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M END











45.8590	0.4180	-18.1690	C	0	0	3	0	0	0	0	0	0	0	0	0	0
45.7460	1.3390	-18.7540	H	0	0	0	0	0	0	0	0	0	0	0	0	0
45.6590	0.6970	-16.6690	C	0	0	0	0	0	0	0	0	0	0	0	0	0
44.6140	0.9650	-16.4810	H	0	0	0	0	0	0	0	0	0	0	0	0	0
45.9010	-0.2070	-16.0980	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.5360	1.7980	-16.2520	N	0	0	3	0	0	0	0	0	0	0	0	0	0
47.4970	1.5580	-16.5090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
47.1950	-0.0580	-18.3960	O	0	0	0	0	0	0	0	0	0	0	0	0	0
47.1770	-0.3930	-19.3160	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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201210	2	0	0	0	0
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M END  
> <NAME>  
AA24\_12

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AA28\_12  
MOE2012 3D

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10.0650 -17.9010 -5.5770 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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9.0460 -18.2090 -5.3210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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11.0290 -19.4030 -4.3760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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9.7190 -17.9110 -2.8410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
11.7470 -18.0090 -2.0910 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
11.7110 -19.0900 -1.9100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
12.7550 -17.7530 -2.4380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
11.4310 -17.2830 -0.8620 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
11.4160 -16.2750 -1.0630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
11.0400 -9.0050 1.7620 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
11.2910 -9.0980 0.3880 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
12.1700 -9.6140 0.0100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
10.4100 -8.5170 -0.5260 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
10.6080 -8.5920 -1.5930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
9.2760 -7.8440 -0.0740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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12.7900 -14.5000 2.1970 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
13.0420 -13.1000 1.9940 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
13.7820 -12.9820 1.1920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
12.1030 -12.6310 1.6750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
13.5730 -12.4350 3.2970 C 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
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12.3820 -13.5830 4.7420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
12.8120 -11.7180 5.5110 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
11.7880 -11.3640 6.3340 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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13.1900 -10.8310 8.3290 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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13.8390 -11.6130 7.9150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
12.2390 -14.6740 -0.0310 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
10.6590 -11.8350 6.3170 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
14.8660 -13.1930 3.7400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
14.6180 -14.2350 3.9810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
15.5540 -13.2380 2.8850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
13.9090 -10.9470 2.9970 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
14.0880 -10.3550 3.9020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
14.8380 -10.8950 2.4160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0









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M END
> <NAME>
AA28_12

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AA28_12
MOE2012 3D

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10.7730 -22.3280 1.9720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.9270 -22.6790 0.6590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.5160 -21.0960 0.2050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.6320 -21.2030 -0.8810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.4500 -20.8950 0.3740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.3610 -19.9350 0.7180 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.2510 -19.8640 1.8080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.4220 -20.1290 0.5130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.9380 -18.6170 0.0680 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.1120 -18.6630 -1.0130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.8660 -18.4600 0.2360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.7100 -17.5210 0.6560 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
11.5870 -17.5430 1.6750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.1750 -15.9700 8.7950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.5780 -16.8580 7.8900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.5510 -16.6470 6.8240 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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30.1220	-4.3880	6.7660	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.5920	-5.8320	7.6120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.7600	-7.7210	5.9070	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.7700	-7.8210	6.3150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.0660	-8.1500	6.6400	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.6710	-5.4210	7.7910	C	0	0	0	0	0	0	0	0	0	0	0	0	0
32.4800	-4.9000	7.2740	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.0040	-6.4290	8.0500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.4980	-4.8850	8.7310	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.7500	-8.4530	4.6660	O	0	0	0	0	0	0	0	0	0	0	0	0	0
30.0210	-9.5960	4.6110	C	0	0	0	0	0	0	0	0	0	0	0	0	0
29.4200	-10.1270	5.5340	O	0	0	0	0	0	0	0	0	0	0	0	0	0
40.2600	-3.8890	9.2060	O	0	0	0	0	0	0	0	0	0	0	0	0	0
40.6220	-4.3120	10.0030	H	0	0	0	0	0	0	0	0	0	0	0	0	0
39.5690	-4.9010	8.4840	C	0	0	0	0	0	0	0	0	0	0	0	0	0
40.2380	-5.7570	8.3590	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.7010	-5.2170	9.0700	H	0	0	0	0	0	0	0	0	0	0	0	0	0
39.1390	-4.3490	7.1300	C	0	0	0	0	0	0	0	0	0	0	0	0	0
38.4520	-3.5080	7.2830	H	0	0	0	0	0	0	0	0	0	0	0	0	0
40.0120	-3.9330	6.6130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.4800	-5.4240	6.2630	C	0	0	0	0	0	0	0	0	0	0	0	0	0
39.1840	-6.2530	6.1270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.6050	-5.8320	6.7860	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.0500	-4.8600	4.9030	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.3080	-4.0700	5.0750	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.8950	-4.3530	4.4210	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.5080	-5.9420	4.0570	N	0	0	3	0	0	0	0	0	0	0	0	0	0
43.1270	-5.5520	6.4380	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.2390	-5.4430	5.0460	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1450	-6.3160	4.4040	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.4770	-4.2000	4.4560	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.5610	-4.1180	3.3750	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.6060	-3.0630	5.2510	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.7910	-2.0950	4.7910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.4940	-3.1630	6.6370	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.5880	-2.2760	7.2570	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.2550	-4.4040	7.2300	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1640	-4.4640	8.3130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.3910	-6.2440	2.9070	C	0	0	0	0	0	0	0	0	0	0	0	0	0
38.5440	-5.3350	2.3100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.8910	-6.9650	2.2460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
39.7540	-6.8350	3.2740	C	0	0	0	0	0	0	0	0	0	0	0	0	0
40.3660	-6.8960	2.3660	H	0	0	0	0	0	0	0	0	0	0	0	0	0
40.2810	-6.1940	3.9870	H	0	0	0	0	0	0	0	0	0	0	0	0	0
39.6580	-8.2340	3.8360	C	0	0	0	0	0	0	0	0	0	0	0	0	0
40.8670	-8.5820	4.3690	O	0	0	0	0	0	0	0	0	0	0	0	0	0
40.9140	-9.8840	4.9740	C	0	0	0	0	0	0	0	0	0	0	0	0	0
40.1350	-9.9290	5.7430	H	0	0	0	0	0	0	0	0	0	0	0	0	0
40.6940	-10.6370	4.2060	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.3070	-10.1670	5.6030	C	0	0	3	0	0	0	0	0	0	0	0	0	0
43.3850	-10.0420	4.4910	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1860	-10.7580	3.6850	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.3660	-9.0490	4.0280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.7120	-10.2030	5.0350	O	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4480	-11.2750	4.6180	C	0	0	0	0	0	0	0	0	0	0	0	0	0
46.8160	-11.2140	5.2600	C	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2330	-10.2200	5.0650	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.6790	-11.3370	6.3390	H	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7570	-12.2830	4.6860	C	0	0	0	0	0	0	0	0	0	0	0	0	0
47.3590	-13.2910	4.8630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7640	-12.1420	3.5970	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.6790	-8.9640	3.7900	O	0	0	0	0	0	0	0	0	0	0	0	0	0
45.0600	-12.1510	3.8600	O	0	0	0	0	0	0	0	0	0	0	0	0	0
42.3470	-11.6170	6.1730	C	0	0	0	0	0	0	0	0	0	0	0	0	0
42.2200	-12.3310	5.3490	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.3390	-11.8160	6.5990	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.5930	-9.1530	6.7430	C	0	0	0	0	0	0	0	0	0	0	0	0	0
41.7410	-9.1130	7.4330	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.4840	-9.4540	7.3080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.3150	-11.9480	7.2450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
40.2930	-11.8750	6.8610	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.4110	-11.2950	8.1160	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.4590	-12.9770	7.5900	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.8310	-7.8430	6.2070	O	0	0	0	0	0	0	0	0	0	0	0	0	0
42.8690	-6.8350	7.1120	C	0	0	0	0	0	0	0	0	0	0	0	0	0
42.7080	-6.9430	8.3190	O	0	0	0	0	0	0	0	0	0	0	0	0	0
49.7930	-8.0860	7.0350	O	0	0	0	0	0	0	0	0	0	0	0	0	0
50.3860	-7.8840	7.7790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0740	-9.4210	6.6270	C	0	0	0	0	0	0	0	0	0	0	0	0	0
49.5010	-9.6110	5.7190	H	0	0	0	0	0	0	0	0	0	0	0	0	0
51.1390	-9.4850	6.3820	H	0	0	0	0	0	0	0	0	0	0	0	0	0

49.7020	-10.3810	7.7500	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1780	-10.0270	8.6740	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.6240	-10.3300	7.9450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1440	-11.8270	7.5120	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.1780	-11.8400	7.1620	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1560	-12.3310	8.4880	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2240	-12.6530	6.6000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.5300	-13.7060	6.6280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.2360	-12.6490	7.0770	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.1430	-12.1640	5.2100	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
56.6470	-17.2540	8.2630	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.9320	-17.4110	6.9000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.9520	-16.5590	6.2250	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.1980	-18.6800	6.3800	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.4220	-18.7970	5.3230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.1780	-19.7950	7.2160	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.3840	-20.7830	6.8100	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.8920	-19.6460	8.5720	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.8740	-20.5170	9.2230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.6270	-18.3800	9.0960	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.4040	-18.2800	10.1570	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0700	-12.8960	4.3070	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.8240	-12.6040	3.2770	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.8980	-13.9780	4.3610	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.5540	-12.5390	4.4660	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.0460	-12.6280	3.4890	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.6630	-11.5010	4.7950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.3040	-13.4570	5.3990	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.4840	-12.8690	5.7680	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.2230	-13.6010	6.7590	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.5820	-13.7300	7.6410	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.4610	-14.5930	6.3560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.5240	-12.8470	7.1670	C	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
56.4760	-12.8340	5.9410	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.5260	-13.8360	5.4960	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.1070	-12.1370	5.1780	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.8060	-12.4350	6.3230	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.7560	-12.5730	5.3520	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0910	-12.1310	5.8920	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0060	-11.0880	6.2150	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.3160	-12.7590	6.7600	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.1830	-12.2620	4.8270	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.2330	-13.2880	4.4430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9140	-11.6360	3.9670	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.9300	-14.5620	5.7640	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.5530	-12.9930	4.2220	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.1450	-11.4030	7.6110	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.6680	-10.8730	6.7760	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.3850	-11.4660	8.4010	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.1600	-13.6240	8.3450	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.1080	-13.1800	8.6630	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.4760	-13.6170	9.2030	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.2750	-10.5200	8.1250	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.0060	-10.3000	7.3430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.7920	-10.9690	8.9780	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.8670	-9.5600	8.4610	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.4410	-14.9690	7.9200	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.3610	-15.9400	8.8630	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.0950	-15.7810	10.0450	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.0440	-13.7320	8.9720	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.9290	-13.4200	9.2270	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.5240	-12.7960	8.0390	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.4750	-11.8150	8.5210	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.2030	-12.7410	7.1830	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.1430	-13.2630	7.6110	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.2180	-14.2650	7.1700	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.5070	-13.3740	8.4980	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.5030	-12.2950	6.6190	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.4370	-11.2980	7.0730	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.1380	-12.2050	5.7290	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1090	-12.7790	6.2190	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1900	-13.7660	5.7480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.4980	-12.8830	7.1220	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.5060	-11.8270	5.2870	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
62.4390	-10.9080	5.7220	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END  
> <NAME>  
AA28\_12

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AA36\_12  
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24.8740 -22.3790 14.2600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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M END
> <NAME>
AA36_12

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$$$$
AA60_12
MOE2012 3D

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22.6660 -7.8090 0.8920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.8250 -8.8200 -0.2860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.2420 -6.8100 -0.3130 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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22.0080 -5.4600 1.1190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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19.7120 -4.6000 -0.7440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.4870 -3.2240 0.6820 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.2600 -3.3110 1.4820 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.2700 -4.1850 2.1400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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19.1700 -2.4420 2.1450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.2960 -5.3050 3.3890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.2650 -6.1430 2.9500 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.5060 -5.7900 2.2560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.1970 -7.4640 3.4000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.3950 -8.1140 3.0580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.1540 -7.9510 4.2890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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29.9310 -7.5020 5.4230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.2570 -5.8020 4.2800 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.0680 -5.1660 4.6290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.4810 -1.9640 -0.0870 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.1650 -1.1430 0.5710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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218220	2	0	0	0	0
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220222	1	0	0	0	0
222223	1	0	0	0	0
224225	1	0	0	0	0
224226	1	0	0	0	0
224227	1	0	0	0	0
227228	1	0	0	0	0
227229	1	0	0	0	0
227230	1	0	0	0	0
230231	1	0	0	0	0
230247	2	0	0	0	0
231232	1	0	0	0	0
232233	1	0	0	0	0
232234	1	0	0	0	0
232235	1	0	0	0	0
235236	1	0	0	0	0
235249	1	0	0	0	0
235252	1	0	0	0	0
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236239	1	0	0	0	0
239240	1	0	0	0	0
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240248	2	0	0	0	0
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244245	1	0	0	0	0
244246	1	0	0	0	0
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259260	1	0	0	0	0
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270271	1	0	0	0	0
270272	1	0	0	0	0
270273	1	0	0	0	0
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278279	1	0	0	0	0
278287	2	0	0	0	0
278325	1	0	0	0	0
279280	1	0	0	0	0
279281	2	0	0	0	0
281282	1	0	0	0	0
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283284	1	0	0	0	0
283285	2	0	0	0	0
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295296	1	0	0	0	0
295312	2	0	0	0	0
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309310	1	0	0	0	0
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324325	1	0	0	0	0
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327328	1	0	0	0	0
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327330	1	0	0	0	0
327331	1	0	0	0	0
331332	1	0	0	0	0

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338340 1 0 0 0 0  
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340343 1 0 0 0 0

M END  
> <NAME>  
AA60\_12

\$\$\$\$  
AA61\_12  
MOE2012 3D

379383 0 0 1 0 0 0 0 0999 V2000  
32.5490 -13.1330 -3.8890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
32.7440 -13.2810 -4.9570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
33.1270 -12.2650 -3.5530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
31.1200 -12.9210 -3.6600 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0  
30.9490 -12.8140 -2.6590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
30.6480 -11.7240 -4.3680 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
31.1900 -10.8400 -4.0100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
30.8580 -11.8370 -5.4360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
29.1360 -11.5180 -4.1340 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.5690 -12.4030 -4.4570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.9910 -11.4420 -3.0500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.6280 -10.2990 -4.8060 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0  
27.3820 -9.8290 -4.1680 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.8560 -9.1290 -4.8230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.6920 -10.6610 -3.9840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
33.0140 -14.3650 -3.1280 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
32.8660 -14.2460 -2.0490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
32.4720 -15.2600 -3.4530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
34.0820 -14.5350 -3.3040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.6560 -9.0680 -2.8740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.3360 -8.2280 -3.0500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.0890 -9.7050 -2.0980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.7200 -8.6610 -2.4780 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.9000 -7.3580 -6.9420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.0960 -8.0330 -5.7300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.9420 -7.8050 -5.0860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.1940 -9.0200 -5.3240 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.3480 -9.5400 -4.3820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.0960 -9.3370 -6.1220 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.3950 -10.1040 -5.8040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.8960 -8.6670 -7.3280 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.0390 -8.9140 -7.9500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.7930 -7.6800 -7.7380 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.6210 -7.1660 -8.6820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.4120 -10.5580 -6.2490 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.4800 -11.1150 -6.4110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
29.2120 -11.2010 -6.6310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.4840 -9.2740 -7.0790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
29.0130 -8.4740 -6.5480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
29.0530 -9.4490 -8.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.1160 -8.8190 -7.5010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.8500 -7.5830 -6.9950 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.5470 -7.0680 -7.3080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.5010 -6.8740 -8.3870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.7930 -7.8260 -7.0590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.2800 -5.7550 -6.5170 C 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0  
25.3130 -6.1010 -5.0050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.6860 -6.9800 -4.8070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.3380 -6.3320 -4.6870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.8310 -5.0000 -4.2170 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.6610 -5.2650 -2.8900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.2120 -4.0110 -2.1790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.9360 -3.2240 -2.4140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.2270 -3.7310 -2.5680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.1390 -4.2390 -0.6650 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.5040 -5.1190 -0.4970 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.1320 -4.5050 -0.2810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.3530 -9.4810 -8.1910 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.8500 -6.3490 -2.3580 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.3850 -4.7220 -6.8920 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.3710 -5.1260 -6.6310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0





45.4260	4.8500	11.6290	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.3580	3.9650	11.8180	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0
46.6110	2.7030	11.9690	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2980	1.9130	12.3000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8380	2.7950	12.7420	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2720	8.5160	10.4530	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.9500	7.8900	11.0360	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7360	8.7170	9.4820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.1690	9.4730	10.9760	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.9850	2.2100	10.6680	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.7380	2.1200	9.8780	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.1910	2.8740	10.3160	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.5410	1.2210	10.8200	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.7850	8.8700	13.4130	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.9630	9.8000	12.7660	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0620	9.9970	11.7020	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.9890	10.4970	13.4850	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.3630	11.2280	12.9790	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.8250	10.2620	14.8480	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.0700	10.8070	15.4090	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.6330	9.3280	15.4960	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.5030	9.1430	16.5590	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.6100	8.6330	14.7820	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.2330	7.9080	15.3040	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.1600	4.2260	13.0300	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.6680	3.3040	13.3400	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.5070	4.5160	13.8630	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2370	5.2920	12.8250	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.7930	6.2520	12.5440	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.7810	5.4550	13.7620	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.2480	4.8740	11.7880	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.6330	5.9580	11.0500	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.7070	5.7070	10.1340	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.5150	5.1960	10.6710	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.3340	5.0400	9.3460	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.2430	7.0190	9.5020	C	0	0	3	0	0	0	0	0	0	0	0	0	0	0
51.0620	7.7810	8.8400	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.5920	7.1430	8.0800	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.2990	8.0580	9.5760	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.5460	8.9830	8.2140	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.6420	9.6450	7.4360	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.2920	10.8420	6.7870	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.3500	10.8870	7.0630	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.2710	10.6750	5.7040	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.5610	12.1420	7.1310	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.0350	12.9820	6.6070	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.5490	12.0540	6.7190	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.6990	3.7420	11.6670	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.4800	9.3050	7.2580	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.2890	6.6710	8.3960	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.7930	6.1040	7.5980	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.6540	7.5960	7.9300	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.9150	7.9140	10.5790	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.6470	7.3480	11.1670	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.4730	8.7250	10.0960	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.5090	5.8760	8.8500	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.2310	4.8900	9.2330	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.0750	6.4050	9.6210	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.1810	5.7160	8.0010	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.9500	8.5580	11.4300	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.8300	8.1120	12.7040	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.4680	7.2080	13.2240	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.4810	13.4330	8.8940	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.6360	13.8210	9.9090	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.5600	14.2920	8.2160	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.4960	12.4080	8.5810	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0
51.8140	12.8140	9.1260	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.6230	12.4290	8.5020	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.9280	13.9060	9.1200	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.9830	12.2480	10.5540	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.1360	12.6100	11.1510	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.9070	11.1540	10.5300	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.2440	12.6580	11.2210	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0
53.1140	12.3820	12.6710	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.2020	12.8650	13.0440	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.0000	11.3060	12.8540	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.0680	12.8590	8.8670	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7620	12.5530	7.8630	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.9830	11.9930	9.5320	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.3530	13.6140	9.2110	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.2590	12.9210	13.5190	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0





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20	23	1	0	0	0	0
24	25	1	0	0	0	0
24	33	2	0	0	0	0
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25	26	1	0	0	0	0
25	27	2	0	0	0	0
27	28	1	0	0	0	0
27	29	1	0	0	0	0
29	30	1	0	0	0	0
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38	41	1	0	0	0	0
41	42	1	0	0	0	0
41	58	2	0	0	0	0
42	43	1	0	0	0	0
43	44	1	0	0	0	0
43	45	1	0	0	0	0
43	46	1	0	0	0	0
46	47	1	0	0	0	0
46	60	1	0	0	0	0
46	63	1	0	0	0	0
47	48	1	0	0	0	0
47	49	1	0	0	0	0
47	50	1	0	0	0	0
50	51	1	0	0	0	0
51	52	1	0	0	0	0
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55	56	1	0	0	0	0
55	57	1	0	0	0	0
55	76	1	0	0	0	0
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60	66	1	0	0	0	0
63	64	1	0	0	0	0
63	65	1	0	0	0	0
63	70	1	0	0	0	0
66	67	1	0	0	0	0
66	68	1	0	0	0	0
66	69	1	0	0	0	0
70	71	1	0	0	0	0
71	72	2	0	0	0	0
73	74	1	0	0	0	0
73	75	1	0	0	0	0
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73	87	1	0	0	0	0
76	77	1	0	0	0	0
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77	79	1	0	0	0	0
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80	82	1	0	0	0	0
80	83	1	0	0	0	0
83	84	1	0	0	0	0
83	106	1	0	0	0	0
84	85	1	0	0	0	0

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84	91	1	0	0	0	0
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87	89	1	0	0	0	0
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91	94	1	0	0	0	0
95	96	1	0	0	0	0
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95	142	1	0	0	0	0
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315317	1	0	0	0	0
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319321	1	0	0	0	0
319322	1	0	0	0	0
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322325	1	0	0	0	0
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325342 2 0 0 0 0
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376377 1 0 0 0 0
376378 1 0 0 0 0
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M END
> <NAME>
AA61_12

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$$$$
AA94_12
MOE2012 3D

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337347 0 0 1 0 0 0 0 0 0999 V2000
26.9270 3.2970 17.3620 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.5980 4.0110 16.2450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.6130 3.9840 15.7980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.7510 4.6810 15.9040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.9030 5.3520 15.0700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.7630 4.3970 16.7870 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.2350 3.5610 17.6530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.7500 3.1230 18.4980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.0440 2.4210 18.1080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.3700 2.4460 19.1550 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.0370 2.8540 18.0640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.0520 0.9890 17.5630 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.7160 1.0000 16.5200 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.0770 0.6000 17.5750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.1780 0.1310 18.3750 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
25.5170 0.1400 19.3400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.6500 0.6880 17.9470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.6550 1.6490 18.1160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.5910 1.5930 17.5650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```









39.3890	10.9060	-5.0680	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.1410	10.0960	-5.7810	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.2170	9.0240	-5.6460	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.7660	10.1930	-7.6920	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.3420	9.2310	-7.9940	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.7740	10.8390	-8.5790	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1810	10.0620	-7.1090	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.4990	11.0730	-6.8280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1680	9.4930	-6.1710	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.1380	9.4850	-8.0710	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
41.5660	15.1780	-14.2150	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.8340	14.6570	-13.1410	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.3240	14.1350	-12.3230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.4450	14.8020	-13.1040	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.8790	14.3950	-12.2700	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.7830	15.4650	-14.1360	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37.7030	15.5760	-14.1040	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.5060	15.9840	-15.2090	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.9880	16.5000	-16.0140	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.8940	15.8410	-15.2500	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.4450	16.2540	-16.0930	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.5400	9.7750	-7.7160	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2090	9.0880	-8.2520	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.7180	9.6100	-6.6460	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.9590	11.1970	-8.0900	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3810	11.9440	-7.5360	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.0100	11.3650	-7.8270	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8230	11.4310	-9.5740	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.0000	12.4930	-9.8050	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.6880	12.8000	-11.1770	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.9020	11.9510	-11.8380	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.6020	12.9400	-11.2060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4180	14.0840	-11.6700	C	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
45.0120	15.2600	-10.7420	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9220	15.2930	-10.6260	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4640	15.1370	-9.7500	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4500	16.5110	-11.2990	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.1040	17.6260	-10.5950	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.6450	18.8540	-11.2910	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.6870	18.6580	-11.5710	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.0560	19.0200	-12.1990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.5850	20.0730	-10.3690	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.5490	20.3000	-10.0910	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.0950	19.8290	-9.4290	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.3940	10.7700	-10.4320	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.4440	17.6310	-9.5660	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.9560	13.8330	-11.6260	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2650	13.6360	-10.5920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.1770	12.9180	-12.1920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.9640	14.3700	-13.1250	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4350	15.2790	-13.5130	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.2340	13.5320	-13.7790	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.8650	14.9310	-12.1660	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.8080	15.8400	-11.5630	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.6390	15.1780	-13.2070	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.9060	14.5910	-12.1330	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.5330	14.5230	-13.1600	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.0300	15.0540	-14.3040	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.6770	15.4050	-15.2800	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3560	24.0410	-13.2740	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2930	24.8580	-13.0150	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.8980	25.0100	-12.0190	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9300	25.3640	-14.2420	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1300	26.0570	-14.4630	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.7420	24.8740	-15.2330	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.5890	24.0770	-14.6190	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.3820	23.5160	-15.0960	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.1120	23.2840	-12.2960	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.1200	23.1320	-12.7010	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2080	23.9180	-11.4050	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4550	21.9440	-11.9460	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.4370	22.1280	-11.5820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3780	21.3230	-12.8460	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2430	21.2640	-10.9160	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
47.1670	21.0210	-11.2720	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0													
1	7	1	0	0	0	0													
1	9	1	0	0	0	0													
2	3	1	0	0	0	0													
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4	5	1	0	0	0	0													

4	6	1	0	0	0	0
6	7	2	0	0	0	0
7	8	1	0	0	0	0
9	10	1	0	0	0	0
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9	12	1	0	0	0	0
12	13	1	0	0	0	0
12	14	1	0	0	0	0
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44	52	2	0	0	0	0
45	46	1	0	0	0	0
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69	70	1	0	0	0	0
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80	92	1	0	0	0	0
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216218	1	0	0	0	0
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223226	1	0	0	0	0
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228229	1	0	0	0	0
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258259	1	0	0	0	0
258264	1	0	0	0	0
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259260	1	0	0	0	0
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263264	2	0	0	0	0
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269272	1	0	0	0	0
272284	1	0	0	0	0
273274	1	0	0	0	0
273282	2	0	0	0	0
273320	1	0	0	0	0
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274276	2	0	0	0	0
276277	1	0	0	0	0
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278280	2	0	0	0	0
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292295	1	0	0	0	0
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304305	1	0	0	0	0
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304336	1	0	0	0	0
309310	1	0	0	0	0
309311	1	0	0	0	0
309315	1	0	0	0	0
312313	1	0	0	0	0
312314	1	0	0	0	0
312319	1	0	0	0	0
315316	1	0	0	0	0
315317	1	0	0	0	0
315318	1	0	0	0	0
319320	1	0	0	0	0

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322323 1 0 0 0 0  
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322330 1 0 0 0 0  
323324 1 0 0 0 0  
323325 2 0 0 0 0  
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325327 1 0 0 0 0  
327328 2 0 0 0 0  
328329 1 0 0 0 0  
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333335 1 0 0 0 0  
333336 1 0 0 0 0  
336337 1 0 0 0 0

M END  
> <NAME>  
AA94\_12

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B17\_12  
MOE2012 3D

308313 0 0 1 0 0 0 0 0999 V2000  
25.3990 -8.7140 -1.5930 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.3340 -7.8960 -2.2440 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.0410 -7.4440 -3.5360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.7320 -6.8050 -4.0770 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.8460 -7.8160 -4.1790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.9350 -8.6440 -3.5130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.0060 -8.9430 -3.9930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.2160 -9.1010 -2.2270 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.5170 -9.7590 -1.7190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.6320 -9.2380 -0.3450 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.4790 -7.6020 -1.5500 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.4720 -6.8380 -2.2240 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
29.3220 -6.7240 -1.5440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.1030 -5.8360 -2.4640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.8300 -7.3560 -3.1200 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.3680 -8.2630 0.6640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.4070 -7.7600 0.5050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.1810 -7.5340 0.7210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.3190 -8.7840 1.6250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.5330 -7.3010 -5.5650 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.4690 -7.1880 -6.1290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.9410 -8.0490 -6.1090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.7810 -5.9680 -5.5010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.8380 -6.1100 -4.9600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.3850 -5.2460 -4.9420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.5190 -5.4630 -6.8490 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
24.3970 -5.2250 -7.3110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.6090 -4.3130 -6.8710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.6440 -4.5950 -6.4330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.4060 -4.1080 -7.9290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.1700 -3.0370 -6.2470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.2640 -3.0420 -6.1810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.9160 -2.1700 -6.8700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.5580 -2.7890 -4.8930 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.4270 -3.1420 -3.9090 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.9600 -3.0350 -2.5510 C 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
22.3920 -2.1040 -2.4260 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.1880 -2.9580 -1.6370 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.7370 -2.0320 -1.8510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.8690 -2.8800 -0.5930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.1640 -4.1220 -1.8000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.6800 -5.0970 -1.6800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.6130 -4.1080 -2.7990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.2470 -3.9910 -0.8620 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.0010 -4.4800 0.3900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.2480 -4.3600 1.2290 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.8910 -5.2100 0.9730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.7820 -3.4440 0.9570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.9360 -4.3970 2.7270 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.8580 -4.5830 3.2930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.2880 -5.2620 2.9160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.4250 -2.3580 -4.7290 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.9510 -4.9930 0.7510 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.0660 -4.2270 -2.2130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.1370 -4.1890 -2.7920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0









31.4860	-9.7820	28.4920	H	0	0	0	0	0	0	0	0	0	0	0	0
29.9940	-10.5980	28.9780	H	0	0	0	0	0	0	0	0	0	0	0	0
33.1670	-7.2010	23.2700	C	0	0	0	0	0	0	0	0	0	0	0	0
34.0050	-6.6850	23.7570	H	0	0	0	0	0	0	0	0	0	0	0	0
33.6160	-7.9920	22.6550	H	0	0	0	0	0	0	0	0	0	0	0	0
32.3760	-6.2270	22.3870	C	0	0	0	0	0	0	0	0	0	0	0	0
31.5500	-6.7680	21.9110	H	0	0	0	0	0	0	0	0	0	0	0	0
31.9420	-5.4350	23.0100	H	0	0	0	0	0	0	0	0	0	0	0	0
33.2560	-5.6420	21.3710	N	0	0	3	0	0	0	0	0	0	0	0	0
34.0540	-5.2060	21.8350	H	0	0	0	0	0	0	0	0	0	0	0	0
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1	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END









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144	151	2	0	0	0	0
145	146	1	0	0	0	0
145	147	1	0	0	0	0
145	148	1	0	0	0	0
148	149	1	0	0	0	0
148	150	1	0	0	0	0
148	181	1	0	0	0	0
152	153	1	0	0	0	0
152	154	1	0	0	0	0
152	155	1	0	0	0	0
155	156	1	0	0	0	0
155	157	1	0	0	0	0
155	158	1	0	0	0	0
158	159	1	0	0	0	0
158	166	2	0	0	0	0
159	160	1	0	0	0	0
160	161	1	0	0	0	0
160	162	1	0	0	0	0
160	163	1	0	0	0	0
163	164	1	0	0	0	0
163	165	1	0	0	0	0
163	167	1	0	0	0	0
167	168	1	0	0	0	0
167	169	1	0	0	0	0
170	171	1	0	0	0	0
170	172	1	0	0	0	0
172	173	1	0	0	0	0
172	174	1	0	0	0	0

```

172175 1 0 0 0 0
175176 1 0 0 0 0
175177 1 0 0 0 0
175178 1 0 0 0 0
178179 1 0 0 0 0
178180 1 0 0 0 0
178181 1 0 0 0 0
181194 1 0 0 0 0
182183 1 0 0 0 0
182184 1 0 0 0 0
182185 1 0 0 0 0
182209 1 0 0 0 0
185186 1 0 0 0 0
186187 1 0 0 0 0
186193 2 0 0 0 0
187188 1 0 0 0 0
187189 1 0 0 0 0
187190 1 0 0 0 0
190191 1 0 0 0 0
190192 1 0 0 0 0
190223 1 0 0 0 0
194195 1 0 0 0 0
194196 1 0 0 0 0
194197 1 0 0 0 0
197198 1 0 0 0 0
197199 1 0 0 0 0
197200 1 0 0 0 0
200201 1 0 0 0 0
200208 2 0 0 0 0
201202 1 0 0 0 0
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202204 1 0 0 0 0
202205 1 0 0 0 0
205206 1 0 0 0 0
205207 1 0 0 0 0
205209 1 0 0 0 0
209210 1 0 0 0 0
209211 1 0 0 0 0
212213 1 0 0 0 0
212214 1 0 0 0 0
214215 1 0 0 0 0
214216 1 0 0 0 0
214217 1 0 0 0 0
217218 1 0 0 0 0
217219 1 0 0 0 0
217220 1 0 0 0 0
220221 1 0 0 0 0
220222 1 0 0 0 0
220223 1 0 0 0 0
223224 1 0 0 0 0

```

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M END
> <NAME>
C20_12

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$$$$
C25_12
MOE2012 3D

```

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230229 0 0 1 0 0 0 0 0999 V2000
30.5270 -0.6530 -28.7730 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.9750 -0.0380 -29.2840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.6860 -1.7190 -28.3430 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.9760 -1.2830 -27.6340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.1150 -2.0920 -29.2010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.5190 -2.8430 -27.6880 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.4050 -2.4000 -27.2140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.0320 -3.8430 -28.7470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.6000 -4.6450 -28.2610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.1990 -4.2990 -29.2940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.8940 -3.2180 -29.6890 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.2350 -3.9190 -30.2690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.7400 -3.6160 -26.6980 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
28.8000 -3.7960 -27.0530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.5170 -5.0850 -17.6990 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.1000 -6.0140 -17.6900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.5130 -5.2840 -18.0910 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.4130 -4.5730 -16.3630 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.8270 -5.4250 -15.4740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.7860 -4.7790 -14.1070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.8190 -4.6140 -13.7870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.2760 -3.8130 -14.2040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```





41.4290	16.1780	-14.0310	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.6890	15.3330	-11.4140	N	0	0	3	0	0	0	0	0	0	0	0	0	0
29.0080	15.0020	-12.2260	C	0	0	0	0	0	0	0	0	0	0	0	0	0
28.9330	14.7560	-11.1600	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.1240	14.0810	-12.8090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
27.8180	15.6840	-12.6430	O	0	0	0	0	0	0	0	0	0	0	0	0	0
26.6700	14.9680	-12.4770	C	0	0	0	0	0	0	0	0	0	0	0	0	0
25.5000	15.7880	-12.9580	C	0	0	0	0	0	0	0	0	0	0	0	0	0
25.4830	16.7270	-12.3930	H	0	0	0	0	0	0	0	0	0	0	0	0	0
25.6650	16.0070	-14.0180	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.1840	15.0370	-12.7620	C	0	0	0	0	0	0	0	0	0	0	0	0	0
24.1920	14.0860	-13.3060	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.0880	14.7570	-11.7050	H	0	0	0	0	0	0	0	0	0	0	0	0	0
26.6010	13.8390	-12.0150	O	0	0	0	0	0	0	0	0	0	0	0	0	0
37.5140	16.1680	-11.7450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.5430	17.1190	-11.1980	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.5230	16.4310	-12.8090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.1930	15.4390	-11.4810	C	0	0	0	0	0	0	0	0	0	0	0	0	0
36.1870	14.4810	-12.0140	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.0440	15.2570	-10.4130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.0240	16.2580	-11.9750	C	0	0	0	0	0	0	0	0	0	0	0	0	0
33.8770	15.5320	-11.8460	O	0	0	0	0	0	0	0	0	0	0	0	0	0
32.6920	16.2120	-12.2800	C	0	0	0	0	0	0	0	0	0	0	0	0	0
32.5680	17.1350	-11.7020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.7780	16.4520	-13.3460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.5060	15.2830	-12.0440	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.6640	14.3470	-12.5930	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.4680	15.0060	-10.9830	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.0910	17.3980	-12.4130	O	0	0	0	0	0	0	0	0	0	0	0	0	0
30.1930	15.9290	-12.4680	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.2280	16.2040	-13.5300	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.0360	16.8680	-11.9210	H	0	0	0	0	0	0	0	0	0	0	0	0	0
21.4870	17.5100	-16.0470	O	0	0	0	0	0	0	0	0	0	0	0	0	0
20.7370	18.1340	-16.0760	H	0	0	0	0	0	0	0	0	0	0	0	0	0
21.6240	17.1090	-14.6790	C	0	0	0	0	0	0	0	0	0	0	0	0	0
21.6940	18.0130	-14.0630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
20.7210	16.5570	-14.3970	H	0	0	0	0	0	0	0	0	0	0	0	0	0
22.8890	16.2350	-14.5130	C	0	0	0	0	0	0	0	0	0	0	0	0	0
23.7360	16.8770	-14.7850	H	0	0	0	0	0	0	0	0	0	0	0	0	0
22.8460	15.0640	-15.5220	C	0	0	0	0	0	0	0	0	0	0	0	0	0
23.7330	14.4300	-15.4430	H	0	0	0	0	0	0	0	0	0	0	0	0	0
21.9620	14.4380	-15.3610	H	0	0	0	0	0	0	0	0	0	0	0	0	0
22.8110	15.5450	-16.8680	O	0	0	0	0	0	0	0	0	0	0	0	0	0
22.2410	16.3540	-16.8500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
22.9920	15.8200	-13.1050	N	0	0	3	0	0	0	0	0	0	0	0	0	0
22.9550	16.6440	-12.5030	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0										
1	3	1	0	0	0	0										
3	4	1	0	0	0	0										
3	5	1	0	0	0	0										
3	6	1	0	0	0	0										
6	7	1	0	0	0	0										
6	8	1	0	0	0	0										
6	13	1	0	0	0	0										
8	9	1	0	0	0	0										
8	10	1	0	0	0	0										
8	11	1	0	0	0	0										
11	12	1	0	0	0	0										
13	14	1	0	0	0	0										
13	27	1	0	0	0	0										
15	16	1	0	0	0	0										
15	17	1	0	0	0	0										
15	18	1	0	0	0	0										
15	42	1	0	0	0	0										
18	19	1	0	0	0	0										
19	20	1	0	0	0	0										
19	26	2	0	0	0	0										
20	21	1	0	0	0	0										
20	22	1	0	0	0	0										
20	23	1	0	0	0	0										
23	24	1	0	0	0	0										
23	25	1	0	0	0	0										
23	57	1	0	0	0	0										
27	28	1	0	0	0	0										
27	29	1	0	0	0	0										
27	30	1	0	0	0	0										
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30	32	1	0	0	0	0										
30	33	1	0	0	0	0										
33	34	1	0	0	0	0										
33	41	2	0	0	0	0										

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35	36	1	0	0	0	0
35	37	1	0	0	0	0
35	38	1	0	0	0	0
38	39	1	0	0	0	0
38	40	1	0	0	0	0
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52	54	1	0	0	0	0
52	55	1	0	0	0	0
55	56	1	0	0	0	0
57	70	1	0	0	0	0
58	59	1	0	0	0	0
58	60	1	0	0	0	0
58	61	1	0	0	0	0
58	85	1	0	0	0	0
61	62	1	0	0	0	0
62	63	1	0	0	0	0
62	69	2	0	0	0	0
63	64	1	0	0	0	0
63	65	1	0	0	0	0
63	66	1	0	0	0	0
66	67	1	0	0	0	0
66	68	1	0	0	0	0
66	100	1	0	0	0	0
70	71	1	0	0	0	0
70	72	1	0	0	0	0
70	73	1	0	0	0	0
73	74	1	0	0	0	0
73	75	1	0	0	0	0
73	76	1	0	0	0	0
76	77	1	0	0	0	0
76	84	2	0	0	0	0
77	78	1	0	0	0	0
78	79	1	0	0	0	0
78	80	1	0	0	0	0
78	81	1	0	0	0	0
81	82	1	0	0	0	0
81	83	1	0	0	0	0
81	85	1	0	0	0	0
85	86	1	0	0	0	0
85	87	1	0	0	0	0
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88	90	1	0	0	0	0
90	91	1	0	0	0	0
90	92	1	0	0	0	0
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93	94	1	0	0	0	0
93	95	1	0	0	0	0
93	100	1	0	0	0	0
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95	97	1	0	0	0	0
95	98	1	0	0	0	0
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101	103	1	0	0	0	0
101	104	1	0	0	0	0
101	128	1	0	0	0	0
104	105	1	0	0	0	0
105	106	1	0	0	0	0
105	112	2	0	0	0	0
106	107	1	0	0	0	0
106	108	1	0	0	0	0
106	109	1	0	0	0	0
109	110	1	0	0	0	0
109	111	1	0	0	0	0
109	143	1	0	0	0	0
113	114	1	0	0	0	0
113	115	1	0	0	0	0
113	116	1	0	0	0	0

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116118	1	0	0	0	0
116119	1	0	0	0	0
119120	1	0	0	0	0
119127	2	0	0	0	0
120121	1	0	0	0	0
121122	1	0	0	0	0
121123	1	0	0	0	0
121124	1	0	0	0	0
124125	1	0	0	0	0
124126	1	0	0	0	0
124128	1	0	0	0	0
128129	1	0	0	0	0
128130	1	0	0	0	0
131132	1	0	0	0	0
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133134	1	0	0	0	0
133135	1	0	0	0	0
133136	1	0	0	0	0
136137	1	0	0	0	0
136138	1	0	0	0	0
136143	1	0	0	0	0
138139	1	0	0	0	0
138140	1	0	0	0	0
138141	1	0	0	0	0
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143156	1	0	0	0	0
144145	1	0	0	0	0
144146	1	0	0	0	0
144147	1	0	0	0	0
144171	1	0	0	0	0
147148	1	0	0	0	0
148149	1	0	0	0	0
148155	2	0	0	0	0
149150	1	0	0	0	0
149151	1	0	0	0	0
149152	1	0	0	0	0
152153	1	0	0	0	0
152154	1	0	0	0	0
152186	1	0	0	0	0
156157	1	0	0	0	0
156158	1	0	0	0	0
156159	1	0	0	0	0
159160	1	0	0	0	0
159161	1	0	0	0	0
159162	1	0	0	0	0
162163	1	0	0	0	0
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164165	1	0	0	0	0
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179181	1	0	0	0	0
179186	1	0	0	0	0
181182	1	0	0	0	0
181183	1	0	0	0	0
181184	1	0	0	0	0
184185	1	0	0	0	0
186199	1	0	0	0	0
187188	1	0	0	0	0
187189	1	0	0	0	0
187190	1	0	0	0	0
187214	1	0	0	0	0
190191	1	0	0	0	0
191192	1	0	0	0	0
191198	2	0	0	0	0
192193	1	0	0	0	0
192194	1	0	0	0	0
192195	1	0	0	0	0
195196	1	0	0	0	0









65.1810	-14.9170	8.4430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.5840	-13.8200	8.3070	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.6950	-13.9160	10.2900	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.0550	-12.9380	10.6340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.6890	-14.0270	10.7130	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.1700	-12.0010	8.9420	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.7260	-9.6360	-1.4070	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4230	-10.6700	-1.6160	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.6780	-9.5170	-1.9440	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.0050	-9.4590	0.0890	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5070	-8.5040	0.2790	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0780	-9.4960	0.6660	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.9080	-10.5500	0.5980	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.0280	-10.4430	1.9520	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.8650	-11.4390	2.5550	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.4580	-12.4350	2.3450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.8790	-11.3620	2.1450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.8870	-11.1870	4.0580	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.2530	-10.1710	4.2510	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.8600	-11.2140	4.4450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.4530	-11.3980	-0.0930	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.7530	-12.2080	4.7880	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.7790	-12.1810	4.4010	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.3860	-13.2240	4.5950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72.4450	-16.5730	11.3330	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72.9550	-17.2970	11.7360	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71.0760	-16.8170	11.6200	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70.7970	-17.7860	11.1930	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70.9470	-16.8550	12.7070	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70.2510	-15.6950	11.0130	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70.5810	-14.7350	11.4280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70.4540	-15.6400	9.9360	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.7580	-15.8950	11.2600	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.4450	-16.8600	10.8430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.5640	-15.9280	12.3390	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.9520	-14.7650	10.6200	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.2570	-13.8080	11.0600	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.1770	-14.7330	9.5480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.5260	-14.9860	10.8460	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
66.2450	-15.8870	10.4600	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
C28_12

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$$$$
C32_12
MOE2012 3D

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42.1300 -27.1300 -11.5470 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.9290 -26.8190 -12.0050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.5220 -25.9930 -10.9500 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.2350 -25.5430 -10.2520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.2870 -25.2700 -11.7370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.2590 -26.4380 -10.2260 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.5870 -26.9320 -10.9390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.5180 -27.2020 -9.4810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.5470 -25.2660 -9.5540 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.2240 -24.7860 -8.8370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.2870 -24.5130 -10.3080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.2790 -25.7270 -8.8320 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.6030 -26.2060 -9.5510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.5430 -26.4860 -8.0830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.5660 -24.5540 -8.1530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.2430 -24.0890 -7.4270 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.3100 -23.8070 -8.9110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.3570 -25.0390 -7.4830 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
36.6140 -25.7980 -6.8500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.3950 -17.3990 -8.3010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.7250 -18.0190 -8.9080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.1290 -16.9070 -8.9500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.6290 -16.4060 -7.6070 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.9530 -15.5440 -8.4180 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.2190 -14.5350 -7.5710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.5340 -15.0730 -6.9060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.9730 -14.0130 -6.9730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.4360 -13.5520 -8.4450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.1190 -13.0400 -9.1360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.7580 -14.1440 -9.0750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.9560 -15.5750 -9.6400 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.6780 -23.9960 -6.7080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.9320 -24.4930 -6.0750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.3800 -23.5070 -6.0210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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212239	1	0	0	0	0
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216217	1	0	0	0	0
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217218	1	0	0	0	0
217219	1	0	0	0	0
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224226	1	0	0	0	0
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M END











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46	50	1	0	0	0	0
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M END  
> <NAME>  
C36\_12











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281282 1 0 0 0 0  
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281284 1 0 0 0 0  
M END  
> <NAME>  
C75\_12

\$\$\$  
C80\_12  
MOE2012 3D

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19.1270 -6.3890 -26.7050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.9270 -6.0610 -24.9690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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19.0470 -3.7310 -26.2500 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.5860 -3.9420 -27.2240 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.2680 -3.8810 -25.4910 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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19.9950 -2.0860 -25.2290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.1800 -2.0260 -26.9870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.2610 -1.3330 -26.2950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.7310 -1.5620 -27.2280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.5420 -1.5390 -25.4940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.1580 -4.6540 -27.0460 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.7250 -4.8960 -28.0230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.9500 -5.3810 -26.8340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.6560 -3.6820 -27.1160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.5920 0.0930 -26.3280 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.1770 0.2790 -27.1440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.7160 1.5130 -16.7300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.6070 0.4280 -16.6130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
16.7300 1.9680 -16.8810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.3160 2.0720 -15.5540 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.7030 1.7350 -14.3830 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.4560 2.3470 -13.2260 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.5230 2.2840 -13.4620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.1720 3.4010 -13.1500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.1570 1.5950 -11.9230 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.0860 1.6830 -11.6890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.2990 0.5180 -12.0800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
16.6950 1.0510 -14.2860 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.2740 0.6120 -25.1380 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.2650 0.1560 -25.0310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.4600 1.6790 -25.3150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.4700 0.4630 -23.8480 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.4900 0.9410 -23.9590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.3320 -0.5940 -23.5980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.1840 1.1120 -22.6890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.4390 0.9570 -21.5580 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.0220 1.5280 -20.3790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.0020 1.0710 -20.1970 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.1400 2.6090 -20.5180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.0870 1.2460 -19.2090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.0960 1.6650 -19.4260 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.9410 0.1630 -19.1160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.2640 1.6810 -22.7510 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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18.7590 2.9070 -17.9950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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21.0160 3.8280 -5.9190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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19.3310 3.0030 -7.8090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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19.6380 1.9570 -7.9370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.1640 3.3290 -8.7520 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.3430 2.6170 -8.6010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.7690 4.3220 -8.5010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.5370 3.3390 -10.2450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.6500 3.7020 -10.7810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.3150 4.0900 -10.4330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.9800 2.3910 -5.8720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.8010 2.5880 -4.8090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.2410 1.3330 -5.9850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0





44.9240	-3.2810	-19.7190	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.4620	-2.5240	-20.3120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
45.1610	-2.3820	-21.6410	C	0	0	0	0	0	0	0	0	0	0	0	0	0
44.7630	-1.5690	-22.2580	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2500	-2.2600	-21.6100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.8290	-3.6660	-22.3460	C	0	0	0	0	0	0	0	0	0	0	0	0	0
45.6320	-4.6690	-21.9010	O	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3610	-5.9500	-22.4810	C	0	0	0	0	0	0	0	0	0	0	0	0	0
44.3010	-6.1990	-22.3540	H	0	0	0	0	0	0	0	0	0	0	0	0	0
45.6080	-5.9240	-23.5480	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2270	-6.9740	-21.7600	C	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2840	-6.7010	-21.8680	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.0150	-6.9340	-20.6840	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9470	-3.7810	-23.1860	O	0	0	0	0	0	0	0	0	0	0	0	0	0
45.9850	-8.3790	-22.2940	C	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2250	-8.4280	-23.3630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.9220	-8.6380	-22.2130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.5040	-18.6120	-25.6400	C	0	0	0	0	0	0	0	0	0	0	0	0	0
42.8530	-19.4370	-25.9520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.5090	-18.7960	-26.0370	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1050	-17.7080	-26.1130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.5010	-18.4760	-24.1800	N	0	0	0	0	0	0	0	0	0	0	0	0	0
44.3360	-17.3210	-23.7810	C	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3940	-17.5160	-23.9990	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.0400	-16.4570	-24.3880	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.1690	-16.9330	-22.3030	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1110	-16.7310	-22.0910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.4620	-17.7720	-21.6620	H	0	0	0	0	0	0	0	0	0	0	0	0	0
45.0180	-15.7240	-21.8750	C	0	0	0	0	0	0	0	0	0	0	0	0	0
44.9200	-15.6280	-20.7860	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.0730	-15.9210	-22.0940	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9580	-19.7260	-23.5700	C	0	0	0	0	0	0	0	0	0	0	0	0	0
45.0050	-19.9450	-23.8090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.3460	-20.5680	-23.9160	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.8450	-19.7040	-22.4820	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.5840	-14.4850	-22.5190	N	0	0	3	0	0	0	0	0	0	0	0	0	0
44.8380	-14.4920	-23.5060	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
C80_12

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C86_12
MOE2012 3D

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25.2540 -20.2700 26.8420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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25.0980 -19.2220 24.3290 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
24.4650 -18.7910 25.0040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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C86\_12

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D24\_12  
MOE2012 3D

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199200	2	0	0	0	0
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M END  
> <NAME>  
D24\_12

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D25\_12  
MOE2012 3D

385394 0 0 1 0 0 0 0 0999 V2000  
37.9670 22.6400 -12.7110 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
38.6200 23.3480 -12.8660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0







88.2830	6.1850	-17.5090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
87.4110	4.7210	-17.4030	H	0	0	0	0	0	0	0	0	0	0	0	0	0
85.5140	6.4820	-17.8190	O	0	0	0	0	0	0	0	0	0	0	0	0	0
82.9140	5.3460	-19.3660	C	0	0	0	0	0	0	0	0	0	0	0	0	0
83.0530	4.5270	-20.0830	H	0	0	0	0	0	0	0	0	0	0	0	0	0
83.2890	5.0230	-18.3870	H	0	0	0	0	0	0	0	0	0	0	0	0	0
67.7760	5.3260	-14.6190	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.4460	5.0110	-15.4300	H	0	0	0	0	0	0	0	0	0	0	0	0	0
67.7390	6.4220	-14.6620	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.4320	4.8720	-13.3120	C	0	0	0	0	0	0	0	0	0	0	0	0	0
67.9820	5.3480	-12.4360	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.3300	3.7840	-13.2140	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.9000	5.2220	-13.3330	C	0	0	0	0	0	0	0	0	0	0	0	0	0
70.6120	4.2840	-12.6480	O	0	0	0	0	0	0	0	0	0	0	0	0	0
72.0360	4.4640	-12.6400	C	0	0	0	0	0	0	0	0	0	0	0	0	0
72.3050	5.5110	-12.4550	H	0	0	0	0	0	0	0	0	0	0	0	0	0
72.4310	3.8980	-11.7890	H	0	0	0	0	0	0	0	0	0	0	0	0	0
72.6500	3.9450	-13.9350	C	0	0	0	0	0	0	0	0	0	0	0	0	0
72.3310	2.9060	-14.0880	H	0	0	0	0	0	0	0	0	0	0	0	0	0
72.2960	4.5490	-14.7790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.3780	6.2010	-13.8890	O	0	0	0	0	0	0	0	0	0	0	0	0	0
74.0690	4.0270	-13.8290	O	0	0	0	0	0	0	0	0	0	0	0	0	0
74.7940	3.5100	-14.8680	C	0	0	0	0	0	0	0	0	0	0	0	0	0
76.1720	3.4650	-14.6620	C	0	0	0	0	0	0	0	0	0	0	0	0	0
76.5910	3.8290	-13.7280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
77.0210	2.9480	-15.6450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
78.0910	2.9260	-15.4450	H	0	0	0	0	0	0	0	0	0	0	0	0	0
76.5150	2.4660	-16.8680	C	0	0	0	0	0	0	0	0	0	0	0	0	0
75.1270	2.5270	-17.0610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
74.6630	2.1720	-17.9780	H	0	0	0	0	0	0	0	0	0	0	0	0	0
74.2770	3.0450	-16.0750	C	0	0	0	0	0	0	0	0	0	0	0	0	0
73.2130	3.0680	-16.2900	H	0	0	0	0	0	0	0	0	0	0	0	0	0
77.4830	1.8770	-17.9200	C	0	0	0	0	0	0	0	0	0	0	0	0	0
78.6230	2.8690	-18.2510	C	0	0	0	0	0	0	0	0	0	0	0	0	0
77.9800	0.5250	-17.3420	C	0	0	0	0	0	0	0	0	0	0	0	0	0
78.5740	0.6570	-16.4290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
78.5990	-0.0220	-18.0630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
77.1370	-0.1290	-17.0850	H	0	0	0	0	0	0	0	0	0	0	0	0	0
76.8020	1.5370	-19.2730	C	0	0	0	0	0	0	0	0	0	0	0	0	0
76.0340	0.7630	-19.1570	H	0	0	0	0	0	0	0	0	0	0	0	0	0
76.3230	2.4120	-19.7290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
77.5320	1.1560	-19.9990	H	0	0	0	0	0	0	0	0	0	0	0	0	0
78.3120	4.1870	-18.6360	C	0	0	0	0	0	0	0	0	0	0	0	0	0
77.2760	4.5170	-18.6830	H	0	0	0	0	0	0	0	0	0	0	0	0	0
79.3170	5.1020	-18.9630	C	0	0	0	0	0	0	0	0	0	0	0	0	0
79.0450	6.1130	-19.2560	H	0	0	0	0	0	0	0	0	0	0	0	0	0
80.6590	4.7270	-18.9240	C	0	0	0	0	0	0	0	0	0	0	0	0	0
80.9860	3.4270	-18.5430	C	0	0	0	0	0	0	0	0	0	0	0	0	0
82.0160	3.0880	-18.4910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
79.9800	2.5100	-18.2120	C	0	0	0	0	0	0	0	0	0	0	0	0	0
80.2910	1.5080	-17.9290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
81.5410	5.7110	-19.2750	O	0	0	0	0	0	0	0	0	0	0	0	0	0
87.7760	1.0620	-18.8050	O	0	0	0	0	0	0	0	0	0	0	0	0	0
86.9650	0.6730	-18.4270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
87.8580	2.3980	-18.2880	C	0	0	0	0	0	0	0	0	0	0	0	0	0
86.9040	2.8820	-18.5150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
87.9790	2.3280	-17.2020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
89.0530	3.1670	-18.9310	C	0	0	0	0	0	0	0	0	0	0	0	0	0
88.8210	3.2480	-20.0020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
90.3120	2.2610	-18.8090	C	0	0	0	0	0	0	0	0	0	0	0	0	0
91.2060	2.7170	-19.2370	H	0	0	0	0	0	0	0	0	0	0	0	0	0
90.5240	2.0270	-17.7600	H	0	0	0	0	0	0	0	0	0	0	0	0	0
90.1300	1.0310	-19.5150	O	0	0	0	0	0	0	0	0	0	0	0	0	0
89.1970	0.7540	-19.3310	H	0	0	0	0	0	0	0	0	0	0	0	0	0
89.2840	4.5320	-18.3620	N	0	0	3	0	0	0	0	0	0	0	0	0	0
103.4410	8.8100	-27.5610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
103.2250	9.5040	-26.7400	H	0	0	0	0	0	0	0	0	0	0	0	0	0
102.6360	8.8940	-28.3010	H	0	0	0	0	0	0	0	0	0	0	0	0	0
104.6980	9.1450	-28.1620	O	0	0	0	0	0	0	0	0	0	0	0	0	0
104.7680	10.4040	-28.6820	C	0	0	0	0	0	0	0	0	0	0	0	0	0
106.1440	10.6250	-29.2550	C	0	0	0	0	0	0	0	0	0	0	0	0	0
106.8460	10.5740	-28.4180	H	0	0	0	0	0	0	0	0	0	0	0	0	0
106.3550	9.8160	-29.9630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
106.2410	11.9740	-29.9590	C	0	0	0	0	0	0	0	0	0	0	0	0	0
105.4220	12.0410	-30.6870	H	0	0	0	0	0	0	0	0	0	0	0	0	0
106.0680	12.7960	-29.2540	H	0	0	0	0	0	0	0	0	0	0	0	0	0
103.8650	11.2280	-28.6600	O	0	0	0	0	0	0	0	0	0	0	0	0	0
103.5210	7.3790	-27.0450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
103.7170	6.7150	-27.8970	H	0	0	0	0	0	0	0	0	0	0	0	0	0
104.3730	7.2220	-26.3730	H	0	0	0	0	0	0	0	0	0	0	0	0	0
90.2420	5.3040	-19.1890	C	0	0	0	0	0	0	0	0	0	0	0	0	0





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36	37	1	0	0	0	0
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37	38	1	0	0	0	0
38	39	1	0	0	0	0
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66	68	2	0	0	0	0
68	69	1	0	0	0	0
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70	71	2	0	0	0	0
70	75	1	0	0	0	0
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86	87	1	0	0	0	0
88	104	1	0	0	0	0
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89	91	1	0	0	0	0
89	92	1	0	0	0	0
89	101	1	0	0	0	0
92	93	1	0	0	0	0
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94	95	1	0	0	0	0
94	96	1	0	0	0	0
94	97	1	0	0	0	0
97	98	1	0	0	0	0
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97	162	1	0	0	0	0

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M END
> <NAME>
D25_12

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D28_12
MOE2012 3D

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396397 1 0 0 0 0

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M END
> <NAME>
D28_12

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$$$$
D32_12
MOE2012 3D

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44.5210 9.1790 -55.0400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
45.4580 8.6130 -55.0290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.6510 10.0960 -54.4560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.3740 8.3430 -54.4900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.4400 8.9140 -54.5650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.2350 7.4580 -55.1250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.6210 7.9220 -53.0430 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.5550 7.3500 -52.9810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.7450 8.8140 -52.4170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.4650 7.0740 -52.5070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.5320 7.6480 -52.5720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.3420 6.1850 -53.1380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.7120 6.6490 -51.0570 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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42.8190 7.5420 -50.4320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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40.7240 6.3520 -50.6500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.0030 -1.7200 -34.6170 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.1910 -0.6420 -34.6480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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M END  
> <NAME>  
D32\_12

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D36\_12  
MOE2012 3D

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-0.2090 -5.3440 -19.3970 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
-0.6670 -6.1830 -19.9300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
-0.1820 -4.4730 -20.0610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
1.1920 -5.7040 -18.9190 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
1.6080 -4.8640 -18.3500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
1.1300 -6.5420 -18.2140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
2.1130 -6.0610 -20.0850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
1.6880 -6.9050 -20.6420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
2.1720 -5.2140 -20.7790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
3.5200 -6.4240 -19.6010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
3.9480 -5.5780 -19.0510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
3.4600 -7.2680 -18.9020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
4.4360 -6.7930 -20.7720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
4.0000 -7.6360 -21.3220 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
4.4950 -5.9480 -21.4690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
5.8420 -7.1620 -20.2870 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
6.2750 -6.3110 -19.7490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
5.7780 -8.0080 -19.5930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
6.6860 -7.5100 -21.4330 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
6.2530 -8.2780 -21.9460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.2060 -8.3950 -17.3390 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.8730 -8.7840 -18.3080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.8110 -9.0920 -16.5890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.6430 -8.4030 -17.3530 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.2540 -8.4510 -16.1340 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.7520 -8.4660 -16.3240 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.0220 -9.4260 -16.7750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.0080 -7.6580 -17.0170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.4700 -8.2620 -14.9840 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.1210 -7.3220 -14.5350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.1540 -9.0380 -14.2750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.6780 -8.4800 -15.0560 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.6720 -6.9830 -17.1200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.9550 -6.6480 -16.1150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.1360 -6.2530 -17.7940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
8.0310 -7.8940 -21.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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7.9820 -8.7670 -20.3390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
8.8930 -8.2160 -22.2190 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
8.4480 -9.0430 -22.7860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
8.9720 -7.3370 -22.8690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
10.2830 -8.6250 -21.8050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
11.0100 -8.9460 -22.9140 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
12.3440 -9.4170 -22.6750 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
12.3760 -10.1060 -21.8210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
12.6390 -10.0130 -23.5470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
13.3180 -8.2580 -22.4930 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
13.2580 -7.5990 -23.3680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
13.0470 -7.6830 -21.6000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
10.7000 -8.6600 -20.6560 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
14.6290 -8.8020 -22.3570 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
15.6640 -7.9180 -22.2310 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
16.9280 -8.5020 -22.1700 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.0260 -9.5840 -22.2240 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.0730 -7.7110 -22.0460 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.0420 -8.2060 -22.0040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.9870 -6.3070 -21.9750 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
16.7050 -5.7360 -22.0340 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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15.5570 -6.5310 -22.1590 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
14.5970 -6.0280 -22.1970 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.2780 -5.4650 -21.8550 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.1250 -5.9060 -20.6380 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0











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119.0540	35.4370	11.8090	C	0	0	0	0	0	0	0	0	0	0	0	0
119.3330	35.1900	12.8380	H	0	0	0	0	0	0	0	0	0	0	0	0
118.1770	36.0910	11.8490	H	0	0	0	0	0	0	0	0	0	0	0	0
119.8940	35.9850	11.3730	H	0	0	0	0	0	0	0	0	0	0	0	0
118.0580	33.6860	11.5880	H	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0
5	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0
5	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0
7	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0
7	9	1	0	0	0	0	0	0	0	0	0	0	0	0	0
7	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0
10	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0
10	12	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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13	14	1	0	0	0	0	0	0	0	0	0	0	0	0	0
13	33	1	0	0	0	0	0	0	0	0	0	0	0	0	0
14	15	1	0	0	0	0	0	0	0	0	0	0	0	0	0
14	16	1	0	0	0	0	0	0	0	0	0	0	0	0	0
14	17	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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18	20	1	0	0	0	0	0	0	0	0	0	0	0	0	0
18	21	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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21	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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22	29	2	0	0	0	0	0	0	0	0	0	0	0	0	0
23	24	1	0	0	0	0	0	0	0	0	0	0	0	0	0
23	25	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END  
> <NAME>  
D60\_12

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D61\_12  
MOE2012 3D

445454 0 0 1 0 0 0 0 0999 V2000  
60.0120 -19.8660 -46.5070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
60.0310 -18.8940 -47.0130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
60.8270 -19.8850 -45.7730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
58.7230 -20.0690 -45.8480 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
58.7070 -20.9900 -45.4090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
58.4750 -19.0340 -44.8360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.2620 -19.0610 -44.0730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
58.4980 -18.0520 -45.3210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
57.1040 -19.2530 -44.1630 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
56.3090 -19.2230 -44.9210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
57.1110 -20.2730 -43.7550 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
56.7970 -18.3100 -43.0590 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
55.5660 -18.7600 -42.3770 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
54.6810 -18.5900 -43.0030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
55.6230 -19.8410 -42.1950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
60.2430 -20.9620 -47.5360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
60.2630 -21.9510 -47.0650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.4580 -20.9610 -48.2990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
61.2030 -20.8100 -48.0390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
55.3790 -18.1110 -41.0090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
55.1620 -17.0420 -41.0850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
56.2690 -18.2420 -40.3850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
54.5350 -18.5780 -40.4890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
58.6810 -8.3120 -29.1790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.2820 -9.2010 -29.3950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
57.6480 -8.6700 -29.0870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.1570 -7.7720 -27.9360 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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58.6390 -5.0100 -25.7440 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
57.6460 -4.7170 -26.1050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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58.1470 -6.4460 -30.1030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.8180 -6.8440 -30.3420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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56.5250 -16.8910 -44.6280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
55.7930 -16.4190 -43.1260 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
57.9160 -16.0970 -43.1850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
58.8430 -16.6170 -43.4490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
57.9210 -15.1580 -43.7510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
57.9270 -15.7290 -41.7250 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.0180 -16.2550 -41.1020 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.0980 -16.0330 -39.6860 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
58.1200 -16.1690 -39.2080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.7410 -16.8180 -39.2710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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M END
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D61_12

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D70_12
MOE2012 3D

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22.0150 28.5550 19.8660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.1630 16.6770 14.5970 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.2790 16.8000 13.9630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.8110 16.1660 15.5010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.0980 15.8650 13.8690 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.0100 15.1950 14.6260 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.9530 14.4130 13.7520 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.7290 13.3510 13.8940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.7730 14.6570 12.6990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.3910 14.7650 14.1330 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.4950 15.8550 14.0440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.5610 14.5360 15.1890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.0760 15.2260 15.8480 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.7730 18.0370 14.9270 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.6600 17.8890 15.5540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.1500 18.5500 14.0350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.2390 26.1730 20.8590 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.2830 26.4160 21.0970 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.0170 25.2240 21.3650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.0670 25.9200 19.3590 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.0170 25.6920 19.1420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.3770 26.7850 18.7650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.9050 24.7500 18.9160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.5960 24.4360 17.6250 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```









108.5290	22.5230	-8.7700	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108.4840	20.8730	-7.3580	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108.1980	19.5040	-7.2430	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108.2990	18.9800	-6.2960	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107.7630	18.7550	-8.3450	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107.5590	17.7000	-8.1890	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108.9510	21.7370	-6.1630	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
110.2890	22.4490	-6.4760	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107.7850	22.7130	-5.8470	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107.5970	23.4170	-6.6660	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107.9840	23.3040	-4.9440	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
106.8500	22.1660	-5.6710	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
109.1870	20.9260	-4.8610	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108.2650	20.4470	-4.5100	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
109.9390	20.1390	-4.9910	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
109.5400	21.5750	-4.0490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
111.3930	21.6970	-6.9190	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
111.3050	20.6220	-7.0640	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
112.6250	22.3040	-7.1810	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
113.4590	21.6950	-7.5220	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
112.7980	23.6750	-7.0000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
111.7140	24.4380	-6.5750	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
111.7860	25.5120	-6.4390	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
110.4760	23.8320	-6.3130	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
109.6680	24.4750	-5.9740	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
114.0530	24.1350	-7.2860	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
118.2210	31.7130	-6.7290	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
118.5330	32.6090	-6.1740	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
117.2850	32.0270	-7.2110	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
119.2460	31.4450	-7.8350	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
118.7650	30.8850	-8.6470	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
119.5190	32.4170	-8.2660	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120.5310	30.7100	-7.4510	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120.4280	29.6350	-7.6400	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
121.3150	31.0330	-8.1470	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
117.9140	30.6450	-5.7780	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
121.0200	30.9490	-6.1000	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
120.9270	31.9330	-5.8510	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
118.9250	30.5440	-4.7160	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
118.9910	31.5140	-4.2040	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
118.5570	29.8550	-3.9450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120.3460	30.1030	-5.1120	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120.3470	29.0550	-5.4350	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
120.9590	30.1240	-4.2030	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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346349 1 0 0 0 0
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M END
> <NAME>
D70_12

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$$$$
D86_12
MOE2012 3D

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451460 0 0 1 0 0 0 0 0999 V2000
28.3950 38.4840 -15.1750 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.7830 37.5730 -15.1430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.9220 39.1790 -14.4690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.7800 38.1720 -14.7730 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.7660 37.3430 -13.5470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.3940 37.9270 -12.6940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.0670 36.5080 -13.6890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.1410 36.7270 -13.2150 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.4790 36.1350 -14.0740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```













99.7500	14.5070	0.6790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
100.2910	15.3570	-0.7690	H	0	0	0	0	0	0	0	0	0	0	0	0	0
102.3140	13.2680	0.9680	C	0	0	0	0	0	0	0	0	0	0	0	0	0
101.5170	13.0820	1.6860	H	0	0	0	0	0	0	0	0	0	0	0	0	0
103.6190	13.4220	1.4540	C	0	0	0	0	0	0	0	0	0	0	0	0	0
103.7730	13.3520	2.5250	H	0	0	0	0	0	0	0	0	0	0	0	0	0
104.6690	13.6570	0.5700	C	0	0	0	0	0	0	0	0	0	0	0	0	0
104.4000	13.7320	-0.7960	C	0	0	0	0	0	0	0	0	0	0	0	0	0
105.2120	13.9150	-1.4950	H	0	0	0	0	0	0	0	0	0	0	0	0	0
103.0960	13.5790	-1.2830	C	0	0	0	0	0	0	0	0	0	0	0	0	0
102.9510	13.6540	-2.3560	H	0	0	0	0	0	0	0	0	0	0	0	0	0
105.9830	13.8310	0.9070	O	0	0	0	0	0	0	0	0	0	0	0	0	0
114.2190	15.1650	11.2840	C	0	0	0	0	0	0	0	0	0	0	0	0	0
113.3310	15.7020	11.6440	H	0	0	0	0	0	0	0	0	0	0	0	0	0
114.1670	14.1710	11.7480	H	0	0	0	0	0	0	0	0	0	0	0	0	0
114.1890	15.0740	9.8110	N	0	0	0	0	0	0	0	0	0	0	0	0	0
112.8350	14.6730	9.3650	C	0	0	0	0	0	0	0	0	0	0	0	0	0
112.6070	13.6550	9.7090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
112.0970	15.3390	9.8320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
112.6290	14.7740	7.8380	C	0	0	0	0	0	0	0	0	0	0	0	0	0
112.8470	15.8000	7.5160	H	0	0	0	0	0	0	0	0	0	0	0	0	0
113.3180	14.1000	7.3180	H	0	0	0	0	0	0	0	0	0	0	0	0	0
111.2480	14.4240	7.4690	N	0	0	3	0	0	0	0	0	0	0	0	0	0
111.0470	13.4730	7.7800	H	0	0	0	0	0	0	0	0	0	0	0	0	0
115.2270	14.1590	9.3000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
115.8820	13.7860	10.0990	H	0	0	0	0	0	0	0	0	0	0	0	0	0
114.8030	13.2420	8.8710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
115.4360	15.9340	11.8140	C	0	0	0	0	0	0	0	0	0	0	0	0	0
116.3760	15.4330	11.5650	H	0	0	0	0	0	0	0	0	0	0	0	0	0
115.4590	16.9490	11.4040	H	0	0	0	0	0	0	0	0	0	0	0	0	0
115.3510	16.0260	13.2330	O	0	0	0	0	0	0	0	0	0	0	0	0	0
116.1260	16.5300	13.5330	H	0	0	0	0	0	0	0	0	0	0	0	0	0
116.1020	14.8630	8.2600	C	0	0	0	0	0	0	0	0	0	0	0	0	0
115.5110	15.2190	7.4110	H	0	0	0	0	0	0	0	0	0	0	0	0	0
116.6260	15.7140	8.7080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
117.0760	13.9470	7.7690	O	0	0	0	0	0	0	0	0	0	0	0	0	0
117.6620	14.4450	7.1730	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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421426	1	0	0	0	0
422423	1	0	0	0	0
422424	1	0	0	0	0
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427430	1	0	0	0	0
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431433	1	0	0	0	0
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447450 1 0 0 0 0  
450451 1 0 0 0 0

M END  
> <NAME>  
D86\_12

\$\$\$  
D87\_12  
MOE2012 3D

469478 0 0 1 0 0 0 0 0999 V2000  
74.7210 -0.4400 -37.2580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
75.6880 -0.8930 -37.5080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
74.3530 -0.0180 -38.2030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
73.7870 -1.4530 -36.7210 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
72.3940 -0.9620 -36.7900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
72.3530 0.1060 -36.5430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
71.9970 -1.0560 -37.8090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
71.4870 -1.6840 -35.7830 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
71.4580 -2.7600 -35.9860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
71.8940 -1.5580 -34.7720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
70.0620 -1.1240 -35.8380 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
70.0840 -0.0490 -35.6230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
69.6530 -1.2620 -36.8460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
73.9250 -2.7240 -37.4640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
73.0480 -3.3650 -37.3130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
73.9630 -2.5510 -38.5490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
69.2250 -1.8110 -34.8530 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0  
69.2310 -2.8140 -35.0410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
75.0190 0.6820 -36.2560 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
74.1240 1.2580 -36.0040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
75.4460 0.2720 -35.3350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
75.9670 1.5780 -36.8280 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
76.1730 2.2480 -36.1530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
75.1400 -3.5430 -37.0150 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
76.0820 -3.0320 -37.2330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
75.0900 -3.7500 -35.9410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
75.1460 -4.7880 -37.7080 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
75.9230 -5.2830 -37.3950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
53.5010 6.7760 -31.7060 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
53.5930 5.7000 -31.5250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
53.2210 6.8830 -32.7610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
52.4550 7.2580 -30.8440 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
51.9260 8.4760 -31.1500 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
50.9270 8.8850 -30.0940 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
49.9200 8.7660 -30.5080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
51.0220 8.2000 -29.2450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
51.1970 10.3290 -29.6580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
52.2760 10.4860 -29.5340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
50.9350 11.0020 -30.4860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
52.2310 9.1550 -32.1190 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
54.8200 7.4840 -31.4040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
54.8050 8.4770 -31.8680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
54.9490 7.6800 -30.3320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
67.8500 -1.3090 -34.8830 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
67.8390 -0.2280 -34.6930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
67.4050 -1.4780 -35.8710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
67.0250 -2.0200 -33.8130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
67.0220 -3.1000 -33.9980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
67.4500 -1.8270 -32.8210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
65.5960 -1.5410 -33.8140 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
64.8930 -2.2260 -32.8660 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
63.4910 -1.9290 -32.7870 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
63.0490 -1.8280 -33.7870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
63.0000 -2.7980 -32.3330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
63.2330 -0.6910 -31.9360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
63.6810 -0.8380 -30.9460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
63.6950 0.1850 -32.4060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
65.1320 -0.6750 -34.5420 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
61.8220 -0.5160 -31.8320 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
61.3740 0.5270 -31.0700 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.9870 0.6190 -30.9630 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0













57.5560	36.6040	-45.2960	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.1130	37.6170	-47.0230	O	0	0	0	0	0	0	0	0	0	0	0	0	0
56.5250	38.1810	-46.4900	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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1	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	19	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	14	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	9	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	12	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	13	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	17	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	15	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	16	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	24	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	18	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	44	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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19	21	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	23	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	25	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	26	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	27	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	28	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	30	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	31	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	32	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	41	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	33	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	34	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	40	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	35	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	36	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	37	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	38	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	39	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	106	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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41	43	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	89	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44	45	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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44	47	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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47	49	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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50	51	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	58	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51	52	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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55	57	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55	59	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59	60	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	61	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	68	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	62	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	63	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	64	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	65	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	66	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	70	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66	67	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66	68	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68	69	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	71	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	72	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	76	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	80	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	87	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72	73	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72	74	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0

72	75	1	0	0	0	0
76	77	1	0	0	0	0
76	78	1	0	0	0	0
76	79	1	0	0	0	0
80	81	1	0	0	0	0
80	82	2	0	0	0	0
82	83	1	0	0	0	0
82	84	1	0	0	0	0
84	85	2	0	0	0	0
84	89	1	0	0	0	0
85	86	1	0	0	0	0
85	87	1	0	0	0	0
87	88	1	0	0	0	0
90	91	1	0	0	0	0
90	92	1	0	0	0	0
90	93	1	0	0	0	0
90	107	1	0	0	0	0
93	94	1	0	0	0	0
93	103	1	0	0	0	0
94	95	1	0	0	0	0
94	96	1	0	0	0	0
94	97	1	0	0	0	0
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97	99	1	0	0	0	0
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100	101	1	0	0	0	0
100	102	1	0	0	0	0
100	106	1	0	0	0	0
103	104	1	0	0	0	0
103	105	1	0	0	0	0
103	112	1	0	0	0	0
106	132	1	0	0	0	0
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107	109	1	0	0	0	0
107	110	1	0	0	0	0
110	111	1	0	0	0	0
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112	114	1	0	0	0	0
112	115	1	0	0	0	0
115	116	1	0	0	0	0
117	118	1	0	0	0	0
117	119	1	0	0	0	0
117	120	1	0	0	0	0
117	129	1	0	0	0	0
120	121	1	0	0	0	0
121	122	1	0	0	0	0
121	128	2	0	0	0	0
122	123	1	0	0	0	0
122	124	1	0	0	0	0
122	125	1	0	0	0	0
125	126	1	0	0	0	0
125	127	1	0	0	0	0
125	194	1	0	0	0	0
129	130	1	0	0	0	0
129	131	1	0	0	0	0
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132	133	1	0	0	0	0
132	134	1	0	0	0	0
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135	136	1	0	0	0	0
135	137	1	0	0	0	0
135	138	1	0	0	0	0
138	139	1	0	0	0	0
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139	140	1	0	0	0	0
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149	151	2	0	0	0	0
151	152	1	0	0	0	0
151	153	1	0	0	0	0
153	154	2	0	0	0	0
153	158	1	0	0	0	0
154	155	1	0	0	0	0

154156	1	0	0	0	0
156157	1	0	0	0	0
158159	1	0	0	0	0
158160	1	0	0	0	0
158164	1	0	0	0	0
159168	1	0	0	0	0
159175	2	0	0	0	0
160161	1	0	0	0	0
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160163	1	0	0	0	0
164165	1	0	0	0	0
164166	1	0	0	0	0
164167	1	0	0	0	0
168169	1	0	0	0	0
168170	2	0	0	0	0
170171	1	0	0	0	0
170172	1	0	0	0	0
172173	2	0	0	0	0
172177	1	0	0	0	0
173174	1	0	0	0	0
173175	1	0	0	0	0
175176	1	0	0	0	0
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178180	1	0	0	0	0
178181	1	0	0	0	0
178195	1	0	0	0	0
181182	1	0	0	0	0
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182183	1	0	0	0	0
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185186	1	0	0	0	0
185187	1	0	0	0	0
185188	1	0	0	0	0
188189	1	0	0	0	0
188190	1	0	0	0	0
188194	1	0	0	0	0
191192	1	0	0	0	0
191193	1	0	0	0	0
191200	1	0	0	0	0
194220	1	0	0	0	0
195196	1	0	0	0	0
195197	1	0	0	0	0
195198	1	0	0	0	0
198199	1	0	0	0	0
200201	1	0	0	0	0
200202	1	0	0	0	0
200203	1	0	0	0	0
203204	1	0	0	0	0
205206	1	0	0	0	0
205207	1	0	0	0	0
205208	1	0	0	0	0
205217	1	0	0	0	0
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260265	1	0	0	0	0
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329330	2	0	0	0	0
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M END  
> <NAME>  
D87\_12

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33.8870	19.6600	1.5950	N	0	0	0	0	0	0	0	0	0	0	0	0
35.1590	19.7250	1.2720	C	0	0	0	0	0	0	0	0	0	0	0	0
35.7090	18.9800	0.7120	H	0	0	0	0	0	0	0	0	0	0	0	0
37.1190	21.2600	1.5580	C	0	0	0	0	0	0	0	0	0	0	0	0
37.3970	21.8970	2.4060	H	0	0	0	0	0	0	0	0	0	0	0	0
37.7120	20.3410	1.6240	H	0	0	0	0	0	0	0	0	0	0	0	0
37.3450	21.9880	0.2340	C	0	0	0	0	0	0	0	0	0	0	0	0
37.0090	21.3600	-0.6020	H	0	0	0	0	0	0	0	0	0	0	0	0
36.7190	22.8890	0.2070	H	0	0	0	0	0	0	0	0	0	0	0	0
38.8010	22.4020	-0.0110	C	0	0	0	0	0	0	0	0	0	0	0	0
38.8390	23.0060	-0.9040	H	0	0	0	0	0	0	0	0	0	0	0	0
39.1430	23.0330	-0.8400	H	0	0	0	0	0	0	0	0	0	0	0	0
39.6700	21.2330	-0.1310	N	0	0	3	0	0	0	0	0	0	0	0	0
39.7340	20.7330	0.7550	H	0	0	0	0	0	0	0	0	0	0	0	0
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1	9	1	0	0	0	0									
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87	88	1	0	0	0	0
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146149	1	0	0	0	0
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D93\_12

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D94\_12  
MOE2012 3D

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61.8490 -6.7430 30.0250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
61.4120 -7.7580 31.9860 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
62.1970 -8.4850 32.1470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
60.3980 -7.5920 32.8950 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.6390 -6.6450 32.3910 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
58.7380 -6.2520 32.8450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.5330 -5.1650 30.3720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
59.0810 -4.4290 31.0480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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58.4960 -5.7300 29.3980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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57.7180 -6.2670 29.9550 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
57.8940 -4.6510 28.6080 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
57.4190 -3.9940 29.2290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
49.0200 -10.1020 13.8930 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
48.8050 -9.1230 14.3340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
48.6230 -10.8400 14.6000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
48.3260 -10.1600 12.6360 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
48.0520 -11.4080 12.1560 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
47.3480 -11.2800 10.8290 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
46.4040 -10.7480 10.9880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
47.9990 -10.6850 10.1800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
47.0800 -12.6550 10.2110 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
48.0250 -13.1960 10.0760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
46.5000 -13.2350 10.9430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
48.3550 -12.4560 12.7050 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
50.5230 -10.2770 13.6920 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
50.7190 -11.3020 13.3540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
50.9130 -9.6440 12.8860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
56.9340 -5.1830 27.6350 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
57.4390 -5.8780 26.9530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0











95.3800	-4.4510	-11.9290	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
94.4450	-4.2180	-11.4260	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
95.3400	-4.6050	-13.3220	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
94.3810	-4.4900	-13.8160	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
96.6680	-4.4100	-9.6780	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
97.2940	-5.6550	-9.0050	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
97.4670	-3.1010	-9.4350	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98.5040	-3.1750	-9.7840	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
97.4970	-2.8360	-8.3710	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
97.0090	-2.2550	-9.9620	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
95.2900	-4.1970	-8.9950	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
94.8000	-3.2810	-9.3480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
94.6020	-5.0310	-9.1770	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
95.3990	-4.1020	-7.9070	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
96.7580	-6.9310	-9.2610	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
95.9210	-7.0500	-9.9460	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
97.2810	-8.0730	-8.6470	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
96.8450	-9.0450	-8.8650	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98.3460	-7.9780	-7.7510	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98.8970	-6.7260	-7.4940	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
99.7380	-6.5960	-6.8220	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98.3750	-5.5780	-8.1120	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98.8380	-4.6270	-7.8650	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98.7530	-9.1700	-7.2210	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107.8300	-11.0760	-1.0090	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108.4730	-9.8720	-1.0600	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107.9660	-8.9270	-0.9300	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
109.7920	-10.1900	-1.2900	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
110.6290	-9.5120	-1.3920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
109.9620	-11.5480	-1.3810	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108.7610	-12.0550	-1.2090	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108.5150	-13.1080	-1.2190	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
106.4150	-11.2830	-0.7730	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
106.3120	-12.2130	-0.2000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
106.0630	-10.4620	-0.1370	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
105.6110	-11.3480	-2.0770	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
105.7550	-10.4110	-2.6270	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
105.9940	-12.1630	-2.7040	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
104.1890	-11.5600	-1.7860	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
104.0820	-12.4180	-1.2420	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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1	7	1	0	0	0	0													
1	9	1	0	0	0	0													
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6	7	2	0	0	0	0													
7	8	1	0	0	0	0													
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73	75	1	0	0	0	0
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93	95	1	0	0	0	0
93	96	1	0	0	0	0
93	105	1	0	0	0	0
96	97	1	0	0	0	0
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98	99	1	0	0	0	0
98	100	1	0	0	0	0
98	101	1	0	0	0	0
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101	168	1	0	0	0	0
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M END  
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D94\_12

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E20\_12  
MOE2012 3D

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34.5650 -20.0200 -35.8910 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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34.2400 -17.5580 -33.8160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
34.1000 -16.7910 -34.5880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
33.2310 -17.8340 -33.4810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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36.0520 -16.7110 -33.0080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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33.0380 -6.3590 -24.4310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
33.8300 -6.4400 -22.5160 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
33.0600 -5.4740 -21.9470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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34.4070 -6.3010 -19.3450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
31.9330 -5.1520 -22.3130 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0









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M END  
> <NAME>  
E20\_12









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68.7210	8.9980	-15.4240	C	0	0	0	0	0	0	0	0	0	0	0	0
68.8420	9.9280	-15.9930	H	0	0	0	0	0	0	0	0	0	0	0	0
69.6890	8.4810	-15.4410	H	0	0	0	0	0	0	0	0	0	0	0	0
67.6610	8.1210	-16.0950	C	0	0	0	0	0	0	0	0	0	0	0	0
66.6930	8.6370	-16.0760	H	0	0	0	0	0	0	0	0	0	0	0	0
67.5430	7.1900	-15.5270	H	0	0	0	0	0	0	0	0	0	0	0	0
67.6580	3.4000	-27.9630	O	0	0	0	0	0	0	0	0	0	0	0	0
68.4950	2.9220	-28.1000	H	0	0	0	0	0	0	0	0	0	0	0	0
67.4210	3.4190	-26.5500	C	0	0	0	0	0	0	0	0	0	0	0	0
67.3800	2.3890	-26.1840	H	0	0	0	0	0	0	0	0	0	0	0	0
68.2640	3.9440	-26.0900	H	0	0	0	0	0	0	0	0	0	0	0	0
66.1020	4.1510	-26.3050	C	0	0	3	0	0	0	0	0	0	0	0	0
65.3100	3.6540	-26.8790	H	0	0	0	0	0	0	0	0	0	0	0	0
65.6660	4.2080	-24.8280	C	0	0	0	0	0	0	0	0	0	0	0	0
64.7370	4.7890	-24.7820	H	0	0	0	0	0	0	0	0	0	0	0	0
65.4460	3.1900	-24.4850	H	0	0	0	0	0	0	0	0	0	0	0	0
66.6500	4.8230	-23.9230	N	0	0	3	0	0	0	0	0	0	0	0	0
67.5000	4.2640	-23.8910	H	0	0	0	0	0	0	0	0	0	0	0	0
66.2040	5.4720	-26.8520	O	0	0	0	0	0	0	0	0	0	0	0	0
66.6560	5.3500	-27.7100	H	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
E24_12

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$$$$
E28_12
MOE2012 3D

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14.0410 8.7040 29.3300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.0230 8.7020 29.8140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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14.1580 9.0980 27.8650 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.1550 9.1400 27.4200 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.5600 10.1160 27.7930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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16.0420 8.1010 27.5370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.6270 7.1120 27.1660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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15.9890 7.5730 24.8970 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
16.9140 7.5510 25.3250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.7140 3.2700 14.4820 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.1650 2.3390 14.6670 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.7130 3.2030 14.9290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.8420 3.4790 13.0670 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.4320 2.4510 12.3890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.4870 2.7750 10.9160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.4920 3.1180 10.6180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.2020 3.5930 10.7710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.9180 1.5470 10.1020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.9190 1.2680 10.4510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.2710 0.6870 10.3230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.8600 1.4260 12.9010 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.9510 4.4520 15.0710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.4930 5.3800 14.8510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.9810 4.5440 14.5650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.1050 7.9360 23.4820 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.1090 7.9720 23.0230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.5530 8.9320 23.3830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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182183	1	0	0	0	0
182184	1	0	0	0	0
182203	1	0	0	0	0
185186	1	0	0	0	0
185187	1	0	0	0	0
185188	1	0	0	0	0
188189	1	0	0	0	0
188190	1	0	0	0	0
188191	1	0	0	0	0
191192	1	0	0	0	0
191199	2	0	0	0	0
192193	1	0	0	0	0
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208209	1	0	0	0	0
208210	1	0	0	0	0
208211	1	0	0	0	0
211212	1	0	0	0	0
211213	1	0	0	0	0
211214	1	0	0	0	0
214215	1	0	0	0	0
214216	1	0	0	0	0
214217	1	0	0	0	0
217218	1	0	0	0	0
217219	1	0	0	0	0
217220	1	0	0	0	0
220236	1	0	0	0	0
221222	1	0	0	0	0
221223	1	0	0	0	0
221224	1	0	0	0	0
221233	1	0	0	0	0
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225232	2	0	0	0	0
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229230	1	0	0	0	0
229231	1	0	0	0	0
229271	1	0	0	0	0
233234	1	0	0	0	0
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233254	1	0	0	0	0
236237	1	0	0	0	0
236238	1	0	0	0	0
236239	1	0	0	0	0
239240	1	0	0	0	0
239241	1	0	0	0	0
239242	1	0	0	0	0
242243	1	0	0	0	0
242250	2	0	0	0	0
243244	1	0	0	0	0
244245	1	0	0	0	0
244246	1	0	0	0	0
244247	1	0	0	0	0

```

247248 1 0 0 0 0
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247251 1 0 0 0 0
251252 1 0 0 0 0
251253 1 0 0 0 0
251254 1 0 0 0 0
254255 1 0 0 0 0
254256 1 0 0 0 0
257258 1 0 0 0 0
257259 1 0 0 0 0
259260 1 0 0 0 0
259261 1 0 0 0 0
259262 1 0 0 0 0
262263 1 0 0 0 0
262264 1 0 0 0 0
262265 1 0 0 0 0
265266 1 0 0 0 0
265267 1 0 0 0 0
265268 1 0 0 0 0
268269 1 0 0 0 0
268270 1 0 0 0 0
268271 1 0 0 0 0
271272 1 0 0 0 0

```

```

M END
> <NAME>
E28_12

```

```

$$$$
E32_12
MOE2012 3D

```

```

290289 0 0 1 0 0 0 0 0999 V2000
57.8180 25.9490 -27.3180 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.7810 26.0450 -27.4140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.5890 25.1710 -26.1520 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.0860 24.2040 -26.2750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.0290 25.6910 -25.2940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
56.0890 24.9930 -25.9690 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
55.6110 25.9790 -25.9020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
55.6680 24.5170 -26.8640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
55.7660 24.1640 -24.7280 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
56.2440 23.1810 -24.8080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
56.1820 24.6550 -23.8400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.2560 23.9870 -24.5550 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.7790 24.9720 -24.4780 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.8410 23.4960 -25.4450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.9350 23.1570 -23.3100 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.4140 22.1740 -23.3960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.3400 23.6570 -22.4220 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.4860 22.9960 -23.1850 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0
52.0450 23.9140 -23.1340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.6720 18.4330 -17.5120 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.3800 17.9170 -18.4350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.2310 19.4370 -17.4970 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.1990 17.6870 -16.3800 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.8430 17.5430 -16.3200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.4790 16.7510 -15.0840 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.9280 15.7570 -15.1790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.9160 17.2610 -14.2200 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.9570 16.6370 -14.9290 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.5030 17.6350 -15.0010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.5490 16.0880 -15.7880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.0520 17.9880 -17.1390 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.1920 18.5260 -17.4210 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.4690 18.9950 -16.4680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.6160 17.5150 -17.3920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.1440 22.2140 -21.9940 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.6240 21.2290 -22.0430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.5120 22.7190 -21.0920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50.6310 22.0370 -21.9070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50.1380 23.0130 -21.8330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50.2620 21.5150 -22.7980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50.2520 21.2260 -20.6940 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.8980 21.0550 -20.6670 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.4170 20.2970 -19.5470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.8610 19.2950 -19.5690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.6990 20.8040 -18.6170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
46.8980 20.2000 -19.6500 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
46.4710 21.2100 -19.6790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
46.6280 19.7330 -20.6060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.0330 20.7930 -19.8580 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```







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18	35	1	0	0	0	0
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79	80	1	0	0	0	0
79	81	1	0	0	0	0
79	82	1	0	0	0	0



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82	127	1	0	0	0	0
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86	88	1	0	0	0	0
86	107	1	0	0	0	0
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136	138	1	0	0	0	0
136	181	1	0	0	0	0
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140	142	1	0	0	0	0
140	161	1	0	0	0	0
143	144	1	0	0	0	0
143	145	1	0	0	0	0
143	146	1	0	0	0	0
146	147	1	0	0	0	0
146	148	1	0	0	0	0
146	149	1	0	0	0	0
149	150	1	0	0	0	0
149	157	2	0	0	0	0
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158	159	1	0	0	0	0
158	160	1	0	0	0	0
158	161	1	0	0	0	0
161	162	1	0	0	0	0
161	163	1	0	0	0	0
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182194	1	0	0	0	0
185186	1	0	0	0	0
186187	1	0	0	0	0
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187189	1	0	0	0	0
187190	1	0	0	0	0
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190192	1	0	0	0	0
190235	1	0	0	0	0
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194196	1	0	0	0	0
194215	1	0	0	0	0
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205207	1	0	0	0	0
205208	1	0	0	0	0
208209	1	0	0	0	0
208210	1	0	0	0	0
208212	1	0	0	0	0
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212214	1	0	0	0	0
212215	1	0	0	0	0
215216	1	0	0	0	0
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220222	1	0	0	0	0
220223	1	0	0	0	0
223224	1	0	0	0	0
223225	1	0	0	0	0
223226	1	0	0	0	0
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226228	1	0	0	0	0
226229	1	0	0	0	0
229230	1	0	0	0	0
229231	1	0	0	0	0
229232	1	0	0	0	0
232233	1	0	0	0	0
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239240	1	0	0	0	0
240241	1	0	0	0	0
240247	2	0	0	0	0
241242	1	0	0	0	0
241243	1	0	0	0	0
241244	1	0	0	0	0

```

244245 1 0 0 0 0
244246 1 0 0 0 0
244289 1 0 0 0 0
248249 1 0 0 0 0
248250 1 0 0 0 0
248269 1 0 0 0 0
251252 1 0 0 0 0
251253 1 0 0 0 0
251254 1 0 0 0 0
254255 1 0 0 0 0
254256 1 0 0 0 0
254257 1 0 0 0 0
257258 1 0 0 0 0
257265 2 0 0 0 0
258259 1 0 0 0 0
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259261 1 0 0 0 0
259262 1 0 0 0 0
262263 1 0 0 0 0
262264 1 0 0 0 0
262266 1 0 0 0 0
266267 1 0 0 0 0
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280283 1 0 0 0 0
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286288 1 0 0 0 0
286289 1 0 0 0 0
289290 1 0 0 0 0

```

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M END
> <NAME>
E32_12

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E36_12
MOE2012 3D

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```

308307 0 0 1 0 0 0 0 0999 V2000
20.2470 -5.2220 -19.8040 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8640 -5.6010 -20.6130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.5730 -4.8220 -20.1200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.1290 -5.7010 -20.4620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.5310 -4.0890 -20.9330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.2210 -4.2180 -18.8810 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.6200 -3.3680 -18.5340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.2000 -4.9530 -18.0660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.6580 -3.7730 -19.1530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.2490 -4.6320 -19.4920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.6660 -3.0350 -19.9650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.3050 -3.1670 -17.9050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.7200 -2.3020 -17.5710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.2900 -3.9020 -17.0910 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.7500 -2.7350 -18.1770 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.3310 -3.6020 -18.5150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.7640 -1.9990 -18.9910 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.3970 -2.1330 -16.9260 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.8190 -1.2590 -16.6030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.3810 -2.8720 -16.1160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.7770 -1.7370 -17.2220 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
28.2940 -2.5500 -17.5570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.3570 3.4180 -13.9370 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.2300 4.1440 -14.7480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.9080 2.5450 -14.3070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.0930 4.0260 -12.8650 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.3340 4.4720 -13.2090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.9990 5.0820 -12.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```









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46	48	1	0	0	0	0
46	49	1	0	0	0	0
49	50	1	0	0	0	0
49	51	1	0	0	0	0
49	53	1	0	0	0	0
53	54	1	0	0	0	0
53	55	1	0	0	0	0
53	56	1	0	0	0	0
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M END
> <NAME>
E80_12

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E86_12
MOE2012 3D

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15.5280 21.3500 -21.4030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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16.2230 18.8080 -20.5840 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7000 19.3100 -19.7590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.4500 18.3510 -21.2180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.0970 17.6570 -20.0430 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.5900 17.1610 -20.8880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.8730 18.0570 -19.3840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.2730 16.6900 -19.3100 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
15.8360 17.1400 -18.5060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.9410 20.5520 -20.5600 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.7840 21.6360 -20.6320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.8220 20.3480 -19.4880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.7160 21.4960 -23.2150 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.4700 22.1840 -22.8220 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.1900 20.8330 -23.9470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7250 22.2680 -23.8870 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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 E94\_12  
 MOE2012 3D

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22.4050	30.8210	7.9880	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21.2590	31.5290	7.7560	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20.2960	31.0590	7.6200	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21.6560	32.8470	7.7550	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21.0400	33.7240	7.6080	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23.0060	32.9530	7.9750	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23.4290	31.7160	8.1100	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0







68.4770	25.5560	1.9440	C	0	0	0	0	0	0	0	0	0	0	0	0
69.1940	25.4490	2.7670	H	0	0	0	0	0	0	0	0	0	0	0	0
69.0030	26.0510	1.1190	H	0	0	0	0	0	0	0	0	0	0	0	0
67.3020	26.4240	2.3980	C	0	0	0	0	0	0	0	0	0	0	0	0
66.7740	25.9260	3.2200	H	0	0	0	0	0	0	0	0	0	0	0	0
66.5860	26.5330	1.5730	H	0	0	0	0	0	0	0	0	0	0	0	0
68.4990	36.0290	7.9580	N	0	0	0	0	0	0	0	0	0	0	0	0
69.8530	35.8740	8.0500	C	0	0	0	0	0	0	0	0	0	0	0	0
70.4800	35.6490	7.1980	H	0	0	0	0	0	0	0	0	0	0	0	0
70.1390	36.0740	9.3810	C	0	0	0	0	0	0	0	0	0	0	0	0
71.1060	36.0410	9.8640	H	0	0	0	0	0	0	0	0	0	0	0	0
68.9980	36.3420	10.0940	N	0	0	0	0	0	0	0	0	0	0	0	0
68.0260	36.3060	9.2090	C	0	0	0	0	0	0	0	0	0	0	0	0
66.9780	36.4720	9.4180	H	0	0	0	0	0	0	0	0	0	0	0	0
67.7040	35.9290	6.7500	C	0	0	0	0	0	0	0	0	0	0	0	0
66.8810	36.6480	6.8410	H	0	0	0	0	0	0	0	0	0	0	0	0
68.3350	36.2520	5.9130	H	0	0	0	0	0	0	0	0	0	0	0	0
67.1730	34.5100	6.5200	C	0	0	0	0	0	0	0	0	0	0	0	0
68.0230	33.8220	6.4510	H	0	0	0	0	0	0	0	0	0	0	0	0
66.5660	34.2010	7.3800	H	0	0	0	0	0	0	0	0	0	0	0	0
66.3710	34.4630	5.2930	N	0	0	3	0	0	0	0	0	0	0	0	0
65.6040	35.1340	5.3680	H	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
E94_12

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$$$$
F28_12
MOE2012 3D

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 22.9830 9.9960 -8.6790 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 22.0540 10.1260 -8.9380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 23.4890 8.9230 -9.4610 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 22.8820 8.0330 -9.2660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 23.4010 9.1900 -10.5190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 24.9420 8.6840 -9.0790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 25.5140 9.6070 -9.2340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 25.0050 8.4700 -8.0040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 25.5550 7.5400 -9.8840 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 24.9800 6.6220 -9.7100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 25.4750 7.7750 -10.9520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 27.0190 7.3170 -9.4960 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 27.6080 8.2260 -9.6670 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 27.0720 7.1190 -8.4190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 27.6310 6.1770 -10.1790 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0
 27.0330 5.3560 -10.0800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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M END  
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F28\_12

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F32\_12  
MOE2012 3D

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25.5310 -23.5870 0.2100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.4730 -22.7580 -1.5480 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.1270 -23.5210 -1.9830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.4300 -23.0490 -1.7100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.7570 -21.3900 -2.1540 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.1200 -20.6390 -1.6700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.7900 -21.0990 -1.9250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.5290 -21.3840 -3.6650 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.1720 -22.1380 -4.1350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.4910 -21.6650 -3.8810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.8240 -20.0100 -4.2720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.1720 -19.2580 -3.8100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.8590 -19.7250 -4.0420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.6150 -20.0190 -5.7880 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.2680 -20.7770 -6.2380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.5770 -20.2890 -6.0140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.9290 -18.7010 -6.3410 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0  
25.3020 -18.0010 -5.9290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.7460 -18.6820 -7.7960 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.7110 -18.9420 -8.0520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.4050 -19.4300 -8.2530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.0980 -17.3150 -8.3850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
27.0800 -16.9770 -8.0370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.1320 -17.4140 -9.4760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.0730 -16.2580 -8.0470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.2170 -15.1960 -8.8910 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.2990 -14.1140 -8.6660 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.2730 -14.4980 -8.7330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.4620 -13.7190 -7.6550 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.5130 -12.9970 -9.7130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.4950 -11.8680 -9.4290 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.4720 -12.2580 -9.5040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.6480 -11.4730 -8.4160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.6530 -10.7980 -10.3740 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.8200 -9.7380 -10.1780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.0860 -8.6770 -11.2150 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.1190 -8.7790 -11.5630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.4180 -8.8600 -12.0630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.8630 -7.2890 -10.6090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.4040 -7.2130 -9.6560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.8060 -7.1820 -10.3300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.2550 -16.3340 -7.1400 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.9650 -9.6660 -9.3060 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.9500 -12.4500 -9.6160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.1270 -11.6510 -10.3460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.6920 -13.2330 -9.8060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.1470 -12.0390 -8.6190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.3000 -13.5550 -11.1330 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.0070 -14.3610 -11.3590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.4390 -12.7790 -11.8950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.2880 -13.9570 -11.2480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.8980 -1.8680 -17.0260 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.2960 -1.8210 -17.7880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.7600 -3.1620 -16.4600 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.7150 -3.3050 -16.1660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.0220 -3.9050 -17.2190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.6820 -3.2660 -15.2560 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.7140 -3.0630 -15.5700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.4290 -2.4770 -14.5360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.5940 -4.6370 -14.5900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0









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257262 0 0 1 0 0 0 0 0999 V2000
18.1660 -10.4540 -18.6480 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.5750 -10.6140 -19.8690 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.6290 -11.5370 -20.4310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.9780 -9.4030 -20.1300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.4080 -9.1200 -21.0040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.1890 -8.5200 -19.1010 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.9030 -9.1840 -18.2200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```

18.2520	-8.7960	-17.2730	H	0	0	0	0	0	0	0	0	0	0	0	0	0
18.9350	-11.4500	-17.9290	C	0	0	0	0	0	0	0	0	0	0	0	0	0
18.7600	-11.2880	-16.8580	H	0	0	0	0	0	0	0	0	0	0	0	0	0
18.5260	-12.4340	-18.1870	H	0	0	0	0	0	0	0	0	0	0	0	0	0
20.4260	-11.3670	-18.2640	C	0	0	0	0	0	0	0	0	0	0	0	0	0
20.5660	-11.5400	-19.3380	H	0	0	0	0	0	0	0	0	0	0	0	0	0
20.7990	-10.3600	-18.0410	H	0	0	0	0	0	0	0	0	0	0	0	0	0
21.1760	-12.3640	-17.4950	N	0	0	3	0	0	0	0	0	0	0	0	0	0
21.0750	-12.1700	-16.4900	H	0	0	0	0	0	0	0	0	0	0	0	0	0
22.6070	-12.3110	-17.8160	C	0	0	0	0	0	0	0	0	0	0	0	0	0
22.9990	-11.3020	-17.6400	H	0	0	0	0	0	0	0	0	0	0	0	0	0
22.7500	-12.5490	-18.8770	H	0	0	0	0	0	0	0	0	0	0	0	0	0
23.3980	-13.3200	-16.9830	C	0	0	0	0	0	0	0	0	0	0	0	0	0
22.9710	-14.3260	-17.0710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.4260	-13.3450	-17.3640	H	0	0	0	0	0	0	0	0	0	0	0	0	0
23.4460	-12.9420	-15.5220	C	0	0	0	0	0	0	0	0	0	0	0	0	0
24.4810	-13.5900	-14.9150	O	0	0	0	0	0	0	0	0	0	0	0	0	0
24.6260	-13.3260	-13.5100	C	0	0	0	0	0	0	0	0	0	0	0	0	0
24.7650	-12.2470	-13.3640	H	0	0	0	0	0	0	0	0	0	0	0	0	0
23.7070	-13.6360	-12.9960	H	0	0	0	0	0	0	0	0	0	0	0	0	0
25.8390	-14.0980	-12.9400	C	0	0	0	0	0	0	0	0	0	0	0	0	0
25.9470	-13.7820	-11.4310	C	0	0	0	0	0	0	0	0	0	0	0	0	0
26.0860	-12.7030	-11.2820	H	0	0	0	0	0	0	0	0	0	0	0	0	0
25.0290	-14.0930	-10.9160	H	0	0	0	0	0	0	0	0	0	0	0	0	0
27.0640	-14.4750	-10.8510	O	0	0	0	0	0	0	0	0	0	0	0	0	0
27.2290	-14.2750	-9.5120	C	0	0	0	0	0	0	0	0	0	0	0	0	0
28.4260	-15.0580	-9.0360	C	0	0	0	0	0	0	0	0	0	0	0	0	0
28.2810	-16.1010	-9.3320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.3130	-14.6620	-9.5440	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.5950	-14.9340	-7.5180	C	0	0	0	0	0	0	0	0	0	0	0	0	0
27.7160	-15.3310	-6.9930	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.6290	-13.8620	-7.2880	H	0	0	0	0	0	0	0	0	0	0	0	0	0
22.6560	-12.1900	-14.9650	O	0	0	0	0	0	0	0	0	0	0	0	0	0
26.5190	-13.5650	-8.8140	O	0	0	0	0	0	0	0	0	0	0	0	0	0
25.6470	-15.6130	-13.1500	C	0	0	0	0	0	0	0	0	0	0	0	0	0
26.4910	-16.1840	-12.7480	H	0	0	0	0	0	0	0	0	0	0	0	0	0
25.5620	-15.8640	-14.2120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.7380	-15.9660	-12.6500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
27.1280	-13.6670	-13.6650	C	0	0	0	0	0	0	0	0	0	0	0	0	0
27.0750	-13.8750	-14.7390	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.0050	-14.1950	-13.2750	H	0	0	0	0	0	0	0	0	0	0	0	0	0
27.3050	-12.5920	-13.5420	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.8860	-19.2210	-7.0810	N	0	0	0	0	0	0	0	0	0	0	0	0	0
30.7030	-20.0310	-8.1660	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.6400	-19.6530	-9.1770	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.6380	-21.3030	-7.6460	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.5000	-22.2320	-8.1820	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.7750	-21.2830	-6.2800	N	0	0	0	0	0	0	0	0	0	0	0	0	0
30.9190	-20.0140	-5.9700	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.0490	-19.6200	-4.9710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.0310	-17.7780	-7.1010	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.7050	-17.5140	-6.2790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.5360	-17.5130	-8.0380	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.6770	-17.0610	-6.9930	C	0	0	0	0	0	0	0	0	0	0	0	0	0
29.0620	-17.4150	-7.8290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.1420	-17.3660	-6.0840	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.8350	-15.5900	-7.0460	N	0	0	3	0	0	0	0	0	0	0	0	0	0
30.2120	-15.0640	-5.7100	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.9850	-15.7110	-5.2790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.3620	-15.1190	-5.0200	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.8360	-13.6630	-5.7870	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.8130	-13.6890	-5.2870	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.0030	-13.3510	-6.8250	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.0110	-12.6020	-5.0980	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.7070	-11.4270	-5.1010	O	0	0	0	0	0	0	0	0	0	0	0	0	0
30.0640	-10.2730	-4.5260	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.2030	-9.4570	-5.2460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.9810	-10.4200	-4.4340	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.6860	-9.8820	-3.1630	C	0	0	0	0	0	0	0	0	0	0	0	0	0
29.9650	-8.6080	-2.6590	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.0500	-7.7960	-3.3920	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.8930	-8.8080	-2.5420	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.4420	-8.2040	-1.3620	O	0	0	0	0	0	0	0	0	0	0	0	0	0
31.1870	-7.0630	-1.2900	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.5800	-6.8220	0.1470	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.6750	-6.8590	0.7630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.2540	-7.6340	0.4400	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.2610	-5.4600	0.3160	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.5770	-4.6960	-0.0760	H	0	0	0	0	0	0	0	0	0	0	0	0	0
33.1640	-5.4210	-0.3080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.9010	-12.7610	-4.6120	O	0	0	0	0	0	0	0	0	0	0	0	0	0







68.1490		-4.7000		-4.3370	H	0	0	0	0	0	0	0	0	0	0	0	0
66.4010		-4.4250		-4.2930	H	0	0	0	0	0	0	0	0	0	0	0	0
67.5430		-3.1380		-2.9420	C	0	0	0	0	0	0	0	0	0	0	0	0
66.6930		-2.8950		-2.2940	H	0	0	0	0	0	0	0	0	0	0	0	0
68.3990		-3.2670		-2.2670	H	0	0	0	0	0	0	0	0	0	0	0	0
67.8650		-2.0210		-3.8340	N	0	0	3	0	0	0	0	0	0	0	0	0
68.2140		-1.2380		-3.2780	H	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	9	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	4	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	7	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	12	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	13	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	14	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	15	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	16	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	17	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	18	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	19	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	20	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	21	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	23	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	24	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	40	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	25	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	26	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	27	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	28	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	29	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	42	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	46	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	30	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	31	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	32	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	33	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	34	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	41	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	35	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	36	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	37	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	38	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	39	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	64	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42	43	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42	44	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42	45	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46	47	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46	48	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46	49	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	51	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	56	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	58	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51	52	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51	53	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53	54	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53	55	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55	56	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56	57	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58	59	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58	60	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58	61	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	62	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	63	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	64	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64	65	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	66	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	67	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	68	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68	69	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68	70	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68	71	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	72	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	88	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

72	73	1	0	0	0	0
73	74	1	0	0	0	0
73	75	1	0	0	0	0
73	76	1	0	0	0	0
76	77	1	0	0	0	0
76	90	1	0	0	0	0
76	94	1	0	0	0	0
77	78	1	0	0	0	0
77	79	1	0	0	0	0
77	80	1	0	0	0	0
80	81	1	0	0	0	0
81	82	1	0	0	0	0
81	89	2	0	0	0	0
82	83	1	0	0	0	0
82	84	1	0	0	0	0
82	85	1	0	0	0	0
85	86	1	0	0	0	0
85	87	1	0	0	0	0
85	112	1	0	0	0	0
90	91	1	0	0	0	0
90	92	1	0	0	0	0
90	93	1	0	0	0	0
94	95	1	0	0	0	0
94	96	1	0	0	0	0
94	97	1	0	0	0	0
98	99	1	0	0	0	0
98	104	1	0	0	0	0
98	106	1	0	0	0	0
99	100	1	0	0	0	0
99	101	2	0	0	0	0
101	102	1	0	0	0	0
101	103	1	0	0	0	0
103	104	2	0	0	0	0
104	105	1	0	0	0	0
106	107	1	0	0	0	0
106	108	1	0	0	0	0
106	109	1	0	0	0	0
109	110	1	0	0	0	0
109	111	1	0	0	0	0
109	112	1	0	0	0	0
112	113	1	0	0	0	0
113	114	1	0	0	0	0
113	115	1	0	0	0	0
113	116	1	0	0	0	0
116	117	1	0	0	0	0
116	118	1	0	0	0	0
116	119	1	0	0	0	0
119	120	1	0	0	0	0
119	136	2	0	0	0	0
120	121	1	0	0	0	0
121	122	1	0	0	0	0
121	123	1	0	0	0	0
121	124	1	0	0	0	0
124	125	1	0	0	0	0
124	138	1	0	0	0	0
124	142	1	0	0	0	0
125	126	1	0	0	0	0
125	127	1	0	0	0	0
125	128	1	0	0	0	0
128	129	1	0	0	0	0
129	130	1	0	0	0	0
129	137	2	0	0	0	0
130	131	1	0	0	0	0
130	132	1	0	0	0	0
130	133	1	0	0	0	0
133	134	1	0	0	0	0
133	135	1	0	0	0	0
133	160	1	0	0	0	0
138	139	1	0	0	0	0
138	140	1	0	0	0	0
138	141	1	0	0	0	0
142	143	1	0	0	0	0
142	144	1	0	0	0	0
142	145	1	0	0	0	0
146	147	1	0	0	0	0
146	152	1	0	0	0	0
146	154	1	0	0	0	0
147	148	1	0	0	0	0
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234237 1 0 0 0 0
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253255 1 0 0 0 0
253256 1 0 0 0 0
256257 1 0 0 0 0

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M END
> <NAME>
F94_12

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$$$$
II28_12
MOE2012 3D

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7.1300 6.8780 8.8070 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.0890 7.7790 9.1730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.4960 6.0100 9.8690 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.4640 6.3340 10.2660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.7420 6.0880 10.6590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.5770 4.5890 9.3310 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.6110 4.3110 8.8920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.3020 4.5530 8.5080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.9670 3.5960 10.4250 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.9400 3.8800 10.8460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.2330 3.6550 11.2360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.0380 2.1700 9.8720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.0710 1.8690 9.4500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.7530 2.1480 9.0420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.4890 1.1900 10.8610 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
9.3440 1.5230 11.3080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.4770 0.8900 11.8750 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.3020 1.7690 12.5050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.5270 0.6230 11.3960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.9440 -0.2540 12.7660 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.9490 -0.0700 13.1630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.2840 -0.3520 13.6360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.9010 -1.5640 12.0250 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.1620 -2.0300 11.8010 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.2230 -3.2740 11.0900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.7670 -4.0610 11.7030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.6780 -3.1860 10.1430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.6860 -3.5940 10.8230 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.1460 -2.7840 10.2420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.2460 -3.6110 11.7670 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.8530 -4.9200 10.0950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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14.0650 -6.3970 9.0990 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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14.5450 -6.2650 10.0760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.4710 -7.7470 8.5020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.0950 -8.5260 9.1800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.9770 -7.9150 7.5360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.8670 -2.1280 11.6900 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.7740 -7.1970 8.9890 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8870 -12.6720 8.0960 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.8500 -12.7970 8.1320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.6420 -11.2800 8.2260 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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63.3120	-7.5170	3.7110	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.1960	-1.5620	0.3480	O	0	0	0	0	0	0	0	0	0	0	0	0	0
62.4010	-5.3600	2.2140	O	0	0	0	0	0	0	0	0	0	0	0	0	0
67.2280	-9.9380	7.9090	O	0	0	0	0	0	0	0	0	0	0	0	0	0
67.0860	-9.8250	8.8650	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.0070	-9.6040	7.2650	C	0	0	0	0	0	0	0	0	0	0	0	0	0
65.2240	-10.2760	7.6300	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.7440	-8.5740	7.5290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.1910	-9.7490	5.7610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
67.0150	-9.1030	5.4320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.5040	-10.7750	5.5310	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.9110	-9.4010	5.0050	C	0	0	0	0	0	0	0	0	0	0	0	0	0
64.1010	-10.0650	5.3340	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.6160	-8.3780	5.2640	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.1070	-9.5370	3.4930	C	0	0	0	0	0	0	0	0	0	0	0	0	0
65.8980	-8.8650	3.1380	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.4460	-10.5580	3.2780	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.8660	-9.3200	2.7430	N	0	0	3	0	0	0	0	0	0	0	0	0	0
64.0040	-9.6550	1.7890	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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1	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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20	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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67	69	1	0	0	0	0
67	70	1	0	0	0	0
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73	74	1	0	0	0	0
73	75	1	0	0	0	0
73	76	1	0	0	0	0
76	77	1	0	0	0	0
77	78	1	0	0	0	0
77	85	2	0	0	0	0
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78	80	1	0	0	0	0
78	81	1	0	0	0	0
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81	83	1	0	0	0	0
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86	88	1	0	0	0	0
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88	90	1	0	0	0	0
88	91	1	0	0	0	0
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223224	1	0	0	0	0
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41.2670	33.7430	0.1260	H	0	0	0	0	0	0	0	0	0	0	0	0
41.5100	32.6430	1.4660	H	0	0	0	0	0	0	0	0	0	0	0	0
39.7590	32.1940	0.2700	C	0	0	0	0	0	0	0	0	0	0	0	0
39.2370	31.6370	1.0580	H	0	0	0	0	0	0	0	0	0	0	0	0
38.9970	32.7440	-0.2960	H	0	0	0	0	0	0	0	0	0	0	0	0
40.4810	31.2160	-0.6580	C	0	0	0	0	0	0	0	0	0	0	0	0
41.0050	31.7760	-1.4420	H	0	0	0	0	0	0	0	0	0	0	0	0
41.2430	30.6670	-0.0890	H	0	0	0	0	0	0	0	0	0	0	0	0
39.5000	30.2280	-1.2930	C	0	0	0	0	0	0	0	0	0	0	0	0
38.9810	29.6730	-0.5030	H	0	0	0	0	0	0	0	0	0	0	0	0
38.7490	30.7790	-1.8720	H	0	0	0	0	0	0	0	0	0	0	0	0
40.2280	29.3000	-2.1600	N	0	0	3	0	0	0	0	0	0	0	0	0
40.7290	29.8250	-2.8770	H	0	0	0	0	0	0	0	0	0	0	0	0
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M END  
> <NAME>  
II32\_12

\$\$\$\$  
II36\_12  
MOE2012 3D

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14.8050 -19.8960 -16.9830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
16.1440 -21.0720 -16.9680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
16.2240 -19.6510 -18.6050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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17.8280 -19.1580 -17.2480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.8900 -17.7700 -18.9030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.4980 -18.4140 -19.5490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.1820 -17.2390 -19.5500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.7940 -16.7580 -18.1920 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.1840 -16.1140 -17.5460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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19.5690 -15.8990 -19.1960 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.1790 -16.5460 -19.8370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.8600 -15.3580 -19.8340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.4210 -14.9470 -18.4790 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
21.0500 -15.4580 -17.8580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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21.8520 -14.7690 -20.0040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.5260 -13.6010 -20.1050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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22.8170 -12.7010 -19.3400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.2710 -11.9500 -18.1180 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.9190 -11.4220 -17.0370 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.2910 -10.2630 -16.4690 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.1560 -9.5000 -17.2440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.3140 -10.5480 -16.0610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.1900 -9.7270 -15.3630 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.3610 -10.5040 -14.6070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.1870 -9.5060 -15.7640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.6020 -8.4840 -14.7110 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.4700 -7.6920 -15.4570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.6350 -8.7210 -14.2520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.5140 -8.0320 -13.6980 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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23.1400 -6.5390 -11.9910 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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24.0100 -6.1600 -12.5350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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21.8110 -4.1900 -3.8660 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.7460 -3.9880 -4.0330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.3020 -3.2090 -3.8440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.3800 -5.0310 -5.0070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0







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160162	1	0	0	0	0
160163	1	0	0	0	0
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163165	1	0	0	0	0
163166	1	0	0	0	0
166167	1	0	0	0	0
167168	1	0	0	0	0
167169	1	0	0	0	0
167170	1	0	0	0	0
170171	1	0	0	0	0
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170173	1	0	0	0	0
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173192	2	0	0	0	0
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175178	1	0	0	0	0
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178180	1	0	0	0	0
178181	1	0	0	0	0
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181183	1	0	0	0	0
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185193	2	0	0	0	0
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186189	1	0	0	0	0
189190	1	0	0	0	0
189191	1	0	0	0	0
189214	1	0	0	0	0
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194196	1	0	0	0	0
196197	1	0	0	0	0
196198	1	0	0	0	0
196199	1	0	0	0	0
199200	1	0	0	0	0
199201	1	0	0	0	0

```

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202204 1 0 0 0 0
202205 1 0 0 0 0
205206 1 0 0 0 0
205207 1 0 0 0 0
205208 1 0 0 0 0
208209 1 0 0 0 0
208210 1 0 0 0 0
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211212 1 0 0 0 0
211213 1 0 0 0 0
211214 1 0 0 0 0
214215 1 0 0 0 0
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215217 1 0 0 0 0
215218 1 0 0 0 0
218219 1 0 0 0 0
218220 1 0 0 0 0
218221 1 0 0 0 0
221222 1 0 0 0 0
221240 2 0 0 0 0
222223 1 0 0 0 0
223224 1 0 0 0 0
223225 1 0 0 0 0
223226 1 0 0 0 0
226227 1 0 0 0 0
226228 1 0 0 0 0
226229 1 0 0 0 0
229230 1 0 0 0 0
229231 1 0 0 0 0
229232 1 0 0 0 0
232233 1 0 0 0 0
233234 1 0 0 0 0
233241 2 0 0 0 0
234235 1 0 0 0 0
234236 1 0 0 0 0
234237 1 0 0 0 0
237238 1 0 0 0 0
237239 1 0 0 0 0
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242244 1 0 0 0 0
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244247 1 0 0 0 0
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253255 1 0 0 0 0
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256257 1 0 0 0 0
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259260 1 0 0 0 0
259261 1 0 0 0 0
259262 1 0 0 0 0
262263 1 0 0 0 0

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```

M END
> <NAME>
II36_12

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JJ20_12
MOE2012 3D

```

```

239238 0 0 1 0 0 0 0 0999 V2000
18.2580 -9.4820 1.6050 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.8210 -8.7420 1.8880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.8590 -10.0490 0.4490 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.9300 -9.2740 -0.3220 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8670 -10.3840 0.7110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.0050 -11.2150 -0.0300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.8990 -11.9420 0.7860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.9900 -10.8560 -0.2450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.6120 -11.8780 -1.2660 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.6980 -11.1290 -2.0600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```









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17	20	1	0	0	0	0
20	21	1	0	0	0	0
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22	23	1	0	0	0	0
22	24	1	0	0	0	0
22	26	1	0	0	0	0
26	27	1	0	0	0	0
26	28	1	0	0	0	0
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66	67	1	0	0	0	0
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67	69	1	0	0	0	0
67	71	1	0	0	0	0
71	72	1	0	0	0	0
71	73	1	0	0	0	0
71	89	1	0	0	0	0
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74	77	1	0	0	0	0
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77	78	1	0	0	0	0
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77	80	1	0	0	0	0
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89	90	1	0	0	0	0
89	91	1	0	0	0	0
92	93	1	0	0	0	0
92	94	1	0	0	0	0
94	95	1	0	0	0	0
94	96	1	0	0	0	0

94	97	1	0	0	0	0
97	98	1	0	0	0	0
97	99	1	0	0	0	0
97	100	1	0	0	0	0
100	101	1	0	0	0	0
100	102	1	0	0	0	0
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119	134	1	0	0	0	0
122	123	1	0	0	0	0
122	124	1	0	0	0	0
122	125	1	0	0	0	0
125	126	1	0	0	0	0
126	127	1	0	0	0	0
126	133	2	0	0	0	0
127	128	1	0	0	0	0
127	129	1	0	0	0	0
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130	131	1	0	0	0	0
130	132	1	0	0	0	0
130	148	1	0	0	0	0
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134	136	1	0	0	0	0
137	138	1	0	0	0	0
137	139	1	0	0	0	0
139	140	1	0	0	0	0
139	141	1	0	0	0	0
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152	155	1	0	0	0	0
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157	158	1	0	0	0	0
157	159	1	0	0	0	0
157	161	1	0	0	0	0
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161	163	1	0	0	0	0
161	179	1	0	0	0	0
164	165	1	0	0	0	0
164	166	1	0	0	0	0
164	167	1	0	0	0	0
164	179	1	0	0	0	0
167	168	1	0	0	0	0
167	169	1	0	0	0	0
167	170	1	0	0	0	0
170	171	1	0	0	0	0
171	172	1	0	0	0	0
171	178	2	0	0	0	0
172	173	1	0	0	0	0
172	174	1	0	0	0	0
172	175	1	0	0	0	0

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175193 1 0 0 0 0
179180 1 0 0 0 0
179181 1 0 0 0 0
182183 1 0 0 0 0
182184 1 0 0 0 0
184185 1 0 0 0 0
184186 1 0 0 0 0
184187 1 0 0 0 0
187188 1 0 0 0 0
187189 1 0 0 0 0
187190 1 0 0 0 0
190191 1 0 0 0 0
190192 1 0 0 0 0
190193 1 0 0 0 0
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194195 1 0 0 0 0
194196 1 0 0 0 0
194197 1 0 0 0 0
197198 1 0 0 0 0
197199 1 0 0 0 0
197200 1 0 0 0 0
200201 1 0 0 0 0
200205 2 0 0 0 0
201202 1 0 0 0 0
202203 1 0 0 0 0
202204 1 0 0 0 0
202206 1 0 0 0 0
206207 1 0 0 0 0
206208 1 0 0 0 0
206224 1 0 0 0 0
209210 1 0 0 0 0
209211 1 0 0 0 0
209212 1 0 0 0 0
209224 1 0 0 0 0
212213 1 0 0 0 0
212214 1 0 0 0 0
212215 1 0 0 0 0
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216217 1 0 0 0 0
216223 2 0 0 0 0
217218 1 0 0 0 0
217219 1 0 0 0 0
217220 1 0 0 0 0
220221 1 0 0 0 0
220222 1 0 0 0 0
220238 1 0 0 0 0
224225 1 0 0 0 0
224226 1 0 0 0 0
227228 1 0 0 0 0
227229 1 0 0 0 0
229230 1 0 0 0 0
229231 1 0 0 0 0
229232 1 0 0 0 0
232233 1 0 0 0 0
232234 1 0 0 0 0
232235 1 0 0 0 0
235236 1 0 0 0 0
235237 1 0 0 0 0
235238 1 0 0 0 0
238239 1 0 0 0 0

```

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M END
> <NAME>
JJ20_12

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JJ24_12
MOE2012 3D

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```

245244 0 0 1 0 0 0 0 0999 V2000
28.8720 -14.3370 -3.3320 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.3650 -14.5910 -4.1240 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.9190 -14.0890 -2.2970 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.2910 -13.2430 -2.5910 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.3030 -14.9880 -2.1900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.6900 -13.7960 -1.0120 C 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
29.3680 -12.9480 -1.1730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.7420 -13.5200 0.1620 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.0620 -12.7080 -0.1150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.1490 -14.4170 0.3770 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```









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33	36	1	0	0	0	0
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83	84	1	0	0	0	0
83	90	2	0	0	0	0
84	85	1	0	0	0	0
84	86	1	0	0	0	0
84	87	1	0	0	0	0
87	88	1	0	0	0	0

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96 98	1	0	0	0	0
96 99	1	0	0	0	0
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99105	1	0	0	0	0
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101103	1	0	0	0	0
101104	1	0	0	0	0
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161163	1	0	0	0	0
161165	1	0	0	0	0
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165167	1	0	0	0	0
165183	1	0	0	0	0
168169	1	0	0	0	0
168170	1	0	0	0	0
168171	1	0	0	0	0

168183	1	0	0	0	0
171172	1	0	0	0	0
171173	1	0	0	0	0
171174	1	0	0	0	0
174175	1	0	0	0	0
175176	1	0	0	0	0
175182	2	0	0	0	0
176177	1	0	0	0	0
176178	1	0	0	0	0
176179	1	0	0	0	0
179180	1	0	0	0	0
179181	1	0	0	0	0
179196	1	0	0	0	0
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188190	1	0	0	0	0
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191193	1	0	0	0	0
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193196	1	0	0	0	0
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199201	1	0	0	0	0
199202	1	0	0	0	0
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211213	1	0	0	0	0
211229	1	0	0	0	0
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217220	1	0	0	0	0
220221	1	0	0	0	0
221222	1	0	0	0	0
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222225	1	0	0	0	0
225226	1	0	0	0	0
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225242	1	0	0	0	0
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237239	1	0	0	0	0
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242245	1	0	0	0	0
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M END  
> <NAME>  
JJ24\_12

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JJ28\_12  
MOE2012

3D







96.5640	-1.4880	-4.4100	O	0	0	0	0	0	0	0	0	0	0	0	0
96.8250	-0.5820	-4.6460	H	0	0	0	0	0	0	0	0	0	0	0	0
95.2190	-1.4290	-3.9570	C	0	0	0	0	0	0	0	0	0	0	0	0
95.1730	-0.7690	-3.0850	H	0	0	0	0	0	0	0	0	0	0	0	0
94.6010	-1.0070	-4.7570	H	0	0	0	0	0	0	0	0	0	0	0	0
94.7610	-2.8350	-3.6000	C	0	0	0	0	0	0	0	0	0	0	0	0
94.8690	-3.4860	-4.4770	H	0	0	0	0	0	0	0	0	0	0	0	0
95.4270	-3.2520	-2.8340	H	0	0	0	0	0	0	0	0	0	0	0	0
93.3150	-2.8430	-3.1090	C	0	0	0	0	0	0	0	0	0	0	0	0
93.2280	-2.2050	-2.2210	H	0	0	0	0	0	0	0	0	0	0	0	0
92.6780	-2.4060	-3.8870	H	0	0	0	0	0	0	0	0	0	0	0	0
92.8520	-4.2630	-2.7720	C	0	0	0	0	0	0	0	0	0	0	0	0
92.9100	-4.9120	-3.6540	H	0	0	0	0	0	0	0	0	0	0	0	0
93.5400	-4.6850	-2.0290	H	0	0	0	0	0	0	0	0	0	0	0	0
91.5060	-4.2960	-2.1930	N	0	0	3	0	0	0	0	0	0	0	0	0
91.3500	-5.2220	-1.7940	H	0	0	0	0	0	0	0	0	0	0	0	0
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71	72	1	0	0	0	0
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77	95	1	0	0	0	0
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146	147	1	0	0	0	0



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259260 1 0 0 0 0
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259262 1 0 0 0 0
262263 1 0 0 0 0
262264 1 0 0 0 0
262265 1 0 0 0 0
265266 1 0 0 0 0
265267 1 0 0 0 0
265268 1 0 0 0 0
268269 1 0 0 0 0
268270 1 0 0 0 0
268271 1 0 0 0 0
271272 1 0 0 0 0
271273 1 0 0 0 0
271274 1 0 0 0 0
274275 1 0 0 0 0

```

```

M END
> <NAME>
JJ32_12

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$$$$
JJ36_12
MOE2012 3D

```

```

293292 0 0 1 0 0 0 0 0999 V2000
25.3350 -25.7330 -11.0930 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.0840 -25.9170 -10.5010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.7060 -24.5520 -10.6120 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.3760 -24.7280 -9.5830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.4420 -23.7410 -10.6150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.5250 -24.2170 -11.5120 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.8760 -24.0980 -12.5440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.8280 -25.0650 -11.5280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.8060 -22.9510 -11.0490 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.4560 -23.0840 -10.0180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.5120 -22.1100 -11.0430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.6180 -22.6150 -11.9530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.9670 -22.4800 -12.9840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.9110 -23.4540 -11.9570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.9040 -21.3440 -11.4820 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.5610 -21.4830 -10.4490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.6220 -20.5160 -11.4750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.7100 -21.0080 -12.3820 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.0320 -20.8660 -13.4210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.0240 -21.8630 -12.3880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.9490 -19.8460 -11.9150 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
18.8240 -19.9160 -10.8990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.6150 -18.5750 -12.2130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.6020 -18.5270 -11.7390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.7570 -18.4840 -13.2960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.7680 -17.3940 -11.7390 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.2240 -16.4700 -12.1150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.7470 -17.4640 -12.1310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.7050 -17.3020 -10.2330 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.1620 -16.1040 -9.8740 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.0340 -15.8990 -8.4580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.3890 -16.6780 -8.0350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.0250 -15.9490 -7.9920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.0680 -18.1790 -9.4590 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.4150 -14.5230 -8.2360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.0520 -13.7600 -8.7020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.4530 -14.4710 -8.7600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.5980 -12.8360 -6.5460 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.6370 -12.7750 -7.0730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.2330 -12.0600 -6.9920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.3810 -12.5210 -5.0690 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7140 -13.2660 -4.6200 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.3390 -12.5170 -4.5370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7810 -11.2200 -4.9760 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.4770 -10.8210 -3.7080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.8420 -9.4520 -3.7410 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.1280 -8.9310 -4.6610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.7580 -9.6140 -3.7850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.1830 -8.6130 -2.5040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.3320 -7.9490 -2.2960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.2580 -9.2480 -1.6120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.6570 -11.4830 -2.6950 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```







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3	6	1	0	0	0	0
6	7	1	0	0	0	0
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9	12	1	0	0	0	0
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15	18	1	0	0	0	0
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18	20	1	0	0	0	0
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61	63	1	0	0	0	0
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77	79	1	0	0	0	0
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80	82	1	0	0	0	0
80	83	1	0	0	0	0
83	84	1	0	0	0	0

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85	86	1	0	0	0	0
85	87	1	0	0	0	0
85	89	1	0	0	0	0
89	90	1	0	0	0	0
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103	105	1	0	0	0	0
103	130	1	0	0	0	0
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107	109	1	0	0	0	0
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112	113	1	0	0	0	0
112	114	1	0	0	0	0
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146	148	1	0	0	0	0
146	149	1	0	0	0	0
146	161	1	0	0	0	0
149	150	1	0	0	0	0
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154	157	1	0	0	0	0
157	158	1	0	0	0	0
157	159	1	0	0	0	0
157	184	1	0	0	0	0
161	162	1	0	0	0	0
161	163	1	0	0	0	0
164	165	1	0	0	0	0

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166168	1	0	0	0	0
166169	1	0	0	0	0
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169171	1	0	0	0	0
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178180	1	0	0	0	0
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181183	1	0	0	0	0
181184	1	0	0	0	0
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185187	1	0	0	0	0
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188191	1	0	0	0	0
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197199	1	0	0	0	0
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200202	1	0	0	0	0
200203	1	0	0	0	0
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208211	1	0	0	0	0
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211213	1	0	0	0	0
211238	1	0	0	0	0
215216	1	0	0	0	0
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218219	1	0	0	0	0
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220223	1	0	0	0	0
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223225	1	0	0	0	0
223226	1	0	0	0	0
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226228	1	0	0	0	0
226229	1	0	0	0	0
229230	1	0	0	0	0
229231	1	0	0	0	0
229232	1	0	0	0	0
232233	1	0	0	0	0
232234	1	0	0	0	0
232235	1	0	0	0	0
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235237	1	0	0	0	0
235238	1	0	0	0	0
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239240	1	0	0	0	0
239241	1	0	0	0	0
239242	1	0	0	0	0
242243	1	0	0	0	0
242244	1	0	0	0	0
242245	1	0	0	0	0
245246	1	0	0	0	0

```

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247248  1  0  0  0  0
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247251  1  0  0  0  0
251252  1  0  0  0  0
251253  1  0  0  0  0
251269  1  0  0  0  0
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254256  1  0  0  0  0
254257  1  0  0  0  0
254269  1  0  0  0  0
257258  1  0  0  0  0
257259  1  0  0  0  0
257260  1  0  0  0  0
260261  1  0  0  0  0
261262  1  0  0  0  0
261268  2  0  0  0  0
262263  1  0  0  0  0
262264  1  0  0  0  0
262265  1  0  0  0  0
265266  1  0  0  0  0
265267  1  0  0  0  0
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269270  1  0  0  0  0
269271  1  0  0  0  0
272273  1  0  0  0  0
272274  1  0  0  0  0
274275  1  0  0  0  0
274276  1  0  0  0  0
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277278  1  0  0  0  0
277279  1  0  0  0  0
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283286  1  0  0  0  0
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286288  1  0  0  0  0
286289  1  0  0  0  0
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289291  1  0  0  0  0
289292  1  0  0  0  0
292293  1  0  0  0  0

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M  END
>  <NAME>
JJ36_12

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$$$$
JJ80_12
MOE2012          3D

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281280  0  0  1  0  0  0  0  0999  V2000
 37.3470 -7.5050 -32.3740 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 37.9780 -6.6170 -32.2560 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 37.9480 -8.2980 -32.8330 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 37.0680 -7.8660 -31.3780 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 36.1510 -7.2320 -33.1780 N  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 35.3240 -6.2070 -32.5130 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 35.1600 -6.5100 -31.4710 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 35.8540 -5.2470 -32.4870 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 33.9440 -6.0400 -33.1660 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 34.0410 -5.6100 -34.1690 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 33.4800 -7.0280 -33.2870 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 32.9890 -5.1680 -32.3410 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 32.0060 -5.1930 -32.8270 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 32.8750 -5.6040 -31.3430 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 36.5490 -6.8270 -34.5280 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 37.1930 -7.5880 -34.9840 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 37.0910 -5.8740 -34.5320 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 35.6800 -6.7370 -35.1880 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 33.4590 -3.7860 -32.2570 N  0  0  3  0  0  0  0  0  0  0  0  0  0  0
 34.3330 -3.7430 -31.7200 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 32.4940 -2.8870 -31.6150 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 32.8600 -1.8640 -31.7650 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 31.5310 -2.9430 -32.1350 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 32.2830 -3.1140 -30.1160 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0
 31.5510 -2.3760 -29.7660 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0

```









60.8080	-13.2920	-9.2770	H	0	0	0	0	0	0	0	0	0	0	0	0
60.9830	-11.7160	-10.7420	C	0	0	0	0	0	0	0	0	0	0	0	0
60.6070	-12.3130	-11.5810	H	0	0	0	0	0	0	0	0	0	0	0	0
60.6300	-10.6910	-10.8930	H	0	0	0	0	0	0	0	0	0	0	0	0
62.5150	-11.7500	-10.7540	C	0	0	0	0	0	0	0	0	0	0	0	0
62.9330	-11.2310	-9.8830	H	0	0	0	0	0	0	0	0	0	0	0	0
62.8370	-12.7960	-10.6690	H	0	0	0	0	0	0	0	0	0	0	0	0
58.4030	-10.9320	-9.2370	C	0	0	0	0	0	0	0	0	0	0	0	0
57.3470	-10.9780	-8.9490	H	0	0	0	0	0	0	0	0	0	0	0	0
58.4650	-10.4340	-10.2100	H	0	0	0	0	0	0	0	0	0	0	0	0
58.9010	-10.3010	-8.4920	H	0	0	0	0	0	0	0	0	0	0	0	0
63.0360	-11.2160	-12.0160	N	0	0	3	0	0	0	0	0	0	0	0	0
63.7800	-11.8340	-12.3440	H	0	0	0	0	0	0	0	0	0	0	0	0
1 2	1 0	0 0	0 0												
1 3	1 0	0 0	0 0												
1 4	1 0	0 0	0 0												
1 5	1 0	0 0	0 0												
5 6	1 0	0 0	0 0												
5 15	1 0	0 0	0 0												
6 7	1 0	0 0	0 0												
6 8	1 0	0 0	0 0												
6 9	1 0	0 0	0 0												
9 10	1 0	0 0	0 0												
9 11	1 0	0 0	0 0												
9 12	1 0	0 0	0 0												
12 13	1 0	0 0	0 0												
12 14	1 0	0 0	0 0												
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M END
> <NAME>
JJ80_12

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$$$$
JJ86_12
MOE2012 3D

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12.9300 -5.3480 -16.1190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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13.2850 -8.1830 -17.2660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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12.7860 -7.1050 -19.2010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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M END
> <NAME>
JJ86_12

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JJ94_12
MOE2012 3D

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18.8810 -2.0630 -14.7030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.4050 -2.7030 -14.0070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.4680 -0.7530 -14.6240 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.5950 -0.0650 -13.7990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.8310 -0.3690 -15.7770 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.8570 -1.4310 -16.5520 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.4430 -1.4920 -17.5500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.6870 -3.7980 -16.5090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.7710 -3.6770 -17.5960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.6520 -4.1680 -16.1410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.5550 -4.7640 -16.1480 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.5060 -4.8580 -15.0580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.5970 -4.3500 -16.4860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.7840 -6.0740 -16.7700 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0
17.8170 -5.9580 -17.7850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.7270 -7.0410 -16.4530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7400 -6.5940 -16.6210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.8140 -7.8690 -17.1680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.8120 -7.6060 -15.0390 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.7730 -6.8230 -14.2750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.9520 -8.2580 -14.8430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.0510 -8.4450 -14.8690 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.9540 -7.8060 -14.0750 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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19.9880 -9.4740 -13.4040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.6650 -8.6790 -14.8600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.2050 -9.5450 -15.3850 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.0920 -7.6570 -13.0020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.2430 -6.6790 -13.4760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.5810 -7.4540 -12.0530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.3320 -7.4760 -11.8520 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.8340 -7.2780 -10.8950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.4990 -6.4940 -12.3130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.6780 -8.1440 -11.5900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.5310 -9.1070 -11.0880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.2140 -8.2990 -12.5340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.4480 -7.2780 -10.7420 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.6900 -7.7420 -10.4230 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.3880 -6.7480 -9.5230 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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256257	1	0	0	0	0

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> <NAME>  
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86.5600	17.0610	17.3650	H	0	0	0	0	0	0	0	0	0	0	0	0
85.1250	18.3410	16.3450	C	0	0	0	0	0	0	0	0	0	0	0	0
85.6480	19.2810	16.5560	H	0	0	0	0	0	0	0	0	0	0	0	0
84.6740	18.4180	15.3510	H	0	0	0	0	0	0	0	0	0	0	0	0
84.0920	18.1110	17.3570	N	0	0	3	0	0	0	0	0	0	0	0	0
83.6240	17.2220	17.1830	H	0	0	0	0	0	0	0	0	0	0	0	0
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337339	1	0	0	0	0
337340	1	0	0	0	0
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> <NAME>  
LL8\_12

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M17\_12  
MOE2012 3D

393398 0 0 1 0 0 0 0 0999 V2000  
22.6440 -2.8200 -13.3190 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.8910 -4.1410 -12.9080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.5730 -4.3550 -11.7010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.7820 -5.3600 -11.3480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.9920 -3.2770 -10.9030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.7150 -1.9710 -11.3190 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.0180 -1.1220 -10.7100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.0370 -1.7460 -12.5140 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.8190 -0.7280 -12.8280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.9700 -2.4590 -14.4590 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.4090 -5.1440 -13.7070 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.7200 -6.4860 -13.3530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.3030 -7.1390 -14.1260 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.2560 -6.7590 -12.4010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.8030 -6.6490 -13.3300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.4290 -3.1110 -15.6420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.8280 -4.0040 -15.8390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.4960 -3.3570 -15.6050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.2770 -2.4220 -16.4790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.7010 -3.5250 -9.5910 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.4460 -4.3170 -9.7450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.2760 -2.6360 -9.2980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.7560 -3.9410 -8.4530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.1570 -4.8070 -8.7620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.3700 -4.2480 -7.5980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.8810 -2.8370 -8.0430 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0  
22.3440 -2.5210 -8.8530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.5240 10.7960 -2.8850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.9000 10.1150 -3.4730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.3370 11.1250 -3.5400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.6650 11.8980 -2.4990 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.0230 13.2080 -2.4950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.4820 13.5220 -2.7370 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.1210 12.7670 -2.2720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.6430 13.4920 -3.8210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.8930 14.9000 -2.2070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.1680 15.6680 -2.5090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.8230 15.1910 -2.7090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.1700 14.0790 -2.3450 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.9590 -3.2620 -6.9850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.5110 -3.7260 -6.1600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.2670 -4.0120 -7.3860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.1530 -2.0720 -6.4740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.7210 -1.5140 -7.3130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.3210 -2.4190 -5.8500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.0000 -1.1610 -5.6220 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.7110 0.1440 -5.8950 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.4400 1.1230 -5.1320 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.8250 2.0280 -5.1040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.5640 0.7890 -4.0940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.7960 -1.5420 -4.7740 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.7810 1.4120 -5.8010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.3060 0.4750 -6.0210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.5880 1.8910 -6.7690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.6740 2.3020 -4.9480 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.8780 1.8180 -3.9850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.6260 2.4640 -5.4670 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.0370 3.5600 -4.7270 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0











38.0300	-19.1660	17.8710	H	0	0	0	0	0	0	0	0	0	0	0	0
39.4070	-20.2600	17.4500	H	0	0	0	0	0	0	0	0	0	0	0	0
39.1280	-19.7600	19.1210	H	0	0	0	0	0	0	0	0	0	0	0	0
34.3910	-23.1710	14.3400	C	0	0	0	0	0	0	0	0	0	0	0	0
33.4980	-23.6110	14.8030	H	0	0	0	0	0	0	0	0	0	0	0	0
34.0330	-22.3350	13.7250	H	0	0	0	0	0	0	0	0	0	0	0	0
35.1030	-24.2110	13.4660	C	0	0	0	0	0	0	0	0	0	0	0	0
35.9950	-23.7530	13.0250	H	0	0	0	0	0	0	0	0	0	0	0	0
35.4360	-25.0510	14.0880	H	0	0	0	0	0	0	0	0	0	0	0	0
34.1970	-24.6900	12.4160	N	0	0	3	0	0	0	0	0	0	0	0	0
33.3820	-25.1190	12.8560	H	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	8	2	0	0	0	0	0	0	0	0	0	0	0	0	0
1	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0
2	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0
3	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0
3	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0
5	6	2	0	0	0	0	0	0	0	0	0	0	0	0	0
5	20	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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6	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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10	16	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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12	14	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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16	17	1	0	0	0	0	0	0	0	0	0	0	0	0	0
16	18	1	0	0	0	0	0	0	0	0	0	0	0	0	0
16	19	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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20	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0
20	23	1	0	0	0	0	0	0	0	0	0	0	0	0	0
23	24	1	0	0	0	0	0	0	0	0	0	0	0	0	0
23	25	1	0	0	0	0	0	0	0	0	0	0	0	0	0
23	26	1	0	0	0	0	0	0	0	0	0	0	0	0	0
26	27	1	0	0	0	0	0	0	0	0	0	0	0	0	0
26	40	1	0	0	0	0	0	0	0	0	0	0	0	0	0
28	29	1	0	0	0	0	0	0	0	0	0	0	0	0	0
28	30	1	0	0	0	0	0	0	0	0	0	0	0	0	0
28	31	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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32	39	2	0	0	0	0	0	0	0	0	0	0	0	0	0
33	34	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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46	51	2	0	0	0	0	0	0	0	0	0	0	0	0	0
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59	61	1	0	0	0	0	0	0	0	0	0	0	0	0	0
59	62	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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69	72	1	0	0	0	0
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75	76	1	0	0	0	0
75	82	2	0	0	0	0
75	84	1	0	0	0	0
76	77	2	0	0	0	0
76	85	1	0	0	0	0
77	78	1	0	0	0	0
77	79	1	0	0	0	0
79	80	2	0	0	0	0
79	94	1	0	0	0	0
80	81	1	0	0	0	0
80	82	1	0	0	0	0
82	83	1	0	0	0	0
84	90	1	0	0	0	0
85	86	1	0	0	0	0
86	87	1	0	0	0	0
86	88	1	0	0	0	0
86	89	1	0	0	0	0
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90	92	1	0	0	0	0
90	93	1	0	0	0	0
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101	104	1	0	0	0	0
101	145	1	0	0	0	0
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121	122	1	0	0	0	0
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179180	1	0	0	0	0
179181	1	0	0	0	0
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192197	2	0	0	0	0
193194	1	0	0	0	0
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211214	1	0	0	0	0
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218220	1	0	0	0	0
221222	1	0	0	0	0
221228	2	0	0	0	0
221230	1	0	0	0	0
222223	2	0	0	0	0
222231	1	0	0	0	0
223224	1	0	0	0	0
223225	1	0	0	0	0
225226	2	0	0	0	0
225240	1	0	0	0	0

226227	1	0	0	0	0
226228	1	0	0	0	0
228229	1	0	0	0	0
230236	1	0	0	0	0
231232	1	0	0	0	0
232233	1	0	0	0	0
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236237	1	0	0	0	0
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236239	1	0	0	0	0
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243246	1	0	0	0	0
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247249	1	0	0	0	0
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247291	1	0	0	0	0
250251	1	0	0	0	0
251252	1	0	0	0	0
251258	2	0	0	0	0
252253	1	0	0	0	0
252254	1	0	0	0	0
252255	1	0	0	0	0
255256	1	0	0	0	0
255257	1	0	0	0	0
255319	1	0	0	0	0
259260	1	0	0	0	0
259261	1	0	0	0	0
259262	1	0	0	0	0
262263	1	0	0	0	0
262264	1	0	0	0	0
262265	1	0	0	0	0
265266	1	0	0	0	0
265270	2	0	0	0	0
266267	1	0	0	0	0
267268	1	0	0	0	0
267269	1	0	0	0	0
267271	1	0	0	0	0
271272	1	0	0	0	0
271273	1	0	0	0	0
271274	1	0	0	0	0
274275	1	0	0	0	0
274276	1	0	0	0	0
274277	1	0	0	0	0
277278	1	0	0	0	0
278279	1	0	0	0	0
278280	1	0	0	0	0
278281	1	0	0	0	0
281282	1	0	0	0	0
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281284	1	0	0	0	0
284285	1	0	0	0	0
284286	1	0	0	0	0
284287	1	0	0	0	0
287288	1	0	0	0	0
288289	1	0	0	0	0
288290	1	0	0	0	0
288291	1	0	0	0	0
291292	1	0	0	0	0
291293	1	0	0	0	0
294295	1	0	0	0	0
294301	2	0	0	0	0
294303	1	0	0	0	0
295296	2	0	0	0	0
295304	1	0	0	0	0
296297	1	0	0	0	0
296298	1	0	0	0	0
298299	2	0	0	0	0
298313	1	0	0	0	0
299300	1	0	0	0	0
299301	1	0	0	0	0
301302	1	0	0	0	0
303309	1	0	0	0	0
304305	1	0	0	0	0
305306	1	0	0	0	0
305307	1	0	0	0	0

305308	1	0	0	0	0
309310	1	0	0	0	0
309311	1	0	0	0	0
309312	1	0	0	0	0
313314	1	0	0	0	0
313315	1	0	0	0	0
313316	1	0	0	0	0
316317	1	0	0	0	0
316318	1	0	0	0	0
316319	1	0	0	0	0
319332	1	0	0	0	0
320321	1	0	0	0	0
320322	1	0	0	0	0
320323	1	0	0	0	0
320364	1	0	0	0	0
323324	1	0	0	0	0
324325	1	0	0	0	0
324326	1	0	0	0	0
326327	1	0	0	0	0
326328	1	0	0	0	0
326329	1	0	0	0	0
329330	1	0	0	0	0
329331	1	0	0	0	0
329392	1	0	0	0	0
332333	1	0	0	0	0
332334	1	0	0	0	0
332335	1	0	0	0	0
335336	1	0	0	0	0
335337	1	0	0	0	0
335338	1	0	0	0	0
338339	1	0	0	0	0
338343	2	0	0	0	0
339340	1	0	0	0	0
340341	1	0	0	0	0
340342	1	0	0	0	0
340344	1	0	0	0	0
344345	1	0	0	0	0
344346	1	0	0	0	0
344347	1	0	0	0	0
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347349	1	0	0	0	0
347350	1	0	0	0	0
350351	1	0	0	0	0
351352	1	0	0	0	0
351353	1	0	0	0	0
351354	1	0	0	0	0
354355	1	0	0	0	0
354356	1	0	0	0	0
354357	1	0	0	0	0
357358	1	0	0	0	0
357359	1	0	0	0	0
357360	1	0	0	0	0
360361	1	0	0	0	0
361362	1	0	0	0	0
361363	1	0	0	0	0
361364	1	0	0	0	0
364365	1	0	0	0	0
364366	1	0	0	0	0
367368	1	0	0	0	0
367374	2	0	0	0	0
367376	1	0	0	0	0
368369	2	0	0	0	0
368377	1	0	0	0	0
369370	1	0	0	0	0
369371	1	0	0	0	0
371372	2	0	0	0	0
371386	1	0	0	0	0
372373	1	0	0	0	0
372374	1	0	0	0	0
374375	1	0	0	0	0
376382	1	0	0	0	0
377378	1	0	0	0	0
378379	1	0	0	0	0
378380	1	0	0	0	0
378381	1	0	0	0	0
382383	1	0	0	0	0
382384	1	0	0	0	0
382385	1	0	0	0	0
386387	1	0	0	0	0
386388	1	0	0	0	0
386389	1	0	0	0	0











49.0600	11.2140	-16.9850	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.8340	12.7640	-17.3300	H	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2420	12.9650	-18.1470	C	0	0	0	0	0	0	0	0	0	0	0	0	0
46.4740	13.2780	-18.8630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
47.6370	13.8700	-17.6720	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.7500	12.3740	-17.3670	H	0	0	0	0	0	0	0	0	0	0	0	0	0
45.9870	18.4430	-22.4250	O	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3300	19.1600	-22.4370	H	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2540	19.0420	-22.1880	C	0	0	0	0	0	0	0	0	0	0	0	0	0
47.4350	19.7930	-22.9640	H	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2270	19.5360	-21.2120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
48.3250	17.9590	-22.2220	C	0	0	0	0	0	0	0	0	0	0	0	0	0
48.2990	17.4590	-23.1990	H	0	0	0	0	0	0	0	0	0	0	0	0	0
48.0780	17.1860	-21.4840	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.7130	18.5450	-21.9580	C	0	0	0	0	0	0	0	0	0	0	0	0	0
49.9220	19.3010	-22.7240	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.7300	19.0710	-20.9960	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.7680	17.5370	-22.0470	N	0	0	3	0	0	0	0	0	0	0	0	0	0
50.4340	16.6940	-22.5270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	9	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	12	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	13	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	47	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	15	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	16	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	17	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	56	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	18	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	19	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	25	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	20	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	21	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	23	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	24	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	76	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	27	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	34	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	37	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	40	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	28	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	29	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	30	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	31	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	32	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	33	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	56	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	34	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	35	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	36	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	38	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	39	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	54	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	41	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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40	43	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43	44	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43	45	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43	46	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	48	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	49	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	50	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	51	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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53	54	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53	55	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56	57	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56	61	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57	58	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57	59	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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61	62	1	0	0	0	0
61	63	1	0	0	0	0
61	64	1	0	0	0	0
65	66	1	0	0	0	0
65	67	1	0	0	0	0
67	68	1	0	0	0	0
67	69	1	0	0	0	0
67	70	1	0	0	0	0
70	71	1	0	0	0	0
70	72	1	0	0	0	0
70	73	1	0	0	0	0
73	74	1	0	0	0	0
73	75	1	0	0	0	0
73	76	1	0	0	0	0
76	110	1	0	0	0	0
77	78	1	0	0	0	0
77	79	1	0	0	0	0
77	80	1	0	0	0	0
77	119	1	0	0	0	0
80	81	1	0	0	0	0
81	82	1	0	0	0	0
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85	86	1	0	0	0	0
85	87	1	0	0	0	0
85	139	1	0	0	0	0
89	90	1	0	0	0	0
89	97	1	0	0	0	0
89	100	1	0	0	0	0
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90	91	1	0	0	0	0
90	92	1	0	0	0	0
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94	95	1	0	0	0	0
94	96	1	0	0	0	0
94	119	1	0	0	0	0
96	97	1	0	0	0	0
97	98	1	0	0	0	0
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100	101	1	0	0	0	0
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113	116	1	0	0	0	0
116	117	1	0	0	0	0
116	118	2	0	0	0	0
119	120	1	0	0	0	0
119	124	1	0	0	0	0
120	121	1	0	0	0	0
120	122	1	0	0	0	0
120	123	1	0	0	0	0
124	125	1	0	0	0	0
124	126	1	0	0	0	0
124	127	1	0	0	0	0
128	129	1	0	0	0	0
128	130	1	0	0	0	0
130	131	1	0	0	0	0
130	132	1	0	0	0	0
130	133	1	0	0	0	0
133	134	1	0	0	0	0
133	135	1	0	0	0	0
133	136	1	0	0	0	0
136	137	1	0	0	0	0
136	138	1	0	0	0	0
136	139	1	0	0	0	0
139	173	1	0	0	0	0
140	141	1	0	0	0	0
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140182	1	0	0	0	0
143144	1	0	0	0	0
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144151	2	0	0	0	0
145146	1	0	0	0	0
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148149	1	0	0	0	0
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176179	1	0	0	0	0
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183185	1	0	0	0	0
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191192	1	0	0	0	0
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199202	1	0	0	0	0
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203206	1	0	0	0	0
203245	1	0	0	0	0
206207	1	0	0	0	0
207208	1	0	0	0	0
207214	2	0	0	0	0
208209	1	0	0	0	0
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211212	1	0	0	0	0
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215229	1	0	0	0	0
216217	1	0	0	0	0
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220221	1	0	0	0	0
220222	1	0	0	0	0
220245	1	0	0	0	0
222223	1	0	0	0	0
223224	1	0	0	0	0
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226227	1	0	0	0	0
226228	1	0	0	0	0
226243	1	0	0	0	0
229230	1	0	0	0	0
229231	1	0	0	0	0
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232233	1	0	0	0	0
232234	1	0	0	0	0
232235	1	0	0	0	0
236237	1	0	0	0	0
236238	1	0	0	0	0
236239	1	0	0	0	0
239240	1	0	0	0	0
239241	1	0	0	0	0
239242	1	0	0	0	0
242243	1	0	0	0	0
242244	2	0	0	0	0
245246	1	0	0	0	0
245250	1	0	0	0	0
246247	1	0	0	0	0
246248	1	0	0	0	0
246249	1	0	0	0	0
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254255	1	0	0	0	0
254256	1	0	0	0	0
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256258	1	0	0	0	0
256259	1	0	0	0	0
259260	1	0	0	0	0
259261	1	0	0	0	0
259262	1	0	0	0	0
262263	1	0	0	0	0
262264	1	0	0	0	0
262265	1	0	0	0	0
265299	1	0	0	0	0
266267	1	0	0	0	0
266268	1	0	0	0	0
266269	1	0	0	0	0
266308	1	0	0	0	0
269270	1	0	0	0	0
270271	1	0	0	0	0
270277	2	0	0	0	0
271272	1	0	0	0	0
271273	1	0	0	0	0
271274	1	0	0	0	0
274275	1	0	0	0	0
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278279	1	0	0	0	0
278286	1	0	0	0	0
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279282	1	0	0	0	0
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79	81	1	0	0	0	0
79	82	1	0	0	0	0
79	121	1	0	0	0	0
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230247	1	0	0	0	0
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271274 1 0 0 0 0
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274275 1 0 0 0 0
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275282 2 0 0 0 0
276277 1 0 0 0 0
276278 1 0 0 0 0
276279 1 0 0 0 0
279280 1 0 0 0 0
279281 1 0 0 0 0
279332 1 0 0 0 0
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283291 1 0 0 0 0
283294 1 0 0 0 0
283297 1 0 0 0 0
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284286 1 0 0 0 0
284287 1 0 0 0 0
287288 1 0 0 0 0
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M END
> <NAME>
O24_12

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$$$$
O28_12
MOE2012 3D

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347351 0 0 1 0 0 0 0 0999 V2000
45.2690 -31.1770 6.9890 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
45.5090 -32.1000 7.1790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.2890 -30.7940 7.9420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.4250 -31.4590 7.8400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.7120 -30.9090 8.9450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.9000 -29.3500 7.6780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.7920 -28.7140 7.7460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.5430 -29.2540 6.6440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.8300 -28.8660 8.6530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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40.6340	-21.5390	-6.9030	C	0	0	0	0	0	0	0	0	0	0	0	0
40.8380	-21.2010	-5.8820	H	0	0	0	0	0	0	0	0	0	0	0	0
39.5510	-21.6290	-7.0360	H	0	0	0	0	0	0	0	0	0	0	0	0
41.3210	-22.8680	-7.1760	C	0	0	0	0	0	0	0	0	0	0	0	0
41.1340	-23.1740	-8.2130	H	0	0	0	0	0	0	0	0	0	0	0	0
42.4070	-22.7450	-7.0860	H	0	0	0	0	0	0	0	0	0	0	0	0
40.8190	-23.9330	-6.2050	C	0	0	0	0	0	0	0	0	0	0	0	0
41.0060	-23.5990	-5.1760	H	0	0	0	0	0	0	0	0	0	0	0	0
39.7320	-24.0290	-6.3130	H	0	0	0	0	0	0	0	0	0	0	0	0
41.5000	-25.2840	-6.4320	C	0	0	0	0	0	0	0	0	0	0	0	0
41.3280	-25.6600	-7.4480	H	0	0	0	0	0	0	0	0	0	0	0	0
42.5830	-25.1510	-6.3220	H	0	0	0	0	0	0	0	0	0	0	0	0
41.0570	-26.2440	-5.4220	N	0	0	3	0	0	0	0	0	0	0	0	0
41.7630	-26.9740	-5.3180	H	0	0	0	0	0	0	0	0	0	0	0	0
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3	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0
3	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0
3	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0
6	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0
6	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0
6	9	1	0	0	0	0	0	0	0	0	0	0	0	0	0
9	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0
9	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0
9	12	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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17	19	1	0	0	0	0	0	0	0	0	0	0	0	0	0
17	20	1	0	0	0	0	0	0	0	0	0	0	0	0	0
17	59	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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21	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0
21	28	2	0	0	0	0	0	0	0	0	0	0	0	0	0
22	23	1	0	0	0	0	0	0	0	0	0	0	0	0	0
22	24	1	0	0	0	0	0	0	0	0	0	0	0	0	0
22	25	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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37	39	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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53	56	1	0	0	0	0	0	0	0	0	0	0	0	0	0
56	57	1	0	0	0	0	0	0	0	0	0	0	0	0	0
56	58	2	0	0	0	0	0	0	0	0	0	0	0	0	0
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59	64	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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70	72	1	0	0	0	0
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76	78	1	0	0	0	0
76	79	1	0	0	0	0
79	80	1	0	0	0	0
79	81	1	0	0	0	0
79	82	1	0	0	0	0
82116		1	0	0	0	0
83	84	1	0	0	0	0
83	85	1	0	0	0	0
83	86	1	0	0	0	0
83125		1	0	0	0	0
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87	94	2	0	0	0	0
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88	91	1	0	0	0	0
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91	93	1	0	0	0	0
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95103		1	0	0	0	0
95106		1	0	0	0	0
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112115		1	0	0	0	0
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 U25\_12

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 U28\_12  
 MOE2012 3D

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16.0450	17.1940	7.9820	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15.7580	16.8720	8.8540	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17.4600	17.3100	8.0250	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17.7270	18.0200	8.8140	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17.8830	16.3300	8.2670	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17.9510	17.7940	6.6680	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17.6290	17.0890	5.8920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17.4670	18.7490	6.4250	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19.4710	17.9500	6.6450	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19.7750	18.6670	7.4180	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19.9310	16.9880	6.8970	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0









55.9380	-19.9140	19.3790	H	0	0	0	0	0	0	0	0	0	0	0	0
54.3850	-20.4730	20.0040	H	0	0	0	0	0	0	0	0	0	0	0	0
56.1100	-21.2300	21.0880	C	0	0	0	0	0	0	0	0	0	0	0	0
55.5960	-22.0920	21.5300	H	0	0	0	0	0	0	0	0	0	0	0	0
57.1220	-21.5690	20.8350	H	0	0	0	0	0	0	0	0	0	0	0	0
56.2450	-20.1490	22.0690	N	0	0	3	0	0	0	0	0	0	0	0	0
56.9230	-20.4390	22.7750	H	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
U32_12

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$$$$
U36_12
MOE2012 3D

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39.0310 -17.2700 -25.3990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.5610 -16.8430 -24.2810 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.1870 -17.6030 -24.7590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.7210 -15.8830 -24.7830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.8760 -16.7360 -22.7940 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.2020 -16.0040 -22.3320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.6570 -17.6950 -22.3080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.3330 -16.3400 -22.5510 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.9950 -17.0820 -23.0140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.5370 -15.3780 -23.0360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.6460 -16.2370 -21.0560 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.9880 -15.4910 -20.5940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.4380 -17.1980 -20.5700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.1090 -15.8480 -20.8170 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.7630 -16.5930 -21.2880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.3150 -14.8850 -21.3010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.4260 -15.7520 -19.3200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.7690 -15.0030 -18.8660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.2220 -16.7190 -18.8440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
45.8320 -15.3810 -19.1350 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
46.4120 -16.0430 -19.6520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.6910 -17.2900 -6.8860 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.8370 -18.3690 -7.0170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.8090 -16.8480 -7.8800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.3580 -16.9870 -6.4490 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.8430 -17.8120 -5.4950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.5220 -17.2830 -5.0040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.0960 -16.5800 -5.7280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.8240 -18.1270 -4.9630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.6820 -16.6630 -3.6160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.0210 -17.4680 -2.9500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.7010 -16.3540 -3.2380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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45.7710 -12.1450 -13.0820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
46.2480 -15.3980 -17.7300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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47.3430 -15.3330 -17.7120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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44.5840 -14.2960 -16.8790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
46.2010 -14.2510 -15.5160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
45.6100 -13.2520 -14.8000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
47.0180 -15.0480 -15.0760 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
45.2290 -14.1710 -12.5740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.1540 -14.0040 -12.6960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
45.4470 -15.1920 -12.9060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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68.9290	-23.7170	22.9240	C	0	0	0	0	0	0	0	0	0	0	0	0
68.7110	-22.6440	22.8680	H	0	0	0	0	0	0	0	0	0	0	0	0
68.5350	-24.0550	23.8900	H	0	0	0	0	0	0	0	0	0	0	0	0
70.3680	-23.9980	22.9000	N	0	0	3	0	0	0	0	0	0	0	0	0
70.6640	-24.2100	23.8550	H	0	0	0	0	0	0	0	0	0	0	0	0
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1	3	1	0	0	0	0									
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3	5	1	0	0	0	0									
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6	8	1	0	0	0	0									
6	9	1	0	0	0	0									
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9	12	1	0	0	0	0									
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M END
> <NAME>
U36_12

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$$$$
U75_12
MOE2012 3D

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384383 0 0 1 0 0 0 0 0999 V2000
13.7450 -9.2700 4.3020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.2420 -8.5330 4.9410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.0590 -9.8560 4.9210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.1420 -8.7250 3.5680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.7660 -10.1480 3.5830 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.2530 -10.8830 2.9500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.3250 -9.4850 2.9110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7030 -10.8090 4.5100 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.8420 -11.3800 3.7620 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.5210 -12.2470 3.1700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.2020 -10.6250 3.0520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.0300 -11.7590 4.6750 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.3530 -10.8880 5.2560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.7050 -12.4970 5.4170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```











43.9140	5.1520	33.8150	O	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1990	4.3700	34.7730	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1040	3.3380	34.4140	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.8160	4.3400	35.6770	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.8370	4.9780	35.1060	C	0	0	0	0	0	0	0	0	0	0	0	0	0
41.9720	6.0240	35.4050	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.2090	4.9980	34.2090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.1150	4.2030	36.2080	C	0	0	0	0	0	0	0	0	0	0	0	0	0
41.0030	3.1540	35.9080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.7170	4.2160	37.1250	H	0	0	0	0	0	0	0	0	0	0	0	0	0
39.7360	4.8060	36.4880	C	0	0	0	0	0	0	0	0	0	0	0	0	0
39.8500	5.8540	36.7920	H	0	0	0	0	0	0	0	0	0	0	0	0	0
39.1420	4.8020	35.5660	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.9920	4.0360	37.5760	C	0	0	0	0	0	0	0	0	0	0	0	0	0
38.8860	2.9820	37.2920	H	0	0	0	0	0	0	0	0	0	0	0	0	0
39.5700	4.0400	38.5080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.6100	4.6290	37.8350	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.7020	5.6720	38.1580	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.0080	4.5910	36.9210	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.9810	3.8680	38.8670	O	0	0	0	0	0	0	0	0	0	0	0	0	0
35.6760	4.3420	39.2000	C	0	0	0	0	0	0	0	0	0	0	0	0	0
35.6420	5.4380	39.2030	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.4730	4.0300	40.2300	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.2600	3.7190	47.4800	C	0	0	0	0	0	0	0	0	0	0	0	0	0
28.3650	4.2770	47.1840	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.9970	4.4290	47.8670	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.9800	3.0540	48.3040	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.8060	2.9000	46.3140	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.7020	2.3500	46.6280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.0400	2.1510	46.0770	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.0770	3.7190	45.1190	N	0	0	0	0	0	0	0	0	0	0	0	0	0
30.3120	2.8440	43.9490	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.2810	2.3350	44.0370	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.5440	2.0580	43.9260	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.2150	3.6030	42.6090	C	0	0	0	0	0	0	0	0	0	0	0	0	0
29.2230	4.0650	42.5360	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.9620	4.4010	42.5710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.4180	2.6800	41.4860	N	0	0	3	0	0	0	0	0	0	0	0	0	0
31.3750	2.3080	41.5120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.1960	4.6550	45.3310	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.6910	4.4970	46.2970	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.9900	4.5290	44.5850	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.6840	6.0880	45.2580	C	0	0	0	0	0	0	0	0	0	0	0	0	0
29.9310	6.2850	46.0280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.2390	6.3010	44.2800	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.5110	6.7900	45.4100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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1	3	1	0	0	0	0										
1	4	1	0	0	0	0										
1	5	1	0	0	0	0										
5	6	1	0	0	0	0										
5	7	1	0	0	0	0										
5	8	1	0	0	0	0										
8	9	1	0	0	0	0										
8	17	1	0	0	0	0										
9	10	1	0	0	0	0										
9	11	1	0	0	0	0										
9	12	1	0	0	0	0										
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17	19	1	0	0	0	0										
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29	30	1	0	0	0	0										
29	31	1	0	0	0	0										
29	32	1	0	0	0	0										
32	33	1	0	0	0	0										
32	34	1	0	0	0	0										

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U80\_12

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U86\_12  
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19.4940 28.1120 13.1570 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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16.7430 27.2480 13.2970 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
17.7180 26.5170 14.6020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
16.3360 27.9150 15.1860 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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18.4630 26.1410 10.1720 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
18.4130 25.1800 10.0280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.0330 17.0160 10.8450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.7930 17.2080 10.0770 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
25.8130 17.9880 11.2980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.8070 16.5510 10.2630 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
24.9290 15.6700 9.2320 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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46.6030	-1.2180	41.2000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.7490	-0.6060	41.5100	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2750	-1.8330	40.3530	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.9670	-2.0220	42.3260	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2150	-3.3920	41.9970	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.3950	-3.8050	41.3980	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.1980	-3.9480	42.9390	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.4520	-3.6140	46.4720	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.9250	-4.5390	46.1970	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.6300	-3.6910	47.5530	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7250	-3.5230	45.7280	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.4140	-4.8340	45.7520	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.6800	-5.1150	46.7800	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7090	-5.5930	45.3860	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.6640	-4.9020	44.8510	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.4200	-4.4300	43.9010	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.4870	-4.3330	45.2980	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0890	-6.2930	44.6380	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
50.4530	-6.6560	45.5200	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.5740	-2.4230	46.2280	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.0360	-1.8050	46.9560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.4510	-2.8050	46.7640	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4830	-2.4610	46.1760	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8900	-1.4950	46.4870	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.2470	-2.4190	45.1080	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2690	-2.6740	46.8960	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.6920	-1.9120	46.7120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.0290	-1.5060	45.0850	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.5610	-2.0490	44.2970	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.7140	-0.7500	45.4820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.9260	-0.8130	44.5090	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.5260	-1.4100	43.8340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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4	13	1	0	0	0	0													
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8	11	1	0	0	0	0													
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83	85	1	0	0	0	0
83	86	1	0	0	0	0
86	115	1	0	0	0	0
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87	89	1	0	0	0	0
87	95	1	0	0	0	0
90	91	1	0	0	0	0
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195197	2	0	0	0	0
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198201	1	0	0	0	0
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269270	1	0	0	0	0
269271	2	0	0	0	0
272273	1	0	0	0	0
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275276	1	0	0	0	0
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279280	1	0	0	0	0
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309317	1	0	0	0	0
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312314	1	0	0	0	0
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67.8930	19.8180	19.4250	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.8840	20.2320	19.6460	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.8660	19.5970	18.3510	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.8190	20.8510	19.7610	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.8230	20.4280	19.5820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.8490	21.0960	20.8300	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.9870	22.1300	18.9460	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.9310	22.6170	19.2150	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.0210	21.9150	17.8710	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.9330	23.0330	19.2770	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.0490	23.3240	18.1960	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.6170	23.6370	17.3120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.4520	24.1940	18.4920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.1570	30.8400	16.9840	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.1390	31.6820	17.6870	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0250	31.0300	16.3380	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.2910	29.5550	17.7030	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.7490	28.4930	16.7840	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.2600	28.5950	15.8090	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.8280	28.5790	16.5970	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.3990	27.0950	17.3130	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8860	26.9110	18.2770	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3160	27.0280	17.4820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8320	26.0170	16.3170	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.3030	26.1620	15.3680	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9070	26.1190	16.1280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.2230	29.6960	18.8420	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.5860	28.7180	19.1800	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.1290	30.2470	18.5520	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5240	24.6990	16.8660	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0360	24.5680	17.7480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.8590	30.9310	16.1720	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.8150	30.1760	15.3820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.9880	30.8110	16.8240	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.7840	32.2130	15.5550	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.9320	32.2560	15.0870	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5660	30.3560	20.0590	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.2750	31.3910	19.8560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.6810	29.7940	20.3730	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4930	30.3660	21.1420	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0470	30.7970	21.8920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0													
1	3	1	0	0	0	0													
1	4	1	0	0	0	0													
1	19	1	0	0	0	0													
4	5	1	0	0	0	0													
4	14	1	0	0	0	0													
5	6	1	0	0	0	0													
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11	13	1	0	0	0	0													
11	17	1	0	0	0	0													
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14	16	1	0	0	0	0													
14	24	1	0	0	0	0													
17	18	1	0	0	0	0													
17	44	1	0	0	0	0													
19	20	1	0	0	0	0													
19	21	1	0	0	0	0													
19	22	1	0	0	0	0													
22	23	1	0	0	0	0													
24	25	1	0	0	0	0													
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24	27	1	0	0	0	0													
27	28	1	0	0	0	0													
29	30	1	0	0	0	0													
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29	32	1	0	0	0	0													
29	76	1	0	0	0	0													
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41	53	1	0	0	0	0
44	45	1	0	0	0	0
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66	67	1	0	0	0	0
66	68	1	0	0	0	0
66	69	1	0	0	0	0
69	70	1	0	0	0	0
69	71	1	0	0	0	0
69	72	1	0	0	0	0
72	73	1	0	0	0	0
72	74	1	0	0	0	0
72	75	1	0	0	0	0
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79	80	1	0	0	0	0
79	81	1	0	0	0	0
79	82	1	0	0	0	0
79	96	1	0	0	0	0
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82	92	1	0	0	0	0
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83	86	1	0	0	0	0
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86	89	1	0	0	0	0
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89	95	1	0	0	0	0
92	93	1	0	0	0	0
92	94	1	0	0	0	0
92101	1	0	0	0	0	0
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96	97	1	0	0	0	0
96	98	1	0	0	0	0
96	99	1	0	0	0	0
99100	1	0	0	0	0	0
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111113	1	0	0	0	0	0
111114	1	0	0	0	0	0
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114116	1	0	0	0	0	0
114172	1	0	0	0	0	0
118119	1	0	0	0	0	0
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137139	1	0	0	0	0
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140143	1	0	0	0	0
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166172	1	0	0	0	0
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169171	1	0	0	0	0
169178	1	0	0	0	0
172198	1	0	0	0	0
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178179	1	0	0	0	0
178180	1	0	0	0	0
178181	1	0	0	0	0
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183185	1	0	0	0	0
183186	1	0	0	0	0
183230	1	0	0	0	0
186187	1	0	0	0	0
187188	1	0	0	0	0
187194	2	0	0	0	0
188189	1	0	0	0	0
188190	1	0	0	0	0
188191	1	0	0	0	0
191192	1	0	0	0	0
191193	1	0	0	0	0
191249	1	0	0	0	0
195196	1	0	0	0	0
195197	1	0	0	0	0
195205	1	0	0	0	0
195207	1	0	0	0	0
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198201	1	0	0	0	0

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201204	1	0	0	0	0
204205	1	0	0	0	0
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207208	1	0	0	0	0
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211214	1	0	0	0	0
214215	1	0	0	0	0
214216	1	0	0	0	0
214217	1	0	0	0	0
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217220	1	0	0	0	0
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220223	1	0	0	0	0
223224	1	0	0	0	0
223225	1	0	0	0	0
223226	1	0	0	0	0
226227	1	0	0	0	0
226228	1	0	0	0	0
226229	1	0	0	0	0
229230	1	0	0	0	0
230231	1	0	0	0	0
230232	1	0	0	0	0
233234	1	0	0	0	0
233235	1	0	0	0	0
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233250	1	0	0	0	0
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236246	1	0	0	0	0
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237239	1	0	0	0	0
237240	1	0	0	0	0
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240242	1	0	0	0	0
240243	1	0	0	0	0
243244	1	0	0	0	0
243245	1	0	0	0	0
243249	1	0	0	0	0
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246248	1	0	0	0	0
246255	1	0	0	0	0
249275	1	0	0	0	0
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250252	1	0	0	0	0
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255257	1	0	0	0	0
255258	1	0	0	0	0
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260263	1	0	0	0	0
260307	1	0	0	0	0
263264	1	0	0	0	0
264265	1	0	0	0	0
264271	2	0	0	0	0
265266	1	0	0	0	0
265267	1	0	0	0	0
265268	1	0	0	0	0
268269	1	0	0	0	0
268270	1	0	0	0	0
268326	1	0	0	0	0
272273	1	0	0	0	0
272274	1	0	0	0	0
272282	1	0	0	0	0
272284	1	0	0	0	0
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278279	1	0	0	0	0
278280	1	0	0	0	0
278281	1	0	0	0	0
281282	1	0	0	0	0

281283	2	0	0	0	0
284285	1	0	0	0	0
284286	1	0	0	0	0
284287	1	0	0	0	0
287288	1	0	0	0	0
288289	1	0	0	0	0
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291292	1	0	0	0	0
291293	1	0	0	0	0
291294	1	0	0	0	0
294295	1	0	0	0	0
294296	1	0	0	0	0
294297	1	0	0	0	0
297298	1	0	0	0	0
297299	1	0	0	0	0
297300	1	0	0	0	0
300301	1	0	0	0	0
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300303	1	0	0	0	0
303304	1	0	0	0	0
303305	1	0	0	0	0
303306	1	0	0	0	0
306307	1	0	0	0	0
307308	1	0	0	0	0
307309	1	0	0	0	0
310311	1	0	0	0	0
310312	1	0	0	0	0
310313	1	0	0	0	0
310327	1	0	0	0	0
313314	1	0	0	0	0
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314315	1	0	0	0	0
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317318	1	0	0	0	0
317319	1	0	0	0	0
317320	1	0	0	0	0
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320322	1	0	0	0	0
320326	1	0	0	0	0
323324	1	0	0	0	0
323325	1	0	0	0	0
323332	1	0	0	0	0
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327330	1	0	0	0	0
330331	1	0	0	0	0
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332334	1	0	0	0	0
332335	1	0	0	0	0
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337338	1	0	0	0	0
337339	1	0	0	0	0
337340	1	0	0	0	0
337384	1	0	0	0	0
340341	1	0	0	0	0
341342	1	0	0	0	0
341348	2	0	0	0	0
342343	1	0	0	0	0
342344	1	0	0	0	0
342345	1	0	0	0	0
345346	1	0	0	0	0
345347	1	0	0	0	0
345403	1	0	0	0	0
349350	1	0	0	0	0
349351	1	0	0	0	0
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349361	1	0	0	0	0
352353	1	0	0	0	0
352354	1	0	0	0	0
352355	1	0	0	0	0
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355358	1	0	0	0	0
358359	1	0	0	0	0
358360	2	0	0	0	0
361362	1	0	0	0	0
361363	1	0	0	0	0
361364	1	0	0	0	0













73.3390	-17.1120	31.4650	C	0	0	0	0	0	0	0	0	0	0	0	0
72.8310	-16.1600	31.5370	H	0	0	0	0	0	0	0	0	0	0	0	0
71.6870	-18.1240	29.8740	C	0	0	0	0	0	0	0	0	0	0	0	0
71.2900	-19.1450	29.8440	H	0	0	0	0	0	0	0	0	0	0	0	0
70.9500	-17.4950	30.3880	H	0	0	0	0	0	0	0	0	0	0	0	0
71.9660	-17.6040	28.4660	C	0	0	0	0	0	0	0	0	0	0	0	0
72.4410	-16.6150	28.5260	H	0	0	0	0	0	0	0	0	0	0	0	0
72.6820	-18.2660	27.9630	H	0	0	0	0	0	0	0	0	0	0	0	0
70.6750	-17.5090	27.6510	C	0	0	0	0	0	0	0	0	0	0	0	0
70.2130	-18.5010	27.5780	H	0	0	0	0	0	0	0	0	0	0	0	0
69.9760	-16.8450	28.1710	H	0	0	0	0	0	0	0	0	0	0	0	0
70.9850	-17.0040	26.3180	N	0	0	3	0	0	0	0	0	0	0	0	0
71.4540	-16.0910	26.3900	H	0	0	0	0	0	0	0	0	0	0	0	0
1	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	9	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	4	2	0	0	0	0	0	0	0	0	0	0	0	0	0
4	5	1	0	0	0	0	0	0	0	0	0	0	0	0	0
4	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0
6	7	2	0	0	0	0	0	0	0	0	0	0	0	0	0
7	8	1	0	0	0	0	0	0	0	0	0	0	0	0	0
9	10	1	0	0	0	0	0	0	0	0	0	0	0	0	0
9	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0
9	12	1	0	0	0	0	0	0	0	0	0	0	0	0	0
12	13	1	0	0	0	0	0	0	0	0	0	0	0	0	0
12	14	1	0	0	0	0	0	0	0	0	0	0	0	0	0
12	15	1	0	0	0	0	0	0	0	0	0	0	0	0	0
15	16	1	0	0	0	0	0	0	0	0	0	0	0	0	0
15	17	1	0	0	0	0	0	0	0	0	0	0	0	0	0
15	18	1	0	0	0	0	0	0	0	0	0	0	0	0	0
18	19	1	0	0	0	0	0	0	0	0	0	0	0	0	0
18	35	1	0	0	0	0	0	0	0	0	0	0	0	0	0
20	21	1	0	0	0	0	0	0	0	0	0	0	0	0	0
20	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0
20	23	1	0	0	0	0	0	0	0	0	0	0	0	0	0
20	67	1	0	0	0	0	0	0	0	0	0	0	0	0	0
23	24	1	0	0	0	0	0	0	0	0	0	0	0	0	0
24	25	1	0	0	0	0	0	0	0	0	0	0	0	0	0
24	31	2	0	0	0	0	0	0	0	0	0	0	0	0	0
25	26	1	0	0	0	0	0	0	0	0	0	0	0	0	0
25	27	1	0	0	0	0	0	0	0	0	0	0	0	0	0
25	28	1	0	0	0	0	0	0	0	0	0	0	0	0	0
28	29	1	0	0	0	0	0	0	0	0	0	0	0	0	0
28	30	1	0	0	0	0	0	0	0	0	0	0	0	0	0
28	87	1	0	0	0	0	0	0	0	0	0	0	0	0	0
32	33	1	0	0	0	0	0	0	0	0	0	0	0	0	0
32	34	1	0	0	0	0	0	0	0	0	0	0	0	0	0
32	42	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
U93_12

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$$$$
U94_12
MOE2012 3D

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342347 0 0 1 0 0 0 0 0999 V2000
 34.8770 0.2220 -31.9750 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 34.0000 -0.4500 -31.1720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 32.9290 -0.3190 -31.2310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 34.7920 -1.2470 -30.3780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 34.4760 -1.9380 -29.6080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 36.1200 -1.0740 -30.6770 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 36.1390 -0.1820 -31.6420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 37.0270 0.2000 -32.1290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 34.5350 1.1830 -33.0040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 35.2680 1.0710 -33.8130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 33.5540 0.9010 -33.4050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 34.5180 2.6210 -32.4730 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 33.7870 2.6880 -31.6600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 35.5010 2.8720 -32.0570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 34.1740 3.5540 -33.5520 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
 34.8480 3.4510 -34.3120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 36.7940 9.5290 -19.6420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 37.8390 9.6580 -19.9520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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323324	1	0	0	0	0
324325	1	0	0	0	0
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327335	1	0	0	0	0
328329	1	0	0	0	0
328330	2	0	0	0	0
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330332	1	0	0	0	0
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333334	1	0	0	0	0
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335337	1	0	0	0	0
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338340	1	0	0	0	0
338341	1	0	0	0	0
341342	1	0	0	0	0

M END  
> <NAME>  
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