	-3.5002760	-0.5401800	-0.0867780	
4	No	Show	4	N	-3.7660240	2.0887700	-0.0052750	
5	No	Show	5	C	-4.7735710	0.0645280	0.0855600	
6	No	Show	6	N	-4.8844510	1.3654260	0.1281740	
7	No	Show	7	Pd	-0.6683590	-1.0982970	-0.4016310	
8	No	Show	8	P	1.4286470	-0.0303290	-0.0285130	
9	No	Show	9	O	-1.5410460	2.4100300	-0.3439090	
10	No	Show	10	H	-5.6929200	-0.5034710	0.1915490	
11	No	Show	11	C	1.4919450	1.0392190	1.4553840	
12	No	Show	12	C	0.6450760	0.7384360	2.5298820	
13	No	Show	13	C	2.3653550	2.1297810	1.5541820	
14	No	Show	14	C	0.6870490	1.5020660	3.6955890	
15	No	Show	15	H	-0.0570410	-0.0885770	2.4458040	
16	No	Show	16	C	2.3985030	2.8987090	2.7175160	
17	No	Show	17	H	3.0142940	2.3849010	0.7205690	
18	No	Show	18	C	1.5637190	2.5842000	3.7910820	
19	No	Show	19	H	0.0249370	1.2601820	4.5230600	
20	No	Show	20	H	3.0749620	3.7472910	2.7825920	
21	No	Show	21	H	1.5888610	3.1872490	4.6952850	
22	No	Show	22	C	2.1158820	1.0022410	-1.3777370	
23	No	Show	23	C	3.4165490	0.8428230	-1.8745620	
24	No	Show	24	C	1.2790280	1.9856960	-1.9284440	
25	No	Show	25	C	3.8749450	1.6557540	-2.9129840	
26	No	Show	26	H	4.0765790	0.0888670	-1.4542980	
27	No	Show	27	C	1.7488940	2.8001430	-2.9575570	
28	No	Show	28	H	0.2716760	2.1209430	-1.5376150	
29	No	Show	29	C	3.0432540	2.6353030	-3.4560870	
30	No	Show	30	H	4.8848270	1.5229240	-3.2933950	
31	No	Show	31	H	1.0963750	3.5633350	-3.3742180	
32	No	Show	32	H	3.4021760	3.2673520	-4.2647020	
33	No	Show	33	C	2.7220360	-1.3044610	0.2673650	
34	No	Show	34	C	3.5691510	-1.2947910	1.3824180	

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35	No	Show	35	C	2.8227100	-2.3622900	-0.6517420
36	No	Show	36	C	4.5034650	-2.3159040	1.5685860
37	No	Show	37	H	3.5020150	-0.4904740	2.1094840
38	No	Show	38	C	3.7637300	-3.3732370	-0.4710620
39	No	Show	39	H	2.1653920	-2.3904460	-1.5196970
40	No	Show	40	C	4.6061750	-3.3542810	0.6434730
41	No	Show	41	H	5.1526990	-2.2960690	2.4404170
42	No	Show	42	H	3.8334490	-4.1807550	-1.1954970
43	No	Show	43	H	5.3339920	-4.1480140	0.7909570
44	No	Show	44	C	-3.9383220	3.5363810	0.0350860
45	No	Show	45	H	-3.3085610	3.9634810	0.8184080
46	No	Show	46	H	-3.6377380	3.9767610	-0.9187110
47	No	Show	47	H	-4.9898180	3.7358870	0.2334520
48	No	Show	48	Br	-3.4044130	-2.4823090	-0.1411340

### 38 (L=NHC)

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	3.7126190	-0.4008850	-0.6711840
2	No	Show	2	C	5.1045140	-0.3305720	-0.3717110
3	No	Show	3	C	2.7453560	-0.0348340	0.2070250
4	No	Show	4	C	3.2299740	0.4386440	1.4974890
5	No	Show	5	N	4.6147390	0.4692370	1.6839780
6	No	Show	6	H	5.8682310	-0.6266390	-1.0847550
7	No	Show	7	N	5.5370250	0.0972630	0.7831760
8	No	Show	8	O	2.4898400	0.8095810	2.4257670
9	No	Show	9	C	-1.4305810	0.0769630	0.0456500
10	No	Show	10	Pd	0.6838440	-0.0060140	0.0696010
11	No	Show	11	C	-3.5670780	0.8604350	-0.0126010
12	No	Show	12	C	-3.6307560	-0.4707230	0.2496260
13	No	Show	13	N	-2.3219490	-0.9281320	0.2796760
14	No	Show	14	N	-2.2214850	1.1731920	-0.1326080
15	No	Show	15	C	-1.9446870	-2.2946190	0.5336250
16	No	Show	16	C	-1.6559590	-2.6815600	1.8554850
17	No	Show	17	C	-1.8888570	-3.1897180	-0.5506580
18	No	Show	18	C	-1.2984910	-4.0169640	2.0708590
19	No	Show	19	C	-1.5307190	-4.5137770	-0.2769500
20	No	Show	20	C	-1.2370310	-4.9250410	1.0191060
21	No	Show	21	H	-1.0615260	-4.3501270	3.0778980
22	No	Show	22	H	-1.4736640	-5.2316920	-1.0911480
23	No	Show	23	H	-0.9544490	-5.9574950	1.2097930
24	No	Show	24	C	-1.7137090	2.4950920	-0.3972530
25	No	Show	25	C	-1.4887280	2.8758740	-1.7330410
26	No	Show	26	C	-1.4662760	3.3521460	0.6911300
27	No	Show	27	C	-1.0005040	4.1665210	-1.9616370
28	No	Show	28	C	-0.9785730	4.6315750	0.4042960

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29	No	Show	29	C	-0.7478550	5.0367910	-0.9061270
30	No	Show	30	H	-0.8078710	4.4929320	-2.9804000
31	No	Show	31	H	-0.7692670	5.3180650	1.2204070
32	No	Show	32	H	-0.3642240	6.0343690	-1.1058190
33	No	Show	33	H	-4.4756110	-1.1225500	0.4158730
34	No	Show	34	H	-4.3451020	1.6015100	-0.1210170
35	No	Show	35	C	-1.7215660	-1.7200240	3.0312080
36	No	Show	36	H	-2.0131710	-0.7372460	2.6506570
37	No	Show	37	C	-2.1881790	-2.7686710	-1.9805800
38	No	Show	38	H	-2.4407600	-1.7046890	-1.9754110
39	No	Show	39	C	-0.3516220	-1.5546050	3.7045690
40	No	Show	40	H	-0.4174550	-0.8276860	4.5205870
41	No	Show	41	H	0.0031720	-2.4994010	4.1302480
42	No	Show	42	H	0.4035730	-1.1932270	3.0011700
43	No	Show	43	C	-2.7934730	-2.1509230	4.0442200
44	No	Show	44	H	-2.8722400	-1.4130540	4.8497480
45	No	Show	45	H	-3.7776200	-2.2445630	3.5735490
46	No	Show	46	H	-2.5512850	-3.1152150	4.5030610
47	No	Show	47	C	-0.9566980	-2.9346100	-2.8829030
48	No	Show	48	H	-1.1757060	-2.5714160	-3.8928050
49	No	Show	49	H	-0.1020150	-2.3723410	-2.4966950
50	No	Show	50	H	-0.6569760	-3.9843920	-2.9669140
51	No	Show	51	C	-3.4007850	-3.5215900	-2.5481420
52	No	Show	52	H	-4.2878540	-3.3835550	-1.9216060
53	No	Show	53	H	-3.6366590	-3.1590630	-3.5543310
54	No	Show	54	H	-3.2099810	-4.5972820	-2.6210820
55	No	Show	55	C	-1.7388730	1.9439560	-2.9076130
56	No	Show	56	H	-2.1327590	1.0021630	-2.5154770
57	No	Show	57	C	-1.7131830	2.9440090	2.1346570
58	No	Show	58	H	-2.0512460	1.9038820	2.1396320
59	No	Show	59	C	-2.8319440	3.7888840	2.7641180
60	No	Show	60	H	-2.5477780	4.8442430	2.8329090
61	No	Show	61	H	-3.7575550	3.7317950	2.1818510
62	No	Show	62	H	-3.0475830	3.4378560	3.7789020
63	No	Show	63	C	-0.4288950	3.0055560	2.9745000
64	No	Show	64	H	-0.0414930	4.0280560	3.0401130
65	No	Show	65	H	-0.6353560	2.6686270	3.9961890
66	No	Show	66	H	0.3603700	2.3687890	2.5657140
67	No	Show	67	C	-0.4321300	1.6153440	-3.6446190
68	No	Show	68	H	0.3083160	1.1793110	-2.9675620
69	No	Show	69	H	-0.6203200	0.8977250	-4.4503740
70	No	Show	70	H	0.0111340	2.5099510	-4.0946060
71	No	Show	71	C	-2.7928490	2.5120700	-3.8696400
72	No	Show	72	H	-3.7329150	2.7294430	-3.3525620
73	No	Show	73	H	-2.4515880	3.4383300	-4.3432460

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74	No	Show	74	H	-3.0035350	1.7925370	-4.6679880
75	No	Show	75	Br	3.2616480	-1.0575520	-2.4311410
76	No	Show	76	C	5.1246070	0.9428340	2.9636210
77	No	Show	77	H	4.7876340	1.9662310	3.1453190
78	No	Show	78	H	4.7475510	0.3139800	3.7738000
79	No	Show	79	H	6.2116020	0.8997430	2.9198340

### 38\*\*

Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	-3.0646870	-2.3127660	0.5495520	
2	No	Show	2	C	-4.2856110	-2.8681270	0.0716000	
3	No	Show	3	C	-2.1245460	-1.7762150	-0.2686950	
4	No	Show	4	N	-4.5798400	-2.8843040	-1.2002320	
5	No	Show	5	C	-2.4454110	-1.8037940	-1.6920000	
6	No	Show	6	N	-3.6783350	-2.3605110	-2.0445130	
7	No	Show	7	Pd	-0.2534420	-0.9382980	0.1351590	
8	No	Show	8	P	-1.0039180	1.3543290	0.0981770	
9	No	Show	9	C	-2.7366700	1.7120210	-0.3851120	
10	No	Show	10	C	-3.7637770	1.2762210	0.4662470	
11	No	Show	11	C	-3.0711010	2.3489140	-1.5857300	
12	No	Show	12	C	-5.0975710	1.4954080	0.1314810	
13	No	Show	13	H	-3.5211580	0.7663690	1.3957110	
14	No	Show	14	C	-4.4097260	2.5618440	-1.9213600	
15	No	Show	15	H	-2.2893130	2.6830000	-2.2616100	
16	No	Show	16	C	-5.4254920	2.1396590	-1.0642640	
17	No	Show	17	H	-5.8825610	1.1547980	0.8019500	
18	No	Show	18	H	-4.6558940	3.0607620	-2.8556680	
19	No	Show	19	H	-6.4671980	2.3059640	-1.3270860	
20	No	Show	20	C	-0.8665840	2.2564240	1.6953700	
21	No	Show	21	C	-1.4157570	3.5341120	1.8821720	
22	No	Show	22	C	-0.2252480	1.6297430	2.7711240	
23	No	Show	23	C	-1.2916970	4.1827830	3.1095520	
24	No	Show	24	H	-1.9615670	4.0145960	1.0738070	
25	No	Show	25	C	-0.1039980	2.2781180	4.0015970	
26	No	Show	26	H	0.1651250	0.6215400	2.6473010	
27	No	Show	27	C	-0.6308670	3.5584020	4.1705580	
28	No	Show	28	H	-1.7208890	5.1730460	3.2420480	
29	No	Show	29	H	0.3922570	1.7764820	4.8285690	
30	No	Show	30	H	-0.5416930	4.0634560	5.1291690	
31	No	Show	31	O	-1.7051870	-1.3763410	-2.5957410	
32	No	Show	32	H	-5.0266570	-3.3022300	0.7363930	
33	No	Show	33	H	1.6927580	4.8681570	-2.4605970	
34	No	Show	34	C	1.1784570	3.9435580	-2.2262330	
35	No	Show	35	C	1.1929320	2.7513400	-3.0122950	
36	No	Show	36	C	0.4269340	3.6861350	-1.0410200	

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37	No	Show	37	C	0.4544160	1.7529480	-2.3158880
38	No	Show	38	H	1.7159300	2.6129120	-3.9507940
39	No	Show	39	C	-0.0301860	2.3250010	-1.0886120
40	No	Show	40	Fe	2.0061130	2.4089590	-1.1584990
41	No	Show	41	C	3.7046690	1.2804350	-1.3371750
42	No	Show	42	C	2.9346580	0.8585900	-0.2021980
43	No	Show	43	C	4.0384740	2.6563950	-1.1640300
44	No	Show	44	H	3.9472070	0.6667780	-2.1955130
45	No	Show	45	C	2.7964260	1.9960900	0.6673260
46	No	Show	46	C	3.4849520	3.0952030	0.0765650
47	No	Show	47	H	4.5809790	3.2699280	-1.8733380
48	No	Show	48	H	2.2398490	2.0231080	1.5954640
49	No	Show	49	H	3.5311770	4.1010460	0.4763540
50	No	Show	50	H	0.2762250	4.3772970	-0.2216030
51	No	Show	51	H	0.2811030	0.7318370	-2.6345320
52	No	Show	52	P	2.1549640	-0.7609860	0.0842230
53	No	Show	53	C	2.7628830	-1.7577650	-1.3396720
54	No	Show	54	C	4.0842260	-2.2211700	-1.4160170
55	No	Show	55	C	1.8680660	-2.0643390	-2.3749220
56	No	Show	56	C	4.5072290	-2.9665930	-2.5154500
57	No	Show	57	H	4.7834540	-2.0100820	-0.6107780
58	No	Show	58	C	2.2974980	-2.8057680	-3.4773480
59	No	Show	59	H	0.8281610	-1.7422700	-2.3217850
60	No	Show	60	C	3.6152470	-3.2568600	-3.5508030
61	No	Show	61	H	5.5326340	-3.3254660	-2.5613030
62	No	Show	62	H	1.5922920	-3.0375450	-4.2713070
63	No	Show	63	H	3.9456310	-3.8417250	-4.4057950
64	No	Show	64	C	3.0926400	-1.4440950	1.5100460
65	No	Show	65	C	4.2828570	-0.8911930	2.0003350
66	No	Show	66	C	2.5616620	-2.5819280	2.1356500
67	No	Show	67	C	4.9335330	-1.4727880	3.0903060
68	No	Show	68	H	4.7026770	-0.0031450	1.5349140
69	No	Show	69	C	3.2182590	-3.1678170	3.2160190
70	No	Show	70	H	1.6270090	-3.0087280	1.7755530
71	No	Show	71	C	4.4061410	-2.6129900	3.6974840
72	No	Show	72	H	5.8553650	-1.0331640	3.4636060
73	No	Show	73	H	2.7967930	-4.0515200	3.6883740
74	No	Show	74	H	4.9147010	-3.0641280	4.5457970
75	No	Show	75	Br	-2.8054780	-2.3665280	2.4637040
76	No	Show	76	C	-4.0353720	-2.3931070	-3.4563740
77	No	Show	77	H	-3.3062180	-2.9848000	-4.0153510
78	No	Show	78	H	-5.0264150	-2.8371320	-3.5332420
79	No	Show	79	H	-4.0347390	-1.3797790	-3.8642290



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**TS1\_Fc**

Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	H	1.4215240		-3.1383270	-3.2847050
2	No	Show	2	C	1.1652600		-3.1759870	-2.2327680
3	No	Show	3	C	0.8183260		-4.3482370	-1.4938270
4	No	Show	4	C	1.1764150		-2.0731040	-1.3286870
5	No	Show	5	C	0.6267320		-3.9691050	-0.1330350
6	No	Show	6	H	0.7521220		-5.3551170	-1.8877860
7	No	Show	7	C	0.8317010		-2.5517510	-0.0229140
8	No	Show	8	Fe	2.5143040		-3.5072830	-0.7420630
9	No	Show	9	C	3.8241950		-4.5167000	0.4578880
10	No	Show	10	C	4.0870370		-3.1128610	0.5030140
11	No	Show	11	C	3.9539780		-4.9449270	-0.8989210
12	No	Show	12	H	3.5455140		-5.1415270	1.2977810
13	No	Show	13	C	4.3773670		-2.6725610	-0.8248370
14	No	Show	14	H	4.0348100		-2.4887440	1.3861760
15	No	Show	15	C	4.2954430		-3.8059560	-1.6911380
16	No	Show	16	H	3.7831570		-5.9486770	-1.2685340
17	No	Show	17	H	4.5849410		-1.6544150	-1.1302750
18	No	Show	18	H	4.4272790		-3.7951830	-2.7661520
19	No	Show	19	H	1.4412170		-1.0522760	-1.5744180
20	No	Show	20	H	0.3549260		-4.6327720	0.6786440
21	No	Show	21	C	0.6731570		-1.7645160	1.2138560
22	No	Show	22	C	1.1155580		-2.3485130	2.4463460
23	No	Show	23	C	0.0794110		-0.5247310	1.2667640
24	No	Show	24	N	0.9991920		-1.7901700	3.6186420
25	No	Show	25	C	-0.0788920		0.1222790	2.5595990
26	No	Show	26	N	0.4179100		-0.5822230	3.6562220
27	No	Show	27	Pd	-0.6495830		0.5041440	-0.2895300
28	No	Show	28	P	1.1850700		2.1606930	-0.1841680
29	No	Show	29	C	2.3893590		2.0343850	1.1961890
30	No	Show	30	C	3.0960350		0.8344820	1.3716770
31	No	Show	31	C	2.6248690		3.0950180	2.0791920
32	No	Show	32	C	4.0290410		0.7068430	2.3996180
33	No	Show	33	H	2.9196460		-0.0033050	0.7022750
34	No	Show	34	C	3.5532890		2.9615030	3.1126470
35	No	Show	35	H	2.0804390		4.0276820	1.9670030
36	No	Show	36	C	4.2587470		1.7696190	3.2752150
37	No	Show	37	H	4.5722960		-0.2262720	2.5229940
38	No	Show	38	H	3.7227140		3.7936630	3.7915160
39	No	Show	39	H	4.9809440		1.6664420	4.0812930
40	No	Show	40	C	0.4554710		3.8308190	0.0207260
41	No	Show	41	C	0.9708740		4.9679900	-0.6161060
42	No	Show	42	C	-0.6452780		3.9580770	0.8803900
43	No	Show	43	C	0.3893580		6.2172880	-0.4000850

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44	No	Show	44	H	1.8278400	4.8839250	-1.2787650
45	No	Show	45	C	-1.2138830	5.2121490	1.1005670
46	No	Show	46	H	-1.0350570	3.0801220	1.3900070
47	No	Show	47	C	-0.7037180	6.3416670	0.4591980
48	No	Show	48	H	0.7940420	7.0932290	-0.9012720
49	No	Show	49	H	-2.0636950	5.3032300	1.7724230
50	No	Show	50	H	-1.1556390	7.3163190	0.6271640
51	No	Show	51	C	2.2719350	2.3369960	-1.6652960
52	No	Show	52	C	3.6701990	2.2718470	-1.5982800
53	No	Show	53	C	1.6670590	2.5374270	-2.9175830
54	No	Show	54	C	4.4439710	2.3913300	-2.7548620
55	No	Show	55	H	4.1665330	2.1391890	-0.6418150
56	No	Show	56	C	2.4424900	2.6654440	-4.0685930
57	No	Show	57	H	0.5866820	2.6161420	-2.9845560
58	No	Show	58	C	3.8347780	2.5856100	-3.9934950
59	No	Show	59	H	5.5275680	2.3404410	-2.6808250
60	No	Show	60	H	1.9563030	2.8306510	-5.0271230
61	No	Show	61	H	4.4387290	2.6819650	-4.8922230
62	No	Show	62	O	-0.6212330	1.2226250	2.7539040
63	No	Show	63	H	1.5973310	-3.3226810	2.4488320
64	No	Show	64	C	0.2977390	0.0329110	4.9708430
65	No	Show	65	H	0.8139380	0.9954850	4.9794980
66	No	Show	66	H	-0.7537940	0.2089110	5.2106540
67	No	Show	67	H	0.7450460	-0.6500070	5.6911510
68	No	Show	68	H	-6.6103750	-2.8230950	-0.3134600
69	No	Show	69	C	-6.3214080	-1.7934280	-0.1424050
70	No	Show	70	C	-6.0627580	-1.1938400	1.1291560
71	No	Show	71	C	-6.0846890	-0.8136400	-1.1513880
72	No	Show	72	C	-5.6561390	0.1548530	0.9117000
73	No	Show	73	H	-6.1133780	-1.6916190	2.0895290
74	No	Show	74	C	-5.6844180	0.3943940	-0.4954140
75	No	Show	75	Fe	-4.3848210	-1.1788430	-0.0224910
76	No	Show	76	C	-2.7173190	-1.4151460	1.1507110
77	No	Show	77	C	-2.2267830	-0.8950370	-0.0920140
78	No	Show	78	C	-3.3954720	-2.6543590	0.9329770
79	No	Show	79	H	-2.5900900	-0.9431610	2.1174660
80	No	Show	80	C	-2.7010280	-1.8134530	-1.0924080
81	No	Show	81	C	-3.3955030	-2.8973750	-0.4727840
82	No	Show	82	H	-3.8757510	-3.2677940	1.6871920
83	No	Show	83	H	-2.5369660	-1.7274550	-2.1604220
84	No	Show	84	H	-3.8670910	-3.7306280	-0.9815350
85	No	Show	85	H	-6.2087240	-0.9539760	-2.2190510
86	No	Show	86	H	-5.3588300	0.8619370	1.6764110
87	No	Show	87	H	-5.5500640	1.3491300	-0.9908890
88	No	Show	88	O	-3.4953030	0.6923050	-2.7771660

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89	No	Show	89	H	-4.0812920	0.1853590	-2.1801920
90	No	Show	90	O	-2.9877840	2.4174100	-1.0879590
91	No	Show	91	H	-3.8645610	2.2517390	-0.7214720
92	No	Show	92	B	-2.6654740	1.5135910	-2.0574520
93	No	Show	93	O	-1.3063300	1.4897080	-2.3849960
94	No	Show	94	H	-1.1742150	0.7959000	-3.0489220

#### TS1\_Ph

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	C	-2.0414700	1.7573420	-0.0290240
2	No	Show	2	C	-2.5004750	2.9335240	-0.7130510
3	No	Show	3	C	-1.1847030	0.9177390	-0.7049050
4	No	Show	4	N	-2.1886930	3.2531300	-1.9376700
5	No	Show	5	C	-0.8145390	1.2499630	-2.0714020
6	No	Show	6	N	-1.3773280	2.4121680	-2.5929150
7	No	Show	7	Pd	-0.4286930	-0.8184990	-0.0270100
8	No	Show	8	P	1.7722230	0.0875090	0.2090800
9	No	Show	9	C	2.1456560	1.8198640	-0.2501790
10	No	Show	10	C	1.3745900	2.8527460	0.3049960
11	No	Show	11	C	3.1730280	2.1425760	-1.1453910
12	No	Show	12	C	1.6370820	4.1827010	-0.0187700
13	No	Show	13	H	0.5664350	2.6240950	0.9937810
14	No	Show	14	C	3.4293960	3.4748220	-1.4720070
15	No	Show	15	H	3.7726410	1.3564130	-1.5944740
16	No	Show	16	C	2.6648550	4.4970000	-0.9097150
17	No	Show	17	H	1.0301430	4.9711690	0.4184110
18	No	Show	18	H	4.2285740	3.7111440	-2.1699970
19	No	Show	19	H	2.8648760	5.5338900	-1.1677710
20	No	Show	20	C	2.8908790	-0.9346770	-0.8231050
21	No	Show	21	C	4.1582350	-1.3383140	-0.3818210
22	No	Show	22	C	2.4492410	-1.3135150	-2.1003360
23	No	Show	23	C	4.9731180	-2.1153170	-1.2058380
24	No	Show	24	H	4.5142140	-1.0511110	0.6038080
25	No	Show	25	C	3.2731110	-2.0842620	-2.9208150
26	No	Show	26	H	1.4771370	-0.9759150	-2.4552820
27	No	Show	27	C	4.5319770	-2.4914850	-2.4751760
28	No	Show	28	H	5.9531710	-2.4263940	-0.8528200
29	No	Show	29	H	2.9257490	-2.3677010	-3.9112180
30	No	Show	30	H	5.1673890	-3.0994910	-3.1143260
31	No	Show	31	C	2.4466190	-0.0986410	1.9089450
32	No	Show	32	C	3.0126360	0.9590620	2.6308480
33	No	Show	33	C	2.3619640	-1.3658490	2.5102340
34	No	Show	34	C	3.4786580	0.7559950	3.9318600
35	No	Show	35	H	3.1012220	1.9430700	2.1799840
36	No	Show	36	C	2.8369060	-1.5665700	3.8039870

37	No	Show	37	H	1.9477360	-2.2003950	1.9506690
38	No	Show	38	C	3.3915680	-0.5038960	4.5220150
39	No	Show	39	H	3.9157790	1.5868360	4.4799680
40	No	Show	40	H	2.7743750	-2.5549190	4.2525720
41	No	Show	41	H	3.7571070	-0.6601810	5.5336950
42	No	Show	42	O	-0.0532000	0.5809450	-2.7914310
43	No	Show	43	H	-3.1396060	3.6533140	-0.2084040
44	No	Show	44	C	-1.0451370	2.7762170	-3.9637150
45	No	Show	45	H	0.0325100	2.9269350	-4.0609200
46	No	Show	46	H	-1.3391080	1.9744140	-4.6448090
47	No	Show	47	H	-1.5833370	3.6936200	-4.1956160
48	No	Show	48	O	-1.8498200	-4.3116860	0.4517000
49	No	Show	49	H	-2.2749060	-4.9221110	-0.1644900
50	No	Show	50	O	-0.6418090	-3.7612230	-1.5736100
51	No	Show	51	H	0.2960140	-3.5580500	-1.6847310
52	No	Show	52	B	-1.0722250	-3.3828320	-0.2805100
53	No	Show	53	O	0.0265010	-2.8633280	0.5695770
54	No	Show	54	H	-0.2275260	-3.0595530	1.4850750
55	No	Show	55	C	-2.5215710	1.5457960	1.3602920
56	No	Show	56	C	-1.6757010	1.0675150	2.3726740
57	No	Show	57	C	-3.8508650	1.8469840	1.7005820
58	No	Show	58	C	-2.1389710	0.8956340	3.6762910
59	No	Show	59	H	-0.6399570	0.8331700	2.1432260
60	No	Show	60	C	-4.3182390	1.6690250	3.0011780
61	No	Show	61	H	-4.5390460	2.1865270	0.9309430
62	No	Show	62	C	-3.4634320	1.1946450	3.9978080
63	No	Show	63	H	-1.4595270	0.5302420	4.4424430
64	No	Show	64	H	-5.3558390	1.8947200	3.2348380
65	No	Show	65	H	-3.8266060	1.0581390	5.0132740
66	No	Show	66	C	-2.2920940	-1.8673610	-0.5369210
67	No	Show	67	C	-3.2926190	-1.7239840	0.4528830
68	No	Show	68	C	-2.7022290	-1.7171980	-1.8807230
69	No	Show	69	C	-4.6249560	-1.4880780	0.1246070
70	No	Show	70	H	-3.0303990	-1.8406450	1.5023290
71	No	Show	71	C	-4.0331990	-1.4822670	-2.2222070
72	No	Show	72	H	-1.9603490	-1.8249260	-2.6670330
73	No	Show	73	C	-4.9975780	-1.3675650	-1.2177650
74	No	Show	74	H	-5.3734580	-1.4010200	0.9089670
75	No	Show	75	H	-4.3210260	-1.3904240	-3.2674380
76	No	Show	76	H	-6.0384230	-1.1881830	-1.4796430

#### TS2\_Fc

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	H	2.1357240	-1.5644780	-3.7419360
2	No	Show	2	C	2.1368170	-1.9289550	-2.7216590

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3	No	Show	3	C	2.6493430	-3.1856340	-2.2760690
4	No	Show	4	C	1.6850590	-1.2124010	-1.5761090
5	No	Show	5	C	2.5267250	-3.2387420	-0.8578740
6	No	Show	6	H	3.1031720	-3.9464680	-2.8998460
7	No	Show	7	C	1.9063460	-2.0201590	-0.4092930
8	No	Show	8	Fe	3.6687720	-1.6457290	-1.4072750
9	No	Show	9	C	5.5028480	-1.9461920	-0.5685570
10	No	Show	10	C	4.9356030	-0.7216810	-0.1029610
11	No	Show	11	C	5.6107050	-1.8662940	-1.9910130
12	No	Show	12	H	5.7398650	-2.8025340	0.0493350
13	No	Show	13	C	4.6878180	0.1158550	-1.2348900
14	No	Show	14	H	4.6862340	-0.5050170	0.9277440
15	No	Show	15	C	5.1049620	-0.5943340	-2.4037830
16	No	Show	16	H	5.9673600	-2.6509080	-2.6473360
17	No	Show	17	H	4.2278090	1.0967640	-1.2210320
18	No	Show	18	H	5.0145860	-0.2462060	-3.4256360
19	No	Show	19	H	1.2840910	-0.2078830	-1.5778500
20	No	Show	20	H	2.8702720	-4.0328360	-0.2112260
21	No	Show	21	C	1.5293870	-1.6815050	0.9705820
22	No	Show	22	C	2.3184800	-2.2766120	2.0553720
23	No	Show	23	C	0.4423970	-0.8970620	1.3017950
24	No	Show	24	N	1.8892140	-1.9708240	3.3481970
25	No	Show	25	C	0.1575030	-0.6930720	2.6874210
26	No	Show	26	N	0.8382350	-1.2112380	3.6772860
27	No	Show	27	Pd	-0.8962720	-0.0232200	0.0642470
28	No	Show	28	P	-0.0082810	2.2541270	0.3049560
29	No	Show	29	C	1.0033890	2.6261820	1.7871280
30	No	Show	30	C	2.2183600	1.9399990	1.9441480
31	No	Show	31	C	0.5992000	3.5327990	2.7740990
32	No	Show	32	C	3.0181670	2.1727860	3.0600360
33	No	Show	33	H	2.5405070	1.2234900	1.1929340
34	No	Show	34	C	1.3983620	3.7529910	3.8979050
35	No	Show	35	H	-0.3362720	4.0753640	2.6715100
36	No	Show	36	C	2.6090670	3.0773430	4.0422320
37	No	Show	37	H	3.9579270	1.6375400	3.1673720
38	No	Show	38	H	1.0720750	4.4583020	4.6581040
39	No	Show	39	H	3.2302090	3.2505610	4.9172320
40	No	Show	40	C	-1.3829100	3.4751340	0.4026420
41	No	Show	41	C	-1.3146900	4.7602000	-0.1576250
42	No	Show	42	C	-2.5502290	3.0928400	1.0851430
43	No	Show	43	C	-2.3891800	5.6428070	-0.0326400
44	No	Show	44	H	-0.4255100	5.0711310	-0.6993030
45	No	Show	45	C	-3.6160860	3.9814000	1.2199970
46	No	Show	46	H	-2.6233870	2.0914960	1.5035280
47	No	Show	47	C	-3.5380340	5.2578670	0.6595620

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48	No	Show	48	H	-2.3262340	6.6319540	-0.4787810
49	No	Show	49	H	-4.5120130	3.6717010	1.7516970
50	No	Show	50	H	-4.3733700	5.9466690	0.7542330
51	No	Show	51	C	1.0195400	2.8838080	-1.0830630
52	No	Show	52	C	2.0679430	3.7974520	-0.9027320
53	No	Show	53	C	0.7190320	2.4421520	-2.3794730
54	No	Show	54	C	2.7965010	4.2596520	-1.9990590
55	No	Show	55	H	2.3219260	4.1451030	0.0949210
56	No	Show	56	C	1.4404570	2.9141910	-3.4751950
57	No	Show	57	H	-0.0805280	1.7223710	-2.5373710
58	No	Show	58	C	2.4829160	3.8223680	-3.2869710
59	No	Show	59	H	3.6115500	4.9622580	-1.8446850
60	No	Show	60	H	1.1933960	2.5628880	-4.4735540
61	No	Show	61	H	3.0535300	4.1827020	-4.1390430
62	No	Show	62	H	-5.8678170	-3.5596420	-1.3676280
63	No	Show	63	C	-5.5638880	-2.9044930	-0.5605250
64	No	Show	64	C	-5.3491540	-3.2876540	0.7986760
65	No	Show	65	C	-5.2653350	-1.5132530	-0.6808340
66	No	Show	66	C	-4.9110300	-2.1354150	1.5210780
67	No	Show	67	H	-5.4579830	-4.2868320	1.2022780
68	No	Show	68	C	-4.8635830	-1.0374900	0.6107210
69	No	Show	69	Fe	-3.6267050	-2.5598990	-0.0101540
70	No	Show	70	C	-1.8311000	-2.9735010	0.8759100
71	No	Show	71	C	-1.6295040	-1.9414240	-0.0939460
72	No	Show	72	C	-2.3655430	-4.1333070	0.2337660
73	No	Show	73	H	-1.6384810	-2.8856070	1.9383130
74	No	Show	74	C	-2.0694550	-2.4884220	-1.3520420
75	No	Show	75	C	-2.5172360	-3.8308530	-1.1521830
76	No	Show	76	H	-2.6469950	-5.0610990	0.7185020
77	No	Show	77	H	-2.0571550	-1.9829820	-2.3115560
78	No	Show	78	H	-2.9284100	-4.4877720	-1.9100820
79	No	Show	79	H	-5.3402790	-0.9295550	-1.5913490
80	No	Show	80	H	-4.6260120	-2.1095460	2.5657440
81	No	Show	81	H	-4.5540680	-0.0280070	0.8514070
82	No	Show	82	O	-4.0450990	0.6533290	-3.2401740
83	No	Show	83	H	-4.3279130	1.2713450	-3.9285390
84	No	Show	84	O	-2.8684430	2.5897490	-2.5429010
85	No	Show	85	H	-2.3938190	2.9712560	-1.7878750
86	No	Show	86	B	-3.2216970	1.2842140	-2.3426340
87	No	Show	87	O	-2.7653200	0.5725540	-1.2471220
88	No	Show	88	H	-3.1819730	-0.3169000	-1.1701700
89	No	Show	89	H	-0.6856830	-0.0861600	3.0044960
90	No	Show	90	O	3.3040520	-3.0135240	1.9220750
91	No	Show	91	C	2.6268660	-2.5602810	4.4577030
92	No	Show	92	H	2.1733650	-2.1944510	5.3772310

93	No	Show	93	H	2.5737130	-3.6508270	4.4111780
94	No	Show	94	H	3.6794050	-2.2727110	4.4057220

# TS2\_Ph

Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	-2.1252640	1.4004470	-0.0010730	
2	No	Show	2	C	-2.7781820	2.5579340	-0.6237970	
3	No	Show	3	C	-1.2163690	0.6781550	-0.7450190	
4	No	Show	4	N	-2.4292760	2.7946860	-1.9562590	
5	No	Show	5	C	-0.9730360	1.0820200	-2.0930550	
6	No	Show	6	N	-1.5579590	2.0910940	-2.6835230	
7	No	Show	7	Pd	-0.2282470	-0.9485080	-0.0816570	
8	No	Show	8	P	1.8581150	0.2410350	0.0883970	
9	No	Show	9	C	1.9208390	2.0254170	-0.3205600	
10	No	Show	10	C	1.0875740	2.9084660	0.3852670	
11	No	Show	11	C	2.7343380	2.5294110	-1.3431240	
12	No	Show	12	C	1.0893330	4.2697720	0.0894720	
13	No	Show	13	H	0.4298290	2.5397760	1.1673530	
14	No	Show	14	C	2.7260750	3.8925440	-1.6432550	
15	No	Show	15	H	3.3734930	1.8622120	-1.9137660	
16	No	Show	16	C	1.9085940	4.7654180	-0.9267940	
17	No	Show	17	H	0.4376700	4.9383650	0.6456560	
18	No	Show	18	H	3.3593840	4.2689030	-2.4425390	
19	No	Show	19	H	1.9020130	5.8262040	-1.1639700	
20	No	Show	20	C	3.0575920	-0.5466950	-1.0551240	
21	No	Show	21	C	4.4417580	-0.4601100	-0.8444340	
22	No	Show	22	C	2.5777870	-1.2400890	-2.1739080	
23	No	Show	23	C	5.3283110	-1.0469100	-1.7459330	
24	No	Show	24	H	4.8282390	0.0614700	0.0274770	
25	No	Show	25	C	3.4678210	-1.8213260	-3.0782980	
26	No	Show	26	H	1.5063490	-1.3424440	-2.3297560	
27	No	Show	27	C	4.8432530	-1.7253730	-2.8663250	
28	No	Show	28	H	6.3989820	-0.9758210	-1.5717840	
29	No	Show	29	H	3.0830580	-2.3552620	-3.9434180	
30	No	Show	30	H	5.5363340	-2.1832020	-3.5675550	
31	No	Show	31	C	2.6927180	0.0909520	1.7189210	
32	No	Show	32	C	3.1463120	1.1865550	2.4629090	
33	No	Show	33	C	2.8619920	-1.2044620	2.2352960	
34	No	Show	34	C	3.7561460	0.9900730	3.7041580	
35	No	Show	35	H	3.0354730	2.1954450	2.0762240	
36	No	Show	36	C	3.4783560	-1.3957110	3.4694130	
37	No	Show	37	H	2.5256630	-2.0631690	1.6596680	
38	No	Show	38	C	3.9232280	-0.2979050	4.2105930	
39	No	Show	39	H	4.1045560	1.8493720	4.2715340	
40	No	Show	40	H	3.6109200	-2.4038870	3.8540150	

41	No	Show	41	H	4.3997780	-0.4477770	5.1759410
42	No	Show	42	O	-1.1842380	-4.6012570	0.2675640
43	No	Show	43	H	-1.7686250	-5.0425370	-0.3629300
44	No	Show	44	O	-0.0446140	-3.6678680	-1.7015750
45	No	Show	45	H	0.8713200	-3.9790790	-1.6655320
46	No	Show	46	B	-0.5133540	-3.5410820	-0.3681280
47	No	Show	47	O	0.4803270	-2.9568190	0.5337140
48	No	Show	48	H	0.2150610	-3.1786840	1.4403450
49	No	Show	49	C	-2.5023340	1.0818930	1.3979600
50	No	Show	50	C	-1.5462070	0.6648680	2.3382830
51	No	Show	51	C	-3.8398670	1.1720040	1.8206630
52	No	Show	52	C	-1.9070090	0.3346000	3.6446010
53	No	Show	53	H	-0.4988080	0.6065150	2.0547670
54	No	Show	54	C	-4.2039700	0.8288010	3.1204230
55	No	Show	55	H	-4.5977120	1.5074710	1.1226820
56	No	Show	56	C	-3.2417020	0.4096540	4.0419090
57	No	Show	57	H	-1.1405400	0.0247870	4.3511500
58	No	Show	58	H	-5.2479220	0.8953540	3.4174750
59	No	Show	59	H	-3.5284000	0.1517920	5.0585750
60	No	Show	60	C	-1.9860750	-2.1338530	-0.5733520
61	No	Show	61	C	-2.9734400	-2.1859690	0.4375620
62	No	Show	62	C	-2.4412930	-2.1535560	-1.9087870
63	No	Show	63	C	-4.3284600	-2.2874620	0.1351890
64	No	Show	64	H	-2.6771640	-2.1695070	1.4842600
65	No	Show	65	C	-3.7961150	-2.2633340	-2.2234700
66	No	Show	66	H	-1.7128410	-2.1248460	-2.7146030
67	No	Show	67	C	-4.7430650	-2.3283890	-1.1999300
68	No	Show	68	H	-5.0626020	-2.3300960	0.9363520
69	No	Show	69	H	-4.1132190	-2.2936010	-3.2637250
70	No	Show	70	H	-5.8011920	-2.4089560	-1.4396510
71	No	Show	71	O	-3.5851670	3.3202940	-0.0796380
72	No	Show	72	H	-0.2749370	0.5436150	-2.7273990
73	No	Show	73	C	-3.0652100	3.9216350	-2.6258360
74	No	Show	74	H	-2.6744660	3.9564390	-3.6411720
75	No	Show	75	H	-4.1497690	3.7904910	-2.6353130
76	No	Show	76	H	-2.8418960	4.8497940	-2.0947570

**TS\_33a\_to\_34a+32**

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	H	2.7200984	-3.2892776	1.7405450
2	No	Show	2	C	3.0934324	-2.3341296	1.3933000
3	No	Show	3	C	4.4134494	-2.0648646	0.9308910
4	No	Show	4	C	2.3720544	-1.0942026	1.3884700
5	No	Show	5	C	4.5122804	-0.6749506	0.6258060
6	No	Show	6	H	5.1981764	-2.7995746	0.7968450



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7	No	Show	7	C	3.2492004	-0.0643636	0.8923330
8	No	Show	8	Fe	3.0546924	-1.5654186	-0.5078160
9	No	Show	9	C	3.8574214	-1.3464946	-2.3631960
10	No	Show	10	C	2.5687914	-0.7358596	-2.3248280
11	No	Show	11	C	3.6999624	-2.7309616	-2.0456800
12	No	Show	12	H	4.7934034	-0.8349806	-2.5503160
13	No	Show	13	C	1.6115664	-1.7373416	-1.9911750
14	No	Show	14	H	2.3624154	0.3174984	-2.4696950
15	No	Show	15	C	2.3117204	-2.9730706	-1.8133730
16	No	Show	16	H	4.5002764	-3.4556496	-1.9601650
17	No	Show	17	H	0.5426974	-1.6122136	-1.8815950
18	No	Show	18	H	1.8640094	-3.9272956	-1.5614750
19	No	Show	19	H	1.4233274	-0.9318206	1.9162530
20	No	Show	20	H	5.3714284	-0.1566456	0.2250980
21	No	Show	21	C	2.8124524	1.3183864	0.6839630
22	No	Show	22	C	3.6524196	2.4749683	0.7248710
23	No	Show	23	C	1.4743354	1.5897894	0.4544390
24	No	Show	24	N	3.2045844	3.7091490	0.7103643
25	No	Show	25	C	0.9548676	2.9513178	0.4342233
26	No	Show	26	N	1.9189897	3.9225525	0.5863212
27	No	Show	27	Pd	0.1299494	-0.1036986	0.4340640
28	No	Show	28	P	-1.9208956	0.7279714	-0.1039770
29	No	Show	29	C	-1.8586386	2.3919474	-0.8861280
30	No	Show	30	C	-0.9192046	2.5979344	-1.9072560
31	No	Show	31	C	-2.7300306	3.4312464	-0.5409320
32	No	Show	32	C	-0.8640666	3.8147594	-2.5828930
33	No	Show	33	H	-0.2170956	1.8059654	-2.1580440
34	No	Show	34	C	-2.6607666	4.6567004	-1.2074680
35	No	Show	35	H	-3.4556446	3.2968654	0.2560070
36	No	Show	36	C	-1.7337296	4.8493604	-2.2314420
37	No	Show	37	H	-0.1275666	3.9618584	-3.3683880
38	No	Show	38	H	-3.3335476	5.4612304	-0.9214610
39	No	Show	39	H	-1.6805406	5.8051164	-2.7463140
40	No	Show	40	C	-2.9858946	0.9494254	1.3725130
41	No	Show	41	C	-4.3853586	0.9576144	1.2932620
42	No	Show	42	C	-2.3690036	1.1583674	2.6128590
43	No	Show	43	C	-5.1523806	1.1691174	2.4393340
44	No	Show	44	H	-4.8796156	0.7904364	0.3400730
45	No	Show	45	C	-3.1377466	1.3805734	3.7544200
46	No	Show	46	H	-1.2833006	1.1409314	2.6798940
47	No	Show	47	C	-4.5310706	1.3832004	3.6705170
48	No	Show	48	H	-6.2371526	1.1659934	2.3678380
49	No	Show	49	H	-2.6471316	1.5425054	4.7107260
50	No	Show	50	H	-5.1306706	1.5472884	4.5623140
51	No	Show	51	C	-2.9877716	-0.1808866	-1.2959780

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52	No	Show	52	C	-3.3138756	0.3405754	-2.5549210
53	No	Show	53	C	-3.5476496	-1.4035636	-0.9009470
54	No	Show	54	C	-4.1875436	-0.3453236	-3.4003260
55	No	Show	55	H	-2.9081496	1.2926144	-2.8796150
56	No	Show	56	C	-4.4469526	-2.0655996	-1.7331650
57	No	Show	57	H	-3.2936656	-1.8345416	0.0638480
58	No	Show	58	C	-4.7645256	-1.5448916	-2.9885470
59	No	Show	59	H	-4.4283346	0.0735484	-4.3741090
60	No	Show	60	H	-4.8979736	-2.9969306	-1.4022070
61	No	Show	61	H	-5.4573856	-2.0710526	-3.6405270
62	No	Show	62	O	-0.8293040	-3.1263490	-0.7891580
63	No	Show	63	C	-0.7890870	-3.4713640	0.3801320
64	No	Show	64	H	-0.9401746	-1.2966046	0.7334730
65	No	Show	65	O	0.3462650	-3.4781790	1.1079830
66	No	Show	66	H	1.0578270	-3.1875000	0.4970730
67	No	Show	67	N	-1.8831740	-3.9253870	1.0964760
68	No	Show	68	C	-2.6527550	-4.9740110	0.4372640
69	No	Show	69	H	-2.1886450	-5.9613490	0.5786630
70	No	Show	70	H	-3.6631470	-5.0052800	0.8559560
71	No	Show	71	H	-2.7147890	-4.7607350	-0.6290990
72	No	Show	72	C	-1.7419100	-4.0985420	2.5374010
73	No	Show	73	H	-2.7419570	-4.1400690	2.9789240
74	No	Show	74	H	-1.2016180	-5.0175540	2.8059470
75	No	Show	75	H	-1.2148240	-3.2460760	2.9641180
76	No	Show	76	H	4.7314319	2.3865081	0.7918132
77	No	Show	77	O	-0.2302655	3.2508665	0.3292546
78	No	Show	78	C	1.4179206	5.2892765	0.6049986
79	No	Show	79	H	1.1188498	5.5730364	-0.3823904
80	No	Show	80	H	0.5773801	5.3520215	1.2641305
81	No	Show	81	H	2.2022263	5.9583706	0.9527364

#### TS\_33b\_to\_34b+32

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	C	2.8124524	1.3183864	0.6839630
2	No	Show	2	C	3.6524196	2.4749683	0.7248710
3	No	Show	3	C	1.4743354	1.5897894	0.4544390
4	No	Show	4	N	3.2045844	3.7091490	0.7103643
5	No	Show	5	C	0.9548676	2.9513178	0.4342233
6	No	Show	6	N	1.9189897	3.9225525	0.5863212
7	No	Show	7	Pd	0.1318111	-0.1013534	0.4340922
8	No	Show	8	P	-1.9194780	0.7304967	-0.1040653
9	No	Show	9	C	-1.8572210	2.3944727	-0.8862163
10	No	Show	10	C	-0.9177870	2.6004597	-1.9073443
11	No	Show	11	C	-2.7286130	3.4337717	-0.5410203
12	No	Show	12	C	-0.8626490	3.8172847	-2.5829813

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13	No	Show	13	H	-0.2156780	1.8084907	-2.1581323
14	No	Show	14	C	-2.6593490	4.6592257	-1.2075563
15	No	Show	15	H	-3.4542270	3.2993907	0.2559187
16	No	Show	16	C	-1.7323120	4.8518857	-2.2315303
17	No	Show	17	H	-0.1261490	3.9643837	-3.3684763
18	No	Show	18	H	-3.3321300	5.4637557	-0.9215493
19	No	Show	19	H	-1.6791230	5.8076417	-2.7464023
20	No	Show	20	C	-2.9844770	0.9519507	1.3724247
21	No	Show	21	C	-4.3839410	0.9601397	1.2931737
22	No	Show	22	C	-2.3675860	1.1608927	2.6127707
23	No	Show	23	C	-5.1509630	1.1716427	2.4392457
24	No	Show	24	H	-4.8781980	0.7929617	0.3399847
25	No	Show	25	C	-3.1363290	1.3830987	3.7543317
26	No	Show	26	H	-1.2818830	1.1434567	2.6798057
27	No	Show	27	C	-4.5296530	1.3857257	3.6704287
28	No	Show	28	H	-6.2357350	1.1685187	2.3677497
29	No	Show	29	H	-2.6457140	1.5450307	4.7106377
30	No	Show	30	H	-5.1292530	1.5498137	4.5622257
31	No	Show	31	C	-2.9863540	-0.1783613	-1.2960663
32	No	Show	32	C	-3.3124580	0.3431007	-2.5550093
33	No	Show	33	C	-3.5462320	-1.4010383	-0.9010353
34	No	Show	34	C	-4.1861260	-0.3427983	-3.4004143
35	No	Show	35	H	-2.9067320	1.2951397	-2.8797033
36	No	Show	36	C	-4.4455350	-2.0630743	-1.7332533
37	No	Show	37	H	-3.2922480	-1.8320163	0.0637597
38	No	Show	38	C	-4.7631080	-1.5423663	-2.9886353
39	No	Show	39	H	-4.4269170	0.0760737	-4.3741973
40	No	Show	40	H	-4.8965560	-2.9944053	-1.4022953
41	No	Show	41	H	-5.4559680	-2.0685273	-3.6406153
42	No	Show	42	O	-0.8037578	-3.0900962	-0.7952733
43	No	Show	43	C	-0.7608717	-3.4414453	0.3720340
44	No	Show	44	H	-0.9531143	-1.3110288	0.7370934
45	No	Show	45	O	0.3731583	-3.4368852	1.1019606
46	No	Show	46	H	1.0817277	-3.1327872	0.4941123
47	No	Show	47	N	-1.8498593	-3.9147790	1.0836330
48	No	Show	48	C	-2.6036823	-4.9700117	0.4168028
49	No	Show	49	H	-2.1262182	-5.9516633	0.5532442
50	No	Show	50	H	-3.6142949	-5.0177190	0.8334069
51	No	Show	51	H	-2.6667463	-4.7512980	-0.6483977
52	No	Show	52	C	-1.7087999	-4.0945010	2.5237737
53	No	Show	53	H	-2.7089675	-4.1524575	2.9631673
54	No	Show	54	H	-1.1563341	-5.0075352	2.7879057
55	No	Show	55	H	-1.1943186	-3.2373771	2.9565011
56	No	Show	56	H	4.7314319	2.3865081	0.7918132
57	No	Show	57	O	-0.2302655	3.2508665	0.3292546

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58	No	Show	58	C	1.4179206	5.2892765	0.6049986
59	No	Show	59	H	1.1188498	5.5730364	-0.3823904
60	No	Show	60	H	0.5773801	5.3520215	1.2641305
61	No	Show	61	H	2.2022263	5.9583706	0.9527364
62	No	Show	62	C	3.3053564	-0.0977732	0.9042360
63	No	Show	63	C	2.9164258	-1.1123703	0.0291377
64	No	Show	64	C	4.1460312	-0.3878783	1.9787838
65	No	Show	65	C	3.3675725	-2.4168778	0.2290096
66	No	Show	66	H	2.2530261	-0.8834783	-0.8174739
67	No	Show	67	C	4.5981982	-1.6925444	2.1782859
68	No	Show	68	H	4.4528107	0.4116958	2.6684915
69	No	Show	69	C	4.2090205	-2.7070395	1.3037132
70	No	Show	70	H	3.0605502	-3.2167661	-0.4603469
71	No	Show	71	H	5.2613562	-1.9209049	3.0253674
72	No	Show	72	H	4.5646533	-3.7356603	1.4610694

#### TS\_36a\_to\_35a+32

Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	H	-2.5707780	-3.3060920	-1.7228600	
2	No	Show	2	C	-2.9995750	-2.3691750	-1.3935450	
3	No	Show	3	C	-4.3392530	-2.1586390	-0.9641880	
4	No	Show	4	C	-2.3327410	-1.0942880	-1.3779270	
5	No	Show	5	C	-4.5057460	-0.7753550	-0.6617560	
6	No	Show	6	H	-5.0951450	-2.9262330	-0.8503050	
7	No	Show	7	C	-3.2687650	-0.1083990	-0.9051810	
8	No	Show	8	Fe	-3.0275120	-1.6093570	0.5019290	
9	No	Show	9	C	-3.8830910	-1.4481720	2.3390620	
10	No	Show	10	C	-2.6247700	-0.7742060	2.3353470	
11	No	Show	11	C	-3.6471940	-2.8196750	2.0163820	
12	No	Show	12	H	-4.8486590	-0.9874580	2.5069360	
13	No	Show	13	C	-1.6097460	-1.7250000	2.0192780	
14	No	Show	14	H	-2.4755650	0.2862610	2.4965770	
15	No	Show	15	C	-2.2437620	-2.9898060	1.8126780	
16	No	Show	16	H	-4.4052190	-3.5854400	1.9057400	
17	No	Show	17	H	-0.5444590	-1.5472940	1.9422300	
18	No	Show	18	H	-1.7424530	-3.9161550	1.5601200	
19	No	Show	19	H	-1.3869820	-0.8972210	-1.9030130	
20	No	Show	20	H	-5.3978640	-0.2967850	-0.2842440	
21	No	Show	21	C	-2.9011550	1.2935760	-0.7096530	
22	No	Show	22	C	-3.9581890	2.2930080	-0.7851580	
23	No	Show	23	C	-1.5822020	1.6305610	-0.4533920	
24	No	Show	24	N	-3.5022080	3.6068850	-0.7183020	
25	No	Show	25	C	-1.3296920	3.0380690	-0.4376610	
26	No	Show	26	N	-2.2269490	3.9871190	-0.5745700	
27	No	Show	27	Pd	-0.2048320	-0.0229690	-0.3566030	

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28	No	Show	28	P	1.8765000	0.8305410	0.0769510
29	No	Show	29	O	-5.1755810	2.0732710	-0.8788330
30	No	Show	30	H	-0.3261520	3.4326820	-0.3328480
31	No	Show	31	C	1.9638280	2.5813730	0.6418160
32	No	Show	32	C	0.9724600	3.0426770	1.5202010
33	No	Show	33	C	2.9871790	3.4546840	0.2529440
34	No	Show	34	C	1.0229660	4.3393220	2.0287030
35	No	Show	35	H	0.1542290	2.3832270	1.8000500
36	No	Show	36	C	3.0285150	4.7575520	0.7523690
37	No	Show	37	H	3.7521190	3.1275260	-0.4448720
38	No	Show	38	C	2.0519590	5.2006230	1.6446010
39	No	Show	39	H	0.2478700	4.6811510	2.7093570
40	No	Show	40	H	3.8250130	5.4272260	0.4379250
41	No	Show	41	H	2.0843950	6.2171610	2.0281390
42	No	Show	42	C	2.9695790	0.7670340	-1.3960280
43	No	Show	43	C	4.3668020	0.7327750	-1.2890190
44	No	Show	44	C	2.3825610	0.7969190	-2.6672330
45	No	Show	45	C	5.1604420	0.7239910	-2.4364470
46	No	Show	46	H	4.8385540	0.7016610	-0.3104290
47	No	Show	47	C	3.1777720	0.7997000	-3.8124070
48	No	Show	48	H	1.2982940	0.8050310	-2.7557250
49	No	Show	49	C	4.5684780	0.7608310	-3.6996690
50	No	Show	50	H	6.2428480	0.6894380	-2.3408260
51	No	Show	51	H	2.7092570	0.8216610	-4.7930230
52	No	Show	52	H	5.1883400	0.7542190	-4.5927080
53	No	Show	53	C	2.8568450	0.0188220	1.4057450
54	No	Show	54	C	3.1035660	0.6499890	2.6316190
55	No	Show	55	C	3.4068590	-1.2485360	1.1678200
56	No	Show	56	C	3.8892110	0.0251230	3.6014370
57	No	Show	57	H	2.6979070	1.6362410	2.8348120
58	No	Show	58	C	4.2114770	-1.8562470	2.1275610
59	No	Show	59	H	3.1959980	-1.7675190	0.2373850
60	No	Show	60	C	4.4519870	-1.2249390	3.3493620
61	No	Show	61	H	4.0682490	0.5262990	4.5493430
62	No	Show	62	H	4.6410420	-2.8334510	1.9236800
63	No	Show	63	H	5.0716420	-1.7066460	4.1017570
64	No	Show	64	O	0.9950830	-3.0949710	0.8674540
65	No	Show	65	C	-4.4880540	4.6736410	-0.8187690
66	No	Show	66	H	-5.0763390	4.5539890	-1.7312840
67	No	Show	67	H	-5.1742460	4.6383080	0.0314980
68	No	Show	68	H	-3.9446480	5.6168810	-0.8307820
69	No	Show	69	C	0.9628460	-3.4330430	-0.3017030
70	No	Show	70	H	0.9579130	-1.2166970	-0.7197750
71	No	Show	71	O	-0.1714390	-3.3911950	-1.0400130
72	No	Show	72	H	-0.8836010	-3.1219840	-0.4175820

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73	No	Show	73	N	2.0404260	-3.9709480	-0.9888750
74	No	Show	74	C	2.7088020	-5.0908320	-0.3396890
75	No	Show	75	H	2.1893810	-6.0396410	-0.5413960
76	No	Show	76	H	3.7353170	-5.1720200	-0.7098670
77	No	Show	77	H	2.7376030	-4.9213370	0.7368350
78	No	Show	78	C	1.9664280	-4.0472790	-2.4421210
79	No	Show	79	H	2.9839430	-4.1247400	-2.8363760
80	No	Show	80	H	1.3845240	-4.9105630	-2.7960230
81	No	Show	81	H	1.5145910	-3.1382660	-2.8380520

### TS\_36b\_to\_35b+32

Row	Highlight		Display Tag	Symbol	X	Y	Z
1	No	Show	1	C	-2.9011550	1.2935760	-0.7096530
2	No	Show	2	C	-3.9581890	2.2930080	-0.7851580
3	No	Show	3	C	-1.5822020	1.6305610	-0.4533920
4	No	Show	4	N	-3.5022080	3.6068850	-0.7183020
5	No	Show	5	C	-1.3296920	3.0380690	-0.4376610
6	No	Show	6	N	-2.2269490	3.9871190	-0.5745700
7	No	Show	7	Pd	-0.2048320	-0.0229690	-0.3566030
8	No	Show	8	P	1.8765000	0.8305410	0.0769510
9	No	Show	9	O	-5.1755810	2.0732710	-0.8788330
10	No	Show	10	H	-0.3261520	3.4326820	-0.3328480
11	No	Show	11	C	1.9638280	2.5813730	0.6418160
12	No	Show	12	C	0.9724600	3.0426770	1.5202010
13	No	Show	13	C	2.9871790	3.4546840	0.2529440
14	No	Show	14	C	1.0229660	4.3393220	2.0287030
15	No	Show	15	H	0.1542290	2.3832270	1.8000500
16	No	Show	16	C	3.0285150	4.7575520	0.7523690
17	No	Show	17	H	3.7521190	3.1275260	-0.4448720
18	No	Show	18	C	2.0519590	5.2006230	1.6446010
19	No	Show	19	H	0.2478700	4.6811510	2.7093570
20	No	Show	20	H	3.8250130	5.4272260	0.4379250
21	No	Show	21	H	2.0843950	6.2171610	2.0281390
22	No	Show	22	C	2.9695790	0.7670340	-1.3960280
23	No	Show	23	C	4.3668020	0.7327750	-1.2890190
24	No	Show	24	C	2.3825610	0.7969190	-2.6672330
25	No	Show	25	C	5.1604420	0.7239910	-2.4364470
26	No	Show	26	H	4.8385540	0.7016610	-0.3104290
27	No	Show	27	C	3.1777720	0.7997000	-3.8124070
28	No	Show	28	H	1.2982940	0.8050310	-2.7557250
29	No	Show	29	C	4.5684780	0.7608310	-3.6996690
30	No	Show	30	H	6.2428480	0.6894380	-2.3408260
31	No	Show	31	H	2.7092570	0.8216610	-4.7930230
32	No	Show	32	H	5.1883400	0.7542190	-4.5927080
33	No	Show	33	C	2.8568450	0.0188220	1.4057450

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34	No	Show	34	C	3.1035660	0.6499890	2.6316190
35	No	Show	35	C	3.4068590	-1.2485360	1.1678200
36	No	Show	36	C	3.8892110	0.0251230	3.6014370
37	No	Show	37	H	2.6979070	1.6362410	2.8348120
38	No	Show	38	C	4.2114770	-1.8562470	2.1275610
39	No	Show	39	H	3.1959980	-1.7675190	0.2373850
40	No	Show	40	C	4.4519870	-1.2249390	3.3493620
41	No	Show	41	H	4.0682490	0.5262990	4.5493430
42	No	Show	42	H	4.6410420	-2.8334510	1.9236800
43	No	Show	43	H	5.0716420	-1.7066460	4.1017570
44	No	Show	44	O	0.9958361	-3.0641146	0.8612168
45	No	Show	45	C	-4.4880540	4.6736410	-0.8187690
46	No	Show	46	H	-5.0763390	4.5539890	-1.7312840
47	No	Show	47	H	-5.1742460	4.6383080	0.0314980
48	No	Show	48	H	-3.9446480	5.6168810	-0.8307820
49	No	Show	49	C	0.9635991	-3.4021866	-0.3079402
50	No	Show	50	H	1.0154954	-1.2758138	-0.7377603
51	No	Show	51	O	-0.1706859	-3.3603386	-1.0462502
52	No	Show	52	H	-0.8828479	-3.0911276	-0.4238192
53	No	Show	53	N	2.0411791	-3.9400916	-0.9951122
54	No	Show	54	C	2.7095551	-5.0599756	-0.3459262
55	No	Show	55	H	2.1901341	-6.0087846	-0.5476332
56	No	Show	56	H	3.7360701	-5.1411636	-0.7161042
57	No	Show	57	H	2.7383561	-4.8904806	0.7305978
58	No	Show	58	C	1.9671811	-4.0164226	-2.4483582
59	No	Show	59	H	2.9846961	-4.0938836	-2.8426132
60	No	Show	60	H	1.3852771	-4.8797066	-2.8022602
61	No	Show	61	H	1.5153441	-3.1074096	-2.8442892
62	No	Show	62	C	-3.2706505	-0.1155899	-0.9061839
63	No	Show	63	C	-4.4782430	-0.5971830	-0.3999627
64	No	Show	64	C	-2.4140778	-0.9712082	-1.5988228
65	No	Show	65	C	-4.8287920	-1.9342700	-0.5858006
66	No	Show	66	H	-5.1529752	0.0774387	0.1467217
67	No	Show	67	C	-2.7650389	-2.3084923	-1.7856578
68	No	Show	68	H	-1.4623498	-0.5917608	-1.9980251
69	No	Show	69	C	-3.9721073	-2.7901548	-1.2791755
70	No	Show	70	H	-5.7803242	-2.3140906	-0.1862767
71	No	Show	71	H	-2.0896593	-2.9827778	-2.3321700
72	No	Show	72	H	-4.2487429	-3.8443467	-1.4256286

Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	H	3.1320070		1.6607800	1.2503350
2	No	Show	2	C	2.2476910		1.6511140	0.6218690
3	No	Show	3	C	2.2318780		1.5604800	-0.8068450

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4	No	Show	4	C	0.8881950	1.6722070	1.0683350
5	No	Show	5	C	0.8602640	1.5220820	-1.2201910
6	No	Show	6	H	3.1001510	1.4860290	-1.4531510
7	No	Show	7	C	0.0086900	1.5794540	-0.0613140
8	No	Show	8	Fe	1.2599850	-0.0314140	0.0138720
9	No	Show	9	C	0.8337250	-1.6907510	-1.0810000
10	No	Show	10	C	-0.1004250	-1.5770740	0.0015510
11	No	Show	11	C	2.1673130	-1.7607840	-0.5638500
12	No	Show	12	H	0.5670340	-1.6719540	-2.1318680
13	No	Show	13	C	0.6881220	-1.5890110	1.1990890
14	No	Show	14	C	2.0763490	-1.6943110	0.8636850
15	No	Show	15	H	3.0824730	-1.8119500	-1.1447620
16	No	Show	16	H	0.2841920	-1.4765060	2.1988040
17	No	Show	17	H	2.9101760	-1.6874610	1.5579670
18	No	Show	18	H	0.5550560	1.6826690	2.0994960
19	No	Show	19	H	0.5197640	1.3766390	-2.2405230
20	No	Show	20	O	-2.4210280	-1.4172960	1.1632030
21	No	Show	21	H	-2.3612500	-0.5193300	1.5421660
22	No	Show	22	O	-1.9178230	0.0778420	-0.7569500
23	No	Show	23	H	-2.8343150	0.1168640	-1.0734550
24	No	Show	24	O	-2.3259980	-2.3236010	-1.0298430
25	No	Show	25	H	-3.1224890	-2.6228400	-0.5700760
26	No	Show	26	B	-1.7076300	-1.4035310	-0.0929040
27	No	Show	27	B	-1.5924270	1.4352540	-0.0142720
28	No	Show	28	O	-2.3476330	2.4605580	-0.7401670
29	No	Show	29	H	-1.7466470	2.9020970	-1.3516760
30	No	Show	30	O	-2.0983420	1.3579780	1.3602040
31	No	Show	31	H	-2.8696970	1.9388450	1.3924050

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Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	H	3.1320070		1.6607800	1.2503350
2	No	Show	2	C	2.2476910		1.6511140	0.6218690
3	No	Show	3	C	2.2318780		1.5604800	-0.8068450
4	No	Show	4	C	0.8881950		1.6722070	1.0683350
5	No	Show	5	C	0.8602640		1.5220820	-1.2201910
6	No	Show	6	H	3.1001510		1.4860290	-1.4531510
7	No	Show	7	C	0.0086900		1.5794540	-0.0613140
8	No	Show	8	Fe	1.2599850		-0.0314140	0.0138720
9	No	Show	9	C	0.8337250		-1.6907510	-1.0810000
10	No	Show	10	C	-0.1004250		-1.5770740	0.0015510
11	No	Show	11	C	2.1673130		-1.7607840	-0.5638500
12	No	Show	12	H	0.5670340		-1.6719540	-2.1318680
13	No	Show	13	C	0.6881220		-1.5890110	1.1990890
14	No	Show	14	C	2.0763490		-1.6943110	0.8636850



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15	No	Show	15	H	3.0824730	-1.8119500	-1.1447620
16	No	Show	16	H	0.2841920	-1.4765060	2.1988040
17	No	Show	17	H	2.9101760	-1.6874610	1.5579670
18	No	Show	18	H	0.5550560	1.6826690	2.0994960
19	No	Show	19	H	0.5197640	1.3766390	-2.2405230
20	No	Show	20	O	-2.4210280	-1.4172960	1.1632030
21	No	Show	21	H	-2.3612500	-0.5193300	1.5421660
22	No	Show	22	O	-1.9178230	0.0778420	-0.7569500
23	No	Show	23	H	-2.8343150	0.1168640	-1.0734550
24	No	Show	24	O	-2.3259980	-2.3236010	-1.0298430
25	No	Show	25	H	-3.1224890	-2.6228400	-0.5700760
26	No	Show	26	B	-1.7076300	-1.4035310	-0.0929040
27	No	Show	27	B	-1.5924270	1.4352540	-0.0142720
28	No	Show	28	O	-2.3476330	2.4605580	-0.7401670
29	No	Show	29	H	-1.7466470	2.9020970	-1.3516760
30	No	Show	30	O	-2.0983420	1.3579780	1.3602040
31	No	Show	31	H	-2.8696970	1.9388450	1.3924050

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Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	H	2.2974260		1.2939360	0.2637920
2	No	Show	2	C	1.2711210		1.6697420	0.1996320
3	No	Show	3	C	0.5943980		2.0811880	-0.9916010
4	No	Show	4	C	0.2989330		1.6486590	1.2503560
5	No	Show	5	C	-0.7887700		2.3040710	-0.6771940
6	No	Show	6	H	1.0421300		2.1304260	-1.9767340
7	No	Show	7	C	-0.9745140		2.0329770	0.7131500
8	No	Show	8	Fe	-0.2645560		0.3704070	-0.2432310
9	No	Show	9	C	-1.2598420		-0.9222930	-1.4654130
10	No	Show	10	C	-1.8043090		-0.9885790	-0.1381310
11	No	Show	11	C	0.1406160		-1.2362200	-1.4355660
12	No	Show	12	H	-1.8190900		-0.5821440	-2.3293660
13	No	Show	13	C	-0.6991050		-1.3714800	0.7031230
14	No	Show	14	C	0.4987680		-1.5126880	-0.0789530
15	No	Show	15	H	0.8451850		-1.1821590	-2.2574970
16	No	Show	16	H	-0.7520870		-1.4308830	1.7840560
17	No	Show	17	H	1.5232790		-1.6492870	0.2687230
18	No	Show	18	H	0.4817160		1.3021420	2.2598240
19	No	Show	19	H	-1.5880180		2.5202430	-1.3748590
20	No	Show	20	H	-1.9291550		1.9681090	1.2213890
21	No	Show	21	O	-4.2435430		-1.7611050	0.0819050
22	No	Show	22	H	-4.1112850		-2.3469030	0.8384020
23	No	Show	23	O	-3.2865390		-0.1765810	1.7009040
24	No	Show	24	H	-4.1565870		0.1983450	1.8977710
25	No	Show	25	O	-3.8476960		0.4751920	-0.6027520

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26	No	Show	26	H	-4.6495820	0.1171240	-1.0061090
27	No	Show	27	B	-3.3515050	-0.5924240	0.2840940
28	No	Show	28	Br	4.1088710	-0.5582770	0.2113500

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Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	H	2.2974260	1.2939360	0.2637920
2	No	Show	2	C	1.2711210	1.6697420	0.1996320
3	No	Show	3	C	0.5943980	2.0811880	-0.9916010
4	No	Show	4	C	0.2989330	1.6486590	1.2503560
5	No	Show	5	C	-0.7887700	2.3040710	-0.6771940
6	No	Show	6	H	1.0421300	2.1304260	-1.9767340
7	No	Show	7	C	-0.9745140	2.0329770	0.7131500
8	No	Show	8	Fe	-0.2645560	0.3704070	-0.2432310
9	No	Show	9	C	-1.2598420	-0.9222930	-1.4654130
10	No	Show	10	C	-1.8043090	-0.9885790	-0.1381310
11	No	Show	11	C	0.1406160	-1.2362200	-1.4355660
12	No	Show	12	H	-1.8190900	-0.5821440	-2.3293660
13	No	Show	13	C	-0.6991050	-1.3714800	0.7031230
14	No	Show	14	C	0.4987680	-1.5126880	-0.0789530
15	No	Show	15	H	0.8451850	-1.1821590	-2.2574970
16	No	Show	16	H	-0.7520870	-1.4308830	1.7840560
17	No	Show	17	H	1.5232790	-1.6492870	0.2687230
18	No	Show	18	H	0.4817160	1.3021420	2.2598240
19	No	Show	19	H	-1.5880180	2.5202430	-1.3748590
20	No	Show	20	H	-1.9291550	1.9681090	1.2213890
21	No	Show	21	O	-4.2435430	-1.7611050	0.0819050
22	No	Show	22	H	-4.1112850	-2.3469030	0.8384020
23	No	Show	23	O	-3.2865390	-0.1765810	1.7009040
24	No	Show	24	H	-4.1565870	0.1983450	1.8977710
25	No	Show	25	O	-3.8476960	0.4751920	-0.6027520
26	No	Show	26	H	-4.6495820	0.1171240	-1.0061090
27	No	Show	27	B	-3.3515050	-0.5924240	0.2840940
28	No	Show	28	Br	4.1088710	-0.5582770	0.2113500

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Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	O	3.2937030	1.4392210	-0.7330770
2	No	Show	2	H	4.2584260	1.5031350	-0.7307610
3	No	Show	3	O	3.1738830	-0.9243380	-1.4356220
4	No	Show	4	H	2.7997620	-0.5097960	-2.2235850
5	No	Show	5	B	3.0090850	0.0566640	-0.3259720
6	No	Show	6	Br	-3.2343930	0.0358470	-0.5176460
7	No	Show	7	C	1.4670120	0.0165900	0.2490570
8	No	Show	8	C	0.8012170	-1.2247780	0.4328360

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9	No	Show	9	C	0.7570420	1.1844080	0.6249650
10	No	Show	10	C	-0.4744080	-1.3048540	0.9573760
11	No	Show	11	H	1.3232000	-2.1325380	0.1365880
12	No	Show	12	C	-0.5208820	1.1271600	1.1520500
13	No	Show	13	H	1.2531880	2.1414500	0.4831950
14	No	Show	14	C	-1.1596550	-0.1241820	1.3351290
15	No	Show	15	H	-0.9685910	-2.2654110	1.0858520
16	No	Show	16	H	-1.0526220	2.0348700	1.4293600
17	No	Show	17	H	-2.0744270	-0.1877490	1.9146280
18	No	Show	18	O	3.9287090	-0.3784270	0.7505790
19	No	Show	19	H	4.2270750	-1.2596400	0.4886640

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Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	O	3.0094840	-1.5707020	-0.0637030
2	No	Show	2	H	3.1866200	-2.5230590	-0.1021430
3	No	Show	3	O	0.8410200	-2.4189190	0.3211490
4	No	Show	4	H	-0.0979680	-2.1597710	0.2718900
5	No	Show	5	B	1.6746260	-1.3501300	0.1450790
6	No	Show	6	Br	-1.9736630	-0.5682020	-0.2766610
7	No	Show	7	C	1.1644810	0.1414280	0.1650380
8	No	Show	8	C	0.0847540	0.5413340	1.0037830
9	No	Show	9	C	1.7339360	1.1089210	-0.6618290
10	No	Show	10	C	-0.3869150	1.8753490	0.9982450
11	No	Show	11	H	-0.2530660	-0.1228690	1.7946550
12	No	Show	12	C	1.2480420	2.4235020	-0.6827910
13	No	Show	13	H	2.5682320	0.8359880	-1.3024110
14	No	Show	14	C	0.1847520	2.8068360	0.1436560
15	No	Show	15	H	-1.1977110	2.1569380	1.6636440
16	No	Show	16	H	1.7031150	3.1541960	-1.3469140
17	No	Show	17	H	-0.1824780	3.8290610	0.1228550

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Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	H	1.0339800	-1.8562650	-0.9547030
2	No	Show	2	C	0.0477450	-1.8162560	-0.5107530
3	No	Show	3	C	-0.2079050	-1.7106650	0.8910970
4	No	Show	4	C	-1.1906320	-1.7199640	-1.1960370
5	No	Show	5	C	-1.6188820	-1.5944090	1.0710940
6	No	Show	6	H	0.5544810	-1.6890100	1.6585950
7	No	Show	7	C	-2.2280960	-1.5856970	-0.2219170
8	No	Show	8	Fe	-0.9413670	0.0000530	-0.0149050
9	No	Show	9	C	-1.6185110	1.5947920	1.0709640
10	No	Show	10	C	-2.2275480	1.5862310	-0.2221310
11	No	Show	11	C	-0.2074600	1.7105540	0.8911480

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12	No	Show	12	H	-2.1347030	1.4835850	2.0165900
13	No	Show	13	C	-1.1898610	1.7201350	-1.1960840
14	No	Show	14	C	0.0484540	1.8160260	-0.5106380
15	No	Show	15	H	0.5546660	1.6886640	1.6588960
16	No	Show	16	H	-1.3212600	1.7089720	-2.2711110
17	No	Show	17	H	1.0348920	1.8550370	-0.9542450
18	No	Show	18	H	-1.3223240	-1.7089860	-2.2710280
19	No	Show	19	H	-2.1350280	-1.4830710	2.0167310
20	No	Show	20	H	-3.2841620	-1.4643120	-0.4296670
21	No	Show	21	Br	2.7752780	-0.0001610	-0.0015060
22	No	Show	22	H	-3.2835640	1.4651460	-0.43029

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Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	H	2.9954070	-2.7054490	2.6331510	
2	No	Show	2	C	3.2483110	-1.8207280	2.0617290	
3	No	Show	3	C	4.5241510	-1.5125810	1.5019010	
4	No	Show	4	C	2.3619960	-0.7522350	1.7354120	
5	No	Show	5	C	4.4252430	-0.2628160	0.8208620	
6	No	Show	6	H	5.4078400	-2.1372080	1.5530370	
7	No	Show	7	C	3.0872450	0.2183640	0.9514660	
8	No	Show	8	Fe	3.1249230	-1.6448330	0.0289570	
9	No	Show	9	C	3.8803240	-1.9251530	-1.8447210	
10	No	Show	10	C	2.5238660	-1.5004330	-1.9422410	
11	No	Show	11	C	3.9098320	-3.1441930	-1.0986500	
12	No	Show	12	H	4.7413100	-1.3925770	-2.2289730	
13	No	Show	13	C	1.7098350	-2.4622370	-1.2622300	
14	No	Show	14	H	2.1731850	-0.5923270	-2.4172220	
15	No	Show	15	C	2.5708850	-3.4699520	-0.7267780	
16	No	Show	16	H	4.7973250	-3.7011390	-0.8247930	
17	No	Show	17	H	0.6233460	-2.4759000	-1.2205010	
18	No	Show	18	H	2.2618160	-4.3226100	-0.1347950	
19	No	Show	19	H	1.3503670	-0.6322170	2.1189300	
20	No	Show	20	H	5.2107210	0.2384290	0.2731500	
21	No	Show	21	C	2.4888580	1.4337510	0.3784470	
22	No	Show	22	C	3.3316550	2.6065790	0.1813710	
23	No	Show	23	C	1.1592810	1.4590540	0.0144820	
24	No	Show	24	N	2.6485120	3.7216580	-0.3153410	
25	No	Show	25	C	0.6446730	2.6854890	-0.4917530	
26	No	Show	26	N	1.3534140	3.7798600	-0.6495460	
27	No	Show	27	Pd	0.2095180	-0.4326150	0.1004850	
28	No	Show	28	P	-2.1234330	-0.0990430	0.0419450	
29	No	Show	29	O	4.5475020	2.6872170	0.4010840	
30	No	Show	30	H	-0.3944440	2.7872250	-0.7945110	
31	No	Show	31	C	-2.6989280	1.0119050	-1.3012330	

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32	No	Show	32	C	-2.0963710	0.8745590	-2.5610630
33	No	Show	33	C	-3.6882610	1.9875880	-1.1233400
34	No	Show	34	C	-2.4928520	1.6787500	-3.6276200
35	No	Show	35	H	-1.3040820	0.1416810	-2.6998480
36	No	Show	36	C	-4.0739040	2.8025760	-2.1895010
37	No	Show	37	H	-4.1545440	2.1203280	-0.1508970
38	No	Show	38	C	-3.4821010	2.6473570	-3.4431750
39	No	Show	39	H	-2.0176820	1.5607290	-4.5981280
40	No	Show	40	H	-4.8363850	3.5622890	-2.0365950
41	No	Show	41	H	-3.7816850	3.2853840	-4.2706440
42	No	Show	42	C	-2.8240270	0.6360280	1.5730930
43	No	Show	43	C	-4.1030820	0.3177600	2.0513950
44	No	Show	44	C	-2.0380260	1.5538960	2.2851300
45	No	Show	45	C	-4.5884250	0.9133130	3.2162420
46	No	Show	46	H	-4.7208290	-0.4010470	1.5192910
47	No	Show	47	C	-2.5301900	2.1559300	3.4425970
48	No	Show	48	H	-1.0357920	1.7891290	1.9338010
49	No	Show	49	C	-3.8054060	1.8358750	3.9119500
50	No	Show	50	H	-5.5799200	0.6547370	3.5798520
51	No	Show	51	H	-1.9111910	2.8675550	3.9830150
52	No	Show	52	H	-4.1847820	2.2984760	4.8196310
53	No	Show	53	C	-3.1354770	-1.6185560	-0.1903170
54	No	Show	54	C	-4.1590370	-1.7330310	-1.1396030
55	No	Show	55	C	-2.8296340	-2.7284060	0.6140970
56	No	Show	56	C	-4.8648790	-2.9306490	-1.2764500
57	No	Show	57	H	-4.4097840	-0.8878720	-1.7747570
58	No	Show	58	C	-3.5441680	-3.9169240	0.4865680
59	No	Show	59	H	-2.0277290	-2.6579790	1.3473110
60	No	Show	60	C	-4.5632450	-4.0230240	-0.4638390
61	No	Show	61	H	-5.6547800	-3.0058300	-2.0198010
62	No	Show	62	H	-3.2999510	-4.7642850	1.1223750
63	No	Show	63	H	-5.1146370	-4.9534940	-0.5719880
64	No	Show	64	C	3.4197620	4.9401190	-0.5234350
65	No	Show	65	H	3.9075440	5.2370790	0.4076110
66	No	Show	66	H	4.1975140	4.7726420	-1.2729470
67	No	Show	67	H	2.7265710	5.7096360	-0.8583270

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Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	H	1.5570560	1.7671020	2.1305080
2	No	Show	2	C	0.8774140	1.7492490	1.2867890
3	No	Show	3	C	1.2744140	1.5963120	-0.0777450
4	No	Show	4	C	-0.5548580	1.7581950	1.3371250
5	No	Show	5	C	0.0708600	1.5131190	-0.8551920
6	No	Show	6	H	2.3003040	1.4220620	-0.4147860

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7	No	Show	7	C	-1.0811870	1.5940370	0.0107770
8	No	Show	8	Fe	0.1124460	0.0091640	0.5007350
9	No	Show	9	C	0.0941470	-1.6083360	-0.7300140
10	No	Show	10	C	-1.1015540	-1.5896680	0.0735410
11	No	Show	11	C	1.2549680	-1.6430130	0.1119830
12	No	Show	12	H	0.1147350	-1.5260450	-1.8098300
13	No	Show	13	C	-0.6483080	-1.6444340	1.4349200
14	No	Show	14	C	0.7857700	-1.6691640	1.4630220
15	No	Show	15	H	2.2972160	-1.5180660	-0.1922280
16	No	Show	16	H	-1.3056920	-1.5917190	2.2950240
17	No	Show	17	H	1.4188850	-1.6302940	2.3417290
18	No	Show	18	H	-1.1682260	1.7858320	2.2299170
19	No	Show	19	H	0.0396160	1.3077840	-1.9191740
20	No	Show	20	O	-3.6178250	-1.4689090	0.6498780
21	No	Show	21	H	-3.7123050	-0.5604960	0.9945740
22	No	Show	22	O	-2.7059400	0.0115810	-1.1315510
23	No	Show	23	H	-3.4832070	0.0132690	-1.7134390
24	No	Show	24	O	-2.9767230	-2.3954420	-1.4497350
25	No	Show	25	H	-3.8348300	-2.7621290	-1.1964290
26	No	Show	26	B	-2.6523410	-1.4483730	-0.4128960
27	No	Show	27	B	-2.6433350	1.3965700	-0.3694050
28	No	Show	28	O	-3.2020330	2.3789500	-1.2811150
29	No	Show	29	H	-2.5053060	2.7708500	-1.8206650
30	No	Show	30	O	-3.4648480	1.3203840	0.8326570
31	No	Show	31	H	-4.2419490	1.8735450	0.6775420
32	No	Show	32	Br	4.5139270	-0.0126070	-0.4572190

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Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	H	0.6282460	2.5446660	0.8242200	
2	No	Show	2	C	0.3338510	2.0015940	-0.0676930	
3	No	Show	3	C	1.2220010	1.3022410	-0.9280990	
4	No	Show	4	C	-1.0234300	1.7966080	-0.4635350	
5	No	Show	5	C	0.4250560	0.6408680	-1.8974150	
6	No	Show	6	H	2.2991230	1.1914100	-0.8056320	
7	No	Show	7	C	-0.9423580	0.9339120	-1.6200550	
8	No	Show	8	Fe	-0.0829230	-0.0177080	-0.0191210	
9	No	Show	9	C	0.2670260	-2.0579540	0.1029100	
10	No	Show	10	C	-1.0838710	-1.7839780	0.4715240	
11	No	Show	11	C	1.1667060	-1.3572450	0.9478060	
12	No	Show	12	H	0.5466530	-2.6432030	-0.7659680	
13	No	Show	13	C	-0.9886360	-0.8799720	1.5960220	
14	No	Show	14	C	0.3823810	-0.6326090	1.8824610	
15	No	Show	15	H	2.2478350	-1.2864860	0.8367390	
16	No	Show	16	H	-1.8292280	-0.3857030	2.0696380	

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17	No	Show	17	H	0.7689760	0.0670510	2.6157040
18	No	Show	18	H	0.7906000	-0.0501660	-2.6497500
19	No	Show	19	H	-1.7942930	0.5044460	-2.1332840
20	No	Show	20	O	-2.8257470	-3.6597140	0.4486250
21	No	Show	21	H	-3.6402620	-3.4402690	0.9192510
22	No	Show	22	O	-3.5577350	-1.4032110	-0.0230600
23	No	Show	23	H	-3.8280210	-1.1381540	-0.9123110
24	No	Show	24	O	-2.1923110	-2.6487730	-1.6499980
25	No	Show	25	H	-2.5841950	-3.5210390	-1.7907990
26	No	Show	26	B	-2.4469580	-2.3802470	-0.2219920
27	No	Show	27	Br	5.0754630	-0.0423880	0.0052630
28	No	Show	28	B	-2.3938330	2.4369460	0.2079630
29	No	Show	29	O	-3.5764180	1.6206830	-0.0333450
30	No	Show	30	H	-3.3964940	0.6984000	0.2170640
31	No	Show	31	O	-2.0821880	2.6124820	1.6633270
32	No	Show	32	H	-2.9507490	2.7721480	2.0603390
33	No	Show	33	O	-2.6503790	3.7560240	-0.4346230
34	No	Show	34	H	-2.0135750	4.3466680	-0.0130850

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Row	Highlight		Display Tag		Symbol	X	Y	Z
1	No	Show	1	H	-	3.5862740	-2.3822810	-2.4282920
2	No	Show	2	C	-	3.6594900	-1.4022500	-1.9728500
3	No	Show	3	C	-	4.8593630	-0.7629490	-1.5388820
4	No	Show	4	C	-	2.5697260	-0.5336690	-1.6787900
5	No	Show	5	C	-	4.5072220	0.5000730	-0.9737670
6	No	Show	6	H	-	5.8580490	-1.1798850	-1.5886800
7	No	Show	7	C	-	3.0873490	0.6521500	-1.0485330
8	No	Show	8	Fe	-	3.6044420	-1.0318900	0.0412970
9	No	Show	9	C	-	4.7433880	-1.2578140	1.7151060
10	No	Show	10	C	-	3.4855070	-0.6876130	2.0679620
11	No	Show	11	C	-	4.5003050	-2.5256750	1.1013870
12	No	Show	12	H	-	5.7120790	-0.7906890	1.8447480
13	No	Show	13	C	-	2.4629290	-1.6102420	1.6873510
14	No	Show	14	H	-	3.3235590	0.2835570	2.5188000
15	No	Show	15	C	-	3.0911030	-2.7396480	1.0724160
16	No	Show	16	H	-	5.2513240	-3.1880300	0.6882970
17	No	Show	17	H	-	1.4033780	-1.5177430	1.9342640
18	No	Show	18	H	-	2.5848570	-3.6000030	0.6522610
19	No	Show	19	H	-	1.5300220	-0.7120360	-1.9338620
20	No	Show	20	H	-	5.1917830	1.1966360	-0.5044010
21	No	Show	21	C	-	2.2851850	1.7868540	-0.5482410
22	No	Show	22	C	-	2.7829590	3.1193280	-0.7030530
23	No	Show	23	C	-	1.0713290	1.5836030	0.0652320
24	No	Show	24	N	-	2.1491580	4.1809420	-0.2832430

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25	No	Show	25	C	-0.3600830	2.7419570	0.5686900
26	No	Show	26	N	-0.9728800	3.9812740	0.3280990
27	No	Show	27	Pd	-0.4066920	-0.3944090	0.2739650
28	No	Show	28	P	1.9512480	-0.3956890	-0.0150360
29	No	Show	29	C	2.9703680	-0.4046560	1.5123990
30	No	Show	30	C	4.0120210	-1.3176980	1.7265580
31	No	Show	31	C	2.6562400	0.5311510	2.5114800
32	No	Show	32	C	4.7306130	-1.2973540	2.9233910
33	No	Show	33	H	4.2682440	-2.0467440	0.9628570
34	No	Show	34	C	3.3864200	0.5521120	3.6989890
35	No	Show	35	H	1.8571080	1.2497890	2.3391030
36	No	Show	36	C	4.4203200	-0.3629800	3.9116370
37	No	Show	37	H	5.5354140	-2.0118060	3.0793490
38	No	Show	38	H	3.1417210	1.2857070	4.4633030
39	No	Show	39	H	4.9814210	-0.3476730	4.8429250
40	No	Show	40	C	2.6236370	0.9774820	-1.0245620
41	No	Show	41	C	3.8541370	1.5874960	-0.7533690
42	No	Show	42	C	1.8719630	1.4135230	-2.1235160
43	No	Show	43	C	4.3285260	2.6098180	-1.5763430
44	No	Show	44	H	4.4408970	1.2717680	0.1050550
45	No	Show	45	C	2.3518210	2.4273070	-2.9509040
46	No	Show	46	H	0.9011400	0.9654780	-2.3228480
47	No	Show	47	C	3.5820860	3.0287700	-2.6784610
48	No	Show	48	H	5.2827540	3.0806440	-1.3528450
49	No	Show	49	H	1.7581130	2.7568290	-3.7999650
50	No	Show	50	H	3.9528030	3.8267460	-3.3170940
51	No	Show	51	C	2.5213710	-1.8997580	-0.9168460
52	No	Show	52	C	3.4458700	-1.8651680	-1.9688720
53	No	Show	53	C	1.9754150	-3.1371550	-0.5400070
54	No	Show	54	C	3.8183200	-3.0412450	-2.6236520
55	No	Show	55	H	3.8770660	-0.9184350	-2.2819320
56	No	Show	56	C	2.3579110	-4.3122680	-1.1834960
57	No	Show	57	H	1.2471870	-3.1800270	0.2686950
58	No	Show	58	C	3.2798400	-4.2668000	-2.2321320
59	No	Show	59	H	4.5337130	-2.9964740	-3.4412390
60	No	Show	60	H	1.9298970	-5.2622700	-0.8729390
61	No	Show	61	H	3.5718000	-5.1808160	-2.7430670
62	No	Show	62	H	-3.7287170	3.3180280	-1.2024250
63	No	Show	63	O	0.7132060	2.7318020	1.1930180
64	No	Show	64	C	-0.2930660	5.1773700	0.8073750
65	No	Show	65	H	-0.2082290	5.1526880	1.8969220
66	No	Show	66	H	0.7160830	5.2230800	0.3921930
67	No	Show	67	H	-0.8811050	6.0369940	0.4898970