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M END
> <NAME>
AA20_1

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$$$$
AA24_1
MOE2012 3D

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  11.1710 -14.2030 4.9480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  19.3640 -14.1570 8.2130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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M END
> <NAME>
AA24_1

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AA28_1
MOE2012 3D

322326 0 0 1 0 0 0 0 0 0999 V2000
39.5490 -2.0540 19.6260 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.9260 -2.2720 20.4950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.4410 -2.9180 19.4190 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.7940 -3.9530 19.4620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.7170 -2.7540 20.2230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.8280 -2.6080 18.0610 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.5320 -1.5520 18.0290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.5910 -2.7300 17.2820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.6260 -3.5040 17.7710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.9390 -4.5560 17.7980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.8810 -3.3680 18.5630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.0160 -3.1810 16.4040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.6960 -2.1330 16.3590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.7910 -3.2960 15.6360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.9130 -4.0710 16.0440 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
35.1890 -5.0420 16.1850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.8310 -4.2680 8.8590 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.1690 -2.9970 8.3750 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.4140 -2.2190 8.2810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.4860 -2.7100 8.0160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.7460 -1.7230 7.6450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.4680 -3.6920 8.1340 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.4920 -3.4670 7.8540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.1370 -4.9610 8.6050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.9020 -5.7300 8.6840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.8210 -5.2490 8.9710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.5910 -6.2480 9.3350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

46.6940	-13.8060	3.0920	H	0	0	0	0	0	0	0	0	0	0	0	0
47.5290	-12.6040	1.5430	N	0	0	3	0	0	0	0	0	0	0	0	0
51.8870	-7.8290	-5.1830	C	0	0	0	0	0	0	0	0	0	0	0	0
51.0320	-8.6460	-5.9320	C	0	0	0	0	0	0	0	0	0	0	0	0
50.0250	-8.8710	-5.5860	H	0	0	0	0	0	0	0	0	0	0	0	0
51.4590	-9.1750	-7.1510	C	0	0	0	0	0	0	0	0	0	0	0	0
50.7930	-9.8080	-7.7310	H	0	0	0	0	0	0	0	0	0	0	0	0
52.7380	-8.8880	-7.6260	C	0	0	0	0	0	0	0	0	0	0	0	0
53.0690	-9.3020	-8.5750	H	0	0	0	0	0	0	0	0	0	0	0	0
53.5900	-8.0660	-6.8880	C	0	0	0	0	0	0	0	0	0	0	0	0
54.5850	-7.8410	-7.2610	H	0	0	0	0	0	0	0	0	0	0	0	0
53.1650	-7.5320	-5.6700	C	0	0	0	0	0	0	0	0	0	0	0	0
53.8380	-6.8900	-5.1060	H	0	0	0	0	0	0	0	0	0	0	0	0
46.9510	-13.3480	0.4050	C	0	0	0	0	0	0	0	0	0	0	0	0
45.9930	-13.8000	0.6940	H	0	0	0	0	0	0	0	0	0	0	0	0
47.6250	-14.1820	0.1690	H	0	0	0	0	0	0	0	0	0	0	0	0
46.7370	-12.5650	-0.8890	C	0	0	0	0	0	0	0	0	0	0	0	0
46.3830	-13.2340	-1.6820	H	0	0	0	0	0	0	0	0	0	0	0	0
45.9540	-11.8070	-0.7670	H	0	0	0	0	0	0	0	0	0	0	0	0
48.0090	-11.9230	-1.3770	C	0	0	0	0	0	0	0	0	0	0	0	0
47.8710	-10.5690	-1.3610	O	0	0	0	0	0	0	0	0	0	0	0	0
49.0410	-9.8220	-1.7240	C	0	0	0	0	0	0	0	0	0	0	0	0
49.8300	-10.0210	-0.9890	H	0	0	0	0	0	0	0	0	0	0	0	0
49.3860	-10.1560	-2.7100	H	0	0	0	0	0	0	0	0	0	0	0	0
48.6870	-8.3080	-1.7410	C	0	0	3	0	0	0	0	0	0	0	0	0
47.5900	-8.1180	-2.8200	C	0	0	0	0	0	0	0	0	0	0	0	0
47.8730	-8.6170	-3.7550	H	0	0	0	0	0	0	0	0	0	0	0	0
46.6570	-8.5930	-2.5000	H	0	0	0	0	0	0	0	0	0	0	0	0
47.2880	-6.7320	-3.0320	O	0	0	0	0	0	0	0	0	0	0	0	0
47.5920	-6.2070	-4.2520	C	0	0	0	0	0	0	0	0	0	0	0	0
47.2100	-4.7460	-4.2650	C	0	0	0	0	0	0	0	0	0	0	0	0
46.1270	-4.6700	-4.1210	H	0	0	0	0	0	0	0	0	0	0	0	0
47.7190	-4.2480	-3.4320	H	0	0	0	0	0	0	0	0	0	0	0	0
47.5990	-4.0660	-5.5660	C	0	0	0	0	0	0	0	0	0	0	0	0
48.6790	-4.1290	-5.7350	H	0	0	0	0	0	0	0	0	0	0	0	0
47.3170	-3.0090	-5.5420	H	0	0	0	0	0	0	0	0	0	0	0	0
47.0980	-4.5350	-6.4190	H	0	0	0	0	0	0	0	0	0	0	0	0
49.0020	-12.5320	-1.7480	O	0	0	0	0	0	0	0	0	0	0	0	0
48.0930	-6.8110	-5.1900	O	0	0	0	0	0	0	0	0	0	0	0	0
48.1700	-7.9050	-0.3250	C	0	0	0	0	0	0	0	0	0	0	0	0
47.2270	-8.4270	-0.1170	H	0	0	0	0	0	0	0	0	0	0	0	0
48.8860	-8.2660	0.4260	H	0	0	0	0	0	0	0	0	0	0	0	0
49.9570	-7.5090	-2.1040	C	0	0	0	0	0	0	0	0	0	0	0	0
49.7470	-6.4360	-2.1680	H	0	0	0	0	0	0	0	0	0	0	0	0
50.7370	-7.6700	-1.3490	H	0	0	0	0	0	0	0	0	0	0	0	0
47.9440	-6.4220	-0.0560	C	0	0	0	0	0	0	0	0	0	0	0	0
47.1740	-5.9980	-0.7030	H	0	0	0	0	0	0	0	0	0	0	0	0
48.8630	-5.8420	-0.1720	H	0	0	0	0	0	0	0	0	0	0	0	0
47.6050	-6.2870	0.9770	H	0	0	0	0	0	0	0	0	0	0	0	0
50.4480	-7.9640	-3.3740	O	0	0	0	0	0	0	0	0	0	0	0	0
51.4830	-7.2560	-3.8910	C	0	0	0	0	0	0	0	0	0	0	0	0
52.0420	-6.3030	-3.3680	O	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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M END
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AA28_1

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AA36_1
MOE2012 3D

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352356 0 0 1 0 0 0 0 0999 V2000
13.8140 -4.0400 -15.5220 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.3890 -4.8230 -15.4830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.0100 -3.3210 -14.3110 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.7480 -3.9750 -13.4730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.0690 -3.0520 -14.2340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.1330 -2.0760 -14.3220 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.3850 -1.4620 -15.1960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.0850 -2.3710 -14.4560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.2930 -1.2600 -13.0390 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.0330 -1.8830 -12.1750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.3420 -0.9640 -12.9210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.4080 -0.0110 -13.0530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.6730 0.6180 -13.9120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.3590 -0.3060 -13.1790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.5600 0.7970 -11.7610 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.3010 0.1630 -10.9040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.6090 1.0940 -11.6370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.6680 2.0430 -11.7710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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11.9420	2.6770	-12.6230	H	0	0	0	0	0	0	0	0	0	0	0	0
10.6210	1.7420	-11.8920	H	0	0	0	0	0	0	0	0	0	0	0	0
11.8400	2.7850	-10.5200	N	0	0	3	0	0	0	0	0	0	0	0	0
11.6190	2.1700	-9.7360	H	0	0	0	0	0	0	0	0	0	0	0	0
17.7200	9.2190	-7.1120	C	0	0	0	0	0	0	0	0	0	0	0	0
16.4550	9.6390	-6.6840	C	0	0	0	0	0	0	0	0	0	0	0	0
15.6560	8.9240	-6.5020	H	0	0	0	0	0	0	0	0	0	0	0	0
16.1990	10.9970	-6.4790	C	0	0	0	0	0	0	0	0	0	0	0	0
15.2160	11.3220	-6.1490	H	0	0	0	0	0	0	0	0	0	0	0	0
17.2030	11.9390	-6.7010	C	0	0	0	0	0	0	0	0	0	0	0	0
17.0010	12.9960	-6.5450	H	0	0	0	0	0	0	0	0	0	0	0	0
18.4660	11.5260	-7.1230	C	0	0	0	0	0	0	0	0	0	0	0	0
19.2480	12.2610	-7.2960	H	0	0	0	0	0	0	0	0	0	0	0	0
18.7260	10.1700	-7.3250	C	0	0	0	0	0	0	0	0	0	0	0	0
19.7170	9.8630	-7.6560	H	0	0	0	0	0	0	0	0	0	0	0	0
10.9790	3.9690	-10.4810	C	0	0	0	0	0	0	0	0	0	0	0	0
9.9280	3.6570	-10.4960	H	0	0	0	0	0	0	0	0	0	0	0	0
11.1560	4.5950	-11.3640	H	0	0	0	0	0	0	0	0	0	0	0	0
11.2350	4.7760	-9.2150	C	0	0	0	0	0	0	0	0	0	0	0	0
10.4450	5.5230	-9.0750	H	0	0	0	0	0	0	0	0	0	0	0	0
11.2180	4.1420	-8.3200	H	0	0	0	0	0	0	0	0	0	0	0	0
12.5400	5.5230	-9.3060	C	0	0	0	0	0	0	0	0	0	0	0	0
13.4590	4.9910	-8.4520	O	0	0	0	0	0	0	0	0	0	0	0	0
14.7440	5.6330	-8.4790	C	0	0	0	0	0	0	0	0	0	0	0	0
15.1310	5.6180	-9.5070	H	0	0	0	0	0	0	0	0	0	0	0	0
14.6080	6.6780	-8.1750	H	0	0	0	0	0	0	0	0	0	0	0	0
15.7440	4.9110	-7.5310	C	0	0	3	0	0	0	0	0	0	0	0	0
15.1650	4.9550	-6.0920	C	0	0	0	0	0	0	0	0	0	0	0	0
14.8020	5.9630	-5.8580	H	0	0	0	0	0	0	0	0	0	0	0	0
14.3240	4.2570	-6.0030	H	0	0	0	0	0	0	0	0	0	0	0	0
16.1820	4.6350	-5.1270	O	0	0	0	0	0	0	0	0	0	0	0	0
15.7420	4.3120	-3.8760	C	0	0	0	0	0	0	0	0	0	0	0	0
16.9330	4.0550	-2.9840	C	0	0	0	0	0	0	0	0	0	0	0	0
17.5310	3.2640	-3.4420	H	0	0	0	0	0	0	0	0	0	0	0	0
17.5250	4.9770	-2.9590	H	0	0	0	0	0	0	0	0	0	0	0	0
16.4910	3.6650	-1.5660	C	0	0	0	0	0	0	0	0	0	0	0	0
15.9540	4.5220	-1.1350	H	0	0	0	0	0	0	0	0	0	0	0	0
15.7360	2.8690	-1.6130	H	0	0	0	0	0	0	0	0	0	0	0	0
12.7300	6.4810	-10.0440	O	0	0	0	0	0	0	0	0	0	0	0	0
14.5700	4.2490	-3.5330	O	0	0	0	0	0	0	0	0	0	0	0	0
15.9070	3.4400	-8.0210	C	0	0	0	0	0	0	0	0	0	0	0	0
14.9300	2.9400	-8.0180	H	0	0	0	0	0	0	0	0	0	0	0	0
16.2360	3.4520	-9.0690	H	0	0	0	0	0	0	0	0	0	0	0	0
17.1040	5.6500	-7.6040	C	0	0	0	0	0	0	0	0	0	0	0	0
17.8350	5.2220	-6.9110	H	0	0	0	0	0	0	0	0	0	0	0	0
17.5090	5.5800	-8.6220	H	0	0	0	0	0	0	0	0	0	0	0	0
16.8760	2.5570	-7.2430	C	0	0	0	0	0	0	0	0	0	0	0	0
16.5310	2.3810	-6.2210	H	0	0	0	0	0	0	0	0	0	0	0	0
17.8820	2.9820	-7.2090	H	0	0	0	0	0	0	0	0	0	0	0	0
16.9520	1.5790	-7.7290	H	0	0	0	0	0	0	0	0	0	0	0	0
16.9200	7.0380	-7.2770	O	0	0	0	0	0	0	0	0	0	0	0	0
18.0380	7.8040	-7.3630	C	0	0	0	0	0	0	0	0	0	0	0	0
19.1630	7.4040	-7.6290	O	0	0	0	0	0	0	0	0	0	0	0	0
24.5880	1.5240	3.1060	O	0	0	0	0	0	0	0	0	0	0	0	0
25.0370	1.5050	3.9690	H	0	0	0	0	0	0	0	0	0	0	0	0
23.5990	2.5430	3.1690	C	0	0	0	0	0	0	0	0	0	0	0	0
22.9930	2.3870	4.0670	H	0	0	0	0	0	0	0	0	0	0	0	0
24.0980	3.5150	3.2360	H	0	0	0	0	0	0	0	0	0	0	0	0
22.7470	2.4440	1.9150	C	0	0	0	0	0	0	0	0	0	0	0	0
23.3820	2.5740	1.0300	H	0	0	0	0	0	0	0	0	0	0	0	0
22.3390	1.4290	1.8450	H	0	0	0	0	0	0	0	0	0	0	0	0
21.6050	3.4540	1.9050	C	0	0	0	0	0	0	0	0	0	0	0	0
20.9740	3.3040	2.7900	H	0	0	0	0	0	0	0	0	0	0	0	0
22.0060	4.4730	1.9570	H	0	0	0	0	0	0	0	0	0	0	0	0
20.7620	3.2920	0.6380	C	0	0	0	0	0	0	0	0	0	0	0	0
21.3810	3.5110	-0.2400	H	0	0	0	0	0	0	0	0	0	0	0	0
20.4480	2.2490	0.5560	H	0	0	0	0	0	0	0	0	0	0	0	0
19.5460	4.2170	0.6530	C	0	0	0	0	0	0	0	0	0	0	0	0
18.9100	4.0010	1.5210	H	0	0	0	0	0	0	0	0	0	0	0	0
19.9050	5.2450	0.7910	H	0	0	0	0	0	0	0	0	0	0	0	0
18.7190	4.1770	-0.6430	C	0	0	0	0	0	0	0	0	0	0	0	0
18.3530	5.2040	-0.7750	H	0	0	0	0	0	0	0	0	0	0	0	0
19.3580	3.9720	-1.5080	H	0	0	0	0	0	0	0	0	0	0	0	0
17.5490	3.2990	-0.6100	N	0	0	3	0	0	0	0	0	0	0	0	0
17.9370	-3.2570	-1.3180	C	0	0	0	0	0	0	0	0	0	0	0	0
17.7580	-2.7800	-0.0130	C	0	0	0	0	0	0	0	0	0	0	0	0
18.5790	-2.3340	0.5430	H	0	0	0	0	0	0	0	0	0	0	0	0
16.5060	-2.8640	0.6000	C	0	0	0	0	0	0	0	0	0	0	0	0
16.3730	-2.4940	1.6140	H	0	0	0	0	0	0	0	0	0	0	0	0
15.4290	-3.4240	-0.0840	C	0	0	0	0	0	0	0	0	0	0	0	0
14.4550	-3.4910	0.3940	H	0	0	0	0	0	0	0	0	0	0	0	0

28.0410	-5.1160	3.4700	O	0	0	0	0	0	0	0	0	0	0	0
29.2070	-5.5020	2.7170	C	0	0	0	0	0	0	0	0	0	0	0
29.1330	-6.5300	2.3440	H	0	0	0	0	0	0	0	0	0	0	0
29.2180	-4.8560	1.8300	H	0	0	0	0	0	0	0	0	0	0	0
30.5230	-5.2920	3.5260	C	0	0	3	0	0	0	0	0	0	0	0
31.6870	-5.6220	2.5520	C	0	0	0	0	0	0	0	0	0	0	0
31.5200	-6.6060	2.0980	H	0	0	0	0	0	0	0	0	0	0	0
31.7170	-4.8830	1.7420	H	0	0	0	0	0	0	0	0	0	0	0
32.9630	-5.5880	3.2120	O	0	0	0	0	0	0	0	0	0	0	0
33.9500	-6.3410	2.6510	C	0	0	0	0	0	0	0	0	0	0	0
35.2490	-6.1730	3.3960	C	0	0	0	0	0	0	0	0	0	0	0
35.9500	-5.7290	2.6830	H	0	0	0	0	0	0	0	0	0	0	0
35.1240	-5.4610	4.2210	H	0	0	0	0	0	0	0	0	0	0	0
35.7290	-7.5230	3.9300	C	0	0	0	0	0	0	0	0	0	0	0
34.9850	-7.8420	4.6650	H	0	0	0	0	0	0	0	0	0	0	0
35.7200	-8.2810	3.1360	H	0	0	0	0	0	0	0	0	0	0	0
27.1070	-7.2120	3.2770	O	0	0	0	0	0	0	0	0	0	0	0
33.8300	-7.0380	1.6510	O	0	0	0	0	0	0	0	0	0	0	0
30.5700	-3.8120	4.0140	C	0	0	0	0	0	0	0	0	0	0	0
30.4400	-3.1460	3.1510	H	0	0	0	0	0	0	0	0	0	0	0
29.7100	-3.6250	4.6700	H	0	0	0	0	0	0	0	0	0	0	0
30.5510	-6.2470	4.7460	C	0	0	0	0	0	0	0	0	0	0	0
31.4920	-6.1720	5.2980	H	0	0	0	0	0	0	0	0	0	0	0
29.7530	-5.9880	5.4510	H	0	0	0	0	0	0	0	0	0	0	0
31.8150	-3.3600	4.7670	C	0	0	0	0	0	0	0	0	0	0	0
32.6890	-3.3160	4.1130	H	0	0	0	0	0	0	0	0	0	0	0
32.0390	-4.0050	5.6200	H	0	0	0	0	0	0	0	0	0	0	0
31.6600	-2.3470	5.1560	H	0	0	0	0	0	0	0	0	0	0	0
30.3020	-7.6080	4.3370	O	0	0	0	0	0	0	0	0	0	0	0
31.3510	-8.4660	4.3240	C	0	0	0	0	0	0	0	0	0	0	0
32.5050	-8.2110	4.6370	O	0	0	0	0	0	0	0	0	0	0	0
39.5300	-4.0890	9.7090	O	0	0	0	0	0	0	0	0	0	0	0
38.9910	-4.0520	10.5170	H	0	0	0	0	0	0	0	0	0	0	0
38.6970	-4.6040	8.6790	C	0	0	0	0	0	0	0	0	0	0	0
38.3230	-5.5840	8.9910	H	0	0	0	0	0	0	0	0	0	0	0
37.8510	-3.9230	8.5440	H	0	0	0	0	0	0	0	0	0	0	0
39.5090	-4.7220	7.3980	C	0	0	0	0	0	0	0	0	0	0	0
39.9310	-3.7430	7.1410	H	0	0	0	0	0	0	0	0	0	0	0
40.3660	-5.3840	7.5710	H	0	0	0	0	0	0	0	0	0	0	0
38.6540	-5.2510	6.2470	C	0	0	0	0	0	0	0	0	0	0	0
38.2200	-6.2080	6.5480	H	0	0	0	0	0	0	0	0	0	0	0
37.8240	-4.5580	6.0610	H	0	0	0	0	0	0	0	0	0	0	0
39.4820	-5.4230	4.9730	C	0	0	0	0	0	0	0	0	0	0	0
40.0270	-4.4890	4.7850	H	0	0	0	0	0	0	0	0	0	0	0
40.2390	-6.2020	5.1210	H	0	0	0	0	0	0	0	0	0	0	0
38.6520	-5.7310	3.7210	C	0	0	0	0	0	0	0	0	0	0	0
37.8350	-5.0070	3.6350	H	0	0	0	0	0	0	0	0	0	0	0
39.2980	-5.5580	2.8500	H	0	0	0	0	0	0	0	0	0	0	0
38.1320	-7.1740	3.6110	C	0	0	0	0	0	0	0	0	0	0	0
37.7930	-7.3550	2.5830	H	0	0	0	0	0	0	0	0	0	0	0
38.9940	-7.8420	3.7400	H	0	0	0	0	0	0	0	0	0	0	0
37.0590	-7.4750	4.5810	N	0	0	3	0	0	0	0	0	0	0	0
33.7980	-5.5440	9.3760	C	0	0	0	0	0	0	0	0	0	0	0
34.9310	-6.0950	9.9850	C	0	0	0	0	0	0	0	0	0	0	0
35.1850	-7.1450	9.8570	H	0	0	0	0	0	0	0	0	0	0	0
35.7550	-5.2950	10.7790	C	0	0	0	0	0	0	0	0	0	0	0
36.6280	-5.7270	11.2630	H	0	0	0	0	0	0	0	0	0	0	0
35.4570	-3.9440	10.9590	C	0	0	0	0	0	0	0	0	0	0	0
36.0960	-3.3230	11.5820	H	0	0	0	0	0	0	0	0	0	0	0
34.3360	-3.3880	10.3450	C	0	0	0	0	0	0	0	0	0	0	0
34.0980	-2.3380	10.4980	H	0	0	0	0	0	0	0	0	0	0	0
33.5090	-4.1840	9.5500	C	0	0	0	0	0	0	0	0	0	0	0
32.6280	-3.7430	9.0870	H	0	0	0	0	0	0	0	0	0	0	0
37.3500	-8.7480	5.2830	C	0	0	0	0	0	0	0	0	0	0	0
38.3960	-8.7130	5.6160	H	0	0	0	0	0	0	0	0	0	0	0
37.2700	-9.6020	4.5990	H	0	0	0	0	0	0	0	0	0	0	0
36.5290	-8.9350	6.5640	C	0	0	0	0	0	0	0	0	0	0	0
37.1700	-9.3820	7.3340	H	0	0	0	0	0	0	0	0	0	0	0
36.1790	-7.9680	6.9450	H	0	0	0	0	0	0	0	0	0	0	0
35.3500	-9.8640	6.4000	C	0	0	0	0	0	0	0	0	0	0	0
34.5470	-9.7460	7.4970	O	0	0	0	0	0	0	0	0	0	0	0
33.3470	-10.5340	7.4850	C	0	0	0	0	0	0	0	0	0	0	0
32.8790	-10.4550	6.4980	H	0	0	0	0	0	0	0	0	0	0	0
33.6190	-11.5820	7.6560	H	0	0	0	0	0	0	0	0	0	0	0
32.3700	-10.0320	8.5790	C	0	0	3	0	0	0	0	0	0	0	0
33.0440	-10.1640	9.9710	C	0	0	0	0	0	0	0	0	0	0	0
34.0250	-9.6760	9.9970	H	0	0	0	0	0	0	0	0	0	0	0
32.4050	-9.6940	10.7300	H	0	0	0	0	0	0	0	0	0	0	0
33.2290	-11.5490	10.2960	O	0	0	0	0	0	0	0	0	0	0	0
33.5100	-11.7950	11.6050	C	0	0	0	0	0	0	0	0	0	0	0
33.5580	-13.2770	11.8640	C	0	0	0	0	0	0	0	0	0	0	0

29.4960	-6.2840	11.0620	C	0	0	0	0	0	0	0	0	0	0	0	0
29.5050	-5.2030	11.2420	H	0	0	0	0	0	0	0	0	0	0	0	0
30.1820	-6.5020	10.2350	H	0	0	0	0	0	0	0	0	0	0	0	0
31.8570	-5.3840	12.8720	C	0	0	0	0	0	0	0	0	0	0	0	0
31.4300	-4.9820	13.7940	H	0	0	0	0	0	0	0	0	0	0	0	0
31.5820	-4.7310	12.0400	H	0	0	0	0	0	0	0	0	0	0	0	0
32.9460	-5.3400	12.9790	H	0	0	0	0	0	0	0	0	0	0	0	0
28.1710	-6.6790	10.6750	O	0	0	0	0	0	0	0	0	0	0	0	0
27.6850	-6.0580	9.5710	C	0	0	0	0	0	0	0	0	0	0	0	0
28.2590	-5.2060	8.9080	O	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
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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M END
> <NAME>
AA36_1

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$$$$
AA61_1
MOE2012 3D

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21.1340 -5.4080 -7.0470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.9850 -5.8670 -5.1680 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
22.5830 -5.0400 -5.1470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.7530 -5.6000 -4.4140 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.2110 -4.7620 -4.8700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.1070 -6.4820 -4.4630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.0800 -5.2520 -2.9450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.6570 -6.0590 -2.4740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.7410 -4.3770 -2.9680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8590 -4.9540 -2.1580 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
20.1880 -4.1340 -0.9740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.3650 -4.1560 -0.2530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.0690 -4.5270 -0.4520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.9790 -6.4720 -7.3140 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.6140 -5.5800 -7.3270 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.5480 -7.2930 -6.8630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.7600 -6.7440 -8.3520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.3940 -2.6660 -1.3340 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.5230 -2.2650 -1.8640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.2780 -2.5090 -1.9590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.5290 -2.0750 -0.4220 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.6410 -2.2250 5.5640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.8600 -2.5600 4.9610 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.9340 -2.7250 3.8890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.0170 -2.6770 5.7350 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.9610 -2.9360 5.2620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.9630 -2.4620 7.1110 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.8640 -2.5560 7.7120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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M END
> <NAME>
AA61_1

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B17_1
MOE2012 3D

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19.0650 3.2480 -5.4040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.6100 4.1490 -6.3340 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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19.4290 4.9070 -8.3610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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17.4140 2.5310 -7.0210 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.5500 1.9170 -7.2640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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17.5350 1.7830 -5.0110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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21.2900 5.7660 -6.8690 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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20.6180 6.5440 -7.2460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.7000 5.1640 -7.6870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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15.6610 4.6140 -8.4180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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13.4130 5.6890 -9.4780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.8330 5.9090 -8.4910 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

11.9380	3.5560	18.9180	H	0	0	0	0	0	0	0	0	0	0	0	0
19.7480	9.7120	16.5280	O	0	0	0	0	0	0	0	0	0	0	0	0
13.3710	5.8600	18.2640	O	0	0	0	0	0	0	0	0	0	0	0	0
17.6350	7.5790	15.3950	C	0	0	0	0	0	0	0	0	0	0	0	0
16.5560	7.7180	15.2750	H	0	0	0	0	0	0	0	0	0	0	0	0
17.9230	6.6380	14.9140	H	0	0	0	0	0	0	0	0	0	0	0	0
18.1370	8.3790	14.8420	H	0	0	0	0	0	0	0	0	0	0	0	0
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110	113	1	0	0	0	0
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114	121	2	0	0	0	0
114	123	1	0	0	0	0
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115	124	1	0	0	0	0
116	117	1	0	0	0	0
116	118	1	0	0	0	0
118	119	2	0	0	0	0
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140	143	1	0	0	0	0
143	144	1	0	0	0	0
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143	146	1	0	0	0	0
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146	164	2	0	0	0	0
147	148	1	0	0	0	0
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174189	1	0	0	0	0
175176	1	0	0	0	0
175177	1	0	0	0	0
177178	1	0	0	0	0
179185	1	0	0	0	0
180181	1	0	0	0	0
181182	1	0	0	0	0
181183	1	0	0	0	0
181184	1	0	0	0	0
185186	1	0	0	0	0
185187	1	0	0	0	0
185188	1	0	0	0	0
189190	1	0	0	0	0
189191	1	0	0	0	0
189192	1	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
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
199202	1	0	0	0	0
202203	1	0	0	0	0
202220	2	0	0	0	0
203204	1	0	0	0	0
204205	1	0	0	0	0
204206	1	0	0	0	0
204222	1	0	0	0	0
206207	1	0	0	0	0
206208	1	0	0	0	0
206209	1	0	0	0	0
209210	1	0	0	0	0
209211	1	0	0	0	0
209212	1	0	0	0	0
212213	1	0	0	0	0
213214	1	0	0	0	0
213221	2	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
217251	1	0	0	0	0
222223	1	0	0	0	0
222224	1	0	0	0	0
222225	1	0	0	0	0
226227	1	0	0	0	0
226233	2	0	0	0	0
226235	1	0	0	0	0
227228	2	0	0	0	0
227236	1	0	0	0	0
228229	1	0	0	0	0
228230	1	0	0	0	0


```

230231 2 0 0 0 0
230245 1 0 0 0 0
231232 1 0 0 0 0
231233 1 0 0 0 0
233234 1 0 0 0 0
235241 1 0 0 0 0
236237 1 0 0 0 0
237238 1 0 0 0 0
237239 1 0 0 0 0
237240 1 0 0 0 0
241242 1 0 0 0 0
241243 1 0 0 0 0
241244 1 0 0 0 0
245246 1 0 0 0 0
245247 1 0 0 0 0
245248 1 0 0 0 0
248249 1 0 0 0 0
248250 1 0 0 0 0
248251 1 0 0 0 0
251252 1 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
255258 1 0 0 0 0
258259 1 0 0 0 0
258277 2 0 0 0 0
259260 1 0 0 0 0
260261 1 0 0 0 0
260262 1 0 0 0 0
260279 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
269270 1 0 0 0 0
269278 2 0 0 0 0
270271 1 0 0 0 0
270272 1 0 0 0 0
270273 1 0 0 0 0
273274 1 0 0 0 0
273275 1 0 0 0 0
273276 1 0 0 0 0
279280 1 0 0 0 0
279281 1 0 0 0 0
279282 1 0 0 0 0

```

```

M END
> <NAME>
B17_1

```

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$$$$
C20_1
MOE2012 3D

```

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212211 0 0 1 0 0 0 0 0999 V2000
3.3690 -3.3600 13.0030 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.8350 -4.1610 12.8640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.6870 -3.6510 12.5570 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5.0730 -4.4930 13.1400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.6410 -3.9400 11.5020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5.5570 -2.4160 12.7440 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5.1220 -1.5790 12.1810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5.5320 -2.1130 13.7990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.9950 -2.6730 12.2950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.4200 -3.4950 12.8830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.9990 -2.9710 11.2400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.7930 -1.4580 12.4720 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
7.7520 -1.1630 13.4480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.0900 3.4410 11.6040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.9760 3.7560 12.6470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.5840 4.1570 10.9460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.4830 3.3880 11.2680 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.1510 4.5660 11.4340 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.6000 4.3800 11.0500 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.9870 3.5100 11.5930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.6380 4.1780 9.9750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.4260 5.6180 11.4140 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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68.3110	16.9110	-7.7280	O	0	0	0	0	0	0	0	0	0	0	0	0	0
69.5380	17.4540	-7.4830	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.7360	18.6590	-8.3710	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.6420	18.3400	-9.4140	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.9510	19.3880	-8.1460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.0960	19.3020	-8.1650	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.2190	19.6380	-7.1300	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.2120	20.1700	-8.8220	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.9030	18.5960	-8.3850	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.3470	17.0310	-6.6690	O	0	0	0	0	0	0	0	0	0	0	0	0	0
61.6790	10.0520	-5.6540	C	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5260	9.6850	-6.6770	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9820	10.8900	-5.5140	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.0960	10.6230	-5.5070	C	0	0	0	0	0	0	0	0	0	0	0	0	0
63.2640	10.9310	-4.4680	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.8480	9.8820	-5.7940	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.2940	11.8320	-6.3940	C	0	0	0	0	0	0	0	0	0	0	0	0	0
64.5200	12.3810	-6.1500	O	0	0	0	0	0	0	0	0	0	0	0	0	0
64.8230	13.5400	-6.9390	C	0	0	0	0	0	0	0	0	0	0	0	0	0
64.8050	13.2720	-8.0020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.0770	14.3200	-6.7440	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.2110	14.0290	-6.5430	C	0	0	0	0	0	0	0	0	0	0	0	0	0
66.2260	14.2440	-5.4670	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.9380	13.2210	-6.6980	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.4870	12.2490	-7.2130	O	0	0	0	0	0	0	0	0	0	0	0	0	0
66.6190	15.2650	-7.3350	C	0	0	0	0	0	0	0	0	0	0	0	0	0
65.8920	16.0730	-7.1800	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.6020	15.0500	-8.4110	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	9	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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12	26	1	0	0	0	0
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14	16	1	0	0	0	0
14	17	1	0	0	0	0
14	41	1	0	0	0	0
17	18	1	0	0	0	0
18	19	1	0	0	0	0
18	25	2	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
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41	43	1	0	0	0	0
44	45	1	0	0	0	0
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52	54	1	0	0	0	0

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56	57	1	0	0	0	0
56	58	1	0	0	0	0
56	59	1	0	0	0	0
56	83	1	0	0	0	0
59	60	1	0	0	0	0
60	61	1	0	0	0	0
60	67	2	0	0	0	0
61	62	1	0	0	0	0
61	63	1	0	0	0	0
61	64	1	0	0	0	0
64	65	1	0	0	0	0
64	66	1	0	0	0	0
64	97	1	0	0	0	0
68	69	1	0	0	0	0
68	70	1	0	0	0	0
68	71	1	0	0	0	0
71	72	1	0	0	0	0
71	73	1	0	0	0	0
71	74	1	0	0	0	0
74	75	1	0	0	0	0
74	82	2	0	0	0	0
75	76	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
79	80	1	0	0	0	0
79	81	1	0	0	0	0
79	83	1	0	0	0	0
83	84	1	0	0	0	0
83	85	1	0	0	0	0
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88	90	1	0	0	0	0
88	91	1	0	0	0	0
91	92	1	0	0	0	0
91	93	1	0	0	0	0
91	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	110	1	0	0	0	0
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98	100	1	0	0	0	0
98	101	1	0	0	0	0
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103	104	1	0	0	0	0
103	105	1	0	0	0	0
103	106	1	0	0	0	0
106	107	1	0	0	0	0
106	108	1	0	0	0	0
106	139	1	0	0	0	0
110	111	1	0	0	0	0
110	112	1	0	0	0	0
110	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	124	2	0	0	0	0
117	118	1	0	0	0	0
118	119	1	0	0	0	0
118	120	1	0	0	0	0
118	121	1	0	0	0	0
121	122	1	0	0	0	0
121	123	1	0	0	0	0
121	125	1	0	0	0	0
125	126	1	0	0	0	0
125	127	1	0	0	0	0
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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

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136139	1	0	0	0	0
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140141	1	0	0	0	0
140142	1	0	0	0	0
140143	1	0	0	0	0
140167	1	0	0	0	0
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145146	1	0	0	0	0
145147	1	0	0	0	0
145148	1	0	0	0	0
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148150	1	0	0	0	0
148181	1	0	0	0	0
152153	1	0	0	0	0
152154	1	0	0	0	0
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158159	1	0	0	0	0
158166	2	0	0	0	0
159160	1	0	0	0	0
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160163	1	0	0	0	0
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163165	1	0	0	0	0
163167	1	0	0	0	0
167168	1	0	0	0	0
167169	1	0	0	0	0
170171	1	0	0	0	0
170172	1	0	0	0	0
172173	1	0	0	0	0
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175178	1	0	0	0	0
178179	1	0	0	0	0
178180	1	0	0	0	0
178181	1	0	0	0	0
181195	1	0	0	0	0
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182185	1	0	0	0	0
182210	1	0	0	0	0
185186	1	0	0	0	0
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187188	1	0	0	0	0
187189	1	0	0	0	0
187190	1	0	0	0	0
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190193	1	0	0	0	0
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195197	1	0	0	0	0
195198	1	0	0	0	0
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203205	1	0	0	0	0
203206	1	0	0	0	0
206207	1	0	0	0	0
206208	1	0	0	0	0
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210211	1	0	0	0	0
210212	1	0	0	0	0

M END
> <NAME>
C20_1

45.0820	9.7000	3.3250	H	0	0	0	0	0	0	0	0	0	0	0	0
46.4650	8.9980	4.7790	C	0	0	0	0	0	0	0	0	0	0	0	0
45.7500	8.6270	5.5240	H	0	0	0	0	0	0	0	0	0	0	0	0
47.3760	8.4000	4.8820	H	0	0	0	0	0	0	0	0	0	0	0	0
46.8000	10.4210	5.1470	C	0	0	0	0	0	0	0	0	0	0	0	0
47.7540	10.9230	4.3150	O	0	0	0	0	0	0	0	0	0	0	0	0
48.1430	12.2730	4.6020	C	0	0	0	0	0	0	0	0	0	0	0	0
47.2550	12.9160	4.6370	H	0	0	0	0	0	0	0	0	0	0	0	0
48.6540	12.3000	5.5710	H	0	0	0	0	0	0	0	0	0	0	0	0
49.0790	12.7410	3.4960	C	0	0	0	0	0	0	0	0	0	0	0	0
49.9400	12.0640	3.4340	H	0	0	0	0	0	0	0	0	0	0	0	0
48.5660	12.6630	2.5290	H	0	0	0	0	0	0	0	0	0	0	0	0
46.2930	11.0200	6.0870	O	0	0	0	0	0	0	0	0	0	0	0	0
49.5460	14.1710	3.7350	C	0	0	0	0	0	0	0	0	0	0	0	0
50.0810	14.2400	4.6910	H	0	0	0	0	0	0	0	0	0	0	0	0
48.6840	14.8430	3.8260	H	0	0	0	0	0	0	0	0	0	0	0	0
52.7100	20.1030	4.6270	O	0	0	0	0	0	0	0	0	0	0	0	0
52.7960	21.0620	4.7570	H	0	0	0	0	0	0	0	0	0	0	0	0
53.8370	19.5020	5.2630	C	0	0	0	0	0	0	0	0	0	0	0	0
54.7530	19.9290	4.8390	H	0	0	0	0	0	0	0	0	0	0	0	0
53.7880	19.8050	6.3130	H	0	0	0	0	0	0	0	0	0	0	0	0
53.8260	17.9520	5.1050	C	0	0	0	0	0	0	0	0	0	0	0	0
52.7920	17.6070	5.2390	H	0	0	0	0	0	0	0	0	0	0	0	0
54.6650	17.3640	6.2740	C	0	0	0	0	0	0	0	0	0	0	0	0
54.6110	16.2740	6.3030	H	0	0	0	0	0	0	0	0	0	0	0	0
55.7140	17.6680	6.1900	H	0	0	0	0	0	0	0	0	0	0	0	0
54.1660	17.8050	7.5350	O	0	0	0	0	0	0	0	0	0	0	0	0
54.7500	17.4370	8.2210	H	0	0	0	0	0	0	0	0	0	0	0	0
54.3210	17.5060	3.7560	N	0	0	3	0	0	0	0	0	0	0	0	0
57.7330	10.1500	-1.6900	C	0	0	0	0	0	0	0	0	0	0	0	0
58.7310	10.6010	-1.6520	H	0	0	0	0	0	0	0	0	0	0	0	0
57.1790	10.5520	-2.5460	H	0	0	0	0	0	0	0	0	0	0	0	0
57.8570	8.7280	-1.8260	O	0	0	0	0	0	0	0	0	0	0	0	0
58.5180	8.3240	-2.9490	C	0	0	0	0	0	0	0	0	0	0	0	0
58.5800	6.8160	-2.9750	C	0	0	0	0	0	0	0	0	0	0	0	0
59.0980	6.4740	-2.0730	H	0	0	0	0	0	0	0	0	0	0	0	0
57.5560	6.4260	-2.9690	H	0	0	0	0	0	0	0	0	0	0	0	0
59.3090	6.2950	-4.2010	C	0	0	0	0	0	0	0	0	0	0	0	0
58.8100	6.6170	-5.1220	H	0	0	0	0	0	0	0	0	0	0	0	0
59.3370	5.2010	-4.1920	H	0	0	0	0	0	0	0	0	0	0	0	0
60.3390	6.6640	-4.2330	H	0	0	0	0	0	0	0	0	0	0	0	0
58.9840	9.0690	-3.7990	O	0	0	0	0	0	0	0	0	0	0	0	0
54.4270	16.0380	3.6330	C	0	0	0	0	0	0	0	0	0	0	0	0
55.0540	15.6520	4.4430	H	0	0	0	0	0	0	0	0	0	0	0	0
53.4470	15.5650	3.7600	H	0	0	0	0	0	0	0	0	0	0	0	0
55.1110	15.5430	2.3520	C	0	0	0	0	0	0	0	0	0	0	0	0
54.5560	15.8210	1.4540	H	0	0	0	0	0	0	0	0	0	0	0	0
56.1240	15.9570	2.2920	H	0	0	0	0	0	0	0	0	0	0	0	0
55.2090	14.0380	2.3490	C	0	0	0	0	0	0	0	0	0	0	0	0
55.9190	13.6360	1.2570	O	0	0	0	0	0	0	0	0	0	0	0	0
56.0420	12.2140	1.1220	C	0	0	0	0	0	0	0	0	0	0	0	0
56.5900	11.8130	1.9820	H	0	0	0	0	0	0	0	0	0	0	0	0
55.0440	11.7620	1.0780	H	0	0	0	0	0	0	0	0	0	0	0	0
56.8020	11.9300	-0.1670	C	0	0	0	0	0	0	0	0	0	0	0	0
56.2680	12.3840	-1.0110	H	0	0	0	0	0	0	0	0	0	0	0	0
57.7800	12.4270	-0.1290	H	0	0	0	0	0	0	0	0	0	0	0	0
54.7150	13.2940	3.1840	O	0	0	0	0	0	0	0	0	0	0	0	0
56.9780	10.4340	-0.3960	C	0	0	0	0	0	0	0	0	0	0	0	0
56.0010	9.9360	-0.4300	H	0	0	0	0	0	0	0	0	0	0	0	0
57.5170	9.9810	0.4450	H	0	0	0	0	0	0	0	0	0	0	0	0

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M END
> <NAME>
C25_1

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C28_1
MOE2012 3D

227226 0 0 1 0 0 0 0 0999 V2000
21.1570 -1.1850 -27.7480 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.1490 -1.0610 -28.7130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.9860 0.0960 -27.1610 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.8080 0.7410 -27.4860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.0390 0.5200 -27.5120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.9820 -0.0640 -25.6500 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.1740 -0.7470 -25.3580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.9130 -0.5530 -25.3360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.8250 1.2780 -24.9400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.6370 1.9490 -25.2450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8820 1.7480 -25.2450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.8470 1.0890 -23.4230 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.0180 0.4350 -23.1280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.7840 0.5980 -23.1410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.7200 2.3870 -22.7640 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
21.4790 3.0030 -23.0530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.2660 0.9480 -14.8960 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.9080 1.7640 -15.2500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.6210 -0.0040 -15.3070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.3080 0.8930 -13.4630 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.5550 0.7190 -12.9370 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.4750 0.6950 -11.4300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.9420 1.5980 -11.1170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.8920 -0.1840 -11.1300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.8770 0.6300 -10.8100 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.3430 -0.2950 -11.1700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.5060 1.4510 -11.1800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.5830 0.5980 -13.5880 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.6870 2.2740 -21.3040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.3480 3.2400 -20.9080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.9270 1.5450 -20.9960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.0460 1.9370 -20.6920 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.4020 0.9630 -21.0420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.7780 2.7060 -20.9620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.9570 1.8720 -19.1900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.1970 1.6300 -18.6750 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.2390 1.5480 -17.2440 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.8860 2.4920 -16.8140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.5960 0.7270 -16.9070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

38.7130	-16.9140	-9.7160	C	0	0	0	0	0	0	0	0	0	0	0	0
39.0740	-17.6930	-10.3960	H	0	0	0	0	0	0	0	0	0	0	0	0
37.8990	-17.3180	-9.1060	H	0	0	0	0	0	0	0	0	0	0	0	0
38.1980	-15.7380	-10.5270	C	0	0	0	0	0	0	0	0	0	0	0	0
37.8260	-14.9420	-9.8730	H	0	0	0	0	0	0	0	0	0	0	0	0
37.3790	-16.0540	-11.1800	H	0	0	0	0	0	0	0	0	0	0	0	0
38.9900	-15.3130	-11.1530	H	0	0	0	0	0	0	0	0	0	0	0	0
40.3200	-15.3950	-8.6990	O	0	0	0	0	0	0	0	0	0	0	0	0
46.4960	-21.5500	-1.7520	C	0	0	0	0	0	0	0	0	0	0	0	0
46.7780	-22.1700	-2.6140	H	0	0	0	0	0	0	0	0	0	0	0	0
45.7810	-22.1430	-1.1660	H	0	0	0	0	0	0	0	0	0	0	0	0
45.8130	-20.2970	-2.3060	C	0	0	0	0	0	0	0	0	0	0	0	0
45.3970	-19.6830	-1.5020	H	0	0	0	0	0	0	0	0	0	0	0	0
46.5370	-19.7070	-2.8800	H	0	0	0	0	0	0	0	0	0	0	0	0
44.6760	-20.6750	-3.2220	C	0	0	0	0	0	0	0	0	0	0	0	0
44.2530	-19.5730	-3.9040	O	0	0	0	0	0	0	0	0	0	0	0	0
43.1680	-19.8170	-4.8100	C	0	0	0	0	0	0	0	0	0	0	0	0
43.4710	-20.5670	-5.5500	H	0	0	0	0	0	0	0	0	0	0	0	0
42.3010	-20.1840	-4.2480	H	0	0	0	0	0	0	0	0	0	0	0	0
42.8280	-18.5030	-5.5030	C	0	0	0	0	0	0	0	0	0	0	0	0
42.5700	-17.7500	-4.7480	H	0	0	0	0	0	0	0	0	0	0	0	0
43.7190	-18.1210	-6.0160	H	0	0	0	0	0	0	0	0	0	0	0	0
44.1950	-21.7950	-3.3230	O	0	0	0	0	0	0	0	0	0	0	0	0
41.6810	-18.6740	-6.4930	C	0	0	0	0	0	0	0	0	0	0	0	0
40.7900	-19.0560	-5.9800	H	0	0	0	0	0	0	0	0	0	0	0	0
41.9390	-19.4280	-7.2470	H	0	0	0	0	0	0	0	0	0	0	0	0
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67	70	1	0	0	0	0
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115	151	1	0	0	0	0
119	120	1	0	0	0	0
119	121	1	0	0	0	0
119	122	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
125	133	2	0	0	0	0
126	127	1	0	0	0	0
127	128	1	0	0	0	0
127	129	1	0	0	0	0
127	130	1	0	0	0	0
130	131	1	0	0	0	0
130	132	1	0	0	0	0
130	134	1	0	0	0	0
134	135	1	0	0	0	0
134	136	1	0	0	0	0

137138	1	0	0	0	0
137139	1	0	0	0	0
139140	1	0	0	0	0
139141	1	0	0	0	0
139142	1	0	0	0	0
142143	1	0	0	0	0
142144	1	0	0	0	0
142145	1	0	0	0	0
145146	1	0	0	0	0
145147	1	0	0	0	0
145148	1	0	0	0	0
148149	1	0	0	0	0
148150	1	0	0	0	0
148151	1	0	0	0	0
151164	1	0	0	0	0
152153	1	0	0	0	0
152154	1	0	0	0	0
152155	1	0	0	0	0
152179	1	0	0	0	0
155156	1	0	0	0	0
156157	1	0	0	0	0
156163	2	0	0	0	0
157158	1	0	0	0	0
157159	1	0	0	0	0
157160	1	0	0	0	0
160161	1	0	0	0	0
160162	1	0	0	0	0
160196	1	0	0	0	0
164165	1	0	0	0	0
164166	1	0	0	0	0
164167	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
170178	2	0	0	0	0
171172	1	0	0	0	0
172173	1	0	0	0	0
172174	1	0	0	0	0
172175	1	0	0	0	0
175176	1	0	0	0	0
175177	1	0	0	0	0
175179	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
193194	1	0	0	0	0
193195	1	0	0	0	0
193196	1	0	0	0	0
196210	1	0	0	0	0
197198	1	0	0	0	0
197199	1	0	0	0	0
197200	1	0	0	0	0
197225	1	0	0	0	0
200201	1	0	0	0	0
201202	1	0	0	0	0
201209	2	0	0	0	0
202203	1	0	0	0	0
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
210211	1	0	0	0	0
210212	1	0	0	0	0
210213	1	0	0	0	0
213214	1	0	0	0	0
213215	1	0	0	0	0
213216	1	0	0	0	0
216217	1	0	0	0	0
216224	2	0	0	0	0

217218 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
221223 1 0 0 0 0
221225 1 0 0 0 0
225226 1 0 0 0 0
225227 1 0 0 0 0

M END
> <NAME>
C28_1

\$\$\$
C32_1
MOE2012 3D

242241 0 0 1 0 0 0 0 0999 V2000
16.6850 23.7080 -29.1770 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.8030 23.9270 -29.5240 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.5140 22.6550 -28.2380 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.8390 22.9990 -27.4480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.0600 21.8010 -28.7500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.8750 22.2850 -27.6660 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.5470 21.9970 -28.4850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.3290 23.1710 -27.2050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.7700 21.1530 -26.6460 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.1010 21.4550 -25.8310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.3250 20.2710 -27.1210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.1430 20.7910 -26.0750 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8110 20.4930 -26.8930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.5870 21.6760 -25.6010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.0360 19.6560 -25.0540 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.3690 19.9630 -24.2390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.6030 18.7710 -25.5340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.3640 19.3460 -24.5220 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
20.9850 19.0900 -25.2890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.1090 14.3710 -18.5370 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.4200 15.3180 -18.0810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.7580 14.1440 -19.3920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.2120 13.3190 -17.5680 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.4720 13.1190 -17.0810 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.4490 11.9900 -16.0790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.6800 12.2160 -15.3310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.1750 11.0760 -16.6160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.8080 11.8330 -15.3890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.5780 11.5620 -16.1230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.0920 12.8220 -15.0050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.4610 13.7570 -17.4140 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.2990 18.2540 -23.5490 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.6230 18.5230 -22.7270 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.9030 17.3470 -24.0220 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.6920 17.9780 -22.9890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.3730 17.6830 -23.7960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.0840 18.8770 -22.4990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.6570 16.8640 -21.9740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.9090 16.6770 -21.4660 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.0050 15.6330 -20.4870 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.3540 15.8690 -19.6370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.6940 14.6830 -20.9360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.4570 15.5490 -20.0310 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.1000 15.3670 -20.9010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.7670 16.5210 -19.6280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.6650 16.2230 -21.6580 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.6560 14.4550 -18.9890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.3440 13.4840 -19.3920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.0150 14.6380 -18.1170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.5570 4.6890 -18.4220 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.1670 3.8120 -18.5820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.8240 5.2950 -17.3640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.7720 5.3500 -17.6600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.9110 4.6620 -16.4750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.3850 6.6870 -17.0970 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.4510 6.6080 -16.8460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.3370 7.2790 -18.0190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.6280 7.3950 -15.9730 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.5640 7.4540 -16.2320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.7050 6.8050 -15.0510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.1720 8.8080 -15.7230 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.2300 8.7420 -15.4500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.1120 9.3770 -16.6580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

58.3460	-10.3140	-5.4270	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3120	-10.3010	-7.1810	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.6920	-11.7160	-6.3830	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.3840	-11.7730	-7.2310	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.2760	-11.9270	-5.4820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.6590	-12.8010	-6.5200	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.2800	-12.9240	-7.8210	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.2500	-13.8920	-8.0540	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.6210	-14.8890	-7.7900	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.3720	-13.6510	-7.4430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.8910	-13.8350	-9.5330	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.5840	-12.8140	-9.7920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.7870	-14.0400	-10.1330	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.2060	-13.4410	-5.5810	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.7850	-14.8230	-9.8800	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.8910	-14.6220	-9.2760	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.0940	-15.8450	-9.6290	H	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											
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	9	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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15	18	1	0	0	0	0											
18	19	1	0	0	0	0											
18	32	1	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											
20	47	1	0	0	0	0											
23	24	1	0	0	0	0											
24	25	1	0	0	0	0											
24	31	2	0	0	0	0											
25	26	1	0	0	0	0											
25	27	1	0	0	0	0											
25	28	1	0	0	0	0											
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28	30	1	0	0	0	0											
28	67	1	0	0	0	0											
32	33	1	0	0	0	0											
32	34	1	0	0	0	0											
32	35	1	0	0	0	0											
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											
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40	41	1	0	0	0	0											
40	42	1	0	0	0	0											
40	43	1	0	0	0	0											
43	44	1	0	0	0	0											
43	45	1	0	0	0	0											
43	47	1	0	0	0	0											
47	48	1	0	0	0	0											
47	49	1	0	0	0	0											
50	51	1	0	0	0	0											
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58	61	1	0	0	0	0											
61	62	1	0	0	0	0											
61	63	1	0	0	0	0											
61	64	1	0	0	0	0											
64	65	1	0	0	0	0											

64	66	1	0	0	0	0
64	67	1	0	0	0	0
67	80	1	0	0	0	0
68	69	1	0	0	0	0
68	70	1	0	0	0	0
68	71	1	0	0	0	0
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71	72	1	0	0	0	0
72	73	1	0	0	0	0
72	79	2	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	78	1	0	0	0	0
76	115	1	0	0	0	0
80	81	1	0	0	0	0
80	82	1	0	0	0	0
80	83	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
86	87	1	0	0	0	0
86	94	2	0	0	0	0
87	88	1	0	0	0	0
88	89	1	0	0	0	0
88	90	1	0	0	0	0
88	91	1	0	0	0	0
91	92	1	0	0	0	0
91	93	1	0	0	0	0
91	95	1	0	0	0	0
95	96	1	0	0	0	0
95	97	1	0	0	0	0
98	99	1	0	0	0	0
98	100	1	0	0	0	0
100	101	1	0	0	0	0
100	102	1	0	0	0	0
100	103	1	0	0	0	0
103	104	1	0	0	0	0
103	105	1	0	0	0	0
103	106	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
112	114	1	0	0	0	0
112	115	1	0	0	0	0
115	128	1	0	0	0	0
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116	118	1	0	0	0	0
116	119	1	0	0	0	0
116	143	1	0	0	0	0
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120	121	1	0	0	0	0
120	127	2	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	126	1	0	0	0	0
124	163	1	0	0	0	0
128	129	1	0	0	0	0
128	130	1	0	0	0	0
128	131	1	0	0	0	0
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134	135	1	0	0	0	0
134	142	2	0	0	0	0
135	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
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139	143	1	0	0	0	0
143	144	1	0	0	0	0
143	145	1	0	0	0	0

146147	1	0	0	0	0
146148	1	0	0	0	0
148149	1	0	0	0	0
148150	1	0	0	0	0
148151	1	0	0	0	0
151152	1	0	0	0	0
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157158	1	0	0	0	0
157159	1	0	0	0	0
157160	1	0	0	0	0
160161	1	0	0	0	0
160162	1	0	0	0	0
160163	1	0	0	0	0
163176	1	0	0	0	0
164165	1	0	0	0	0
164166	1	0	0	0	0
164167	1	0	0	0	0
164191	1	0	0	0	0
167168	1	0	0	0	0
168169	1	0	0	0	0
168175	2	0	0	0	0
169170	1	0	0	0	0
169171	1	0	0	0	0
169172	1	0	0	0	0
172173	1	0	0	0	0
172174	1	0	0	0	0
172211	1	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
179182	1	0	0	0	0
182183	1	0	0	0	0
182190	2	0	0	0	0
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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
187191	1	0	0	0	0
191192	1	0	0	0	0
191193	1	0	0	0	0
194195	1	0	0	0	0
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
199202	1	0	0	0	0
202203	1	0	0	0	0
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
208211	1	0	0	0	0
211225	1	0	0	0	0
212213	1	0	0	0	0
212214	1	0	0	0	0
212215	1	0	0	0	0
212240	1	0	0	0	0
215216	1	0	0	0	0
216217	1	0	0	0	0
216224	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
220223	1	0	0	0	0
225226	1	0	0	0	0
225227	1	0	0	0	0

225228 1 0 0 0 0
228229 1 0 0 0 0
228230 1 0 0 0 0
228231 1 0 0 0 0
231232 1 0 0 0 0
231239 2 0 0 0 0
232233 1 0 0 0 0
233234 1 0 0 0 0
233235 1 0 0 0 0
233236 1 0 0 0 0
236237 1 0 0 0 0
236238 1 0 0 0 0
236240 1 0 0 0 0
240241 1 0 0 0 0
240242 1 0 0 0 0

M END
> <NAME>
C32_1

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C36_1
MOE2012 3D

257256 0 0 1 0 0 0 0 0999 V2000
31.7940 17.3330 -13.9200 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.8510 17.8900 -14.7140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.8750 18.2020 -12.7980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.8260 18.7420 -12.8450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.0530 18.9220 -12.8560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.7830 17.3770 -11.5200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.8430 16.8110 -11.5200 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.5840 16.6270 -11.5140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.8720 18.2540 -10.2720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.8190 18.8090 -10.2810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.0640 18.9960 -10.2870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.7790 17.4220 -8.9900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.8300 16.8740 -8.9760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.5840 16.6770 -8.9770 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.8800 18.3050 -7.7420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.8300 18.8540 -7.7620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.0750 19.0510 -7.7570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.7890 17.4740 -6.4580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.8320 16.9380 -6.4420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.5950 16.7320 -6.4530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.8890 18.3560 -5.2950 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0
32.7730 18.8640 -5.3210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.6020 12.8750 1.2300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.4100 13.6150 1.2010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.7830 12.1010 0.4740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.5520 12.2700 2.5290 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.7030 11.6430 2.9050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.5230 11.0550 4.2810 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.2340 11.8630 4.9630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.7080 10.3260 4.2300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.8150 10.4020 4.7720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.1770 9.6500 4.0590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.5970 11.1750 4.7820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.7180 11.5650 2.2280 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.7390 17.6520 -4.0200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.5660 18.4120 -3.2480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.8340 17.0310 -4.0320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.9620 16.8210 -3.6320 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.1220 16.0080 -4.3470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.8530 17.4600 -3.6080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.7860 16.2060 -2.2660 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.9280 15.5470 -1.9160 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.8800 14.9180 -0.6280 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.6940 15.6770 0.1410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.0730 14.1760 -0.6140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.2220 14.2390 -0.3820 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.4130 13.5120 -1.1820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.0240 14.9840 -0.4560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.7770 16.2790 -1.5800 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.2600 13.5520 0.9780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.4580 12.8070 1.0500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.0660 14.2800 1.7760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.1170 11.0570 14.0520 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.9480 10.7920 14.9710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.0970 10.4670 13.2560 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.1430 9.3810 13.3820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.1260 10.8250 13.6140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

41.3130	10.8540	11.7980	C	0	0	0	0	0	0	0	0	0	0	0	0
41.3080	11.9480	11.7070	H	0	0	0	0	0	0	0	0	0	0	0	0
42.3130	10.5320	11.4830	H	0	0	0	0	0	0	0	0	0	0	0	0
40.2480	10.2420	10.8890	C	0	0	0	0	0	0	0	0	0	0	0	0
40.2610	9.1500	10.9970	H	0	0	0	0	0	0	0	0	0	0	0	0
39.2550	10.5850	11.2040	H	0	0	0	0	0	0	0	0	0	0	0	0
40.4760	10.6120	9.4210	C	0	0	0	0	0	0	0	0	0	0	0	0
40.4460	11.7030	9.3070	H	0	0	0	0	0	0	0	0	0	0	0	0
41.4750	10.2810	9.1100	H	0	0	0	0	0	0	0	0	0	0	0	0
39.4190	9.9690	8.5150	C	0	0	0	0	0	0	0	0	0	0	0	0
39.4440	8.8860	8.6790	H	0	0	0	0	0	0	0	0	0	0	0	0
38.4230	10.3230	8.8080	H	0	0	0	0	0	0	0	0	0	0	0	0
39.6720	10.2980	7.0350	C	0	0	0	0	0	0	0	0	0	0	0	0
39.7370	11.3920	6.9620	H	0	0	0	0	0	0	0	0	0	0	0	0
40.6470	9.8980	6.7250	H	0	0	0	0	0	0	0	0	0	0	0	0
38.6070	9.8300	6.1200	N	0	0	3	0	0	0	0	0	0	0	0	0
33.3910	2.2110	2.9530	C	0	0	0	0	0	0	0	0	0	0	0	0
33.6540	2.4780	1.9230	H	0	0	0	0	0	0	0	0	0	0	0	0
32.4710	2.7300	3.2450	H	0	0	0	0	0	0	0	0	0	0	0	0
33.1840	0.7960	3.0560	O	0	0	0	0	0	0	0	0	0	0	0	0
32.3220	0.2780	2.1390	C	0	0	0	0	0	0	0	0	0	0	0	0
32.1930	-1.2100	2.3350	C	0	0	0	0	0	0	0	0	0	0	0	0
33.0740	-1.5740	2.8760	H	0	0	0	0	0	0	0	0	0	0	0	0
31.3120	-1.3970	2.9590	H	0	0	0	0	0	0	0	0	0	0	0	0
32.0790	-1.9080	0.9830	C	0	0	0	0	0	0	0	0	0	0	0	0
31.1780	-1.5510	0.4690	H	0	0	0	0	0	0	0	0	0	0	0	0
32.9020	-1.5980	0.3250	H	0	0	0	0	0	0	0	0	0	0	0	0
31.7210	0.9200	1.2880	O	0	0	0	0	0	0	0	0	0	0	0	0
38.5300	8.3540	6.0930	C	0	0	0	0	0	0	0	0	0	0	0	0
39.4770	7.9280	5.7340	H	0	0	0	0	0	0	0	0	0	0	0	0
38.3880	7.9800	7.1130	H	0	0	0	0	0	0	0	0	0	0	0	0
37.3650	7.8030	5.2640	C	0	0	0	0	0	0	0	0	0	0	0	0
36.4220	8.2380	5.6120	H	0	0	0	0	0	0	0	0	0	0	0	0
37.5010	8.0240	4.2010	H	0	0	0	0	0	0	0	0	0	0	0	0
37.2690	6.3040	5.4090	C	0	0	0	0	0	0	0	0	0	0	0	0
36.2040	5.8460	4.6900	O	0	0	0	0	0	0	0	0	0	0	0	0
36.0030	4.4280	4.7630	C	0	0	0	0	0	0	0	0	0	0	0	0
36.9080	3.9100	4.4250	H	0	0	0	0	0	0	0	0	0	0	0	0
35.7840	4.1470	5.8000	H	0	0	0	0	0	0	0	0	0	0	0	0
34.8290	4.0730	3.8600	C	0	0	0	0	0	0	0	0	0	0	0	0
33.9440	4.6440	4.1690	H	0	0	0	0	0	0	0	0	0	0	0	0
35.0510	4.3960	2.8350	H	0	0	0	0	0	0	0	0	0	0	0	0
38.0280	5.6070	6.0670	O	0	0	0	0	0	0	0	0	0	0	0	0
34.5320	2.5800	3.8930	C	0	0	0	0	0	0	0	0	0	0	0	0
34.2800	2.2650	4.9140	H	0	0	0	0	0	0	0	0	0	0	0	0
35.4270	2.0080	3.6160	H	0	0	0	0	0	0	0	0	0	0	0	0
23.4580	-4.8800	0.8210	O	0	0	0	0	0	0	0	0	0	0	0	0
22.6540	-4.6290	1.3060	H	0	0	0	0	0	0	0	0	0	0	0	0
24.5520	-4.2530	1.4780	C	0	0	0	0	0	0	0	0	0	0	0	0
24.3890	-3.1700	1.4660	H	0	0	0	0	0	0	0	0	0	0	0	0
24.5770	-4.5970	2.5170	H	0	0	0	0	0	0	0	0	0	0	0	0
25.8440	-4.6150	0.7560	C	0	0	0	0	0	0	0	0	0	0	0	0
25.9590	-5.7060	0.7440	H	0	0	0	0	0	0	0	0	0	0	0	0
25.7690	-4.3100	-0.2950	H	0	0	0	0	0	0	0	0	0	0	0	0
27.0610	-3.9620	1.4110	C	0	0	0	0	0	0	0	0	0	0	0	0
26.9310	-2.8730	1.4170	H	0	0	0	0	0	0	0	0	0	0	0	0
27.1330	-4.2840	2.4570	H	0	0	0	0	0	0	0	0	0	0	0	0
28.3550	-4.3190	0.6750	C	0	0	0	0	0	0	0	0	0	0	0	0
28.4930	-5.4070	0.6810	H	0	0	0	0	0	0	0	0	0	0	0	0
28.2780	-4.0080	-0.3740	H	0	0	0	0	0	0	0	0	0	0	0	0
29.5710	-3.6420	1.3190	C	0	0	0	0	0	0	0	0	0	0	0	0
29.4040	-2.5590	1.3340	H	0	0	0	0	0	0	0	0	0	0	0	0
29.6590	-3.9670	2.3630	H	0	0	0	0	0	0	0	0	0	0	0	0
30.8660	-3.9870	0.5640	C	0	0	0	0	0	0	0	0	0	0	0	0
30.9670	-5.0800	0.5890	H	0	0	0	0	0	0	0	0	0	0	0	0
30.7850	-3.7010	-0.4920	H	0	0	0	0	0	0	0	0	0	0	0	0
32.0580	-3.3710	1.1820	N	0	0	3	0	0	0	0	0	0	0	0	0
41.4510	-4.7930	3.2330	C	0	0	0	0	0	0	0	0	0	0	0	0
41.1170	-5.1400	4.2180	H	0	0	0	0	0	0	0	0	0	0	0	0
41.6290	-3.7120	3.2650	H	0	0	0	0	0	0	0	0	0	0	0	0
42.6670	-5.4650	2.8760	O	0	0	0	0	0	0	0	0	0	0	0	0
43.6950	-5.2830	3.7550	C	0	0	0	0	0	0	0	0	0	0	0	0
44.9090	-6.0410	3.2750	C	0	0	0	0	0	0	0	0	0	0	0	0
44.6350	-7.1000	3.2340	H	0	0	0	0	0	0	0	0	0	0	0	0
45.1570	-5.6890	2.2670	H	0	0	0	0	0	0	0	0	0	0	0	0
46.1030	-5.8200	4.2130	C	0	0	0	0	0	0	0	0	0	0	0	0
46.2340	-4.7340	4.3160	H	0	0	0	0	0	0	0	0	0	0	0	0
45.8700	-6.2050	5.2150	H	0	0	0	0	0	0	0	0	0	0	0	0
43.6370	-4.6160	4.7780	O	0	0	0	0	0	0	0	0	0	0	0	0
33.2840	-4.0180	0.6670	C	0	0	0	0	0	0	0	0	0	0	0	0
33.1730	-5.1080	0.7460	H	0	0	0	0	0	0	0	0	0	0	0	0

33.4200	-3.7960	-0.4000	H	0	0	0	0	0	0	0	0	0	0	0	0
34.5350	-3.6300	1.4610	C	0	0	0	0	0	0	0	0	0	0	0	0
34.7560	-2.5640	1.3540	H	0	0	0	0	0	0	0	0	0	0	0	0
34.3850	-3.8640	2.5210	H	0	0	0	0	0	0	0	0	0	0	0	0
35.7420	-4.3920	0.9770	C	0	0	0	0	0	0	0	0	0	0	0	0
36.8000	-4.1220	1.7940	O	0	0	0	0	0	0	0	0	0	0	0	0
38.0160	-4.7920	1.4340	C	0	0	0	0	0	0	0	0	0	0	0	0
37.8460	-5.8750	1.4140	H	0	0	0	0	0	0	0	0	0	0	0	0
38.3370	-4.4520	0.4430	H	0	0	0	0	0	0	0	0	0	0	0	0
39.0700	-4.4470	2.4790	C	0	0	0	0	0	0	0	0	0	0	0	0
39.1970	-3.3580	2.5210	H	0	0	0	0	0	0	0	0	0	0	0	0
38.7080	-4.7450	3.4710	H	0	0	0	0	0	0	0	0	0	0	0	0
35.7740	-5.1240	-0.0020	O	0	0	0	0	0	0	0	0	0	0	0	0
40.4020	-5.1230	2.1780	C	0	0	0	0	0	0	0	0	0	0	0	0
40.7700	-4.8160	1.1910	H	0	0	0	0	0	0	0	0	0	0	0	0
40.2730	-6.2120	2.1240	H	0	0	0	0	0	0	0	0	0	0	0	0
50.8850	-14.2270	2.0000	O	0	0	0	0	0	0	0	0	0	0	0	0
51.7750	-14.5860	1.8400	H	0	0	0	0	0	0	0	0	0	0	0	0
51.0200	-12.8170	2.0990	C	0	0	0	0	0	0	0	0	0	0	0	0
51.7650	-12.5920	2.8690	H	0	0	0	0	0	0	0	0	0	0	0	0
51.3740	-12.4330	1.1380	H	0	0	0	0	0	0	0	0	0	0	0	0
49.6680	-12.2150	2.4620	C	0	0	0	0	0	0	0	0	0	0	0	0
48.9240	-12.5010	1.7090	H	0	0	0	0	0	0	0	0	0	0	0	0
49.3210	-12.6480	3.4080	H	0	0	0	0	0	0	0	0	0	0	0	0
49.7560	-10.6970	2.5730	C	0	0	0	0	0	0	0	0	0	0	0	0
50.5340	-10.4310	3.3000	H	0	0	0	0	0	0	0	0	0	0	0	0
50.0650	-10.2770	1.6070	H	0	0	0	0	0	0	0	0	0	0	0	0
48.4260	-10.0720	3.0010	C	0	0	0	0	0	0	0	0	0	0	0	0
47.6450	-10.3160	2.2720	H	0	0	0	0	0	0	0	0	0	0	0	0
48.1170	-10.4900	3.9670	H	0	0	0	0	0	0	0	0	0	0	0	0
48.5730	-8.5530	3.1190	C	0	0	0	0	0	0	0	0	0	0	0	0
49.4120	-8.3500	3.7930	H	0	0	0	0	0	0	0	0	0	0	0	0
48.8270	-8.1420	2.1340	H	0	0	0	0	0	0	0	0	0	0	0	0
47.2970	-7.8790	3.6440	C	0	0	0	0	0	0	0	0	0	0	0	0
46.4900	-8.1650	2.9600	H	0	0	0	0	0	0	0	0	0	0	0	0
47.0480	-8.2930	4.6300	H	0	0	0	0	0	0	0	0	0	0	0	0
47.3740	-6.3990	3.7170	N	0	0	3	0	0	0	0	0	0	0	0	0
54.1570	-9.2830	8.0380	C	0	0	0	0	0	0	0	0	0	0	0	0
54.3570	-10.0300	7.2610	H	0	0	0	0	0	0	0	0	0	0	0	0
53.2770	-9.5820	8.6200	H	0	0	0	0	0	0	0	0	0	0	0	0
55.2950	-9.1800	8.9060	O	0	0	0	0	0	0	0	0	0	0	0	0
55.6100	-10.3250	9.5780	C	0	0	0	0	0	0	0	0	0	0	0	0
56.8130	-10.0760	10.4580	C	0	0	0	0	0	0	0	0	0	0	0	0
57.6180	-9.7230	9.8060	H	0	0	0	0	0	0	0	0	0	0	0	0
56.5580	-9.2880	11.1740	H	0	0	0	0	0	0	0	0	0	0	0	0
57.2290	-11.3520	11.2000	C	0	0	0	0	0	0	0	0	0	0	0	0
56.4130	-11.6550	11.8710	H	0	0	0	0	0	0	0	0	0	0	0	0
57.2990	-12.1890	10.4940	H	0	0	0	0	0	0	0	0	0	0	0	0
55.0100	-11.3860	9.4760	O	0	0	0	0	0	0	0	0	0	0	0	0
48.4990	-5.9510	4.5670	C	0	0	0	0	0	0	0	0	0	0	0	0
48.2220	-5.0650	5.1570	H	0	0	0	0	0	0	0	0	0	0	0	0
48.7580	-6.7080	5.3190	H	0	0	0	0	0	0	0	0	0	0	0	0
49.6980	-5.5420	3.7110	C	0	0	0	0	0	0	0	0	0	0	0	0
49.9380	-6.2550	2.9180	H	0	0	0	0	0	0	0	0	0	0	0	0
49.4940	-4.5870	3.2110	H	0	0	0	0	0	0	0	0	0	0	0	0
50.9280	-5.3790	4.5620	C	0	0	0	0	0	0	0	0	0	0	0	0
51.3430	-6.5870	5.0380	O	0	0	0	0	0	0	0	0	0	0	0	0
52.5010	-6.5230	5.8810	C	0	0	0	0	0	0	0	0	0	0	0	0
53.3660	-6.2170	5.2810	H	0	0	0	0	0	0	0	0	0	0	0	0
52.3360	-5.7960	6.6840	H	0	0	0	0	0	0	0	0	0	0	0	0
52.7310	-7.9080	6.4730	C	0	0	0	0	0	0	0	0	0	0	0	0
51.8290	-8.2280	7.0100	H	0	0	0	0	0	0	0	0	0	0	0	0
52.8730	-8.6340	5.6630	H	0	0	0	0	0	0	0	0	0	0	0	0
51.4760	-4.3070	4.7790	O	0	0	0	0	0	0	0	0	0	0	0	0
53.9330	-7.9140	7.4090	C	0	0	0	0	0	0	0	0	0	0	0	0
53.7980	-7.1700	8.2050	H	0	0	0	0	0	0	0	0	0	0	0	0
54.8380	-7.6100	6.8670	H	0	0	0	0	0	0	0	0	0	0	0	0
63.7770	-12.1250	5.0610	O	0	0	0	0	0	0	0	0	0	0	0	0
63.8230	-12.6450	4.2410	H	0	0	0	0	0	0	0	0	0	0	0	0
62.6420	-12.5860	5.7810	C	0	0	0	0	0	0	0	0	0	0	0	0
61.7540	-12.4430	5.1570	H	0	0	0	0	0	0	0	0	0	0	0	0
62.7670	-13.6550	5.9830	H	0	0	0	0	0	0	0	0	0	0	0	0
62.5250	-11.8000	7.0810	C	0	0	0	0	0	0	0	0	0	0	0	0
63.4390	-11.9340	7.6730	H	0	0	0	0	0	0	0	0	0	0	0	0
62.4720	-10.7280	6.8510	H	0	0	0	0	0	0	0	0	0	0	0	0
61.3020	-12.2300	7.8870	C	0	0	0	0	0	0	0	0	0	0	0	0
60.4020	-12.1080	7.2710	H	0	0	0	0	0	0	0	0	0	0	0	0
61.3790	-13.2950	8.1360	H	0	0	0	0	0	0	0	0	0	0	0	0
61.1540	-11.4120	9.1720	C	0	0	0	0	0	0	0	0	0	0	0	0
62.0290	-11.5690	9.8140	H	0	0	0	0	0	0	0	0	0	0	0	0
61.1200	-10.3440	8.9240	H	0	0	0	0	0	0	0	0	0	0	0	0

59.8790	-11.8020	9.9270	C	0	0	0	0	0	0	0	0	0	0	0	0	0
59.0330	-11.6960	9.2380	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.9330	-12.8580	10.2190	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.6710	-10.9270	11.1750	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.5680	-11.0450	11.7920	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.6320	-9.8720	10.8790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.4840	-11.2840	11.9770	N	0	0	3	0	0	0	0	0	0	0	0	0	0
62.0610	-9.8600	20.9180	C	0	0	0	0	0	0	0	0	0	0	0	0	0
63.0440	-9.6240	20.4940	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.9770	-10.9420	21.0720	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.9080	-9.1850	22.1740	O	0	0	0	0	0	0	0	0	0	0	0	0	0
62.8390	-9.5230	23.1130	C	0	0	0	0	0	0	0	0	0	0	0	0	0
62.5690	-8.7500	24.3810	C	0	0	0	0	0	0	0	0	0	0	0	0	0
62.6130	-7.6800	24.1510	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5620	-9.0000	24.7320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.5760	-9.0720	25.4710	C	0	0	0	0	0	0	0	0	0	0	0	0	0
63.5520	-10.1360	25.7270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.3560	-8.4970	26.3760	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.5950	-8.8280	25.1500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.7460	-10.3260	22.9490	O	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3390	-10.4270	13.1720	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3230	-9.3660	12.8910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.3710	-10.6360	13.6470	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.4280	-10.6800	14.2210	C	0	0	0	0	0	0	0	0	0	0	0	0	0
59.4600	-11.7460	14.4720	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4100	-10.3650	13.8520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.1590	-9.9070	15.4900	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0890	-10.2400	16.4330	O	0	0	0	0	0	0	0	0	0	0	0	0	0
59.9380	-9.5600	17.6870	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0250	-8.4790	17.5290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.9550	-9.7920	18.1120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.0410	-10.0460	18.6200	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9730	-11.1350	18.7270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.0180	-9.8500	18.1600	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.2560	-9.0970	15.6450	O	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9570	-9.3750	19.9860	C	0	0	0	0	0	0	0	0	0	0	0	0	0
59.9810	-9.5710	20.4460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.0250	-8.2850	19.8790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
C36_1

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$$$$
C75_1
MOE2012 3D

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262261 0 0 1 0 0 0 0 0999 V2000
40.6880 23.1630 -19.2190 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.6200 23.0090 -19.4100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.2500 22.7520 -20.0630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.8710 24.2420 -19.1960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.1020 22.5370 -17.8900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.1730 22.6990 -17.7140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.5640 23.0880 -17.1080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.7610 21.1060 -17.8070 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.8780 20.6380 -16.4090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.9320 20.6120 -16.1000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.3720 21.3530 -15.7470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.2140 19.2630 -16.1730 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.1570 19.3270 -16.4580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.6870 18.4970 -16.7980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.3230 18.8690 -14.7600 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
41.3080 18.8090 -14.5020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.5690 20.2900 -18.7300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.3180 20.8860 -19.2640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.1470 19.5190 -18.2050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.6580 19.6150 -19.7470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
40.1070 20.3520 -20.3410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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43.7270	1.4720	16.6700	C	0	0	0	0	0	0	0	0	0	0	0
44.4390	2.2710	17.7340	C	0	0	0	0	0	0	0	0	0	0	0
44.8630	1.5700	18.4610	H	0	0	0	0	0	0	0	0	0	0	0
45.2590	2.8110	17.2510	H	0	0	0	0	0	0	0	0	0	0	0
43.4710	3.2410	18.4250	C	0	0	0	0	0	0	0	0	0	0	0
42.9560	3.8710	17.6880	H	0	0	0	0	0	0	0	0	0	0	0
42.6920	2.6330	18.9000	H	0	0	0	0	0	0	0	0	0	0	0
42.5160	1.3170	16.6030	O	0	0	0	0	0	0	0	0	0	0	0
46.3040	-3.8440	7.4810	C	0	0	0	0	0	0	0	0	0	0	0
47.1430	-4.3900	7.9290	H	0	0	0	0	0	0	0	0	0	0	0
46.7440	-2.9600	7.0020	H	0	0	0	0	0	0	0	0	0	0	0
45.3640	-3.4450	8.6210	C	0	0	0	0	0	0	0	0	0	0	0
44.5210	-2.8520	8.2530	H	0	0	0	0	0	0	0	0	0	0	0
44.9780	-4.3440	9.1160	H	0	0	0	0	0	0	0	0	0	0	0
46.0880	-2.6170	9.6490	C	0	0	0	0	0	0	0	0	0	0	0
45.2220	-2.2900	10.6500	O	0	0	0	0	0	0	0	0	0	0	0
45.7940	-1.4890	11.6910	C	0	0	0	0	0	0	0	0	0	0	0
46.5680	-2.0680	12.2080	H	0	0	0	0	0	0	0	0	0	0	0
46.2380	-0.5830	11.2610	H	0	0	0	0	0	0	0	0	0	0	0
44.6790	-1.1140	12.6590	C	0	0	0	0	0	0	0	0	0	0	0
43.8930	-0.5760	12.1130	H	0	0	0	0	0	0	0	0	0	0	0
44.2060	-2.0270	13.0420	H	0	0	0	0	0	0	0	0	0	0	0
47.2630	-2.2850	9.5930	O	0	0	0	0	0	0	0	0	0	0	0
45.1970	-0.2640	13.8130	C	0	0	0	0	0	0	0	0	0	0	0
45.6950	0.6350	13.4300	H	0	0	0	0	0	0	0	0	0	0	0
45.9600	-0.8130	14.3770	H	0	0	0	0	0	0	0	0	0	0	0
48.3880	8.6370	19.5790	C	0	0	0	0	0	0	0	0	0	0	0
47.6060	9.3350	19.2610	H	0	0	0	0	0	0	0	0	0	0	0
49.0830	8.4950	18.7460	H	0	0	0	0	0	0	0	0	0	0	0
48.9450	9.1090	20.3950	H	0	0	0	0	0	0	0	0	0	0	0
47.7840	7.3190	20.0580	C	0	0	0	0	0	0	0	0	0	0	0
48.5800	6.6320	20.3700	H	0	0	0	0	0	0	0	0	0	0	0
47.1990	7.5570	20.9550	H	0	0	0	0	0	0	0	0	0	0	0
46.9080	6.6950	19.0510	N	0	0	0	0	0	0	0	0	0	0	0
46.1200	5.6080	19.6710	C	0	0	0	0	0	0	0	0	0	0	0
46.7640	4.7470	19.8970	H	0	0	0	0	0	0	0	0	0	0	0
45.7230	5.9620	20.6290	H	0	0	0	0	0	0	0	0	0	0	0
44.9230	5.1660	18.7950	C	0	0	0	0	0	0	0	0	0	0	0
44.2720	6.0220	18.5700	H	0	0	0	0	0	0	0	0	0	0	0
45.3150	4.8330	17.8300	H	0	0	0	0	0	0	0	0	0	0	0
44.1530	4.0740	19.4400	N	0	0	3	0	0	0	0	0	0	0	0
47.6670	6.2230	17.8790	C	0	0	0	0	0	0	0	0	0	0	0
48.7490	6.3430	18.0100	H	0	0	0	0	0	0	0	0	0	0	0
47.5250	5.1510	17.6960	H	0	0	0	0	0	0	0	0	0	0	0
47.2270	6.9940	16.6410	C	0	0	0	0	0	0	0	0	0	0	0
47.4120	8.0670	16.7500	H	0	0	0	0	0	0	0	0	0	0	0
46.1610	6.8490	16.4390	H	0	0	0	0	0	0	0	0	0	0	0
47.7840	6.6460	15.7650	H	0	0	0	0	0	0	0	0	0	0	0
40.0060	2.3790	28.0510	C	0	0	0	0	0	0	0	0	0	0	0
41.0110	2.1660	28.4330	H	0	0	0	0	0	0	0	0	0	0	0
39.5530	1.4570	27.6690	H	0	0	0	0	0	0	0	0	0	0	0
39.1950	2.9060	29.1100	O	0	0	0	0	0	0	0	0	0	0	0
39.0400	2.0660	30.1740	C	0	0	0	0	0	0	0	0	0	0	0
38.1710	2.7330	31.2130	C	0	0	0	0	0	0	0	0	0	0	0
38.6570	3.6630	31.5260	H	0	0	0	0	0	0	0	0	0	0	0
37.2050	2.9700	30.7550	H	0	0	0	0	0	0	0	0	0	0	0
37.9490	1.8470	32.4260	C	0	0	0	0	0	0	0	0	0	0	0
37.4590	0.9090	32.1440	H	0	0	0	0	0	0	0	0	0	0	0
37.3160	2.3560	33.1590	H	0	0	0	0	0	0	0	0	0	0	0
38.8990	1.5960	32.9090	H	0	0	0	0	0	0	0	0	0	0	0
39.5300	0.9490	30.2680	O	0	0	0	0	0	0	0	0	0	0	0
43.1770	4.6470	20.3960	C	0	0	0	0	0	0	0	0	0	0	0
43.6110	5.5170	20.9050	H	0	0	0	0	0	0	0	0	0	0	0
42.2890	5.0240	19.8690	H	0	0	0	0	0	0	0	0	0	0	0
42.7800	3.6440	21.4820	C	0	0	0	0	0	0	0	0	0	0	0
42.2140	2.8060	21.0650	H	0	0	0	0	0	0	0	0	0	0	0
43.6830	3.2600	21.9710	H	0	0	0	0	0	0	0	0	0	0	0
41.9220	4.3070	22.5330	C	0	0	0	0	0	0	0	0	0	0	0
41.7890	3.4740	23.6040	O	0	0	0	0	0	0	0	0	0	0	0
40.9830	3.9990	24.6670	C	0	0	0	0	0	0	0	0	0	0	0
41.4370	4.9220	25.0470	H	0	0	0	0	0	0	0	0	0	0	0
39.9760	4.2120	24.2910	H	0	0	0	0	0	0	0	0	0	0	0
40.9190	2.9510	25.7720	C	0	0	0	0	0	0	0	0	0	0	0
40.5120	2.0180	25.3640	H	0	0	0	0	0	0	0	0	0	0	0
41.9370	2.7140	26.1070	H	0	0	0	0	0	0	0	0	0	0	0
41.4120	5.4150	22.4360	O	0	0	0	0	0	0	0	0	0	0	0
40.0740	3.4270	26.9470	C	0	0	0	0	0	0	0	0	0	0	0
39.0570	3.6670	26.6120	H	0	0	0	0	0	0	0	0	0	0	0
40.4830	4.3600	27.3570	H	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
C75_1

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C80_1
MOE2012 3D

247246 0 0 1 0 0 0 0 0999 V2000
10.4170 24.0650 -10.4320 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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8.7780 23.2030 -8.5870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.8140 22.0060 -7.8470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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17.7520 11.9800 -11.6090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.4100 11.3280 -9.9750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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20.4330 9.0060 -11.2490 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.1030 9.5140 -11.9510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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18.1630 15.2810 -8.2380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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21.0760 4.7610 -15.1100 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

21.1060	5.0980	-16.1540	H	0	0	0	0	0	0	0	0	0	0	0
20.0470	4.4280	-14.9200	H	0	0	0	0	0	0	0	0	0	0	0
21.3320	5.9700	-14.1930	C	0	0	0	0	0	0	0	0	0	0	0
22.3050	6.4220	-14.4200	H	0	0	0	0	0	0	0	0	0	0	0
20.5820	6.7310	-14.4370	H	0	0	0	0	0	0	0	0	0	0	0
21.2620	5.6090	-12.7010	C	0	0	0	0	0	0	0	0	0	0	0
20.3040	5.1280	-12.4620	H	0	0	0	0	0	0	0	0	0	0	0
22.0320	4.8560	-12.5110	H	0	0	0	0	0	0	0	0	0	0	0
23.3670	3.9540	-15.2810	C	0	0	0	0	0	0	0	0	0	0	0
23.4460	4.2910	-16.3210	H	0	0	0	0	0	0	0	0	0	0	0
24.0190	3.0830	-15.1530	H	0	0	0	0	0	0	0	0	0	0	0
23.7770	4.7330	-14.6300	H	0	0	0	0	0	0	0	0	0	0	0
21.4800	6.8000	-11.8420	N	0	0	3	0	0	0	0	0	0	0	0
29.4880	3.4550	-7.4220	C	0	0	0	0	0	0	0	0	0	0	0
30.0920	4.2580	-7.8600	H	0	0	0	0	0	0	0	0	0	0	0
29.4450	2.6060	-8.1140	H	0	0	0	0	0	0	0	0	0	0	0
30.0830	3.0370	-6.1840	O	0	0	0	0	0	0	0	0	0	0	0
31.3280	2.4910	-6.3080	C	0	0	0	0	0	0	0	0	0	0	0
31.8410	2.0790	-4.9480	C	0	0	0	0	0	0	0	0	0	0	0
31.9520	2.9820	-4.3380	H	0	0	0	0	0	0	0	0	0	0	0
31.0830	1.4260	-4.5030	H	0	0	0	0	0	0	0	0	0	0	0
33.1870	1.3480	-5.0580	C	0	0	0	0	0	0	0	0	0	0	0
33.0720	0.4600	-5.6950	H	0	0	0	0	0	0	0	0	0	0	0
33.8710	2.0230	-5.5860	H	0	0	0	0	0	0	0	0	0	0	0
31.9370	2.3540	-7.3590	O	0	0	0	0	0	0	0	0	0	0	0
22.0140	6.3920	-10.5220	C	0	0	0	0	0	0	0	0	0	0	0
21.8940	7.2050	-9.7970	H	0	0	0	0	0	0	0	0	0	0	0
21.4450	5.5430	-10.1190	H	0	0	0	0	0	0	0	0	0	0	0
23.5130	6.0650	-10.5810	C	0	0	0	0	0	0	0	0	0	0	0
23.7100	5.2320	-11.2620	H	0	0	0	0	0	0	0	0	0	0	0
24.0720	6.9440	-10.9230	H	0	0	0	0	0	0	0	0	0	0	0
24.0360	5.6740	-9.2200	C	0	0	0	0	0	0	0	0	0	0	0
25.3400	5.2840	-9.3250	O	0	0	0	0	0	0	0	0	0	0	0
25.9460	4.8880	-8.0860	C	0	0	0	0	0	0	0	0	0	0	0
25.9700	5.7460	-7.4040	H	0	0	0	0	0	0	0	0	0	0	0
25.3630	4.0760	-7.6350	H	0	0	0	0	0	0	0	0	0	0	0
27.3620	4.4110	-8.3850	C	0	0	0	0	0	0	0	0	0	0	0
27.3210	3.5920	-9.1140	H	0	0	0	0	0	0	0	0	0	0	0
27.9230	5.2180	-8.8720	H	0	0	0	0	0	0	0	0	0	0	0
23.3930	5.7080	-8.1810	O	0	0	0	0	0	0	0	0	0	0	0
28.0810	3.9560	-7.1200	C	0	0	0	0	0	0	0	0	0	0	0
27.5110	3.1590	-6.6250	H	0	0	0	0	0	0	0	0	0	0	0
28.1350	4.7790	-6.3970	H	0	0	0	0	0	0	0	0	0	0	0
29.4760	-0.3000	0.5150	C	0	0	0	0	0	0	0	0	0	0	0
28.8480	0.2270	1.2420	H	0	0	0	0	0	0	0	0	0	0	0
29.9190	-1.1720	1.0090	H	0	0	0	0	0	0	0	0	0	0	0
28.8050	-0.6540	-0.2760	H	0	0	0	0	0	0	0	0	0	0	0
30.4940	0.6000	-0.0360	N	0	0	0	0	0	0	0	0	0	0	0
31.2890	-0.1060	-1.0570	C	0	0	0	0	0	0	0	0	0	0	0
31.8680	-0.9210	-0.6040	H	0	0	0	0	0	0	0	0	0	0	0
30.6010	-0.5670	-1.7780	H	0	0	0	0	0	0	0	0	0	0	0
32.2250	0.8230	-1.8450	C	0	0	0	0	0	0	0	0	0	0	0
31.6490	1.6690	-2.2340	H	0	0	0	0	0	0	0	0	0	0	0
32.9970	1.2360	-1.1850	H	0	0	0	0	0	0	0	0	0	0	0
32.9150	0.0610	-2.9860	C	0	0	0	0	0	0	0	0	0	0	0
33.4920	-0.7540	-2.5280	H	0	0	0	0	0	0	0	0	0	0	0
32.1800	-0.4380	-3.6300	H	0	0	0	0	0	0	0	0	0	0	0
31.3300	1.1220	1.0480	C	0	0	0	0	0	0	0	0	0	0	0
31.9200	0.3350	1.5310	H	0	0	0	0	0	0	0	0	0	0	0
30.7100	1.6030	1.8130	H	0	0	0	0	0	0	0	0	0	0	0
32.0120	1.8970	0.6860	H	0	0	0	0	0	0	0	0	0	0	0
33.7910	0.9690	-3.7590	N	0	0	3	0	0	0	0	0	0	0	0
43.2340	2.9520	-5.1150	C	0	0	0	0	0	0	0	0	0	0	0
43.1340	3.6700	-4.2940	H	0	0	0	0	0	0	0	0	0	0	0
43.0310	3.4520	-6.0690	H	0	0	0	0	0	0	0	0	0	0	0
44.5690	2.4240	-5.1320	O	0	0	0	0	0	0	0	0	0	0	0
45.5530	3.3620	-5.2560	C	0	0	0	0	0	0	0	0	0	0	0
46.9030	2.6840	-5.2760	C	0	0	0	0	0	0	0	0	0	0	0
46.9410	1.9710	-4.4440	H	0	0	0	0	0	0	0	0	0	0	0
46.9790	2.1400	-6.2230	H	0	0	0	0	0	0	0	0	0	0	0
48.0420	3.7020	-5.1310	C	0	0	0	0	0	0	0	0	0	0	0
48.0400	4.3870	-5.9880	H	0	0	0	0	0	0	0	0	0	0	0
47.8210	4.3140	-4.2460	H	0	0	0	0	0	0	0	0	0	0	0
45.3720	4.5670	-5.3590	O	0	0	0	0	0	0	0	0	0	0	0
35.1230	0.3440	-3.9420	C	0	0	0	0	0	0	0	0	0	0	0
35.4720	-0.0240	-2.9670	H	0	0	0	0	0	0	0	0	0	0	0
35.0490	-0.5330	-4.5990	H	0	0	0	0	0	0	0	0	0	0	0
36.2020	1.3030	-4.4590	C	0	0	0	0	0	0	0	0	0	0	0
36.0050	1.6020	-5.4930	H	0	0	0	0	0	0	0	0	0	0	0
36.2320	2.1960	-3.8230	H	0	0	0	0	0	0	0	0	0	0	0
37.5660	0.6520	-4.4270	C	0	0	0	0	0	0	0	0	0	0	0

64.4720	7.4150	-14.4260	H	0	0	0	0	0	0	0	0	0	0	0	0
64.5600	8.1120	-16.3780	O	0	0	0	0	0	0	0	0	0	0	0	0
64.9300	6.9410	-16.9720	C	0	0	0	0	0	0	0	0	0	0	0	0
65.6710	7.2450	-18.2520	C	0	0	0	0	0	0	0	0	0	0	0	0
65.0100	7.8220	-18.9070	H	0	0	0	0	0	0	0	0	0	0	0	0
66.5510	7.8490	-18.0080	H	0	0	0	0	0	0	0	0	0	0	0	0
66.1120	5.9810	-18.9700	C	0	0	0	0	0	0	0	0	0	0	0	0
66.7790	5.3830	-18.3400	H	0	0	0	0	0	0	0	0	0	0	0	0
66.6450	6.2320	-19.8910	H	0	0	0	0	0	0	0	0	0	0	0	0
65.2510	5.3560	-19.2310	H	0	0	0	0	0	0	0	0	0	0	0	0
64.6960	5.8240	-16.5340	O	0	0	0	0	0	0	0	0	0	0	0	0
60.0380	12.6570	-9.0400	C	0	0	0	0	0	0	0	0	0	0	0	0
59.4120	13.1470	-9.7990	H	0	0	0	0	0	0	0	0	0	0	0	0
60.8540	13.3580	-8.8250	H	0	0	0	0	0	0	0	0	0	0	0	0
60.5940	11.3760	-9.6650	C	0	0	0	0	0	0	0	0	0	0	0	0
61.3180	10.8950	-8.9990	H	0	0	0	0	0	0	0	0	0	0	0	0
59.7750	10.6800	-9.8780	H	0	0	0	0	0	0	0	0	0	0	0	0
61.3130	11.6740	-10.9540	C	0	0	0	0	0	0	0	0	0	0	0	0
61.6860	10.5020	-11.5410	O	0	0	0	0	0	0	0	0	0	0	0	0
62.4020	10.6580	-12.7720	C	0	0	0	0	0	0	0	0	0	0	0	0
61.7750	11.1940	-13.4940	H	0	0	0	0	0	0	0	0	0	0	0	0
63.3220	11.2270	-12.5900	H	0	0	0	0	0	0	0	0	0	0	0	0
62.7400	9.2690	-13.3010	C	0	0	0	0	0	0	0	0	0	0	0	0
63.3260	8.7270	-12.5480	H	0	0	0	0	0	0	0	0	0	0	0	0
61.8140	8.6950	-13.4310	H	0	0	0	0	0	0	0	0	0	0	0	0
61.5450	12.7910	-11.3930	O	0	0	0	0	0	0	0	0	0	0	0	0
63.5060	9.3410	-14.6160	C	0	0	0	0	0	0	0	0	0	0	0	0
64.4330	9.9150	-14.4850	H	0	0	0	0	0	0	0	0	0	0	0	0
62.9210	9.8840	-15.3680	H	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
C80_1

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$$$$
C86_1
MOE2012 3D

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16.2060 -17.3600 20.2130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.3220 -17.2070 19.5780 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.0930 -18.3680 20.6340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.4240 -17.2710 19.3770 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.2980 -18.2110 18.2400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.4570 -19.2460 18.5710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.2760 -18.1640 17.8390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.2450 -17.8520 17.0760 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.0270 -16.8240 16.7650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.2910 -17.8890 17.4000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.0450 -18.7860 15.9600 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
18.3210 -19.7210 16.2640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.6470 -17.5400 20.1610 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.4280 -18.0740 21.0950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.3340 -18.2130 19.6320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.1160 -16.3260 21.3420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.8890 -16.4890 22.0980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.2080 -15.3100 20.9450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.8490 -16.4420 21.9820 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.8210 -15.7690 22.6850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.4160 -16.2490 20.4550 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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18.7950 -15.5160 20.9760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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19.1860 -10.7350 5.4610 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.2450 -10.6210 5.7130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.0620 -11.5950 4.7950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.6480 -9.4630 4.8000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.5700 -9.5780 4.6190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.7020 -8.6280 5.5100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.5290 -10.3530 7.1990 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.8290 -18.4290 14.7740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8770 -18.2400 15.0390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.8360 -19.3020 14.1090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


42.0260	-4.6300	9.9780	C	0	0	0	0	0	0	0	0	0	0	0	0
41.4970	-3.6940	9.7650	H	0	0	0	0	0	0	0	0	0	0	0	0
41.2680	-5.4180	10.0200	H	0	0	0	0	0	0	0	0	0	0	0	0
42.6480	-4.5520	11.3420	C	0	0	0	0	0	0	0	0	0	0	0	0
43.1710	-3.3120	11.5410	O	0	0	0	0	0	0	0	0	0	0	0	0
43.8650	-3.1420	12.7820	C	0	0	0	0	0	0	0	0	0	0	0	0
43.1410	-3.1530	13.6040	H	0	0	0	0	0	0	0	0	0	0	0	0
44.5870	-3.9560	12.9190	H	0	0	0	0	0	0	0	0	0	0	0	0
44.5930	-1.8050	12.7290	C	0	0	0	0	0	0	0	0	0	0	0	0
45.2240	-1.7710	11.8320	H	0	0	0	0	0	0	0	0	0	0	0	0
43.8630	-0.9940	12.6130	H	0	0	0	0	0	0	0	0	0	0	0	0
42.6970	-5.4880	12.1290	O	0	0	0	0	0	0	0	0	0	0	0	0
45.4390	-1.5860	13.9760	C	0	0	0	0	0	0	0	0	0	0	0	0
46.1500	-2.4130	14.1000	H	0	0	0	0	0	0	0	0	0	0	0	0
44.8070	-1.5990	14.8730	H	0	0	0	0	0	0	0	0	0	0	0	0
45.3920	6.3870	15.7150	C	0	0	0	0	0	0	0	0	0	0	0	0
45.6760	6.8280	16.6800	H	0	0	0	0	0	0	0	0	0	0	0	0
46.2350	6.5910	15.0400	H	0	0	0	0	0	0	0	0	0	0	0	0
45.1950	4.9300	15.8880	N	0	0	0	0	0	0	0	0	0	0	0	0
46.4110	4.3530	16.5100	C	0	0	0	0	0	0	0	0	0	0	0	0
47.2230	4.3040	15.7740	H	0	0	0	0	0	0	0	0	0	0	0	0
46.7530	5.0160	17.3160	H	0	0	0	0	0	0	0	0	0	0	0	0
46.1430	2.9730	17.1600	C	0	0	0	0	0	0	0	0	0	0	0	0
45.2530	3.1020	17.7860	H	0	0	0	0	0	0	0	0	0	0	0	0
45.8690	2.2240	16.4110	H	0	0	0	0	0	0	0	0	0	0	0	0
47.2630	2.5000	17.9980	N	0	0	3	0	0	0	0	0	0	0	0	0
44.8850	4.2640	14.6060	C	0	0	0	0	0	0	0	0	0	0	0	0
45.2030	4.8630	13.7420	H	0	0	0	0	0	0	0	0	0	0	0	0
45.4360	3.3220	14.4890	H	0	0	0	0	0	0	0	0	0	0	0	0
44.1580	7.1580	15.2310	C	0	0	0	0	0	0	0	0	0	0	0	0
43.8860	6.8790	14.2090	H	0	0	0	0	0	0	0	0	0	0	0	0
43.3060	6.9810	15.8940	H	0	0	0	0	0	0	0	0	0	0	0	0
44.4460	8.5540	15.2380	O	0	0	0	0	0	0	0	0	0	0	0	0
43.6440	9.0160	14.9350	H	0	0	0	0	0	0	0	0	0	0	0	0
43.3950	3.9260	14.5030	C	0	0	0	0	0	0	0	0	0	0	0	0
43.1140	3.1940	15.2670	H	0	0	0	0	0	0	0	0	0	0	0	0
42.7660	4.8120	14.6190	H	0	0	0	0	0	0	0	0	0	0	0	0
43.1260	3.3630	13.2210	O	0	0	0	0	0	0	0	0	0	0	0	0
42.1810	3.1370	13.2040	H	0	0	0	0	0	0	0	0	0	0	0	0
43.1160	0.8450	26.6250	C	0	0	0	0	0	0	0	0	0	0	0	0
42.2060	1.3570	26.2890	H	0	0	0	0	0	0	0	0	0	0	0	0
43.8120	1.5750	27.0540	H	0	0	0	0	0	0	0	0	0	0	0	0
42.7750	-0.1320	27.6180	O	0	0	0	0	0	0	0	0	0	0	0	0
42.1730	0.3800	28.7300	C	0	0	0	0	0	0	0	0	0	0	0	0
41.8680	-0.7430	29.6920	C	0	0	0	0	0	0	0	0	0	0	0	0
41.2140	-1.4630	29.1880	H	0	0	0	0	0	0	0	0	0	0	0	0
42.8080	-1.2370	29.9580	H	0	0	0	0	0	0	0	0	0	0	0	0
41.1870	-0.2440	30.9540	C	0	0	0	0	0	0	0	0	0	0	0	0
41.8190	0.4760	31.4840	H	0	0	0	0	0	0	0	0	0	0	0	0
40.9780	-1.0780	31.6310	H	0	0	0	0	0	0	0	0	0	0	0	0
40.2390	0.2520	30.7200	H	0	0	0	0	0	0	0	0	0	0	0	0
41.9220	1.5620	28.9150	O	0	0	0	0	0	0	0	0	0	0	0	0
46.8670	1.4120	18.9080	C	0	0	0	0	0	0	0	0	0	0	0	0
46.3130	0.6320	18.3700	H	0	0	0	0	0	0	0	0	0	0	0	0
47.7670	0.9300	19.3160	H	0	0	0	0	0	0	0	0	0	0	0	0
46.0550	1.9260	20.1000	C	0	0	0	0	0	0	0	0	0	0	0	0
46.6260	2.6990	20.6280	H	0	0	0	0	0	0	0	0	0	0	0	0
45.0960	2.3440	19.7810	H	0	0	0	0	0	0	0	0	0	0	0	0
45.7600	0.8110	21.0700	C	0	0	0	0	0	0	0	0	0	0	0	0
45.1640	1.3270	22.1830	O	0	0	0	0	0	0	0	0	0	0	0	0
44.8220	0.3530	23.1780	C	0	0	0	0	0	0	0	0	0	0	0	0
44.1240	-0.3760	22.7510	H	0	0	0	0	0	0	0	0	0	0	0	0
45.7300	-0.1600	23.5140	H	0	0	0	0	0	0	0	0	0	0	0	0
44.1690	1.0830	24.3460	C	0	0	0	0	0	0	0	0	0	0	0	0
44.8600	1.8420	24.7320	H	0	0	0	0	0	0	0	0	0	0	0	0
43.2900	1.6320	23.9860	H	0	0	0	0	0	0	0	0	0	0	0	0
46.0020	-0.3730	20.8820	O	0	0	0	0	0	0	0	0	0	0	0	0
43.7700	0.1180	25.4570	C	0	0	0	0	0	0	0	0	0	0	0	0
44.6490	-0.4310	25.8170	H	0	0	0	0	0	0	0	0	0	0	0	0
43.0800	-0.6430	25.0700	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
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 16	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 13	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
C86_1

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D24_1
MOE2012 3D

372381 0 0 1 0 0 0 0 0999 V2000
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28.4920 29.1540 -31.7570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.0630 28.3060 -30.0950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.1750 28.6560 -29.5610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.8880 27.2980 -30.4830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.3020 28.3470 -29.2030 C 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
30.4790 29.3740 -28.8590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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31.3190 28.4750 -30.8340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.0710 17.5130 -12.3480 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.0630 17.8550 -12.6620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.7270 16.8380 -13.1420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.2370 16.8130 -11.1040 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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30.5850 15.2560 -9.4700 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.5130 14.6870 -9.5890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.7450 16.0570 -8.7410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.4360 14.3490 -9.0120 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.5170 14.9480 -8.9350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.2010 13.6230 -9.8010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.3090 15.6320 -11.5080 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.1280 18.7000 -12.1800 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.1400 18.3310 -11.8790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.4350 19.3610 -11.3610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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30.5700 26.4880 -25.5210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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33.5950 26.4970 -26.0160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.7340 27.5200 -24.8330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.8300 25.4610 -24.3290 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.0650 25.5070 -23.7510 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.3450 24.4820 -22.7860 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.9630 23.5090 -23.1180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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34.2190 25.8260 -21.1130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.7100 24.9380 -21.4520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.9500 24.6630 -24.0410 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.1920 23.8360 -20.4930 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.8210 23.9940 -19.1870 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.2480 22.9790 -18.3310 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.8270 22.1480 -18.7260 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.9400 23.0200 -16.9680 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.2890 22.2070 -16.3340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.1930 24.0800 -16.4200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.7710 25.0920 -17.2960 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.1940 25.9430 -16.9420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.0800 25.0500 -18.6630 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.7230 25.8630 -19.2860 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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D24_1

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D25_1
MOE2012 3D

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21.8350 10.9280 23.6410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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22.2040 11.6420 21.6000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.5750 11.7540 20.7060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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23.9840 10.9770 20.5240 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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73.1910	-11.8470	-31.5160	C	0	0	0	0	0	0	0	0	0	0	0	0	0
74.0880	-12.2440	-31.9810	H	0	0	0	0	0	0	0	0	0	0	0	0	0
73.3300	-10.6910	-30.7330	C	0	0	0	0	0	0	0	0	0	0	0	0	0
74.3230	-10.2650	-30.6330	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.7440	-13.7300	-32.5590	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.0730	-14.8620	-31.7440	C	0	0	0	0	0	0	0	0	0	0	0	0	0
70.9270	-13.2890	-33.8030	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.9180	-12.9490	-33.5410	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.8200	-14.1060	-34.5280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.4210	-12.4600	-34.3260	H	0	0	0	0	0	0	0	0	0	0	0	0	0
73.0690	-14.3200	-33.1120	C	0	0	0	0	0	0	0	0	0	0	0	0	0
73.5820	-13.6130	-33.7740	H	0	0	0	0	0	0	0	0	0	0	0	0	0
73.7690	-14.5920	-32.3130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
72.8820	-15.2300	-33.6960	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.6330	-15.2660	-30.5170	C	0	0	0	0	0	0	0	0	0	0	0	0	0
72.5210	-14.7720	-30.1280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.0690	-16.3040	-29.7690	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.5250	-16.5920	-28.8250	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.9380	-16.9800	-30.2260	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.3630	-16.5880	-31.4320	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.4710	-17.0650	-31.8240	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.9260	-15.5440	-32.1830	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.4400	-15.2880	-33.1210	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.4970	-17.9750	-29.4010	O	0	0	0	0	0	0	0	0	0	0	0	0	0
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D25_1

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D28_1
MOE2012 3D

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M END
> <NAME>
D28_1

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D32_1
MOE2012 3D

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-0.8490 5.4220 -26.0820 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-1.0560 4.3570 -26.2420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-0.4670 5.8000 -27.0380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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-0.1860 5.2030 -24.0390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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2.7530 6.1220 -24.1060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.1750 4.6430 -23.3120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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393394 1 0 0 0 0
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395396 1 0 0 0 0

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M END
> <NAME>
D32_1

```

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$$$$
D36_1
MOE2012 3D

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-1.9720 -7.5020 -6.5640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-0.0440 -7.3690 -6.3650 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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1.0500 -6.3460 -6.6430 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.0380 -6.0810 -7.7070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0.8240 -5.4180 -6.1010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.4290 -6.8690 -6.2430 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.4280 -7.1250 -5.1760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.6460 -7.7910 -6.7960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.5250 -5.8360 -6.5200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.5320 -5.5860 -7.5880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.3050 -4.9120 -5.9730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.9040 -6.3600 -6.1080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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M END
> <NAME>
D36_1

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D60_1
MOE2012 3D

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26.2840 4.0970 -41.4110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.9800 3.0520 -39.7360 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
27.2050 3.9140 -39.2370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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25.6860 2.4150 -38.2040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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28.0520 2.5420 -37.2840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.3350 0.5710 -36.8980 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
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27.1060 1.8290 -35.1870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.2360 0.2820 -35.1130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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44.8570 -1.7070 -35.4230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.5390 -0.1100 -36.3840 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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M END
> <NAME>
D60_1

\$\$\$
D61_1
MOE2012 3D

417426 0 0 1 0 0 0 0 0999 V2000
8.1330 14.5630 -11.4110 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

117.4560	7.5460	0.8660	H	0	0	0	0	0	0	0	0	0	0	0	0
115.7490	10.0970	2.3770	C	0	0	0	0	0	0	0	0	0	0	0	0
115.0760	10.2010	1.5280	H	0	0	0	0	0	0	0	0	0	0	0	0
116.2150	11.2590	3.0000	C	0	0	0	0	0	0	0	0	0	0	0	0
115.8980	12.2300	2.6280	H	0	0	0	0	0	0	0	0	0	0	0	0
117.0910	11.1850	4.0830	C	0	0	0	0	0	0	0	0	0	0	0	0
117.4750	9.9320	4.5520	C	0	0	0	0	0	0	0	0	0	0	0	0
118.1360	9.8170	5.4040	H	0	0	0	0	0	0	0	0	0	0	0	0
117.0050	8.7650	3.9300	C	0	0	0	0	0	0	0	0	0	0	0	0
117.3480	7.8150	4.3310	H	0	0	0	0	0	0	0	0	0	0	0	0
117.4730	12.3950	4.5910	O	0	0	0	0	0	0	0	0	0	0	0	0
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79	80	2	0	0	0	0
79	84	1	0	0	0	0
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413415 1 0 0 0 0
415416 1 0 0 0 0

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M END
> <NAME>
D61_1

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$$$$
D70_1
MOE2012 3D

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392406 0 0 1 0 0 0 0 0 0999 V2000
15.7720 -5.4180 25.7480 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.7610 -5.0700 26.0740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.0740 -5.0550 26.5130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.3840 -4.7640 24.4270 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.2900 -4.6960 24.3700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7530 -3.7300 24.4390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.8750 -5.4560 23.1560 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.2070 -6.2890 22.8980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7320 -4.7320 22.3450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.6990 -6.8780 25.7170 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
15.5420 -7.2030 26.6710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.2800 -5.9000 23.2380 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
16.9750 -7.4500 25.2640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.7990 -7.0610 25.8780 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.9390 -8.5270 25.4690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.3220 -7.2840 23.7700 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.6800 -7.9450 23.1720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.3420 -7.6770 23.6620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.6380 -5.7660 9.2450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.0990 -4.8450 9.4900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.8830 -6.4490 8.8350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.6200 -5.4250 8.2500 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.0640 -6.4520 7.4740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.0180 -5.9560 6.4180 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.4130 -6.8360 5.8950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.4430 -5.3680 5.6940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.1670 -5.1500 7.0250 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.7840 -4.2070 7.4290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.5540 -5.7140 7.8850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.7120 -7.6190 7.5800 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.2920 -6.3490 10.4940 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.7380 -7.3190 10.2450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.1350 -5.7410 10.8440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.9170 -5.8730 21.9040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.8350 -6.4750 21.9210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.2650 -6.3260 21.1460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.3260 -4.4520 21.5060 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.4580 -3.7880 21.4590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.0420 -4.0500 22.2320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.9790 -4.4460 20.1470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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37.4320	2.1800	2.3960	H	0	0	0	0	0	0	0	0	0	0	0
38.5630	0.8100	3.6210	C	0	0	0	0	0	0	0	0	0	0	0
38.3040	1.2990	4.5680	H	0	0	0	0	0	0	0	0	0	0	0
38.6260	-0.2720	3.7910	H	0	0	0	0	0	0	0	0	0	0	0
36.6000	-1.4660	2.4940	O	0	0	0	0	0	0	0	0	0	0	0
39.8010	1.3080	3.1190	O	0	0	0	0	0	0	0	0	0	0	0
40.9010	1.1500	3.9160	C	0	0	0	0	0	0	0	0	0	0	0
42.0800	1.6930	3.4060	C	0	0	0	0	0	0	0	0	0	0	0
42.0700	2.1950	2.4420	H	0	0	0	0	0	0	0	0	0	0	0
43.2740	1.6010	4.1260	C	0	0	0	0	0	0	0	0	0	0	0
44.1740	2.0360	3.6930	H	0	0	0	0	0	0	0	0	0	0	0
43.3260	0.9590	5.3780	C	0	0	0	0	0	0	0	0	0	0	0
42.1300	0.4170	5.8750	C	0	0	0	0	0	0	0	0	0	0	0
42.0930	-0.0890	6.8360	H	0	0	0	0	0	0	0	0	0	0	0
40.9320	0.5090	5.1530	C	0	0	0	0	0	0	0	0	0	0	0
40.0440	0.0670	5.5920	H	0	0	0	0	0	0	0	0	0	0	0
44.6650	0.8890	6.1490	C	0	0	0	0	0	0	0	0	0	0	0
45.7710	0.2260	5.2920	C	0	0	0	0	0	0	0	0	0	0	0
44.9990	2.3420	6.5800	C	0	0	0	0	0	0	0	0	0	0	0
45.1910	2.9980	5.7220	H	0	0	0	0	0	0	0	0	0	0	0
45.8840	2.3810	7.2270	H	0	0	0	0	0	0	0	0	0	0	0
44.1710	2.7860	7.1470	H	0	0	0	0	0	0	0	0	0	0	0
44.5860	0.0650	7.4630	C	0	0	0	0	0	0	0	0	0	0	0
43.8800	0.5080	8.1760	H	0	0	0	0	0	0	0	0	0	0	0
44.2720	-0.9710	7.2860	H	0	0	0	0	0	0	0	0	0	0	0
45.5620	0.0230	7.9620	H	0	0	0	0	0	0	0	0	0	0	0
45.5350	-1.0280	4.6970	C	0	0	0	0	0	0	0	0	0	0	0
44.5740	-1.5230	4.8180	H	0	0	0	0	0	0	0	0	0	0	0
46.5210	-1.6680	3.9390	C	0	0	0	0	0	0	0	0	0	0	0
46.3070	-2.6350	3.4910	H	0	0	0	0	0	0	0	0	0	0	0
47.7750	-1.0850	3.7640	C	0	0	0	0	0	0	0	0	0	0	0
48.0250	0.1580	4.3380	C	0	0	0	0	0	0	0	0	0	0	0
48.9770	0.6650	4.2170	H	0	0	0	0	0	0	0	0	0	0	0
47.0350	0.8040	5.0950	C	0	0	0	0	0	0	0	0	0	0	0
47.2890	1.7680	5.5280	H	0	0	0	0	0	0	0	0	0	0	0
48.6440	-1.8180	3.0060	O	0	0	0	0	0	0	0	0	0	0	0
56.9960	-1.3110	1.7180	C	0	0	0	0	0	0	0	0	0	0	0
57.4270	-2.3210	1.6720	H	0	0	0	0	0	0	0	0	0	0	0
56.2890	-1.3540	2.5550	H	0	0	0	0	0	0	0	0	0	0	0
58.0670	-0.3020	2.1240	C	0	0	0	0	0	0	0	0	0	0	0
57.5820	0.5680	2.5860	H	0	0	0	0	0	0	0	0	0	0	0
58.6760	-0.7640	2.9130	H	0	0	0	0	0	0	0	0	0	0	0
58.9920	0.2080	1.0220	C	0	0	0	0	0	0	0	0	0	0	0
58.5340	1.0670	0.5140	H	0	0	0	0	0	0	0	0	0	0	0
59.8760	0.6120	1.5340	H	0	0	0	0	0	0	0	0	0	0	0
56.3130	-0.9600	0.4590	N	0	0	3	0	0	0	0	0	0	0	0
59.3860	-0.8340	0.0650	N	0	0	3	0	0	0	0	0	0	0	0
57.0450	-1.5720	-0.6750	C	0	0	0	0	0	0	0	0	0	0	0
57.1810	-2.6500	-0.5110	H	0	0	0	0	0	0	0	0	0	0	0
56.4350	-1.4820	-1.5840	H	0	0	0	0	0	0	0	0	0	0	0
58.4020	-0.9300	-1.0310	C	0	0	0	0	0	0	0	0	0	0	0
58.2150	0.0570	-1.4750	H	0	0	0	0	0	0	0	0	0	0	0
58.8240	-1.5490	-1.8350	H	0	0	0	0	0	0	0	0	0	0	0
76.0970	1.0200	-2.6410	C	0	0	0	0	0	0	0	0	0	0	0
75.4990	1.8420	-3.0470	H	0	0	0	0	0	0	0	0	0	0	0
75.5940	0.1000	-2.9650	H	0	0	0	0	0	0	0	0	0	0	0
77.4090	1.1270	-3.2160	O	0	0	0	0	0	0	0	0	0	0	0
78.1280	-0.0300	-3.2400	C	0	0	0	0	0	0	0	0	0	0	0
79.4810	0.2040	-3.8560	C	0	0	0	0	0	0	0	0	0	0	0
79.4060	-0.0580	-4.9160	H	0	0	0	0	0	0	0	0	0	0	0
79.7440	1.2650	-3.7760	H	0	0	0	0	0	0	0	0	0	0	0
80.5210	-0.6390	-3.1180	C	0	0	0	0	0	0	0	0	0	0	0
80.4950	-0.3370	-2.0620	H	0	0	0	0	0	0	0	0	0	0	0
80.2230	-1.6910	-3.1310	H	0	0	0	0	0	0	0	0	0	0	0
77.7340	-1.1140	-2.8310	O	0	0	0	0	0	0	0	0	0	0	0
76.1660	1.1120	-1.1180	C	0	0	0	0	0	0	0	0	0	0	0
76.8420	0.3370	-0.7400	H	0	0	0	0	0	0	0	0	0	0	0
76.6130	2.0530	-0.7770	H	0	0	0	0	0	0	0	0	0	0	0
60.7460	-0.6070	-0.4600	C	0	0	0	0	0	0	0	0	0	0	0
61.4530	-0.6560	0.3800	H	0	0	0	0	0	0	0	0	0	0	0
61.0200	-1.4610	-1.0950	H	0	0	0	0	0	0	0	0	0	0	0
60.9680	0.6960	-1.2350	C	0	0	0	0	0	0	0	0	0	0	0
60.3180	0.7380	-2.1150	H	0	0	0	0	0	0	0	0	0	0	0
60.7660	1.5630	-0.5960	H	0	0	0	0	0	0	0	0	0	0	0
62.3910	0.7980	-1.7180	C	0	0	0	0	0	0	0	0	0	0	0
62.5610	1.9860	-2.3670	O	0	0	0	0	0	0	0	0	0	0	0
63.8530	2.2000	-2.9520	C	0	0	0	0	0	0	0	0	0	0	0
64.2250	1.2880	-3.4380	H	0	0	0	0	0	0	0	0	0	0	0
63.7290	2.9340	-3.7560	H	0	0	0	0	0	0	0	0	0	0	0
64.8490	2.7280	-1.9250	C	0	0	0	0	0	0	0	0	0	0	0
64.4530	3.6510	-1.4820	H	0	0	0	0	0	0	0	0	0	0	0

88.9000	-3.1990	-10.3870	C	0	0	0	0	0	0	0	0	0	0	0
90.1000	-3.3450	-11.0810	C	0	0	0	0	0	0	0	0	0	0	0
90.8070	-4.1140	-10.7810	H	0	0	0	0	0	0	0	0	0	0	0
90.4020	-2.5150	-12.1640	C	0	0	0	0	0	0	0	0	0	0	0
91.3500	-2.6600	-12.6790	H	0	0	0	0	0	0	0	0	0	0	0
89.5120	-1.5080	-12.5830	C	0	0	0	0	0	0	0	0	0	0	0
88.3080	-1.3740	-11.8720	C	0	0	0	0	0	0	0	0	0	0	0
87.5720	-0.6230	-12.1440	H	0	0	0	0	0	0	0	0	0	0	0
88.0050	-2.2080	-10.7870	C	0	0	0	0	0	0	0	0	0	0	0
87.0600	-2.0520	-10.2770	H	0	0	0	0	0	0	0	0	0	0	0
89.8760	-0.6160	-13.7930	C	0	0	0	0	0	0	0	0	0	0	0
91.2470	0.0740	-13.5890	C	0	0	0	0	0	0	0	0	0	0	0
89.8220	-1.5350	-15.0440	C	0	0	0	0	0	0	0	0	0	0	0
90.5860	-2.3210	-15.0160	H	0	0	0	0	0	0	0	0	0	0	0
89.9680	-0.9680	-15.9710	H	0	0	0	0	0	0	0	0	0	0	0
88.8480	-2.0340	-15.1250	H	0	0	0	0	0	0	0	0	0	0	0
88.8560	0.5220	-14.0590	C	0	0	0	0	0	0	0	0	0	0	0
87.8620	0.1270	-14.3020	H	0	0	0	0	0	0	0	0	0	0	0
88.7440	1.1910	-13.1970	H	0	0	0	0	0	0	0	0	0	0	0
89.1690	1.1440	-14.9080	H	0	0	0	0	0	0	0	0	0	0	0
91.4890	0.8100	-12.4140	C	0	0	0	0	0	0	0	0	0	0	0
90.7280	0.8790	-11.6400	H	0	0	0	0	0	0	0	0	0	0	0
92.7060	1.4690	-12.2090	C	0	0	0	0	0	0	0	0	0	0	0
92.8630	2.0280	-11.2900	H	0	0	0	0	0	0	0	0	0	0	0
93.7120	1.4250	-13.1740	C	0	0	0	0	0	0	0	0	0	0	0
93.4940	0.6940	-14.3390	C	0	0	0	0	0	0	0	0	0	0	0
94.2490	0.6110	-15.1130	H	0	0	0	0	0	0	0	0	0	0	0
92.2750	0.0300	-14.5440	C	0	0	0	0	0	0	0	0	0	0	0
92.1580	-0.5170	-15.4760	H	0	0	0	0	0	0	0	0	0	0	0
94.8450	2.1150	-12.8470	O	0	0	0	0	0	0	0	0	0	0	0
102.4570	3.7360	-16.8930	C	0	0	0	0	0	0	0	0	0	0	0
102.2040	2.6700	-16.9300	H	0	0	0	0	0	0	0	0	0	0	0
103.1960	3.8490	-16.0900	H	0	0	0	0	0	0	0	0	0	0	0
103.1520	4.0700	-18.2180	C	0	0	0	0	0	0	0	0	0	0	0
104.1670	3.6540	-18.1740	H	0	0	0	0	0	0	0	0	0	0	0
102.6540	3.5420	-19.0430	H	0	0	0	0	0	0	0	0	0	0	0
103.2510	5.5600	-18.5410	C	0	0	0	0	0	0	0	0	0	0	0
103.4860	6.1440	-17.6430	H	0	0	0	0	0	0	0	0	0	0	0
104.1060	5.6710	-19.2210	H	0	0	0	0	0	0	0	0	0	0	0
101.2910	4.5430	-16.5390	N	0	0	3	0	0	0	0	0	0	0	0
102.0460	6.0510	-19.2250	N	0	0	3	0	0	0	0	0	0	0	0
100.4170	4.8720	-17.6670	C	0	0	0	0	0	0	0	0	0	0	0
100.3230	4.0470	-18.3840	H	0	0	0	0	0	0	0	0	0	0	0
99.4000	5.0710	-17.3030	H	0	0	0	0	0	0	0	0	0	0	0
100.8760	6.1750	-18.3460	C	0	0	0	0	0	0	0	0	0	0	0
101.0370	6.9380	-17.5740	H	0	0	0	0	0	0	0	0	0	0	0
100.0300	6.5240	-18.9520	H	0	0	0	0	0	0	0	0	0	0	0
109.0910	19.3540	-28.9350	C	0	0	0	0	0	0	0	0	0	0	0
108.8140	19.5460	-27.8930	H	0	0	0	0	0	0	0	0	0	0	0
108.1480	19.1530	-29.4580	H	0	0	0	0	0	0	0	0	0	0	0
109.7180	20.5480	-29.4310	O	0	0	0	0	0	0	0	0	0	0	0
109.6660	20.7340	-30.7820	C	0	0	0	0	0	0	0	0	0	0	0
110.3390	22.0400	-31.1310	C	0	0	0	0	0	0	0	0	0	0	0
109.8200	22.8490	-30.6050	H	0	0	0	0	0	0	0	0	0	0	0
111.3780	21.9970	-30.7880	H	0	0	0	0	0	0	0	0	0	0	0
110.3130	22.3140	-32.6250	C	0	0	0	0	0	0	0	0	0	0	0
110.8300	21.5230	-33.1780	H	0	0	0	0	0	0	0	0	0	0	0
110.8060	23.2650	-32.8460	H	0	0	0	0	0	0	0	0	0	0	0
109.2850	22.3660	-32.9970	H	0	0	0	0	0	0	0	0	0	0	0
109.1600	19.9600	-31.5800	O	0	0	0	0	0	0	0	0	0	0	0
110.0400	18.1620	-29.0240	C	0	0	0	0	0	0	0	0	0	0	0
110.2560	17.9580	-30.0790	H	0	0	0	0	0	0	0	0	0	0	0
111.0200	18.3750	-28.5800	H	0	0	0	0	0	0	0	0	0	0	0
102.3010	7.2970	-19.9700	C	0	0	0	0	0	0	0	0	0	0	0
103.0620	7.0910	-20.7360	H	0	0	0	0	0	0	0	0	0	0	0
101.4000	7.5560	-20.5440	H	0	0	0	0	0	0	0	0	0	0	0
102.7380	8.5060	-19.1370	C	0	0	0	0	0	0	0	0	0	0	0
101.9640	8.7720	-18.4100	H	0	0	0	0	0	0	0	0	0	0	0
103.6740	8.2960	-18.6080	H	0	0	0	0	0	0	0	0	0	0	0
102.9710	9.7110	-20.0120	C	0	0	0	0	0	0	0	0	0	0	0
103.2550	10.7880	-19.2250	O	0	0	0	0	0	0	0	0	0	0	0
103.4710	12.0290	-19.9130	C	0	0	0	0	0	0	0	0	0	0	0
102.7470	12.1650	-20.7260	H	0	0	0	0	0	0	0	0	0	0	0
103.2700	12.8360	-19.1980	H	0	0	0	0	0	0	0	0	0	0	0
104.9050	12.1340	-20.4180	C	0	0	0	0	0	0	0	0	0	0	0
105.5930	11.9860	-19.5760	H	0	0	0	0	0	0	0	0	0	0	0
105.0920	11.3550	-21.1670	H	0	0	0	0	0	0	0	0	0	0	0
102.9290	9.7210	-21.2340	O	0	0	0	0	0	0	0	0	0	0	0
105.0780	13.4290	-20.9900	O	0	0	0	0	0	0	0	0	0	0	0
106.3200	13.7380	-21.4710	C	0	0	0	0	0	0	0	0	0	0	0
106.4500	15.0380	-21.9580	C	0	0	0	0	0	0	0	0	0	0	0

105.5980	15.7120	-21.9350	H	0	0	0	0	0	0	0	0	0	0	0	0
107.6700	15.4860	-22.4740	C	0	0	0	0	0	0	0	0	0	0	0	0
107.7310	16.5070	-22.8450	H	0	0	0	0	0	0	0	0	0	0	0	0
108.7970	14.6420	-22.5210	C	0	0	0	0	0	0	0	0	0	0	0	0
108.6460	13.3360	-22.0280	C	0	0	0	0	0	0	0	0	0	0	0	0
109.4740	12.6330	-22.0280	H	0	0	0	0	0	0	0	0	0	0	0	0
107.4230	12.8890	-21.5100	C	0	0	0	0	0	0	0	0	0	0	0	0
107.3720	11.8670	-21.1470	H	0	0	0	0	0	0	0	0	0	0	0	0
110.1320	15.1800	-23.0860	C	0	0	0	0	0	0	0	0	0	0	0	0
109.9490	15.7360	-24.5190	C	0	0	0	0	0	0	0	0	0	0	0	0
110.6450	16.2340	-22.0690	C	0	0	0	0	0	0	0	0	0	0	0	0
109.9800	17.1030	-21.9980	H	0	0	0	0	0	0	0	0	0	0	0	0
111.6420	16.6050	-22.3370	H	0	0	0	0	0	0	0	0	0	0	0	0
110.7230	15.8060	-21.0620	H	0	0	0	0	0	0	0	0	0	0	0	0
111.2480	14.1040	-23.1780	C	0	0	0	0	0	0	0	0	0	0	0	0
111.5110	13.7080	-22.1900	H	0	0	0	0	0	0	0	0	0	0	0	0
110.9580	13.2560	-23.8090	H	0	0	0	0	0	0	0	0	0	0	0	0
112.1670	14.5240	-23.6090	H	0	0	0	0	0	0	0	0	0	0	0	0
109.3640	14.9280	-25.5120	C	0	0	0	0	0	0	0	0	0	0	0	0
109.0200	13.9230	-25.2730	H	0	0	0	0	0	0	0	0	0	0	0	0
109.2080	15.3890	-26.8230	C	0	0	0	0	0	0	0	0	0	0	0	0
108.7520	14.7410	-27.5680	H	0	0	0	0	0	0	0	0	0	0	0	0
109.6390	16.6650	-27.1870	C	0	0	0	0	0	0	0	0	0	0	0	0
110.2110	17.4820	-26.2160	C	0	0	0	0	0	0	0	0	0	0	0	0
110.5470	18.4900	-26.4390	H	0	0	0	0	0	0	0	0	0	0	0	0
110.3670	17.0220	-24.8990	C	0	0	0	0	0	0	0	0	0	0	0	0
110.8280	17.7000	-24.1870	H	0	0	0	0	0	0	0	0	0	0	0	0
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> <NAME>
D70_1

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D86_1
MOE2012 3D

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24.2150 8.3220 -7.4100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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20.2050 11.1050 -6.0150 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.2490 11.2810 -5.9700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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31.2830 -12.1230 -6.1020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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31.3480 -15.4350 -5.4890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.0820 -11.7000 -4.9720 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.9190 -9.4700 -6.5450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.2150 -10.0230 -5.6460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.6870 -9.7200 -7.2860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.5130 4.4820 -6.6560 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.4700 4.3340 -6.1420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.7720 3.9270 -6.0680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

68.6940	-0.5180	-3.8870	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.5360	-0.9990	-5.1150	O	0	0	0	0	0	0	0	0	0	0	0	0	0
64.1640	1.8710	-4.7360	C	0	0	0	0	0	0	0	0	0	0	0	0	0
63.6670	0.9090	-4.9050	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.9520	2.2030	-3.7120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1820	-3.7890	-4.1120	C	0	0	0	0	0	0	0	0	0	0	0	0	0
50.7630	-3.5110	-3.2220	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.6900	-4.6570	-4.5540	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.2360	-2.6580	-5.1450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
49.6460	-2.9370	-6.0250	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.8550	-1.7200	-4.7310	H	0	0	0	0	0	0	0	0	0	0	0	0	0
51.6580	-2.4080	-5.5790	C	0	0	0	0	0	0	0	0	0	0	0	0	0
51.6750	-1.6770	-6.7300	O	0	0	0	0	0	0	0	0	0	0	0	0	0
52.9710	-1.4230	-7.2960	C	0	0	0	0	0	0	0	0	0	0	0	0	0
53.6010	-2.3210	-7.2570	H	0	0	0	0	0	0	0	0	0	0	0	0	0
52.8230	-1.2090	-8.3610	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.6490	-0.2370	-6.6210	C	0	0	0	0	0	0	0	0	0	0	0	0	0
52.9810	0.6310	-6.6690	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.8460	-0.4740	-5.5690	H	0	0	0	0	0	0	0	0	0	0	0	0	0
52.6500	-2.7810	-4.9690	O	0	0	0	0	0	0	0	0	0	0	0	0	0
54.8700	0.0260	-7.3090	O	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6000	1.1020	-6.8850	C	0	0	0	0	0	0	0	0	0	0	0	0	0
56.7240	1.3880	-7.6570	C	0	0	0	0	0	0	0	0	0	0	0	0	0
56.9610	0.7710	-8.5200	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.5530	2.4670	-7.3340	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.4190	2.6600	-7.9640	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.2850	3.2850	-6.2190	C	0	0	0	0	0	0	0	0	0	0	0	0	0
56.1500	2.9810	-5.4520	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.8770	3.5750	-4.5840	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.3180	1.9010	-5.7790	C	0	0	0	0	0	0	0	0	0	0	0	0	0
54.4580	1.7160	-5.1440	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.2160	4.4780	-5.9050	C	0	0	0	0	0	0	0	0	0	0	0	0	0
59.6960	4.0300	-5.8490	C	0	0	0	0	0	0	0	0	0	0	0	0	0
57.9300	5.5480	-6.9940	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.1870	5.1960	-8.0000	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.4940	6.4710	-6.8120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.8670	5.8190	-7.0110	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.9140	5.1660	-4.5470	C	0	0	0	0	0	0	0	0	0	0	0	0	0
56.9130	5.6130	-4.5320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.9740	4.4670	-3.7040	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.6280	5.9750	-4.3460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0820	3.0050	-4.9620	C	0	0	0	0	0	0	0	0	0	0	0	0	0
59.3390	2.5220	-4.3290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.4110	2.5740	-4.8710	C	0	0	0	0	0	0	0	0	0	0	0	0	0
61.6420	1.7790	-4.1700	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.3910	3.1590	-5.6690	C	0	0	0	0	0	0	0	0	0	0	0	0	0
62.0250	4.1710	-6.5560	C	0	0	0	0	0	0	0	0	0	0	0	0	0
62.7800	4.6330	-7.1870	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.6970	4.6050	-6.6450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4780	5.4010	-7.3510	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.7190	2.8370	-5.6840	O	0	0	0	0	0	0	0	0	0	0	0	0	0
73.9280	-1.7760	-1.4180	C	0	0	0	0	0	0	0	0	0	0	0	0	0
73.4980	-1.0160	-0.7520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
74.0320	-2.6800	-0.8030	H	0	0	0	0	0	0	0	0	0	0	0	0	0
73.0130	-2.0070	-2.5550	N	0	0	0	0	0	0	0	0	0	0	0	0	0
71.6460	-2.2720	-2.0500	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.5940	-3.2710	-1.6020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.4090	-1.5520	-1.2540	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.5790	-2.0820	-3.1550	C	0	0	0	0	0	0	0	0	0	0	0	0	0
70.7610	-1.0900	-3.5890	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.7090	-2.8060	-3.9690	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.1900	-2.1370	-2.6370	N	0	0	3	0	0	0	0	0	0	0	0	0	0
73.4870	-3.0970	-3.4300	C	0	0	0	0	0	0	0	0	0	0	0	0	0
74.2730	-3.6990	-2.9540	H	0	0	0	0	0	0	0	0	0	0	0	0	0
72.6970	-3.8300	-3.6460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
75.3170	-1.2650	-1.8250	C	0	0	0	0	0	0	0	0	0	0	0	0	0
75.8720	-2.0180	-2.3940	H	0	0	0	0	0	0	0	0	0	0	0	0	0
75.2330	-0.3530	-2.4260	H	0	0	0	0	0	0	0	0	0	0	0	0	0
76.0720	-0.9600	-0.6560	O	0	0	0	0	0	0	0	0	0	0	0	0	0
76.9400	-0.6330	-0.9520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
73.9900	-2.5450	-4.7670	C	0	0	0	0	0	0	0	0	0	0	0	0	0
73.1760	-2.0640	-5.3190	H	0	0	0	0	0	0	0	0	0	0	0	0	0
74.7940	-1.8180	-4.6220	H	0	0	0	0	0	0	0	0	0	0	0	0	0
74.4990	-3.6150	-5.5580	O	0	0	0	0	0	0	0	0	0	0	0	0	0
74.8510	-3.2240	-6.3760	H	0	0	0	0	0	0	0	0	0	0	0	0	0
77.0280	-6.2110	11.9610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
76.8010	-6.3470	13.0260	H	0	0	0	0	0	0	0	0	0	0	0	0	0
77.6180	-5.2930	11.8500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
77.7680	-7.3370	11.4740	O	0	0	0	0	0	0	0	0	0	0	0	0	0
78.9710	-7.5240	12.0830	C	0	0	0	0	0	0	0	0	0	0	0	0	0
79.6640	-8.7370	11.5270	C	0	0	0	0	0	0	0	0	0	0	0	0	0

79.7480	-9.4790	12.3280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
79.0500	-9.1820	10.7360	H	0	0	0	0	0	0	0	0	0	0	0	0	0
81.0280	-8.3230	10.9860	C	0	0	0	0	0	0	0	0	0	0	0	0	0
81.6320	-7.8880	11.7930	H	0	0	0	0	0	0	0	0	0	0	0	0	0
80.9000	-7.4940	10.2760	H	0	0	0	0	0	0	0	0	0	0	0	0	0
79.4440	-6.8110	12.9580	O	0	0	0	0	0	0	0	0	0	0	0	0	0
75.7340	-6.0900	11.1670	C	0	0	0	0	0	0	0	0	0	0	0	0	0
75.9770	-5.9090	10.1130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
75.1750	-7.0310	11.2450	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.7840	-3.5220	-2.3160	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.1430	-3.9360	-3.1040	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.6510	-4.1930	-2.2770	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.0570	-3.6010	-0.9730	C	0	0	0	0	0	0	0	0	0	0	0	0	0
67.2180	-2.9020	-0.9130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
67.6310	-4.6010	-0.8330	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.0100	-3.3610	0.1660	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.6970	-2.2130	0.8260	O	0	0	0	0	0	0	0	0	0	0	0	0	0
69.6080	-1.8250	1.8650	C	0	0	0	0	0	0	0	0	0	0	0	0	0
70.6500	-1.9890	1.5630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.5050	-0.7420	2.0000	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.2850	-2.5390	3.1710	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.2400	-2.3420	3.4400	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.4180	-3.6200	3.0450	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.9430	-4.1040	0.4430	O	0	0	0	0	0	0	0	0	0	0	0	0	0
70.1680	-2.0430	4.1750	O	0	0	0	0	0	0	0	0	0	0	0	0	0
69.9980	-2.5210	5.4450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
70.8090	-1.9230	6.4080	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.5050	-1.1410	6.1150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.7320	-2.3150	7.7470	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.3810	-1.8230	8.4690	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.8410	-3.3240	8.1610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.0340	-3.9180	7.1780	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.3220	-4.6990	7.4270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.1130	-3.5230	5.8350	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.4670	-4.0240	5.1220	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.7700	-3.7150	9.6550	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.1740	-4.0600	10.2030	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.0900	-2.5250	10.3850	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.6830	-1.6040	10.3220	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.9280	-2.7410	11.4470	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.1080	-2.3030	9.9480	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.8710	-4.9500	9.9370	C	0	0	0	0	0	0	0	0	0	0	0	0	0
67.8250	-4.7590	9.6690	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.1950	-5.8370	9.3810	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.8850	-5.2130	11.0020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.9360	-5.0710	9.5830	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.5430	-5.5970	8.7140	H	0	0	0	0	0	0	0	0	0	0	0	0	0
73.2080	-5.4220	10.0500	C	0	0	0	0	0	0	0	0	0	0	0	0	0
73.7430	-6.2070	9.5260	H	0	0	0	0	0	0	0	0	0	0	0	0	0
73.7530	-4.7680	11.1510	C	0	0	0	0	0	0	0	0	0	0	0	0	0
73.0150	-3.7610	11.7730	C	0	0	0	0	0	0	0	0	0	0	0	0	0
73.4310	-3.2410	12.6330	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.7410	-3.4130	11.3110	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.2140	-2.6250	11.8430	H	0	0	0	0	0	0	0	0	0	0	0	0	0
74.9800	-5.0080	11.7060	O	0	0	0	0	0	0	0	0	0	0	0	0	0
79.6480	-9.1800	5.8910	C	0	0	0	0	0	0	0	0	0	0	0	0	0
79.3970	-10.2370	6.0530	H	0	0	0	0	0	0	0	0	0	0	0	0	0
78.7690	-8.6140	6.2290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
80.8450	-8.8320	6.6810	N	0	0	0	0	0	0	0	0	0	0	0	0	0
80.6350	-9.2500	8.0870	C	0	0	0	0	0	0	0	0	0	0	0	0	0
79.8580	-8.6220	8.5390	H	0	0	0	0	0	0	0	0	0	0	0	0	0
80.2550	-10.2800	8.1130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
81.9400	-9.2390	8.9220	C	0	0	0	0	0	0	0	0	0	0	0	0	0
82.5800	-10.0330	8.5150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
82.4950	-8.3010	8.8020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
81.6930	-9.4860	10.3630	N	0	0	3	0	0	0	0	0	0	0	0	0	0
81.1380	-7.3840	6.6120	C	0	0	0	0	0	0	0	0	0	0	0	0	0
80.3790	-6.8280	6.0450	H	0	0	0	0	0	0	0	0	0	0	0	0	0
81.1120	-6.9060	7.6010	H	0	0	0	0	0	0	0	0	0	0	0	0	0
79.8280	-8.9980	4.3800	C	0	0	0	0	0	0	0	0	0	0	0	0	0
79.9800	-7.9480	4.1150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
80.6830	-9.5710	4.0050	H	0	0	0	0	0	0	0	0	0	0	0	0	0
78.6530	-9.4380	3.7050	O	0	0	0	0	0	0	0	0	0	0	0	0	0
78.7100	-10.4050	3.6130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
82.5100	-7.1370	5.9850	C	0	0	0	0	0	0	0	0	0	0	0	0	0
83.2970	-7.6640	6.5340	H	0	0	0	0	0	0	0	0	0	0	0	0	0
82.5290	-7.4610	4.9390	H	0	0	0	0	0	0	0	0	0	0	0	0	0
82.7930	-5.7430	6.0340	O	0	0	0	0	0	0	0	0	0	0	0	0	0
83.6720	-5.6170	5.6370	H	0	0	0	0	0	0	0	0	0	0	0	0	0
96.5410	-16.7120	17.3780	C	0	0	0	0	0	0	0	0	0	0	0	0	0
95.7520	-16.3860	18.0640	H	0	0	0	0	0	0	0	0	0	0	0	0	0

21	22	1	0	0	0	0
21	23	1	0	0	0	0
21	24	1	0	0	0	0
24	25	1	0	0	0	0
26	27	1	0	0	0	0
26	28	1	0	0	0	0
26	29	1	0	0	0	0
26	38	1	0	0	0	0
29	30	1	0	0	0	0
30	31	1	0	0	0	0
30	37	2	0	0	0	0
31	32	1	0	0	0	0
31	33	1	0	0	0	0
31	34	1	0	0	0	0
34	35	1	0	0	0	0
34	36	1	0	0	0	0
34	97	1	0	0	0	0
38	39	1	0	0	0	0
38	40	1	0	0	0	0
38	86	1	0	0	0	0
41	42	1	0	0	0	0
41	43	1	0	0	0	0
41	44	1	0	0	0	0
44	45	1	0	0	0	0
44	46	1	0	0	0	0
44	47	1	0	0	0	0
47	48	1	0	0	0	0
47	55	2	0	0	0	0
48	49	1	0	0	0	0
49	50	1	0	0	0	0
49	51	1	0	0	0	0
49	52	1	0	0	0	0
52	53	1	0	0	0	0
52	54	1	0	0	0	0
52	56	1	0	0	0	0
56	57	1	0	0	0	0
57	58	1	0	0	0	0
57	65	2	0	0	0	0
58	59	1	0	0	0	0
58	60	2	0	0	0	0
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> <NAME>
D86_1

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D87_1
MOE2012 3D

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40.5170 35.3340 -41.0160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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39.2540 23.0570 -30.5780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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38.3010	22.0360	-30.6190	C	0	0	0	0	0	0	0	0	0	0	0
38.4930	21.1260	-30.0520	H	0	0	0	0	0	0	0	0	0	0	0
37.1200	22.1680	-31.3740	C	0	0	0	0	0	0	0	0	0	0	0
36.9380	23.3660	-32.0830	C	0	0	0	0	0	0	0	0	0	0	0
36.0480	23.5400	-32.6810	H	0	0	0	0	0	0	0	0	0	0	0
37.8960	24.3900	-32.0410	C	0	0	0	0	0	0	0	0	0	0	0
37.6960	25.2910	-32.6120	H	0	0	0	0	0	0	0	0	0	0	0
36.0840	21.0200	-31.3810	C	0	0	0	0	0	0	0	0	0	0	0
36.7360	19.6880	-31.8220	C	0	0	0	0	0	0	0	0	0	0	0
35.4710	20.9720	-29.9550	C	0	0	0	0	0	0	0	0	0	0	0
36.2130	20.7140	-29.1900	H	0	0	0	0	0	0	0	0	0	0	0
34.6600	20.2380	-29.8880	H	0	0	0	0	0	0	0	0	0	0	0
35.0470	21.9450	-29.6750	H	0	0	0	0	0	0	0	0	0	0	0
34.8890	21.2620	-32.3430	C	0	0	0	0	0	0	0	0	0	0	0
34.3100	22.1480	-32.0530	H	0	0	0	0	0	0	0	0	0	0	0
35.2110	21.4050	-33.3810	H	0	0	0	0	0	0	0	0	0	0	0
34.1980	20.4100	-32.3360	H	0	0	0	0	0	0	0	0	0	0	0
37.4130	19.6170	-33.0540	C	0	0	0	0	0	0	0	0	0	0	0
37.4950	20.4980	-33.6890	H	0	0	0	0	0	0	0	0	0	0	0
37.9990	18.4260	-33.4920	C	0	0	0	0	0	0	0	0	0	0	0
38.5140	18.4040	-34.4500	H	0	0	0	0	0	0	0	0	0	0	0
37.9260	17.2670	-32.7190	C	0	0	0	0	0	0	0	0	0	0	0
37.2660	17.3190	-31.4950	C	0	0	0	0	0	0	0	0	0	0	0
37.1860	16.4520	-30.8480	H	0	0	0	0	0	0	0	0	0	0	0
36.6770	18.5140	-31.0530	C	0	0	0	0	0	0	0	0	0	0	0
36.1680	18.4930	-30.0930	H	0	0	0	0	0	0	0	0	0	0	0
38.5380	16.1780	-33.2720	O	0	0	0	0	0	0	0	0	0	0	0
37.6140	3.8030	-29.1270	C	0	0	0	0	0	0	0	0	0	0	0
37.5600	2.9820	-28.4020	H	0	0	0	0	0	0	0	0	0	0	0
36.6270	4.2820	-29.0890	H	0	0	0	0	0	0	0	0	0	0	0
38.6870	4.7510	-28.7720	N	0	0	0	0	0	0	0	0	0	0	0
38.4970	6.0480	-29.4610	C	0	0	0	0	0	0	0	0	0	0	0
38.0860	5.9020	-30.4670	H	0	0	0	0	0	0	0	0	0	0	0
37.7760	6.6770	-28.9220	H	0	0	0	0	0	0	0	0	0	0	0
39.8420	6.7690	-29.6260	C	0	0	0	0	0	0	0	0	0	0	0
40.3140	6.8760	-28.6460	H	0	0	0	0	0	0	0	0	0	0	0
40.5020	6.1470	-30.2440	H	0	0	0	0	0	0	0	0	0	0	0
39.6940	8.1580	-30.2730	C	0	0	0	0	0	0	0	0	0	0	0
39.1840	8.0270	-31.2350	H	0	0	0	0	0	0	0	0	0	0	0
39.0440	8.7780	-29.6440	H	0	0	0	0	0	0	0	0	0	0	0
38.7480	4.9470	-27.3080	C	0	0	0	0	0	0	0	0	0	0	0
39.2960	5.8630	-27.0560	H	0	0	0	0	0	0	0	0	0	0	0
37.7460	5.0920	-26.8810	H	0	0	0	0	0	0	0	0	0	0	0
40.9870	8.8340	-30.5070	N	0	0	3	0	0	0	0	0	0	0	0
37.8420	3.1560	-30.4980	C	0	0	0	0	0	0	0	0	0	0	0
37.8290	3.8900	-31.3070	H	0	0	0	0	0	0	0	0	0	0	0
38.7990	2.6230	-30.5180	H	0	0	0	0	0	0	0	0	0	0	0
36.8020	2.2160	-30.7410	O	0	0	0	0	0	0	0	0	0	0	0
36.9830	1.7960	-31.6000	H	0	0	0	0	0	0	0	0	0	0	0
39.4690	3.8000	-26.5910	C	0	0	0	0	0	0	0	0	0	0	0
38.9130	2.8610	-26.6620	H	0	0	0	0	0	0	0	0	0	0	0
40.4700	3.6510	-27.0090	H	0	0	0	0	0	0	0	0	0	0	0
39.6080	4.1280	-25.2110	O	0	0	0	0	0	0	0	0	0	0	0
40.0570	3.3770	-24.7850	H	0	0	0	0	0	0	0	0	0	0	0
47.4060	5.8160	-13.7430	C	0	0	0	0	0	0	0	0	0	0	0
47.1690	4.9410	-14.3570	H	0	0	0	0	0	0	0	0	0	0	0
46.4450	6.3040	-13.5380	H	0	0	0	0	0	0	0	0	0	0	0
48.0130	5.3340	-12.5330	O	0	0	0	0	0	0	0	0	0	0	0
47.9360	6.1670	-11.4560	C	0	0	0	0	0	0	0	0	0	0	0
48.6350	5.5300	-10.2800	C	0	0	0	0	0	0	0	0	0	0	0
48.2240	4.5260	-10.1390	H	0	0	0	0	0	0	0	0	0	0	0
49.6960	5.4530	-10.5390	H	0	0	0	0	0	0	0	0	0	0	0
48.4380	6.3700	-9.0150	C	0	0	0	0	0	0	0	0	0	0	0
48.7440	7.4050	-9.2120	H	0	0	0	0	0	0	0	0	0	0	0
47.3640	6.4620	-8.8130	H	0	0	0	0	0	0	0	0	0	0	0
47.4190	7.2740	-11.4580	O	0	0	0	0	0	0	0	0	0	0	0
48.3540	6.7480	-14.4890	C	0	0	0	0	0	0	0	0	0	0	0
48.5410	7.6370	-13.8760	H	0	0	0	0	0	0	0	0	0	0	0
49.3450	6.3010	-14.6350	H	0	0	0	0	0	0	0	0	0	0	0
41.7600	9.0610	-29.2730	C	0	0	0	0	0	0	0	0	0	0	0
42.3120	10.0090	-29.3300	H	0	0	0	0	0	0	0	0	0	0	0
41.0900	9.1710	-28.4100	H	0	0	0	0	0	0	0	0	0	0	0
42.8120	7.9640	-29.0710	C	0	0	0	0	0	0	0	0	0	0	0
42.5680	7.0600	-29.6400	H	0	0	0	0	0	0	0	0	0	0	0
43.7950	8.2960	-29.4240	H	0	0	0	0	0	0	0	0	0	0	0
42.9250	7.6030	-27.6130	C	0	0	0	0	0	0	0	0	0	0	0
43.0090	6.2500	-27.4630	O	0	0	0	0	0	0	0	0	0	0	0
43.0170	5.7620	-26.1130	C	0	0	0	0	0	0	0	0	0	0	0
42.2680	6.2810	-25.5030	H	0	0	0	0	0	0	0	0	0	0	0
42.7010	4.7130	-26.1460	H	0	0	0	0	0	0	0	0	0	0	0
44.4070	5.8600	-25.4960	C	0	0	0	0	0	0	0	0	0	0	0

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416417	1	0	0	0	0
416418	1	0	0	0	0
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418423	1	0	0	0	0
419420	1	0	0	0	0
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421422 1 0 0 0 0
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M END
> <NAME>
D87_1

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D93_1
MOE2012 3D

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397411 0 0 1 0 0 0 0 0 0999 V2000
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57.8880 43.1640 -9.5870 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.1040 42.3600 -8.8980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.1400 44.5160 -9.5380 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.6340 45.0700 -8.7520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.6710 45.1430 -10.6640 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.1380 44.1870 -11.3920 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
56.6660 44.3200 -12.3560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
56.7700 41.7080 -11.2980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
56.4350 41.1080 -10.4440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
55.8920 41.9180 -11.9200 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.8410 40.9700 -12.0980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.1800 41.6000 -12.9310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.7190 40.7920 -11.4620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.3060 39.6410 -12.6300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
56.9650 39.0250 -11.7900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
56.4470 39.8280 -13.2860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.3620 38.9450 -13.3630 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.6890 39.5290 -14.1340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.3640 21.6590 -16.3030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
55.2360 22.0510 -16.8370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.4940 22.1550 -16.7510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.3300 20.2400 -16.5340 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.1080 19.6430 -16.4150 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.2380 18.1650 -16.6910 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.5220 18.0530 -17.7410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.0360 17.7680 -16.0530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.9240 17.4340 -16.3880 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.6200 17.7160 -15.3700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.1280 17.7870 -17.0570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.0650 20.2150 -16.1320 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.4710 21.9620 -14.8130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.5710 21.5930 -14.3080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
55.2960 21.4180 -14.3360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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57.5240 37.0340 -13.0580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.0450 37.8200 -14.5710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.0190 36.9420 -14.6080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.3770 37.5520 -15.4450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.8500 36.7550 -13.9180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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59.5770 35.0160 -15.8210 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.2670 33.7660 -16.4540 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.2840 33.8010 -16.9410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.9930 33.6210 -17.2620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.3590 32.6070 -15.4680 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
60.3570 32.6030 -15.0120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.6100 32.7320 -14.6770 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.4290 35.1520 -15.0190 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.1270 31.3980 -16.1870 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.2070 30.2270 -15.4860 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


87.1350	-24.1910	3.2150	C	0	0	0	0	0	0	0	0	0	0	0
86.8410	-23.1600	3.3880	H	0	0	0	0	0	0	0	0	0	0	0
89.1720	-26.1170	0.5280	C	0	0	0	0	0	0	0	0	0	0	0
90.4850	-26.8380	0.9190	C	0	0	0	0	0	0	0	0	0	0	0
88.2540	-26.9550	-0.4020	C	0	0	0	0	0	0	0	0	0	0	0
87.9790	-27.9190	0.0420	H	0	0	0	0	0	0	0	0	0	0	0
88.7340	-27.1620	-1.3660	H	0	0	0	0	0	0	0	0	0	0	0
87.3190	-26.4220	-0.6190	H	0	0	0	0	0	0	0	0	0	0	0
89.5930	-24.8750	-0.3040	C	0	0	0	0	0	0	0	0	0	0	0
88.7220	-24.3360	-0.6960	H	0	0	0	0	0	0	0	0	0	0	0
90.1850	-24.1620	0.2830	H	0	0	0	0	0	0	0	0	0	0	0
90.2050	-25.1660	-1.1670	H	0	0	0	0	0	0	0	0	0	0	0
91.3430	-26.2570	1.8720	C	0	0	0	0	0	0	0	0	0	0	0
91.0780	-25.3170	2.3520	H	0	0	0	0	0	0	0	0	0	0	0
92.5520	-26.8650	2.2240	C	0	0	0	0	0	0	0	0	0	0	0
93.1940	-26.3920	2.9630	H	0	0	0	0	0	0	0	0	0	0	0
92.9490	-28.0620	1.6290	C	0	0	0	0	0	0	0	0	0	0	0
92.1070	-28.6590	0.6940	C	0	0	0	0	0	0	0	0	0	0	0
92.3560	-29.6020	0.2190	H	0	0	0	0	0	0	0	0	0	0	0
90.8910	-28.0520	0.3420	C	0	0	0	0	0	0	0	0	0	0	0
90.2800	-28.5580	-0.4010	H	0	0	0	0	0	0	0	0	0	0	0
94.1540	-28.5420	2.0580	O	0	0	0	0	0	0	0	0	0	0	0

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4	5	1	0	0	0	0
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9	12	1	0	0	0	0
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368369	1	0	0	0	0
368376	2	0	0	0	0
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369371 2 0 0 0 0
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373378 1 0 0 0 0
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388390 2 0 0 0 0
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390392 1 0 0 0 0
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393394 1 0 0 0 0
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M END
> <NAME>
D93_1

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$$$$
D94_1
MOE2012 3D

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10.7560 15.2430 -7.8240 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.1250 16.4300 -8.0710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.4280 17.1030 -8.8600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.1170 16.4930 -7.1360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.3860 17.2780 -7.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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10.4250 13.6910 -6.3650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.8830 14.7040 -8.5590 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.8370 13.6120 -8.4790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.7350 14.9640 -9.6140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.2270 15.2350 -8.0470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.2310 16.3290 -8.1200 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.3500 14.9730 -6.9900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.3180 14.6730 -8.8470 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
14.3690 13.6610 -8.7220 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.8980 18.0070 -8.8400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.4580 17.6930 -7.8870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.5440 19.0320 -9.0070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.3250 17.9700 -8.6780 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.0460 18.7490 -9.5370 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.5160 18.5720 -9.2490 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.7180 18.9460 -8.2390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.7230 17.4970 -9.2880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.3700 19.3230 -10.2730 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.1420 18.9660 -11.2860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.0590 20.3770 -10.2470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.5720 19.4570 -10.4120 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.4540 17.0750 -9.9640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.8350 17.4600 -10.9170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.8980 16.0760 -9.8740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.6220 15.2800 -8.5640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.2930 14.9970 -9.3840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.5520 16.3740 -8.6040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.2400 14.8240 -7.2420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.6350 15.1660 -6.3960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.3060 13.7300 -7.2190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.6340 15.3830 -7.0760 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.1910 14.8870 -5.9340 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.5010 15.3780 -5.6070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.5780 16.4570 -5.7940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.6330 15.2550 -4.5260 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.5850 14.6040 -6.3480 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.4740 13.5350 -6.1300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


108.2900	-0.1470	-5.8430	C	0	0	0	0	0	0	0	0	0	0	0	0
107.9440	-0.8510	-5.0770	H	0	0	0	0	0	0	0	0	0	0	0	0
107.5080	-0.0820	-6.6090	H	0	0	0	0	0	0	0	0	0	0	0	0
109.1690	-0.5980	-6.3210	H	0	0	0	0	0	0	0	0	0	0	0	0
108.3680	2.5320	-7.4240	C	0	0	0	0	0	0	0	0	0	0	0	0
107.3040	2.3020	-7.4010	H	0	0	0	0	0	0	0	0	0	0	0	0
108.8630	3.2760	-8.4990	C	0	0	0	0	0	0	0	0	0	0	0	0
108.1840	3.6040	-9.2810	H	0	0	0	0	0	0	0	0	0	0	0	0
110.2200	3.5890	-8.5850	C	0	0	0	0	0	0	0	0	0	0	0	0
111.0720	3.1690	-7.5680	C	0	0	0	0	0	0	0	0	0	0	0	0
112.1310	3.4020	-7.5730	H	0	0	0	0	0	0	0	0	0	0	0	0
110.5760	2.4240	-6.4860	C	0	0	0	0	0	0	0	0	0	0	0	0
111.2890	2.1140	-5.7270	H	0	0	0	0	0	0	0	0	0	0	0	0
110.5680	4.3140	-9.6900	O	0	0	0	0	0	0	0	0	0	0	0	0
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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
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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	29	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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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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35	37	1	0	0	0	0	0	0	0	0	0	0	0	0	0
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72	77	1	0	0	0	0
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73	75	1	0	0	0	0
75	76	1	0	0	0	0
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78	84	1	0	0	0	0
78	86	1	0	0	0	0
79	80	1	0	0	0	0
79	81	2	0	0	0	0
81	82	1	0	0	0	0
81	83	1	0	0	0	0
83	84	2	0	0	0	0
84	85	1	0	0	0	0
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86	89	1	0	0	0	0
89	90	1	0	0	0	0
89	91	1	0	0	0	0
89	92	1	0	0	0	0
92	108	1	0	0	0	0
93	94	1	0	0	0	0
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
97	98	1	0	0	0	0
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230238	1	0	0	0	0
231232	1	0	0	0	0
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233234	1	0	0	0	0
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238241	1	0	0	0	0
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276284	2	0	0	0	0
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279280	1	0	0	0	0
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60.4690	-5.8430	-25.1980	C	0	0	0	0	0	0	0	0	0	0	0	0
59.6730	-5.0900	-25.2330	H	0	0	0	0	0	0	0	0	0	0	0	0
61.4410	-5.3570	-25.3370	H	0	0	0	0	0	0	0	0	0	0	0	0
60.2460	-6.8910	-26.2830	C	0	0	0	0	0	0	0	0	0	0	0	0
61.0210	-7.6640	-26.2070	H	0	0	0	0	0	0	0	0	0	0	0	0
59.2930	-7.4040	-26.1020	H	0	0	0	0	0	0	0	0	0	0	0	0
60.7900	-4.4620	-22.9190	O	0	0	0	0	0	0	0	0	0	0	0	0
60.2540	-6.2670	-27.6780	C	0	0	0	0	0	0	0	0	0	0	0	0
59.4730	-5.4990	-27.7410	H	0	0	0	0	0	0	0	0	0	0	0	0
61.2150	-5.7650	-27.8490	H	0	0	0	0	0	0	0	0	0	0	0	0
60.0260	-7.3190	-28.7640	C	0	0	0	0	0	0	0	0	0	0	0	0
59.0660	-7.8220	-28.5920	H	0	0	0	0	0	0	0	0	0	0	0	0
60.8070	-8.0860	-28.7030	H	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
E20_1

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E24_1
MOE2012 3D

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14.7980 28.4420 5.3940 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.6670 28.9310 5.8440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.1030 28.1270 6.1790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.2150 27.2610 4.5190 C 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
15.8780 27.6090 3.7180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.8810 26.1490 5.3400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.7580 26.5420 5.8660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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16.2810 25.0540 4.4460 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
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19.9980 11.3240 0.8540 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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19.8390 16.2760 2.2380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.1400 15.8110 2.3540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.8950 5.8210 1.5420 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.8190 5.2450 0.7600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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73.6840	3.7370	-13.2940	C	0	0	0	0	0	0	0	0	0	0	0	0	0
73.7290	4.1660	-12.2850	H	0	0	0	0	0	0	0	0	0	0	0	0	0
74.3640	4.3410	-13.9080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.9240	9.2530	-15.9590	C	0	0	0	0	0	0	0	0	0	0	0	0	0
66.6170	9.7820	-16.6270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.8740	9.8500	-15.0390	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.5370	7.8830	-15.6610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
65.9550	7.3450	-14.9070	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.5810	7.2890	-16.5810	H	0	0	0	0	0	0	0	0	0	0	0	0	0
67.9370	8.0250	-15.1190	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.5050	6.7900	-15.0090	O	0	0	0	0	0	0	0	0	0	0	0	0	0
69.8390	6.7930	-14.4810	C	0	0	0	0	0	0	0	0	0	0	0	0	0
70.4860	7.3950	-15.1290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.8290	7.2210	-13.4720	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.3390	5.3530	-14.4340	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.6570	4.7520	-13.8200	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.2950	4.9210	-15.4420	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.4730	9.0780	-14.8040	O	0	0	0	0	0	0	0	0	0	0	0	0	0
71.7620	5.2680	-13.8830	C	0	0	0	0	0	0	0	0	0	0	0	0	0
72.4330	5.8690	-14.5080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.7910	5.6950	-12.8730	H	0	0	0	0	0	0	0	0	0	0	0	0	0
72.2600	3.8220	-13.8420	C	0	0	0	0	0	0	0	0	0	0	0	0	0
72.2300	3.3940	-14.8520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.5900	3.2200	-13.2160	H	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
E24_1

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E32_1
MOE2012 3D

272271 0 0 1 0 0 0 0 0999 V2000
-4.7830 -2.4740 -7.4950 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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-2.2710 -2.4590 -6.7390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-1.2080 -2.1690 -8.6050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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-1.3920 -1.7110 -9.5840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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-0.1820 -0.4570 -7.7830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0.2000 -1.9810 -6.9780 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.2580 -1.6790 -8.8410 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.4510 -2.7450 -9.0090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.0770 -1.2070 -9.8140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.4110 -1.0610 -8.1840 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0
2.2140 -0.0760 -8.0050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.3230 1.6110 -7.7400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.4040 1.0550 -6.7990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.0690 2.6560 -7.5280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.5770 1.5560 -8.4350 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.6280 2.1000 -7.7540 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.8750 2.0010 -8.5930 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.9410 0.9860 -9.0020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.7620 2.7170 -9.4120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.1240 2.2990 -7.7590 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.0680 3.3160 -7.3500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.1080 1.6250 -6.8910 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.5570 2.6120 -6.6460 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.2560 0.9830 -8.6300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.2220 1.5170 -9.5880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.5450 -0.0480 -8.8720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.6150 -1.1840 -9.0090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.8250 -2.2420 -9.2110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.4650 -0.6850 -9.9750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.8060 -0.5610 -8.2850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.6220 0.5040 -8.1000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.9700 -1.0690 -7.3280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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7.1130 -0.1620 -8.4110 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.3720 -0.2220 -9.0980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.6210 -1.2680 -9.3100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.2990 0.3370 -10.0390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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M END
> <NAME>
E32_1

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E36_1
MOE2012 3D

287286 0 0 1 0 0 0 0 0999 V2000
9.9650 2.9840 -15.0650 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.1370 3.4590 -14.8820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.8710 3.3110 -14.0190 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.0180 4.3950 -14.0130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.4250 3.0070 -13.0660 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.1900 2.5850 -14.2560 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.0060 1.5050 -14.3040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.5860 2.8660 -15.2400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.2130 2.9000 -13.1650 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.3910 3.9810 -13.1310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.8090 2.6080 -12.1880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.5380 2.1710 -13.4080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.3620 1.0890 -13.4350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.9400 2.4580 -14.3880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.5640 2.4970 -12.3180 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7310 3.5810 -12.2900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.1620 2.2060 -11.3400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.8940 1.7750 -12.5660 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.7120 0.6950 -12.5850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.2910 2.0730 -13.5430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.8460 2.1140 -11.5040 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
17.9160 3.1310 -11.4440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.3530 -8.2290 -10.5900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.6950 -8.7240 -11.3130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.9470 -8.3530 -9.5790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.6600 -8.8180 -10.6550 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.6920 -10.1500 -10.3650 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.1130 -10.6480 -10.4530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.4710 -10.4820 -11.4760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.7200 -10.0540 -9.7630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.1900 -12.1350 -10.1090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.7290 -12.3410 -9.1340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.5660 -12.6790 -10.8320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.7190 -10.8320 -10.0760 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.4770 -6.7460 -10.9250 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.1800 -6.2740 -10.2270 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.9240 -6.6350 -11.9210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.1850 1.5650 -11.7420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.5490 1.8550 -12.7360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8650 2.0370 -11.0210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.2510 0.0510 -11.5560 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.8780 -0.2180 -10.5610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.6520 -0.4630 -12.3160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.6700 -0.4450 -11.6790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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22.0160 -2.3680 -11.4830 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.4040 -2.2440 -12.5010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.6860 -1.8710 -10.7720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.8960 -3.8500 -11.1450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.4570 -3.9590 -10.1450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.1880 -4.3240 -11.8360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.6350 0.2370 -11.9930 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.2500 -4.5550 -11.2070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.6770 -4.4420 -12.2120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.9450 -4.0770 -10.5060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.1230 -6.0410 -10.8700 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.4310 -6.5190 -11.5740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.6920 -6.1540 -9.8670 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.0590 -18.5530 -14.7770 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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M END
> <NAME>
E36_1

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E80_1
MOE2012 3D

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10.4040 -22.4610 -3.5140 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.9500 -22.9840 -4.3640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.7060 -22.5010 -2.6700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.3030 -23.0270 -3.2470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.7500 -21.0840 -3.8810 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.4200 -20.4130 -2.7480 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.7270 -20.2940 -1.9050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.2400 -21.0530 -2.3980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.0310 -19.0510 -3.1170 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.6920 -19.1680 -3.9850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.2390 -18.3470 -3.4010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.8230 -18.4550 -1.9420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.1610 -18.3650 -1.0730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.6460 -19.1270 -1.6770 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.5440 -20.3720 -4.3100 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.8240 -20.2490 -3.4940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.0480 -20.9130 -5.1250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.7880 -19.3850 -4.7130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.3340 -17.1370 -2.3190 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
13.9550 -17.2170 -3.1230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.1270 -15.9800 3.4040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.6170 -15.9110 2.4260 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.0710 -17.0310 3.7130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.8890 -15.2390 4.3700 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.1610 -15.6980 4.5580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.8570 -14.8430 5.5910 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.8610 -13.8150 5.2130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.2750 -14.8850 6.5170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.2900 -15.3320 5.8360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.2700 -16.3910 6.1310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.8400 -15.3370 4.8860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.6580 -16.6500 3.9740 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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22.2700 -15.4080 4.3310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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13.3780 -16.4420 -0.3210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.4100 -16.9300 -0.9220 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.3760 -17.9490 -0.5230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.0110 -16.9220 -1.8390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.1010 -16.0500 0.0970 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.3950 -16.4600 0.2490 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.1550 -15.6970 1.1990 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.1960 -14.6510 0.8760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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M END
> <NAME>
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E86_1
MOE2012 3D

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18.2510 7.4370 12.6570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.8780 5.8310 13.0390 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.2030 5.6510 14.0710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.8090 5.6110 12.9560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.6140 4.8690 12.1440 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.3050 3.5900 12.5070 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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17.7300 2.7190 10.6690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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52.1020	-21.3890	10.5960	O	0	0	0	0	0	0	0	0	0	0	0	0
56.8720	-22.7870	11.8140	C	0	0	0	0	0	0	0	0	0	0	0	0
56.4230	-23.0240	12.7860	H	0	0	0	0	0	0	0	0	0	0	0	0
56.6610	-23.6320	11.1460	H	0	0	0	0	0	0	0	0	0	0	0	0
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228229	1	0	0	0	0
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229232	1	0	0	0	0
232233	1	0	0	0	0

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289290 1 0 0 0 0
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293294 1 0 0 0 0
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293297 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
300302 1 0 0 0 0

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```

M END
> <NAME>
E86_1

```

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$$$$
F28_1
MOE2012 3D

```

```

242241 0 0 1 0 0 0 0 0 0999 V2000
23.8490 -2.0170 -8.3030 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.2900 -1.4600 -8.8710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.0260 -3.0630 -7.8070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.1920 -2.6190 -7.2540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.6310 -3.6260 -8.6580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


42.4580	-11.9920	5.4920	O	0	0	0	0	0	0	0	0	0	0	0
43.3610	-11.8530	6.6060	C	0	0	0	0	0	0	0	0	0	0	0
43.2930	-10.8530	7.0520	H	0	0	0	0	0	0	0	0	0	0	0
43.0040	-12.5510	7.3730	H	0	0	0	0	0	0	0	0	0	0	0
44.8230	-12.1950	6.2270	C	0	0	0	0	0	0	0	0	0	0	0
45.6860	-12.0950	7.5090	C	0	0	0	0	0	0	0	0	0	0	0
45.6160	-11.0840	7.9300	H	0	0	0	0	0	0	0	0	0	0	0
45.3280	-12.8130	8.2570	H	0	0	0	0	0	0	0	0	0	0	0
47.0660	-12.3710	7.2140	O	0	0	0	0	0	0	0	0	0	0	0
47.8950	-12.3770	8.2970	C	0	0	0	0	0	0	0	0	0	0	0
49.3110	-12.6640	7.8600	C	0	0	0	0	0	0	0	0	0	0	0
49.4340	-13.7510	7.8270	H	0	0	0	0	0	0	0	0	0	0	0
49.4550	-12.2600	6.8500	H	0	0	0	0	0	0	0	0	0	0	0
50.3080	-12.0040	8.8160	C	0	0	0	0	0	0	0	0	0	0	0
50.2270	-12.4390	9.8190	H	0	0	0	0	0	0	0	0	0	0	0
49.9960	-10.9590	8.9220	H	0	0	0	0	0	0	0	0	0	0	0
42.4440	-9.7180	5.1550	O	0	0	0	0	0	0	0	0	0	0	0
47.5430	-12.2070	9.4560	O	0	0	0	0	0	0	0	0	0	0	0
44.8990	-13.6230	5.6540	C	0	0	0	0	0	0	0	0	0	0	0
45.9270	-13.8980	5.3930	H	0	0	0	0	0	0	0	0	0	0	0
44.2950	-13.7240	4.7450	H	0	0	0	0	0	0	0	0	0	0	0
44.5330	-14.3580	6.3800	H	0	0	0	0	0	0	0	0	0	0	0
45.3550	-11.2200	5.1610	C	0	0	0	0	0	0	0	0	0	0	0
44.7800	-11.2860	4.2310	H	0	0	0	0	0	0	0	0	0	0	0
46.3990	-11.4320	4.9050	H	0	0	0	0	0	0	0	0	0	0	0
45.3060	-10.1850	5.5160	H	0	0	0	0	0	0	0	0	0	0	0
54.0030	-17.4830	10.4350	O	0	0	0	0	0	0	0	0	0	0	0
54.1200	-17.9290	11.2920	H	0	0	0	0	0	0	0	0	0	0	0
53.3310	-16.2560	10.6890	C	0	0	0	0	0	0	0	0	0	0	0
52.3720	-16.4770	11.1700	H	0	0	0	0	0	0	0	0	0	0	0
53.9430	-15.6610	11.3740	H	0	0	0	0	0	0	0	0	0	0	0
53.1190	-15.5200	9.3710	C	0	0	0	0	0	0	0	0	0	0	0
54.0880	-15.3800	8.8770	H	0	0	0	0	0	0	0	0	0	0	0
52.5260	-16.1490	8.6950	H	0	0	0	0	0	0	0	0	0	0	0
52.4300	-14.1680	9.5780	C	0	0	0	0	0	0	0	0	0	0	0
51.4550	-14.3330	10.0480	H	0	0	0	0	0	0	0	0	0	0	0
53.0320	-13.5710	10.2720	H	0	0	0	0	0	0	0	0	0	0	0
52.2580	-13.4210	8.2440	C	0	0	0	0	0	0	0	0	0	0	0
53.2330	-13.3570	7.7440	H	0	0	0	0	0	0	0	0	0	0	0
51.6480	-14.0300	7.5660	H	0	0	0	0	0	0	0	0	0	0	0
51.6950	-12.0580	8.3210	N	0	0	3	0	0	0	0	0	0	0	0
52.5950	-11.1440	9.0480	C	0	0	0	0	0	0	0	0	0	0	0
53.6340	-11.3590	8.7630	H	0	0	0	0	0	0	0	0	0	0	0
52.5260	-11.3110	10.1300	H	0	0	0	0	0	0	0	0	0	0	0
52.3540	-9.6630	8.7590	C	0	0	0	0	0	0	0	0	0	0	0
51.3840	-9.3210	9.1330	H	0	0	0	0	0	0	0	0	0	0	0
53.1010	-9.0520	9.2800	H	0	0	0	0	0	0	0	0	0	0	0
52.4770	-9.3650	7.2880	C	0	0	0	0	0	0	0	0	0	0	0
51.2460	-9.1280	6.7530	O	0	0	0	0	0	0	0	0	0	0	0
51.1760	-8.8830	5.3380	C	0	0	0	0	0	0	0	0	0	0	0
52.0840	-9.2240	4.8250	H	0	0	0	0	0	0	0	0	0	0	0
50.3570	-9.5070	4.9600	H	0	0	0	0	0	0	0	0	0	0	0
50.8900	-7.3950	5.0270	C	0	0	0	0	0	0	0	0	0	0	0
50.7830	-7.2440	3.4910	C	0	0	0	0	0	0	0	0	0	0	0
51.7140	-7.5760	3.0180	H	0	0	0	0	0	0	0	0	0	0	0
49.9860	-7.8820	3.0910	H	0	0	0	0	0	0	0	0	0	0	0
50.6100	-5.8670	3.1120	O	0	0	0	0	0	0	0	0	0	0	0
49.4070	-5.5040	2.5810	C	0	0	0	0	0	0	0	0	0	0	0
49.4410	-4.0320	2.2450	C	0	0	0	0	0	0	0	0	0	0	0
49.6500	-3.4720	3.1630	H	0	0	0	0	0	0	0	0	0	0	0
50.2510	-3.8590	1.5280	H	0	0	0	0	0	0	0	0	0	0	0
48.1300	-3.5510	1.6490	C	0	0	0	0	0	0	0	0	0	0	0
47.8960	-4.0900	0.7250	H	0	0	0	0	0	0	0	0	0	0	0
48.1860	-2.4830	1.4170	H	0	0	0	0	0	0	0	0	0	0	0
47.3000	-3.7070	2.3470	H	0	0	0	0	0	0	0	0	0	0	0
53.5390	-9.3300	6.6810	O	0	0	0	0	0	0	0	0	0	0	0
48.4490	-6.2450	2.4110	O	0	0	0	0	0	0	0	0	0	0	0
49.5740	-6.9610	5.6990	C	0	0	0	0	0	0	0	0	0	0	0
49.3500	-5.9070	5.5030	H	0	0	0	0	0	0	0	0	0	0	0
49.6180	-7.0830	6.7870	H	0	0	0	0	0	0	0	0	0	0	0
48.7300	-7.5560	5.3320	H	0	0	0	0	0	0	0	0	0	0	0
52.0240	-6.5030	5.5680	C	0	0	0	0	0	0	0	0	0	0	0
52.1120	-6.5770	6.6570	H	0	0	0	0	0	0	0	0	0	0	0
51.8510	-5.4460	5.3340	H	0	0	0	0	0	0	0	0	0	0	0
52.9880	-6.7860	5.1320	H	0	0	0	0	0	0	0	0	0	0	0

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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	100	1	0	0	0	0
100	101	1	0	0	0	0
100	102	1	0	0	0	0
100	103	1	0	0	0	0
103	104	1	0	0	0	0
103	105	1	0	0	0	0
103	106	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	148	1	0	0	0	0
148	149	1	0	0	0	0
148	150	1	0	0	0	0
148	151	1	0	0	0	0
151	152	1	0	0	0	0
151	153	1	0	0	0	0
151	154	1	0	0	0	0
154	155	1	0	0	0	0
154	156	1	0	0	0	0
154	157	1	0	0	0	0
157	158	1	0	0	0	0
157	159	1	0	0	0	0
157	160	1	0	0	0	0
160	161	1	0	0	0	0
161	162	1	0	0	0	0
161	163	1	0	0	0	0
161	164	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
167	168	1	0	0	0	0
167	184	2	0	0	0	0

168169	1	0	0	0	0
169170	1	0	0	0	0
169171	1	0	0	0	0
169172	1	0	0	0	0
172173	1	0	0	0	0
172186	1	0	0	0	0
172190	1	0	0	0	0
173174	1	0	0	0	0
173175	1	0	0	0	0
173176	1	0	0	0	0
176177	1	0	0	0	0
177178	1	0	0	0	0
177185	2	0	0	0	0
178179	1	0	0	0	0
178180	1	0	0	0	0
178181	1	0	0	0	0
181182	1	0	0	0	0
181183	1	0	0	0	0
181208	1	0	0	0	0
186187	1	0	0	0	0
186188	1	0	0	0	0
186189	1	0	0	0	0
190191	1	0	0	0	0
190192	1	0	0	0	0
190193	1	0	0	0	0
194195	1	0	0	0	0
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
199202	1	0	0	0	0
202203	1	0	0	0	0
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
209210	1	0	0	0	0
209211	1	0	0	0	0
209212	1	0	0	0	0
212213	1	0	0	0	0
212214	1	0	0	0	0
212215	1	0	0	0	0
215216	1	0	0	0	0
215233	2	0	0	0	0
216217	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
220235	1	0	0	0	0
220239	1	0	0	0	0
221222	1	0	0	0	0
221223	1	0	0	0	0
221224	1	0	0	0	0
224225	1	0	0	0	0
225226	1	0	0	0	0
225234	2	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
235236	1	0	0	0	0
235237	1	0	0	0	0
235238	1	0	0	0	0
239240	1	0	0	0	0
239241	1	0	0	0	0
239242	1	0	0	0	0

M END
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19.4120	-4.2130	-2.4530	H	0	0	0	0	0	0	0	0	0	0	0	0
20.6930	-2.5730	-1.7950	C	0	0	0	0	0	0	0	0	0	0	0	0
21.8370	-3.0590	-2.7200	C	0	0	0	0	0	0	0	0	0	0	0	0
22.3490	-3.9160	-2.2650	H	0	0	0	0	0	0	0	0	0	0	0	0
21.4250	-3.3710	-3.6890	H	0	0	0	0	0	0	0	0	0	0	0	0
22.8060	-2.0180	-2.9260	O	0	0	0	0	0	0	0	0	0	0	0	0
23.7950	-2.3210	-3.8140	C	0	0	0	0	0	0	0	0	0	0	0	0
24.8380	-1.2330	-3.8330	C	0	0	0	0	0	0	0	0	0	0	0	0
24.9460	-0.8770	-4.8620	H	0	0	0	0	0	0	0	0	0	0	0	0
24.4780	-0.3880	-3.2370	H	0	0	0	0	0	0	0	0	0	0	0	0
26.1510	-1.7950	-3.2820	C	0	0	0	0	0	0	0	0	0	0	0	0
26.5420	-2.5390	-3.9910	H	0	0	0	0	0	0	0	0	0	0	0	0
25.9530	-2.3880	-2.3800	H	0	0	0	0	0	0	0	0	0	0	0	0
18.2880	-5.5860	-0.1830	O	0	0	0	0	0	0	0	0	0	0	0	0
23.8620	-3.3480	-4.4780	O	0	0	0	0	0	0	0	0	0	0	0	0
19.9090	-1.4420	-2.4850	C	0	0	0	0	0	0	0	0	0	0	0	0
20.5580	-0.5920	-2.7230	H	0	0	0	0	0	0	0	0	0	0	0	0
19.1000	-1.0660	-1.8490	H	0	0	0	0	0	0	0	0	0	0	0	0
19.4610	-1.7910	-3.4230	H	0	0	0	0	0	0	0	0	0	0	0	0
21.2620	-2.0320	-0.4700	C	0	0	0	0	0	0	0	0	0	0	0	0
20.4630	-1.7130	0.2080	H	0	0	0	0	0	0	0	0	0	0	0	0
21.9140	-1.1670	-0.6330	H	0	0	0	0	0	0	0	0	0	0	0	0
21.8500	-2.7990	0.0470	H	0	0	0	0	0	0	0	0	0	0	0	0
24.7570	0.5800	3.9040	O	0	0	0	0	0	0	0	0	0	0	0	0
24.9920	1.1430	4.6690	H	0	0	0	0	0	0	0	0	0	0	0	0
25.4560	1.1280	2.7880	C	0	0	0	0	0	0	0	0	0	0	0	0
24.9510	2.0510	2.4870	H	0	0	0	0	0	0	0	0	0	0	0	0
26.4790	1.3660	3.0980	H	0	0	0	0	0	0	0	0	0	0	0	0
25.4630	0.1090	1.6580	C	0	0	0	0	0	0	0	0	0	0	0	0
25.9700	-0.8020	1.9990	H	0	0	0	0	0	0	0	0	0	0	0	0
24.4330	-0.1900	1.4260	H	0	0	0	0	0	0	0	0	0	0	0	0
26.1440	0.6650	0.4100	C	0	0	0	0	0	0	0	0	0	0	0	0
25.5680	1.5180	0.0290	H	0	0	0	0	0	0	0	0	0	0	0	0
27.1420	1.0400	0.6680	H	0	0	0	0	0	0	0	0	0	0	0	0
26.2700	-0.4030	-0.6780	C	0	0	0	0	0	0	0	0	0	0	0	0
26.9070	-1.2170	-0.3110	H	0	0	0	0	0	0	0	0	0	0	0	0
25.2770	-0.8240	-0.8740	H	0	0	0	0	0	0	0	0	0	0	0	0
26.8660	0.1830	-1.9680	C	0	0	0	0	0	0	0	0	0	0	0	0
26.1750	0.9300	-2.3790	H	0	0	0	0	0	0	0	0	0	0	0	0
27.7760	0.7200	-1.6780	H	0	0	0	0	0	0	0	0	0	0	0	0
27.2170	-0.8180	-2.9890	N	0	0	3	0	0	0	0	0	0	0	0	0
27.7580	-0.2180	-4.2230	C	0	0	0	0	0	0	0	0	0	0	0	0
27.0110	0.4540	-4.6650	H	0	0	0	0	0	0	0	0	0	0	0	0
27.9360	-1.0130	-4.9590	H	0	0	0	0	0	0	0	0	0	0	0	0
29.0690	0.5610	-4.0650	C	0	0	0	0	0	0	0	0	0	0	0	0
29.3170	1.0190	-5.0300	H	0	0	0	0	0	0	0	0	0	0	0	0
28.9610	1.3730	-3.3390	H	0	0	0	0	0	0	0	0	0	0	0	0
30.2460	-0.3050	-3.6800	C	0	0	0	0	0	0	0	0	0	0	0	0
31.2900	0.4980	-3.3120	O	0	0	0	0	0	0	0	0	0	0	0	0
32.5060	-0.1960	-2.9830	C	0	0	0	0	0	0	0	0	0	0	0	0
32.3280	-0.8000	-2.0850	H	0	0	0	0	0	0	0	0	0	0	0	0
32.7740	-0.8650	-3.8110	H	0	0	0	0	0	0	0	0	0	0	0	0
33.6550	0.8100	-2.7300	C	0	0	0	0	0	0	0	0	0	0	0	0
34.9250	0.0070	-2.3670	C	0	0	0	0	0	0	0	0	0	0	0	0
34.7430	-0.5820	-1.4590	H	0	0	0	0	0	0	0	0	0	0	0	0
35.1820	-0.6780	-3.1840	H	0	0	0	0	0	0	0	0	0	0	0	0
36.0400	0.8860	-2.1410	O	0	0	0	0	0	0	0	0	0	0	0	0
37.1790	0.2570	-1.7300	C	0	0	0	0	0	0	0	0	0	0	0	0
38.2880	1.2620	-1.5410	C	0	0	0	0	0	0	0	0	0	0	0	0
38.4690	1.7450	-2.5050	H	0	0	0	0	0	0	0	0	0	0	0	0
37.9540	2.0140	-0.8170	H	0	0	0	0	0	0	0	0	0	0	0	0
39.5480	0.5600	-1.0190	C	0	0	0	0	0	0	0	0	0	0	0	0
39.8770	-0.2210	-1.7180	H	0	0	0	0	0	0	0	0	0	0	0	0
39.2570	0.0400	-0.0960	H	0	0	0	0	0	0	0	0	0	0	0	0
30.2900	-1.5250	-3.7430	O	0	0	0	0	0	0	0	0	0	0	0	0
37.2860	-0.9480	-1.5500	O	0	0	0	0	0	0	0	0	0	0	0	0
33.9050	1.6540	-3.9950	C	0	0	0	0	0	0	0	0	0	0	0	0
34.7180	2.3730	-3.8440	H	0	0	0	0	0	0	0	0	0	0	0	0
33.0150	2.2260	-4.2790	H	0	0	0	0	0	0	0	0	0	0	0	0
34.1770	1.0170	-4.8440	H	0	0	0	0	0	0	0	0	0	0	0	0
33.2840	1.7610	-1.5770	C	0	0	0	0	0	0	0	0	0	0	0	0
32.3840	2.3420	-1.8070	H	0	0	0	0	0	0	0	0	0	0	0	0
34.0880	2.4760	-1.3710	H	0	0	0	0	0	0	0	0	0	0	0	0
33.0910	1.2010	-0.6540	H	0	0	0	0	0	0	0	0	0	0	0	0
46.3900	2.0930	3.9860	O	0	0	0	0	0	0	0	0	0	0	0	0
46.8590	1.6360	4.7050	H	0	0	0	0	0	0	0	0	0	0	0	0
45.3760	1.2160	3.5190	C	0	0	0	0	0	0	0	0	0	0	0	0
45.8490	0.2940	3.1660	H	0	0	0	0	0	0	0	0	0	0	0	0
44.7110	0.9770	4.3550	H	0	0	0	0	0	0	0	0	0	0	0	0
44.6140	1.9020	2.3950	C	0	0	0	0	0	0	0	0	0	0	0	0
44.1950	2.8460	2.7650	H	0	0	0	0	0	0	0	0	0	0	0	0

45.3130	2.1770	1.5960	H	0	0	0	0	0	0	0	0	0	0	0	0
43.5050	1.0090	1.8450	C	0	0	0	0	0	0	0	0	0	0	0	0
43.9370	0.0770	1.4600	H	0	0	0	0	0	0	0	0	0	0	0	0
42.8190	0.7370	2.6570	H	0	0	0	0	0	0	0	0	0	0	0	0
42.7270	1.7140	0.7300	C	0	0	0	0	0	0	0	0	0	0	0	0
42.3010	2.6460	1.1190	H	0	0	0	0	0	0	0	0	0	0	0	0
43.4270	1.9710	-0.0720	H	0	0	0	0	0	0	0	0	0	0	0	0
41.6100	0.8170	0.1870	C	0	0	0	0	0	0	0	0	0	0	0	0
42.0480	-0.0630	-0.3010	H	0	0	0	0	0	0	0	0	0	0	0	0
41.0490	0.4490	1.0560	H	0	0	0	0	0	0	0	0	0	0	0	0
40.6590	1.4940	-0.7240	N	0	0	3	0	0	0	0	0	0	0	0	0
41.3020	1.9720	-1.9670	C	0	0	0	0	0	0	0	0	0	0	0	0
40.6230	1.8670	-2.8220	H	0	0	0	0	0	0	0	0	0	0	0	0
42.1740	1.3560	-2.2240	H	0	0	0	0	0	0	0	0	0	0	0	0
41.7050	3.4450	-1.9030	C	0	0	0	0	0	0	0	0	0	0	0	0
42.5110	3.6230	-1.1860	H	0	0	0	0	0	0	0	0	0	0	0	0
42.0900	3.7750	-2.8750	H	0	0	0	0	0	0	0	0	0	0	0	0
40.5240	4.3120	-1.5640	C	0	0	0	0	0	0	0	0	0	0	0	0
40.7090	4.9160	-0.3580	O	0	0	0	0	0	0	0	0	0	0	0	0
39.5910	5.6840	0.1130	C	0	0	0	0	0	0	0	0	0	0	0	0
39.2610	6.3740	-0.6750	H	0	0	0	0	0	0	0	0	0	0	0	0
38.7700	4.9950	0.3430	H	0	0	0	0	0	0	0	0	0	0	0	0
39.9870	6.4840	1.3740	C	0	0	0	0	0	0	0	0	0	0	0	0
38.7450	7.2580	1.8770	C	0	0	0	0	0	0	0	0	0	0	0	0
38.3460	7.8930	1.0770	H	0	0	0	0	0	0	0	0	0	0	0	0
37.9620	6.5600	2.1990	H	0	0	0	0	0	0	0	0	0	0	0	0
39.1160	8.0920	2.9870	O	0	0	0	0	0	0	0	0	0	0	0	0
38.1340	8.8850	3.4980	C	0	0	0	0	0	0	0	0	0	0	0	0
38.7160	9.8000	4.5470	C	0	0	0	0	0	0	0	0	0	0	0	0
38.0030	9.8690	5.3760	H	0	0	0	0	0	0	0	0	0	0	0	0
39.6200	9.3320	4.9510	H	0	0	0	0	0	0	0	0	0	0	0	0
39.0000	11.1700	3.9270	C	0	0	0	0	0	0	0	0	0	0	0	0
38.0410	11.6470	3.6800	H	0	0	0	0	0	0	0	0	0	0	0	0
39.4770	11.0480	2.9470	H	0	0	0	0	0	0	0	0	0	0	0	0
39.5370	4.4380	-2.2770	O	0	0	0	0	0	0	0	0	0	0	0	0
36.9650	8.9040	3.1390	O	0	0	0	0	0	0	0	0	0	0	0	0
40.4890	5.5290	2.4750	C	0	0	0	0	0	0	0	0	0	0	0	0
40.7560	6.0730	3.3870	H	0	0	0	0	0	0	0	0	0	0	0	0
41.3800	4.9770	2.1540	H	0	0	0	0	0	0	0	0	0	0	0	0
39.7200	4.7950	2.7370	H	0	0	0	0	0	0	0	0	0	0	0	0
41.1250	7.4670	1.0310	C	0	0	0	0	0	0	0	0	0	0	0	0
42.0080	6.9430	0.6500	H	0	0	0	0	0	0	0	0	0	0	0	0
41.4450	8.0390	1.9090	H	0	0	0	0	0	0	0	0	0	0	0	0
40.8060	8.1830	0.2660	H	0	0	0	0	0	0	0	0	0	0	0	0
45.5250	11.2810	0.9800	O	0	0	0	0	0	0	0	0	0	0	0	0
45.8420	12.0510	0.4760	H	0	0	0	0	0	0	0	0	0	0	0	0
44.6550	11.7620	1.9990	C	0	0	0	0	0	0	0	0	0	0	0	0
45.1700	12.5570	2.5480	H	0	0	0	0	0	0	0	0	0	0	0	0
43.7630	12.1760	1.5210	H	0	0	0	0	0	0	0	0	0	0	0	0
44.3060	10.6040	2.9260	C	0	0	0	0	0	0	0	0	0	0	0	0
43.8120	9.8080	2.3540	H	0	0	0	0	0	0	0	0	0	0	0	0
45.2410	10.1600	3.2940	H	0	0	0	0	0	0	0	0	0	0	0	0
43.4490	11.0070	4.1270	C	0	0	0	0	0	0	0	0	0	0	0	0
43.4280	10.1630	4.8280	H	0	0	0	0	0	0	0	0	0	0	0	0
43.9220	11.8440	4.6550	H	0	0	0	0	0	0	0	0	0	0	0	0
42.0070	11.3720	3.7540	C	0	0	0	0	1	0	0	0	0	0	0	0
41.9990	12.2540	3.1040	H	0	0	0	0	0	0	0	0	0	0	0	0
41.5760	10.5380	3.1890	H	0	0	0	0	0	0	0	0	0	0	0	0
41.1680	11.6570	5.0140	C	0	0	0	0	0	0	0	0	0	0	0	0
41.1620	10.7680	5.6570	H	0	0	0	0	0	0	0	0	0	0	0	0
41.6990	12.4330	5.5760	H	0	0	0	0	0	0	0	0	0	0	0	0
39.7910	12.1170	4.7410	N	0	0	3	0	0	0	0	0	0	0	0	0
39.0770	12.4850	5.9820	C	0	0	0	0	0	0	0	0	0	0	0	0
39.2320	11.7050	6.7400	H	0	0	0	0	0	0	0	0	0	0	0	0
37.9950	12.5160	5.7980	H	0	0	0	0	0	0	0	0	0	0	0	0
39.4970	13.8390	6.5680	C	0	0	0	0	0	3	0	0	0	0	0	0
39.1890	13.8630	7.6210	H	0	0	0	0	0	0	0	0	0	0	0	0
40.5800	13.9820	6.5340	H	0	0	0	0	0	0	0	0	0	0	0	0
38.8270	15.0190	5.8990	C	0	0	0	0	0	0	0	0	0	0	0	0
39.3200	16.1760	6.4370	O	0	0	0	0	0	0	0	0	0	0	0	0
38.7140	17.3830	5.9450	C	0	0	0	0	0	0	0	0	0	0	0	0
38.9260	17.4690	4.8720	H	0	0	0	0	0	0	0	0	0	0	0	0
37.6270	17.3220	6.0860	H	0	0	0	0	0	0	0	0	0	0	0	0
39.2730	18.6130	6.6990	C	0	0	0	0	0	0	0	0	0	0	0	0
38.5860	19.8810	6.1410	C	0	0	0	0	0	0	0	0	0	0	0	0
38.7950	19.9790	5.0680	H	0	0	0	0	0	0	0	0	0	0	0	0
37.5000	19.8120	6.2830	H	0	0	0	0	0	0	0	0	0	0	0	0
39.0680	21.0530	6.8170	O	0	0	0	0	0	0	0	0	0	0	0	0
38.5220	22.2270	6.3880	C	0	0	0	0	0	0	0	0	0	0	0	0
39.1140	23.3690	7.1790	C	0	0	0	0	0	0	0	0	0	0	0	0
38.8950	23.2060	8.2400	H	0	0	0	0	0	0	0	0	0	0	0	0

40.1990	23.3660	7.0320	H	0	0	0	0	0	0	0	0	0	0	0
38.5520	24.7130	6.7500	C	0	0	0	0	0	0	0	0	0	0	0
38.7590	24.9060	5.6920	H	0	0	0	0	0	0	0	0	0	0	0
38.9990	25.5190	7.3390	H	0	0	0	0	0	0	0	0	0	0	0
37.4660	24.7480	6.8890	H	0	0	0	0	0	0	0	0	0	0	0
37.9470	14.9620	5.0520	O	0	0	0	0	0	0	0	0	0	0	0
37.6850	22.3340	5.5040	O	0	0	0	0	0	0	0	0	0	0	0
38.9890	18.4800	8.2080	C	0	0	0	0	0	0	0	0	0	0	0
39.3710	19.3420	8.7670	H	0	0	0	0	0	0	0	0	0	0	0
39.4610	17.5860	8.6300	H	0	0	0	0	0	0	0	0	0	0	0
37.9120	18.4100	8.3990	H	0	0	0	0	0	0	0	0	0	0	0
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41.3100	17.8170	6.8830	H	0	0	0	0	0	0	0	0	0	0	0
41.2200	19.5730	7.0200	H	0	0	0	0	0	0	0	0	0	0	0
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> <NAME>
F32_1

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F86_1
MOE2012 3D

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123	124	1	0	0	0	0
123	125	1	0	0	0	0
123	126	1	0	0	0	0
126	140	1	0	0	0	0
127	128	1	0	0	0	0
127	129	1	0	0	0	0
127	135	1	0	0	0	0
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140	143	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	163	2	0	0	0	0
147	148	1	0	0	0	0
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M END
> <NAME>
F86_1

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F94_1
MOE2012 3D

242246 0 0 1 0 0 0 0 0999 V2000
13.4200 -12.5220 -11.2280 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.9010 -13.5020 -12.0490 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.6310 -14.5430 -11.9420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.7290 -12.8470 -12.9310 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.3040 -13.2750 -13.7400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.7600 -11.5010 -12.6680 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.9630 -11.3370 -11.6360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.7490 -10.3930 -11.1510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.4860 -12.6980 -10.1360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.7930 -11.8490 -10.1690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.8980 -13.6010 -10.3370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.1480 -12.7700 -8.7520 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.7550 -11.8710 -8.5980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.3500 -12.7710 -8.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.9770 -13.9710 -8.5950 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
13.4460 -14.7930 -8.8840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.4360 -14.1780 -7.2170 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.8510 -15.1920 -7.1580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.5820 -14.1580 -6.5300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.4950 -13.1850 -6.7540 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.1340 -12.1530 -6.8170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.7420 -13.3590 -5.7000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.7700 -13.3460 -7.5400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.1030 -12.1720 -8.1440 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.3020 -12.2200 -8.9330 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.1390 -12.5200 -8.2900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.1770 -12.9720 -9.7220 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.5840 -10.8370 -9.5580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8810 -10.9380 -10.3900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

20.7210	-11.2230	-9.7430	H	0	0	0	0	0	0	0	0	0	0	0
19.7690	-11.6960	-11.1760	H	0	0	0	0	0	0	0	0	0	0	0
20.1680	-9.6760	-11.0080	O	0	0	0	0	0	0	0	0	0	0	0
21.3390	-9.6240	-11.7020	C	0	0	0	0	0	0	0	0	0	0	0
21.5050	-8.2450	-12.2890	C	0	0	0	0	0	0	0	0	0	0	0
20.7020	-8.0910	-13.0160	H	0	0	0	0	0	0	0	0	0	0	0
21.3980	-7.5170	-11.4760	H	0	0	0	0	0	0	0	0	0	0	0
22.8820	-8.0910	-12.9370	C	0	0	0	0	0	0	0	0	0	0	0
22.9990	-8.7830	-13.7810	H	0	0	0	0	0	0	0	0	0	0	0
23.6290	-8.3980	-12.1950	H	0	0	0	0	0	0	0	0	0	0	0
17.4180	-14.3830	-7.5980	O	0	0	0	0	0	0	0	0	0	0	0
22.1300	-10.5480	-11.8300	O	0	0	0	0	0	0	0	0	0	0	0
17.4090	-10.4150	-10.4590	C	0	0	0	0	0	0	0	0	0	0	0
17.5800	-9.4330	-10.9140	H	0	0	0	0	0	0	0	0	0	0	0
16.4720	-10.3520	-9.8950	H	0	0	0	0	0	0	0	0	0	0	0
17.2650	-11.1370	-11.2710	H	0	0	0	0	0	0	0	0	0	0	0
18.7490	-9.7780	-8.4490	C	0	0	0	0	0	0	0	0	0	0	0
17.8420	-9.6870	-7.8420	H	0	0	0	0	0	0	0	0	0	0	0
18.9600	-8.7870	-8.8670	H	0	0	0	0	0	0	0	0	0	0	0
19.5750	-10.0390	-7.7780	H	0	0	0	0	0	0	0	0	0	0	0
21.4950	-4.6490	-16.0970	N	0	0	0	0	0	0	0	0	0	0	0
20.1410	-4.6180	-16.2680	C	0	0	0	0	0	0	0	0	0	0	0
19.4410	-4.7970	-15.4630	H	0	0	0	0	0	0	0	0	0	0	0
19.9620	-4.3290	-17.6020	C	0	0	0	0	0	0	0	0	0	0	0
19.0290	-4.2180	-18.1370	H	0	0	0	0	0	0	0	0	0	0	0
21.1690	-4.1830	-18.2390	N	0	0	0	0	0	0	0	0	0	0	0
22.0730	-4.3820	-17.3050	C	0	0	0	0	0	0	0	0	0	0	0
23.1450	-4.3470	-17.4480	H	0	0	0	0	0	0	0	0	0	0	0
22.1990	-4.9130	-14.8540	C	0	0	0	0	0	0	0	0	0	0	0
23.1260	-4.3310	-14.8840	H	0	0	0	0	0	0	0	0	0	0	0
21.5820	-4.5130	-14.0400	H	0	0	0	0	0	0	0	0	0	0	0
22.4600	-6.4130	-14.6540	C	0	0	0	0	0	0	0	0	0	0	0
21.4870	-6.9170	-14.7000	H	0	0	0	0	0	0	0	0	0	0	0
23.0460	-6.8220	-15.4870	H	0	0	0	0	0	0	0	0	0	0	0
23.1210	-6.6940	-13.3600	N	0	0	3	0	0	0	0	0	0	0	0
24.5710	-6.4050	-13.4340	C	0	0	0	0	0	0	0	0	0	0	0
24.7640	-5.5320	-14.0680	H	0	0	0	0	0	0	0	0	0	0	0
25.0910	-7.2430	-13.9160	H	0	0	0	0	0	0	0	0	0	0	0
25.2020	-6.1320	-12.0630	C	0	0	0	0	0	0	0	0	0	0	0
24.9130	-6.8870	-11.3260	H	0	0	0	0	0	0	0	0	0	0	0
26.2920	-6.1680	-12.1760	H	0	0	0	0	0	0	0	0	0	0	0
24.8610	-4.7650	-11.5150	C	0	0	0	0	0	0	0	0	0	0	0
25.4450	-4.6220	-10.2870	O	0	0	0	0	0	0	0	0	0	0	0
25.2490	-3.3430	-9.6610	C	0	0	0	0	0	0	0	0	0	0	0
25.5080	-2.5460	-10.3700	H	0	0	0	0	0	0	0	0	0	0	0
24.1880	-3.2470	-9.3960	H	0	0	0	0	0	0	0	0	0	0	0
26.1310	-3.2230	-8.3950	C	0	0	0	0	0	0	0	0	0	0	0
25.8780	-1.8380	-7.7520	C	0	0	0	0	0	0	0	0	0	0	0
26.1140	-1.0420	-8.4690	H	0	0	0	0	0	0	0	0	0	0	0
24.8220	-1.7490	-7.4630	H	0	0	0	0	0	0	0	0	0	0	0
26.7010	-1.6660	-6.5880	O	0	0	0	0	0	0	0	0	0	0	0
26.4950	-0.5020	-5.9110	C	0	0	0	0	0	0	0	0	0	0	0
27.4520	-0.4250	-4.7520	C	0	0	0	0	0	0	0	0	0	0	0
27.4560	-1.3940	-4.2370	H	0	0	0	0	0	0	0	0	0	0	0
28.4490	-0.2420	-5.1630	H	0	0	0	0	0	0	0	0	0	0	0
27.0290	0.6670	-3.7680	C	0	0	0	0	0	0	0	0	0	0	0
26.0320	0.4030	-3.3990	H	0	0	0	0	0	0	0	0	0	0	0
26.9100	1.6380	-4.2680	H	0	0	0	0	0	0	0	0	0	0	0
24.1990	-3.9080	-12.0820	O	0	0	0	0	0	0	0	0	0	0	0
25.6830	0.3590	-6.2160	O	0	0	0	0	0	0	0	0	0	0	0
25.7760	-4.3400	-7.3940	C	0	0	0	0	0	0	0	0	0	0	0
26.3810	-4.2710	-6.4830	H	0	0	0	0	0	0	0	0	0	0	0
25.9470	-5.3330	-7.8220	H	0	0	0	0	0	0	0	0	0	0	0
24.7230	-4.2810	-7.0990	H	0	0	0	0	0	0	0	0	0	0	0
27.6170	-3.3660	-8.7750	C	0	0	0	0	0	0	0	0	0	0	0
27.8220	-4.3360	-9.2410	H	0	0	0	0	0	0	0	0	0	0	0
28.2680	-3.2850	-7.8970	H	0	0	0	0	0	0	0	0	0	0	0
27.9170	-2.5860	-9.4840	H	0	0	0	0	0	0	0	0	0	0	0
25.8540	0.7330	0.4590	N	0	0	0	0	0	0	0	0	0	0	0
24.6950	1.4580	0.4680	C	0	0	0	0	0	0	0	0	0	0	0
24.1680	1.7340	-0.4340	H	0	0	0	0	0	0	0	0	0	0	0
24.4380	1.6920	1.8000	C	0	0	0	0	0	0	0	0	0	0	0
23.6050	2.2320	2.2290	H	0	0	0	0	0	0	0	0	0	0	0
25.4070	1.1310	2.5920	N	0	0	0	0	0	0	0	0	0	0	0
26.2480	0.5650	1.7550	C	0	0	0	0	0	0	0	0	0	0	0
27.1420	0.0220	2.0320	H	0	0	0	0	0	0	0	0	0	0	0
26.5290	0.2190	-0.7180	C	0	0	0	0	0	0	0	0	0	0	0
27.1640	-0.6160	-0.3990	H	0	0	0	0	0	0	0	0	0	0	0
25.7470	-0.1960	-1.3620	H	0	0	0	0	0	0	0	0	0	0	0
27.3700	1.2900	-1.4320	C	0	0	0	0	0	0	0	0	0	0	0
26.7660	2.1780	-1.6600	H	0	0	0	0	0	0	0	0	0	0	0

28	42	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
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71	72	1	0	0	0	0
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101	103	1	0	0	0	0
103	104	2	0	0	0	0
104	105	1	0	0	0	0
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129137	2	0	0	0	0
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130133	1	0	0	0	0
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133135	1	0	0	0	0
133160	1	0	0	0	0
138139	1	0	0	0	0
138140	1	0	0	0	0
138141	1	0	0	0	0
142143	1	0	0	0	0
142144	1	0	0	0	0
142145	1	0	0	0	0
146147	1	0	0	0	0
146152	1	0	0	0	0
146154	1	0	0	0	0
147148	1	0	0	0	0
147149	2	0	0	0	0
149150	1	0	0	0	0
149151	1	0	0	0	0
151152	2	0	0	0	0
152153	1	0	0	0	0
154155	1	0	0	0	0
154156	1	0	0	0	0
154157	1	0	0	0	0
157158	1	0	0	0	0
157159	1	0	0	0	0
157160	1	0	0	0	0
160161	1	0	0	0	0
161162	1	0	0	0	0
161163	1	0	0	0	0
161164	1	0	0	0	0
164165	1	0	0	0	0
164166	1	0	0	0	0
164167	1	0	0	0	0
167168	1	0	0	0	0
167184	2	0	0	0	0
168169	1	0	0	0	0
169170	1	0	0	0	0
169171	1	0	0	0	0
169172	1	0	0	0	0
172173	1	0	0	0	0
172186	1	0	0	0	0
172190	1	0	0	0	0
173174	1	0	0	0	0
173175	1	0	0	0	0
173176	1	0	0	0	0
176177	1	0	0	0	0
177178	1	0	0	0	0
177185	2	0	0	0	0
178179	1	0	0	0	0
178180	1	0	0	0	0
178181	1	0	0	0	0
181182	1	0	0	0	0
181183	1	0	0	0	0
181208	1	0	0	0	0
186187	1	0	0	0	0

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186188 1 0 0 0 0
186189 1 0 0 0 0
190191 1 0 0 0 0
190192 1 0 0 0 0
190193 1 0 0 0 0
194195 1 0 0 0 0
194200 1 0 0 0 0
194202 1 0 0 0 0
195196 1 0 0 0 0
195197 2 0 0 0 0
197198 1 0 0 0 0
197199 1 0 0 0 0
199200 2 0 0 0 0
200201 1 0 0 0 0
202203 1 0 0 0 0
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
209210 1 0 0 0 0
209211 1 0 0 0 0
209212 1 0 0 0 0
212213 1 0 0 0 0
212214 1 0 0 0 0
212215 1 0 0 0 0
215216 1 0 0 0 0
215233 2 0 0 0 0
216217 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
220235 1 0 0 0 0
220239 1 0 0 0 0
221222 1 0 0 0 0
221223 1 0 0 0 0
221224 1 0 0 0 0
224225 1 0 0 0 0
225226 1 0 0 0 0
225234 2 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
235236 1 0 0 0 0
235237 1 0 0 0 0
235238 1 0 0 0 0
239240 1 0 0 0 0
239241 1 0 0 0 0
239242 1 0 0 0 0

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M END
> <NAME>
F94_1

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II28_1
MOE2012 3D

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212211 0 0 1 0 0 0 0 0999 V2000
13.9640 9.2770 -17.6430 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.7490 8.8800 -18.0590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.8240 8.6790 -16.3610 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.7080 7.5990 -16.4920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.7330 8.8740 -15.7840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.6050 9.2780 -15.6740 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.7300 10.3650 -15.5930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.7210 9.1250 -16.3060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.3760 8.6680 -14.2910 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.2510 7.5820 -14.3890 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.2610 8.8370 -13.6640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.1420 9.2750 -13.6200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.2830 10.3570 -13.5120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.2630 9.1090 -14.2550 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.9370 8.6650 -12.3050 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
10.8460 7.6540 -12.4140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.7330 9.2000 -11.6620 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.8020 10.2920 -11.5820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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8.8550	8.9640	-12.2760	H	0	0	0	0	0	0	0	0	0	0	0	0
9.5400	8.5880	-10.2810	C	0	0	0	0	0	0	0	0	0	0	0	0
8.5360	8.8130	-9.9020	H	0	0	0	0	0	0	0	0	0	0	0	0
9.6180	7.4940	-10.3150	H	0	0	0	0	0	0	0	0	0	0	0	0
10.5230	9.1570	-9.2920	C	0	0	0	0	0	0	0	0	0	0	0	0
11.3640	8.1850	-8.8400	O	0	0	0	0	0	0	0	0	0	0	0	0
12.3500	8.6330	-7.8980	C	0	0	0	0	0	0	0	0	0	0	0	0
12.8830	9.5020	-8.3000	H	0	0	0	0	0	0	0	0	0	0	0	0
11.8490	8.9090	-6.9630	H	0	0	0	0	0	0	0	0	0	0	0	0
13.3250	7.4900	-7.6610	C	0	0	0	0	0	0	0	0	0	0	0	0
12.7850	6.5980	-7.3190	H	0	0	0	0	0	0	0	0	0	0	0	0
13.7850	7.1870	-8.6110	H	0	0	0	0	0	0	0	0	0	0	0	0
14.4030	7.8630	-6.6550	C	0	0	0	0	0	0	0	0	0	0	0	0
14.9680	8.7340	-7.0070	H	0	0	0	0	0	0	0	0	0	0	0	0
13.9500	8.0860	-5.6820	H	0	0	0	0	0	0	0	0	0	0	0	0
15.2940	6.7450	-6.5290	O	0	0	0	0	0	0	0	0	0	0	0	0
16.2760	6.8950	-5.5930	C	0	0	0	0	0	0	0	0	0	0	0	0
17.1560	5.6660	-5.5830	C	0	0	0	0	0	0	0	0	0	0	0	0
16.5090	4.7810	-5.5840	H	0	0	0	0	0	0	0	0	0	0	0	0
17.7460	5.6760	-6.5050	H	0	0	0	0	0	0	0	0	0	0	0	0
18.0520	5.6370	-4.3400	C	0	0	0	0	0	0	0	0	0	0	0	0
18.7100	6.5170	-4.3120	H	0	0	0	0	0	0	0	0	0	0	0	0
17.3910	5.7340	-3.4710	H	0	0	0	0	0	0	0	0	0	0	0	0
10.5360	10.3280	-8.9340	O	0	0	0	0	0	0	0	0	0	0	0	0
16.4340	7.8840	-4.8900	O	0	0	0	0	0	0	0	0	0	0	0	0
18.0620	2.1210	1.4700	O	0	0	0	0	0	0	0	0	0	0	0	0
17.3330	1.7660	2.0080	H	0	0	0	0	0	0	0	0	0	0	0	0
17.5030	2.5430	0.2330	C	0	0	0	0	0	0	0	0	0	0	0	0
17.0460	1.6770	-0.2550	H	0	0	0	0	0	0	0	0	0	0	0	0
16.7280	3.2900	0.4350	H	0	0	0	0	0	0	0	0	0	0	0	0
18.6140	3.1300	-0.6260	C	0	0	0	0	0	0	0	0	0	0	0	0
19.0640	3.9840	-0.1040	H	0	0	0	0	0	0	0	0	0	0	0	0
19.4150	2.3880	-0.7320	H	0	0	0	0	0	0	0	0	0	0	0	0
18.1060	3.5610	-2.0030	C	0	0	0	0	0	0	0	0	0	0	0	0
17.6630	2.6950	-2.5120	H	0	0	0	0	0	0	0	0	0	0	0	0
17.3110	4.3030	-1.8750	H	0	0	0	0	0	0	0	0	0	0	0	0
19.2550	4.1230	-2.8550	C	0	0	0	0	0	0	0	0	0	0	0	0
19.6760	5.0260	-2.3920	H	0	0	0	0	0	0	0	0	0	0	0	0
20.0440	3.3650	-2.8330	H	0	0	0	0	0	0	0	0	0	0	0	0
18.8440	4.3870	-4.2510	N	0	0	3	0	0	0	0	0	0	0	0	0
20.0340	4.4580	-5.1380	C	0	0	0	0	0	0	0	0	0	0	0	0
19.7030	4.7910	-6.1290	H	0	0	0	0	0	0	0	0	0	0	0	0
20.7380	5.2200	-4.7810	H	0	0	0	0	0	0	0	0	0	0	0	0
20.7150	3.0980	-5.3700	C	0	0	0	0	0	0	0	0	0	0	0	0
20.0220	2.2760	-5.1580	H	0	0	0	0	0	0	0	0	0	0	0	0
21.0070	3.0260	-6.4260	H	0	0	0	0	0	0	0	0	0	0	0	0
21.9800	2.9060	-4.5630	C	0	0	0	0	0	0	0	0	0	0	0	0
22.3950	1.6080	-4.6640	O	0	0	0	0	0	0	0	0	0	0	0	0
23.5910	1.3000	-3.9320	C	0	0	0	0	0	0	0	0	0	0	0	0
24.4150	1.9210	-4.3040	H	0	0	0	0	0	0	0	0	0	0	0	0
23.4280	1.5060	-2.8680	H	0	0	0	0	0	0	0	0	0	0	0	0
23.9090	-0.1730	-4.1390	C	0	0	0	0	0	0	0	0	0	0	0	0
23.0540	-0.7900	-3.8350	H	0	0	0	0	0	0	0	0	0	0	0	0
24.0360	-0.3830	-5.2090	H	0	0	0	0	0	0	0	0	0	0	0	0
25.1540	-0.5960	-3.3720	C	0	0	0	0	0	0	0	0	0	0	0	0
26.0170	-0.0040	-3.6960	H	0	0	0	0	0	0	0	0	0	0	0	0
24.9990	-0.4610	-2.2950	H	0	0	0	0	0	0	0	0	0	0	0	0
25.3990	-1.9840	-3.6480	O	0	0	0	0	0	0	0	0	0	0	0	0
26.5030	-2.5020	-3.0360	C	0	0	0	0	0	0	0	0	0	0	0	0
26.6530	-3.9540	-3.4130	C	0	0	0	0	0	0	0	0	0	0	0	0
25.7800	-4.4880	-3.0260	H	0	0	0	0	0	0	0	0	0	0	0	0
26.6610	-4.0260	-4.5070	H	0	0	0	0	0	0	0	0	0	0	0	0
27.9580	-4.5280	-2.8500	C	0	0	0	0	0	0	0	0	0	0	0	0
28.7740	-3.8990	-3.2250	H	0	0	0	0	0	0	0	0	0	0	0	0
27.9870	-4.4380	-1.7560	H	0	0	0	0	0	0	0	0	0	0	0	0
22.5580	3.7780	-3.9290	O	0	0	0	0	0	0	0	0	0	0	0	0
27.2520	-1.8830	-2.2940	O	0	0	0	0	0	0	0	0	0	0	0	0
25.1170	-11.2190	-2.2380	O	0	0	0	0	0	0	0	0	0	0	0	0
24.9580	-12.0490	-2.7200	H	0	0	0	0	0	0	0	0	0	0	0	0
25.9080	-10.3910	-3.0780	C	0	0	0	0	0	0	0	0	0	0	0	0
26.8360	-10.9210	-3.3160	H	0	0	0	0	0	0	0	0	0	0	0	0
25.3560	-10.2050	-4.0050	H	0	0	0	0	0	0	0	0	0	0	0	0
26.1960	-9.0900	-2.3460	C	0	0	0	0	0	0	0	0	0	0	0	0
25.2490	-8.6020	-2.0850	H	0	0	0	0	0	0	0	0	0	0	0	0
26.6920	-9.3120	-1.3920	H	0	0	0	0	0	0	0	0	0	0	0	0
27.0630	-8.1570	-3.1870	C	0	0	0	0	0	0	0	0	0	0	0	0
27.9950	-8.6720	-3.4430	H	0	0	0	0	0	0	0	0	0	0	0	0
26.5500	-7.9350	-4.1320	H	0	0	0	0	0	0	0	0	0	0	0	0
27.3460	-6.8470	-2.4400	C	0	0	0	0	0	0	0	0	0	0	0	0
26.3740	-6.3980	-2.2060	H	0	0	0	0	0	0	0	0	0	0	0	0
27.8320	-7.0420	-1.4750	H	0	0	0	0	0	0	0	0	0	0	0	0

28.1600	-5.9320	-3.2670	N	0	0	3	0	0	0	0	0	0	0	0
29.5910	-6.2990	-3.1840	C	0	0	0	0	0	0	0	0	0	0	0
30.0450	-5.9070	-2.2640	H	0	0	0	0	0	0	0	0	0	0	0
29.7090	-7.3880	-3.1260	H	0	0	0	0	0	0	0	0	0	0	0
30.3630	-5.8280	-4.4140	C	0	0	0	0	0	0	0	0	0	0	0
29.9430	-6.2500	-5.3350	H	0	0	0	0	0	0	0	0	0	0	0
30.3340	-4.7390	-4.5260	H	0	0	0	0	0	0	0	0	0	0	0
31.7970	-6.2810	-4.3150	C	0	0	0	0	0	0	0	0	0	0	0
32.6170	-5.2150	-4.0930	O	0	0	0	0	0	0	0	0	0	0	0
34.0120	-5.5410	-4.0140	C	0	0	0	0	0	0	0	0	0	0	0
34.1760	-6.2480	-3.1920	H	0	0	0	0	0	0	0	0	0	0	0
34.3290	-5.9980	-4.9590	H	0	0	0	0	0	0	0	0	0	0	0
34.7940	-4.2590	-3.7640	C	0	0	0	0	0	0	0	0	0	0	0
34.5600	-3.5160	-4.5370	H	0	0	0	0	0	0	0	0	0	0	0
34.4660	-3.7960	-2.8250	H	0	0	0	0	0	0	0	0	0	0	0
36.2940	-4.5170	-3.7270	C	0	0	0	0	0	0	0	0	0	0	0
36.5350	-5.2350	-2.9340	H	0	0	0	0	0	0	0	0	0	0	0
36.6300	-4.9110	-4.6930	H	0	0	0	0	0	0	0	0	0	0	0
36.9630	-3.2760	-3.4550	O	0	0	0	0	0	0	0	0	0	0	0
38.3260	-3.3520	-3.4670	C	0	0	0	0	0	0	0	0	0	0	0
38.9060	-1.9960	-3.1540	C	0	0	0	0	0	0	0	0	0	0	0
38.5510	-1.3110	-3.9300	H	0	0	0	0	0	0	0	0	0	0	0
38.5200	-1.6760	-2.1800	H	0	0	0	0	0	0	0	0	0	0	0
40.4370	-2.0520	-3.1160	C	0	0	0	0	0	0	0	0	0	0	0
40.7060	-2.8640	-2.4270	H	0	0	0	0	0	0	0	0	0	0	0
40.8330	-2.3310	-4.1020	H	0	0	0	0	0	0	0	0	0	0	0
32.1580	-7.4470	-4.4070	O	0	0	0	0	0	0	0	0	0	0	0
38.9720	-4.3630	-3.7030	O	0	0	0	0	0	0	0	0	0	0	0
44.2630	3.8790	-3.1010	O	0	0	0	0	0	0	0	0	0	0	0
44.4820	4.6700	-2.5790	H	0	0	0	0	0	0	0	0	0	0	0
42.9400	3.5020	-2.7470	C	0	0	0	0	0	0	0	0	0	0	0
42.8830	3.4090	-1.6580	H	0	0	0	0	0	0	0	0	0	0	0
42.2530	4.2870	-3.0770	H	0	0	0	0	0	0	0	0	0	0	0
42.6210	2.1750	-3.4190	C	0	0	0	0	0	0	0	0	0	0	0
42.7440	2.2750	-4.5050	H	0	0	0	0	0	0	0	0	0	0	0
43.3720	1.4450	-3.1100	H	0	0	0	0	0	0	0	0	0	0	0
41.2010	1.7130	-3.1000	C	0	0	0	0	0	0	0	0	0	0	0
40.9890	1.7870	-2.0270	H	0	0	0	0	0	0	0	0	0	0	0
40.5100	2.4190	-3.5800	H	0	0	0	0	0	0	0	0	0	0	0
40.8680	0.3010	-3.6120	C	0	0	0	0	0	0	0	0	0	0	0
39.8050	0.3510	-3.8670	H	0	0	0	0	0	0	0	0	0	0	0
41.3950	0.0940	-4.5520	H	0	0	0	0	0	0	0	0	0	0	0
41.0660	-0.7980	-2.6360	N	0	0	3	0	0	0	0	0	0	0	0
42.4980	-1.0430	-2.3490	C	0	0	0	0	0	0	0	0	0	0	0
42.7020	-2.1180	-2.2510	H	0	0	0	0	0	0	0	0	0	0	0
43.1340	-0.7260	-3.1850	H	0	0	0	0	0	0	0	0	0	0	0
42.9160	-0.4050	-1.0220	C	0	0	0	0	0	0	0	0	0	0	0
42.5410	0.6180	-0.9430	H	0	0	0	0	0	0	0	0	0	0	0
42.5170	-0.9720	-0.1750	H	0	0	0	0	0	0	0	0	0	0	0
44.4200	-0.3630	-0.9040	C	0	0	0	0	0	0	0	0	0	0	0
44.7920	0.7230	-0.1650	O	0	0	0	0	0	0	0	0	0	0	0
46.2080	0.9090	-0.0210	C	0	0	0	0	0	0	0	0	0	0	0
46.6170	0.0890	0.5810	H	0	0	0	0	0	0	0	0	0	0	0
46.6840	0.9150	-1.0080	H	0	0	0	0	0	0	0	0	0	0	0
46.4300	2.2430	0.6760	C	0	0	0	0	0	0	0	0	0	0	0
45.9640	3.0510	0.0980	H	0	0	0	0	0	0	0	0	0	0	0
45.9020	2.2530	1.6380	H	0	0	0	0	0	0	0	0	0	0	0
47.9070	2.5410	0.8880	C	0	0	0	0	0	0	0	0	0	0	0
48.3680	1.7460	1.4870	H	0	0	0	0	0	0	0	0	0	0	0
48.4230	2.6210	-0.0760	H	0	0	0	0	0	0	0	0	0	0	0
48.0100	3.7910	1.5830	O	0	0	0	0	0	0	0	0	0	0	0
49.2690	4.1200	1.9870	C	0	0	0	0	0	0	0	0	0	0	0
49.2410	5.3730	2.8250	C	0	0	0	0	0	0	0	0	0	0	0
50.0010	6.0560	2.4290	H	0	0	0	0	0	0	0	0	0	0	0
48.2810	5.8850	2.7000	H	0	0	0	0	0	0	0	0	0	0	0
49.5300	5.0460	4.2910	C	0	0	0	0	0	0	0	0	0	0	0
49.4950	5.9610	4.8960	H	0	0	0	0	0	0	0	0	0	0	0
50.5660	4.6890	4.3390	H	0	0	0	0	0	0	0	0	0	0	0
45.1860	-1.1860	-1.3850	O	0	0	0	0	0	0	0	0	0	0	0
50.2840	3.4860	1.7320	O	0	0	0	0	0	0	0	0	0	0	0
43.8660	1.8980	5.7740	O	0	0	0	0	0	0	0	0	0	0	0
43.2220	1.2200	5.5050	H	0	0	0	0	0	0	0	0	0	0	0
43.7360	2.9740	4.8570	C	0	0	0	0	0	0	0	0	0	0	0
43.8360	2.5850	3.8380	H	0	0	0	0	0	0	0	0	0	0	0
42.7370	3.4060	4.9710	H	0	0	0	0	0	0	0	0	0	0	0
44.8000	4.0290	5.1410	C	0	0	0	0	0	0	0	0	0	0	0
44.6400	4.8840	4.4740	H	0	0	0	0	0	0	0	0	0	0	0
44.6960	4.3850	6.1730	H	0	0	0	0	0	0	0	0	0	0	0
46.2150	3.4760	4.9500	C	0	0	0	0	0	0	0	0	0	0	0
46.3860	2.6620	5.6630	H	0	0	0	0	0	0	0	0	0	0	0
46.2990	3.0430	3.9460	H	0	0	0	0	0	0	0	0	0	0	0

47.2770	4.5710	5.1190	C	0	0	0	0	0	0	0	0	0	0	0	0	0
47.0250	5.3770	4.4200	H	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2350	5.0130	6.1230	H	0	0	0	0	0	0	0	0	0	0	0	0	0
48.6150	4.0260	4.8310	N	0	0	3	0	0	0	0	0	0	0	0	0	0
49.1840	3.3360	6.0020	C	0	0	0	0	0	0	0	0	0	0	0	0	0
49.6730	4.0480	6.6810	H	0	0	0	0	0	0	0	0	0	0	0	0	0
48.3910	2.8590	6.5910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1540	2.2360	5.5630	C	0	0	0	0	0	0	0	0	0	0	0	0	0
49.6500	1.5520	4.8700	H	0	0	0	0	0	0	0	0	0	0	0	0	0
51.0350	2.6590	5.0690	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.6280	1.4340	6.7470	C	0	0	0	0	0	0	0	0	0	0	0	0	0
51.4450	0.4290	6.3180	O	0	0	0	0	0	0	0	0	0	0	0	0	0
51.9680	-0.4020	7.3640	C	0	0	0	0	0	0	0	0	0	0	0	0	0
52.5600	0.2110	8.0540	H	0	0	0	0	0	0	0	0	0	0	0	0	0
51.1380	-0.8690	7.9080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
52.8440	-1.4710	6.7270	C	0	0	0	0	0	0	0	0	0	0	0	0	0
52.2630	-2.0470	5.9960	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.6430	-1.0010	6.1390	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.4410	-2.4030	7.7700	C	0	0	0	0	0	0	0	0	0	0	0	0	0
54.0670	-1.8350	8.4700	H	0	0	0	0	0	0	0	0	0	0	0	0	0
52.6430	-2.9130	8.3230	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.2490	-3.3770	7.0930	O	0	0	0	0	0	0	0	0	0	0	0	0	0
54.8510	-4.2850	7.9140	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6640	-5.2460	7.0800	C	0	0	0	0	0	0	0	0	0	0	0	0	0
54.9940	-5.7450	6.3730	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.4130	-4.6730	6.5220	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.3640	-6.2910	7.9320	C	0	0	0	0	0	0	0	0	0	0	0	0	0
57.0470	-5.8220	8.6480	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.9440	-6.9720	7.3010	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6390	-6.8840	8.5000	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.3350	1.6540	7.9130	O	0	0	0	0	0	0	0	0	0	0	0	0	0
54.7470	-4.3140	9.1320	O	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
6 7	1 0	0 0	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	0	0	0
6 9	1 0	0 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	0	0
9 11	1 0	0 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	0	0
12 13	1 0	0 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	0	0
12 15	1 0	0 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	0	0
15 17	1 0	0 0	0	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	0	0	0	0
17 20	1 0	0 0	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	0	0	0
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23 24	1 0	0 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23 42	2 0	0 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	0	0
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34 35	1 0	0 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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35 43	2 0	0 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36 37	1 0	0 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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119	127	2	0	0	0	0
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123	124	1	0	0	0	0
123	125	1	0	0	0	0
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23	26	1	0	0	0	0
26	27	1	0	0	0	0
26	45	2	0	0	0	0
27	28	1	0	0	0	0
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28	30	1	0	0	0	0
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128	136	2	0	0	0	0
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132	134	1	0	0	0	0
132	154	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
139	142	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
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	151	1	0	0	0	0
151	152	1	0	0	0	0
151	153	1	0	0	0	0
151	154	1	0	0	0	0
154	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	160	1	0	0	0	0
158	161	1	0	0	0	0
161	162	1	0	0	0	0
161	180	2	0	0	0	0
162	163	1	0	0	0	0
163	164	1	0	0	0	0
163	165	1	0	0	0	0
163	166	1	0	0	0	0
166	167	1	0	0	0	0
166	168	1	0	0	0	0
166	169	1	0	0	0	0

```

169170 1 0 0 0 0
169171 1 0 0 0 0
169172 1 0 0 0 0
172173 1 0 0 0 0
173174 1 0 0 0 0
173181 2 0 0 0 0
174175 1 0 0 0 0
174176 1 0 0 0 0
174177 1 0 0 0 0
177178 1 0 0 0 0
177179 1 0 0 0 0
177199 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
193194 1 0 0 0 0
193195 1 0 0 0 0
193196 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
200201 1 0 0 0 0
200202 1 0 0 0 0
200203 1 0 0 0 0
203204 1 0 0 0 0
203205 1 0 0 0 0
203206 1 0 0 0 0
206207 1 0 0 0 0
206226 2 0 0 0 0
207208 1 0 0 0 0
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
218219 1 0 0 0 0
218227 2 0 0 0 0
219220 1 0 0 0 0
219221 1 0 0 0 0
219222 1 0 0 0 0
222223 1 0 0 0 0
222224 1 0 0 0 0
222225 1 0 0 0 0

```

```

M END
> <NAME>
II32_1

```

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$$$$
II36_1
MOE2012 3D

```

```

242241 0 0 1 0 0 0 0 0 0999 V2000
2.8590 -6.5040 2.4400 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.3900 -7.2620 2.7360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.7480 -5.4020 2.3070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.2150 -5.2140 3.2790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.5260 -5.6690 1.5840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.9650 -4.1830 1.8360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.4710 -4.4150 0.8840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.1580 -3.9720 2.5490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.8660 -2.9580 1.6790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.3480 -2.7330 2.6380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
4.6640 -3.1800 0.9600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.0760 -1.7360 1.2040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.6000 -1.9580 0.2410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2.2730 -1.5170 1.9190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3.9790 -0.5080 1.0580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


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18	19	1	0	0	0	0
18	20	1	0	0	0	0
18	21	1	0	0	0	0
21	22	1	0	0	0	0
21	23	1	0	0	0	0
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23	25	1	0	0	0	0
23	26	1	0	0	0	0
26	27	1	0	0	0	0
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26	29	1	0	0	0	0
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34	36	1	0	0	0	0
34	37	1	0	0	0	0
37	38	1	0	0	0	0
37	39	1	0	0	0	0
37	40	1	0	0	0	0
40	41	1	0	0	0	0
41	42	1	0	0	0	0
41	49	2	0	0	0	0
42	43	1	0	0	0	0
42	44	1	0	0	0	0
42	45	1	0	0	0	0
45	46	1	0	0	0	0
45	47	1	0	0	0	0
45	70	1	0	0	0	0
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64	65	1	0	0	0	0
64	66	1	0	0	0	0
64	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
71	72	1	0	0	0	0
71	73	1	0	0	0	0
71	74	1	0	0	0	0
74	75	1	0	0	0	0
74	76	1	0	0	0	0
74	77	1	0	0	0	0
77	78	1	0	0	0	0
77	96	2	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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90	91	1	0	0	0	0
90	92	1	0	0	0	0
90	93	1	0	0	0	0
93	94	1	0	0	0	0
93	95	1	0	0	0	0
93	118	1	0	0	0	0

98 99	1	0	0	0	0
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100101	1	0	0	0	0
100102	1	0	0	0	0
100103	1	0	0	0	0
103104	1	0	0	0	0
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112114	1	0	0	0	0
112115	1	0	0	0	0
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115117	1	0	0	0	0
115118	1	0	0	0	0
118119	1	0	0	0	0
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119121	1	0	0	0	0
119122	1	0	0	0	0
122123	1	0	0	0	0
122124	1	0	0	0	0
122125	1	0	0	0	0
125126	1	0	0	0	0
125144	2	0	0	0	0
126127	1	0	0	0	0
127128	1	0	0	0	0
127129	1	0	0	0	0
127130	1	0	0	0	0
130131	1	0	0	0	0
130132	1	0	0	0	0
130133	1	0	0	0	0
133134	1	0	0	0	0
133135	1	0	0	0	0
133136	1	0	0	0	0
136137	1	0	0	0	0
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148151	1	0	0	0	0
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157159	1	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
170172	1	0	0	0	0
170173	1	0	0	0	0
173174	1	0	0	0	0
173192	2	0	0	0	0
174175	1	0	0	0	0
175176	1	0	0	0	0
175177	1	0	0	0	0
175178	1	0	0	0	0

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178180 1 0 0 0 0
178181 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
185186 1 0 0 0 0
185193 2 0 0 0 0
186187 1 0 0 0 0
186188 1 0 0 0 0
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
199202 1 0 0 0 0
202203 1 0 0 0 0
202204 1 0 0 0 0
202205 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
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208211 1 0 0 0 0
211212 1 0 0 0 0
211213 1 0 0 0 0
211214 1 0 0 0 0
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218220 1 0 0 0 0
218221 1 0 0 0 0
221222 1 0 0 0 0
221241 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
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229232 1 0 0 0 0
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233234 1 0 0 0 0
233242 2 0 0 0 0
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237239 1 0 0 0 0
237240 1 0 0 0 0
M END
> <NAME>
II36_1

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JJ20_1
MOE2012 3D

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```

227226 0 0 1 0 0 0 0 0999 V2000
53.8570 1.2760 -14.6870 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.9820 2.2250 -14.5150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.8760 1.1660 -15.7100 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.9250 1.5360 -15.3150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.1790 1.7930 -16.5540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.7640 -0.2910 -16.1340 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.7350 -0.6320 -16.5160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.5550 -0.9090 -15.2500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.6720 -0.4790 -17.1850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


26	27	1	0	0	0	0
26	28	1	0	0	0	0
26	44	1	0	0	0	0
29	30	1	0	0	0	0
29	31	1	0	0	0	0
29	32	1	0	0	0	0
29	44	1	0	0	0	0
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32	35	1	0	0	0	0
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62	64	1	0	0	0	0
62	65	1	0	0	0	0
65	66	1	0	0	0	0
65	70	2	0	0	0	0
66	67	1	0	0	0	0
67	68	1	0	0	0	0
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
74	89	1	0	0	0	0
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82	83	1	0	0	0	0
82	84	1	0	0	0	0
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85	86	1	0	0	0	0
85	87	1	0	0	0	0
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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
100	103	1	0	0	0	0
103	104	1	0	0	0	0
104	105	1	0	0	0	0
104	106	1	0	0	0	0
104	107	1	0	0	0	0

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107109	1	0	0	0	0
107110	1	0	0	0	0
110111	1	0	0	0	0
110115	2	0	0	0	0
111112	1	0	0	0	0
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112114	1	0	0	0	0
112116	1	0	0	0	0
116117	1	0	0	0	0
116118	1	0	0	0	0
116134	1	0	0	0	0
119120	1	0	0	0	0
119121	1	0	0	0	0
119122	1	0	0	0	0
119134	1	0	0	0	0
122123	1	0	0	0	0
122124	1	0	0	0	0
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134136	1	0	0	0	0
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137139	1	0	0	0	0
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139141	1	0	0	0	0
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152155	1	0	0	0	0
155156	1	0	0	0	0
155160	2	0	0	0	0
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157158	1	0	0	0	0
157159	1	0	0	0	0
157161	1	0	0	0	0
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167170	1	0	0	0	0
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171178	2	0	0	0	0
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172175	1	0	0	0	0
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175177	1	0	0	0	0
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
193194 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
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
206225 1 0 0 0 0
209210 1 0 0 0 0
209211 1 0 0 0 0
209212 1 0 0 0 0
209225 1 0 0 0 0
212213 1 0 0 0 0
212214 1 0 0 0 0
212215 1 0 0 0 0
215216 1 0 0 0 0
216217 1 0 0 0 0
216224 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
220223 1 0 0 0 0
225226 1 0 0 0 0
225227 1 0 0 0 0

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M END
> <NAME>
JJ20_1

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JJ24_1
MOE2012 3D

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```

232231 0 0 1 0 0 0 0 0999 V2000
27.7670 8.0040 -9.6480 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.0100 7.4350 -9.4190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.8670 7.5940 -8.8320 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.5990 7.7240 -7.7800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.0530 6.5350 -9.0390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.0820 8.4470 -9.2100 C 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
29.8610 9.5060 -9.0290 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.3270 8.0050 -8.4290 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.1050 8.0320 -7.3550 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.5860 6.9770 -8.7080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.4720 8.8850 -8.7170 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
32.6510 8.8320 -9.7250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.3030 8.3010 -10.6220 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.4120 8.4030 -11.0170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.6500 8.4700 -7.9520 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.3880 8.4440 -6.8870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.9520 7.4590 -8.2390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.8200 9.4420 -8.1020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.4770 10.4630 -7.9000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.5860 9.1930 -7.3590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.5020 9.4360 -9.4480 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.3630 8.2440 -10.0850 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.9580 8.1870 -11.3890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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37.0150 8.4730 -11.3320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.1460 10.3900 -9.8720 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.8340 6.7570 -11.9010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.3770 6.0860 -11.2250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.7840 6.4410 -11.8570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.3330 5.1680 -13.7890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.3170 4.7640 -13.7030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.9600 4.5530 -13.1310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.8110 5.0120 -15.2270 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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JJ24_1

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JJ28_1
MOE2012 3D

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6.0860 14.5220 -19.5480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.0330 13.3630 -18.3090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.4060 14.2100 -17.7240 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.1060 12.9980 -17.8570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.0750 12.2560 -18.3860 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.6970 11.4470 -19.0250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.9730 12.6380 -18.8870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.4290 11.7150 -17.0020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.8050 12.5330 -16.3750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
7.5220 11.3280 -16.5190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.4820 10.6090 -17.0950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.1000 9.7910 -17.7180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.3850 11.0080 -17.5730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.8020 10.1170 -15.7540 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
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11.1430 8.5740 -14.4030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11.5370 9.4050 -13.8060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
10.2450 8.1750 -13.9170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.1840 7.4830 -14.4400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.4610 7.0810 -13.1670 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.4370 6.0330 -13.0630 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.0890 5.1540 -13.6170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.3890 6.3800 -13.4800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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12.6260 5.4060 -11.1710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
14.7560 4.2420 -9.8780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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15.7580 3.1180 -9.6330 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.4370 2.2060 -10.1500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.7530 3.4110 -9.9850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.8080 2.8750 -8.2190 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.6170 1.8480 -7.8380 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.5750 1.7040 -6.3370 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.1940 2.4990 -5.9100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.5390 1.8330 -6.0020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.0760 0.3190 -5.9270 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.5030 -0.4180 -6.5060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.1220 0.2020 -6.2320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17.2960 1.1620 -8.5890 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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M END
> <NAME>
JJ28_1

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JJ32_1
MOE2012 3D

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37.9560 16.1710 -13.5870 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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37.5810 17.2090 -14.4810 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.1040 18.1250 -14.1900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.8920 16.9270 -15.4920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.0720 17.4000 -14.4110 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.5750 16.4530 -14.6570 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.7820 17.6310 -13.3780 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.6020 18.5060 -15.3530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.1000 19.4470 -15.0920 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.8940 18.2600 -16.3820 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.0850 18.6930 -15.2840 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.5890 17.7490 -15.5440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.7930 18.9380 -14.2550 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.6230 19.8020 -16.2320 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.1210 20.7400 -15.9610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.9090 19.5470 -17.2590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.1710 19.9620 -16.1350 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0
31.7150 19.0780 -16.3610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.6960 21.0120 -17.0400 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.2050 21.9580 -16.8170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.9320 20.7410 -18.0760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.1890 21.1950 -16.9150 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.8180 21.8580 -17.7050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.6580 20.2440 -17.0380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.8330 21.8300 -15.5960 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.2100 20.9280 -14.7890 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.8710 21.4180 -13.4840 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.7760 21.7740 -12.9790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.1540 22.2410 -13.5800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.0830 22.9930 -15.3080 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.2510 20.2650 -12.7020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.3750 19.8900 -13.2460 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.9610 19.4290 -12.6680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.2380 19.5070 -10.5240 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.9450 18.6690 -10.4790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.3590 19.1290 -11.0610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.8300 19.8970 -9.1080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.7070 20.2180 -8.5330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.0920 20.7070 -9.1360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.2520 18.7410 -8.4840 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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86	101	1	0	0	0	0
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M END
> <NAME>
JJ32_1

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$$$$
JJ36_1
MOE2012 3D

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7.1660 -20.3910 16.8300 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6.8360 -20.5110 17.7360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.5330 -20.7820 16.8290 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9.0740 -20.1540 17.5440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8.5960 -21.8250 17.1530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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M END
> <NAME>
JJ36_1

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$$$$
JJ80_1
MOE2012 3D

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50.8510 -3.1860 -21.0090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
49.7190 -1.8200 -20.8980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
49.1670 -3.4870 -20.6170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50.3050 -2.6720 -19.0290 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
49.1230 -2.1930 -18.2920 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.8760 -1.1620 -18.5800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.2620 -2.8150 -18.5680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
49.2870 -2.2860 -16.7680 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
49.5900 -3.3050 -16.4940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50.0760 -1.6060 -16.4270 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
47.9780 -1.9270 -16.0570 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
47.6820 -0.9140 -16.3490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
47.1890 -2.6190 -16.3740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.4640 -1.7940 -18.8470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.2520 -0.7620 -19.1490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.3150 -2.1550 -19.4370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.8020 -1.7920 -17.8070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.1680 -2.0060 -14.6070 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
48.5340 -2.9300 -14.3720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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M END
> <NAME>
JJ80_1

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JJ86_1
MOE2012 3D

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233234	1	0	0	0	0
233241	1	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
237240	1	0	0	0	0
240254	1	0	0	0	0
241242	1	0	0	0	0
241243	1	0	0	0	0
241249	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
249250	1	0	0	0	0
249251	1	0	0	0	0
249252	1	0	0	0	0
252253	1	0	0	0	0
254255	1	0	0	0	0

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254256 1 0 0 0 0
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257258 1 0 0 0 0
257259 1 0 0 0 0
257260 1 0 0 0 0
260261 1 0 0 0 0
260265 2 0 0 0 0
261262 1 0 0 0 0
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266267 1 0 0 0 0
266268 1 0 0 0 0
266285 1 0 0 0 0
269270 1 0 0 0 0
269271 1 0 0 0 0
269272 1 0 0 0 0
269285 1 0 0 0 0
272273 1 0 0 0 0
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272275 1 0 0 0 0
275276 1 0 0 0 0
276277 1 0 0 0 0
276284 2 0 0 0 0
277278 1 0 0 0 0
277279 1 0 0 0 0
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280281 1 0 0 0 0
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280283 1 0 0 0 0
285286 1 0 0 0 0
285287 1 0 0 0 0

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M END
> <NAME>
JJ86_1

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JJ94_1
MOE2012 3D

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242246 0 0 1 0 0 0 0 0999 V2000
20.0270 -14.8510 -17.0890 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.5940 -14.9750 -18.3780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.6710 -15.8960 -18.9390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.0990 -13.7330 -18.7020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18.6630 -13.4180 -19.6400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.2170 -12.8670 -17.6450 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.7740 -13.5710 -16.6860 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.0160 -13.2060 -15.6960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.6450 -15.8880 -16.2870 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.3700 -15.6990 -15.2420 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.1980 -16.8450 -16.5810 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.1650 -15.9100 -16.4640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.4040 -16.1400 -17.5090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.5670 -14.9140 -16.2450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.7620 -16.9110 -15.5790 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
22.6050 -16.6420 -14.5980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.2080 -17.0650 -15.7720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.5270 -17.9060 -15.1430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.4110 -17.3670 -16.8060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.0610 -15.8440 -15.4200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.1160 -16.1210 -15.5310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.8540 -15.0120 -16.1010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.8480 -15.3660 -14.0030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.8140 -14.4610 -13.6810 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.7000 -13.8960 -12.3660 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.7330 -13.3890 -12.2680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.7730 -14.6960 -11.6190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.9240 -15.7110 -13.2770 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.8390 -12.8990 -12.1860 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.7960 -13.4130 -12.3440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
26.7770 -12.1350 -12.9710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.9660 -11.2500 -10.6530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.9030 -10.4740 -11.4260 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.9260 -11.7570 -10.8170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.9780 -10.5910 -9.2780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
27.0560 -10.0210 -9.1190 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
28.0820 -11.3520 -8.4960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.0990 -9.6970 -9.2380 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.3390 -9.1230 -8.0270 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.5670 -8.2550 -8.0940 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


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86	87	1	0	0	0	0
87	88	1	0	0	0	0
87	94	2	0	0	0	0
88	89	1	0	0	0	0
88	90	1	0	0	0	0
88	91	1	0	0	0	0
91	92	1	0	0	0	0
91	93	1	0	0	0	0
91112	1	0	0	0	0	0
95	96	1	0	0	0	0
95	97	1	0	0	0	0
98	99	1	0	0	0	0
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98106	1	0	0	0	0	0
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128143	1	0	0	0	0
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131134	1	0	0	0	0
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157159	1	0	0	0	0
157160	1	0	0	0	0
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191193	1	0	0	0	0
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194200	1	0	0	0	0
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195196	1	0	0	0	0
195197	2	0	0	0	0
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```

197199 1 0 0 0 0
199200 2 0 0 0 0
200201 1 0 0 0 0
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202204 1 0 0 0 0
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212215 1 0 0 0 0
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M END
> <NAME>
JJ94_1

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LL6_1
MOE2012 3D

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312316 0 0 1 0 0 0 0 0 0999 V2000
57.2920 -13.7380 19.8980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.6730 -13.6430 20.9210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.1700 -12.4270 19.3300 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.3150 -12.3010 18.4890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.1300 -11.5830 17.6860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.1530 -11.9530 19.1030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.5310 -13.7060 17.9980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
57.8170 -13.9710 17.2100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.5480 -13.8910 17.6430 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.2410 -14.5070 19.1430 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
55.9390 -14.4430 19.8890 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
55.5840 -14.5330 18.8530 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
56.0610 -15.4670 20.2640 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.9030 -13.6850 20.7190 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
55.2740 -13.5740 21.7450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.7600 -12.6860 20.2960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.6400 -14.4220 20.7190 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
53.2770 -14.4940 19.7680 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.6280 -13.8490 21.6110 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.0300 -13.7410 22.6250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.8310 -14.5990 21.6860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.9890 -12.5550 21.1060 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.8700 -12.5870 20.0170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50.9870 -12.4420 21.5360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.7730 -11.3340 21.5130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
52.8060 -10.4390 20.4860 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.5540 -9.2450 20.7570 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
53.0940 -8.7110 21.5970 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
54.5870 -9.5110 21.0110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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79.6900	12.9040	3.5940	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
80.6490	13.3310	4.4650	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
82.0120	13.1850	4.0300	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
82.1040	13.3880	2.9560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
82.5940	13.9510	4.5520	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
79.9010	12.3910	2.5040	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
82.5280	11.7960	4.3920	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
82.4090	11.6360	5.4710	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
81.9090	11.0320	3.9060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
83.9910	11.6180	3.9880	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
84.0950	11.7780	2.9080	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
84.6050	12.3770	4.4890	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
84.5030	10.2230	4.3510	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
84.4000	10.0630	5.4310	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
83.8880	9.4650	3.8510	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
85.9670	10.0450	3.9430	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
86.0700	10.2090	2.8640	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
86.5820	10.8020	4.4450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
86.4800	8.6490	4.3010	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
86.3780	8.4860	5.3810	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
85.8640	7.8920	3.8000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
87.9430	8.4710	3.8920	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
88.0450	8.6360	2.8120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
88.5590	9.2270	4.3940	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
88.4540	7.0770	4.2460	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
88.3520	6.8960	5.3240	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
87.8410	6.3110	3.7540	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
89.9130	6.8920	3.8410	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90.0230	7.0210	2.7580	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90.5450	7.6180	4.3640	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
90.3110	5.5620	4.2050	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
91.6040	5.2530	3.8980	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
91.8910	3.8350	4.3310	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
91.7240	3.7610	5.4110	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
91.1940	3.1660	3.8130	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
93.3160	3.4180	4.0130	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
93.5130	3.4780	2.9370	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
93.4940	2.3880	4.3370	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
94.0380	4.0660	4.5210	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
92.4020	6.0050	3.3590	O	0	0	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	10	1	0	0	0	0												
1	11	1	0	0	0	0												
3	4	1	0	0	0	0												
4	5	1	0	0	0	0												
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4	7	1	0	0	0	0												
7	8	1	0	0	0	0												
7	9	1	0	0	0	0												
7	10	1	0	0	0	0												
11	12	1	0	0	0	0												
11	13	1	0	0	0	0												
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22	25	1	0	0	0	0												
25	26	1	0	0	0	0												
25	30	2	0	0	0	0												
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27	28	1	0	0	0	0												
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M END
> <NAME>
LL6_1

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LL8_1
MOE2012 3D

337336 0 0 1 0 0 0 0 0999 V2000
63.1510 -14.5460 -4.5870 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63.4800 -13.5080 -4.7230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63.8560 -15.1850 -5.1330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63.1760 -14.9060 -3.0960 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
62.4660 -14.2680 -2.5590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
62.8540 -15.9480 -2.9790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
64.5280 -14.7270 -2.5570 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
65.1830 -15.2420 -3.1480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
61.6880 -14.3840 -6.6710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
62.1620 -13.4050 -6.8180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
60.3410 -14.2490 -7.1360 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.5630 -15.4350 -7.0530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
59.3510 -15.6920 -6.0120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
60.0540 -16.2720 -7.5590 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
58.6080 -15.2470 -7.5520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
62.6610 -14.9690 -8.7470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63.2490 -14.0470 -8.7780 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
61.7190 -14.8350 -9.2860 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63.2330 -15.7600 -9.2410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
62.4260 -15.3660 -7.4020 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
61.7430 -14.7140 -5.1720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
61.4240 -15.7520 -5.0100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
61.0350 -14.0750 -4.6300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
64.6530 -15.2300 -1.1820 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
65.7140 -15.4350 -0.9930 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
64.1440 -16.1970 -1.0910 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
64.1180 -14.2640 -0.1250 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63.1730 -13.8120 -0.4450 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63.9220 -14.8220 0.7990 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
65.1030 -13.1760 0.2310 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
64.4420 -12.1470 0.8410 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
65.2840 -11.0760 1.2930 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
66.0130 -11.4660 2.0120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
65.8100 -10.6400 0.4360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
66.3160 -13.2310 0.0750 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
64.3990 -10.0280 1.9580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63.6540 -9.6710 1.2360 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
63.8290 -10.4980 2.7690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
65.2180 -8.8580 2.4980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
65.9570 -9.2300 3.2170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

65.7740	-8.3870	1.6770	H	0	0	0	0	0	0	0	0	0	0	0
64.3230	-7.8180	3.1740	C	0	0	0	0	0	0	0	0	0	0	0
63.5970	-7.4300	2.4490	H	0	0	0	0	0	0	0	0	0	0	0
63.7520	-8.2940	3.9800	H	0	0	0	0	0	0	0	0	0	0	0
65.1460	-6.6620	3.7460	C	0	0	0	0	0	0	0	0	0	0	0
65.8780	-7.0540	4.4630	H	0	0	0	0	0	0	0	0	0	0	0
65.7110	-6.1770	2.9400	H	0	0	0	0	0	0	0	0	0	0	0
64.2520	-5.6320	4.4380	C	0	0	0	0	0	0	0	0	0	0	0
63.5360	-5.2220	3.7160	H	0	0	0	0	0	0	0	0	0	0	0
63.6700	-6.1230	5.2280	H	0	0	0	0	0	0	0	0	0	0	0
65.0770	-4.4960	5.0450	C	0	0	0	0	0	0	0	0	0	0	0
65.8000	-4.9080	5.7590	H	0	0	0	0	0	0	0	0	0	0	0
65.6510	-3.9950	4.2560	H	0	0	0	0	0	0	0	0	0	0	0
64.1840	-3.4790	5.7520	C	0	0	0	0	0	0	0	0	0	0	0
63.4640	-3.0510	5.0450	H	0	0	0	0	0	0	0	0	0	0	0
63.5840	-3.9730	6.5270	H	0	0	0	0	0	0	0	0	0	0	0
64.9980	-2.3580	6.3880	C	0	0	0	0	0	0	0	0	0	0	0
65.6770	-2.7650	7.1460	H	0	0	0	0	0	0	0	0	0	0	0
65.5760	-1.8290	5.6220	H	0	0	0	0	0	0	0	0	0	0	0
64.0810	-1.4470	7.0110	O	0	0	0	0	0	0	0	0	0	0	0
64.6610	-0.3600	7.5920	C	0	0	0	0	0	0	0	0	0	0	0
63.6090	0.5250	8.2060	C	0	0	0	0	0	0	0	0	0	0	0
62.6100	0.2380	7.8580	H	0	0	0	0	0	0	0	0	0	0	0
63.6330	0.3290	9.2850	H	0	0	0	0	0	0	0	0	0	0	0
63.8620	2.0130	7.9470	C	0	0	0	0	0	0	0	0	0	0	0
63.4040	2.5350	8.7980	H	0	0	0	0	0	0	0	0	0	0	0
64.9300	2.2610	7.9720	H	0	0	0	0	0	0	0	0	0	0	0
65.8650	-0.1440	7.6390	O	0	0	0	0	0	0	0	0	0	0	0
62.9950	1.0600	4.7440	C	0	0	0	0	0	0	0	0	0	0	0
62.6360	0.2760	5.4200	H	0	0	0	0	0	0	0	0	0	0	0
62.1080	1.5950	4.3840	H	0	0	0	0	0	0	0	0	0	0	0
63.9130	2.0350	5.4900	C	0	0	0	0	0	0	0	0	0	0	0
64.8710	1.5560	5.7220	H	0	0	0	0	0	0	0	0	0	0	0
64.1750	2.8560	4.8120	H	0	0	0	0	0	0	0	0	0	0	0
63.2330	2.5170	6.7060	N	0	0	3	0	0	0	0	0	0	0	0
62.8140	-0.5950	2.8230	C	0	0	0	0	0	0	0	0	0	0	0
62.3860	-1.2800	3.5650	H	0	0	0	0	0	0	0	0	0	0	0
63.5540	-1.4080	1.9070	O	0	0	0	0	0	0	0	0	0	0	0
64.1740	-0.6850	0.8530	C	0	0	0	0	0	0	0	0	0	0	0
65.0040	-0.0810	1.2290	H	0	0	0	0	0	0	0	0	0	0	0
63.4550	-0.0580	0.3190	H	0	0	0	0	0	0	0	0	0	0	0
64.5850	-1.4110	0.1440	H	0	0	0	0	0	0	0	0	0	0	0
60.7120	-0.7400	1.7500	C	0	0	0	0	0	0	0	0	0	0	0
60.2660	-1.2700	2.5980	H	0	0	0	0	0	0	0	0	0	0	0
61.0860	-1.4550	1.0120	H	0	0	0	0	0	0	0	0	0	0	0
59.9370	-0.1300	1.2790	H	0	0	0	0	0	0	0	0	0	0	0
61.7500	0.1240	2.1930	O	0	0	0	0	0	0	0	0	0	0	0
63.7170	0.4030	3.5640	C	0	0	0	0	0	0	0	0	0	0	0
64.0440	1.1940	2.8770	H	0	0	0	0	0	0	0	0	0	0	0
64.6200	-0.1120	3.9130	H	0	0	0	0	0	0	0	0	0	0	0
63.1340	3.9900	6.7490	C	0	0	0	0	0	0	0	0	0	0	0
64.1310	4.4410	6.6580	H	0	0	0	0	0	0	0	0	0	0	0
62.7410	4.2990	7.7260	H	0	0	0	0	0	0	0	0	0	0	0
62.2040	4.5830	5.6890	C	0	0	0	0	0	0	0	0	0	0	0
62.1540	5.6720	5.8050	H	0	0	0	0	0	0	0	0	0	0	0
62.5860	4.3860	4.6820	H	0	0	0	0	0	0	0	0	0	0	0
60.7990	4.0510	5.8150	C	0	0	0	0	0	0	0	0	0	0	0
60.2900	3.7990	4.5740	O	0	0	0	0	0	0	0	0	0	0	0
58.9770	3.2280	4.5740	C	0	0	0	0	0	0	0	0	0	0	0
58.9740	2.3160	5.1820	H	0	0	0	0	0	0	0	0	0	0	0
58.2670	3.9510	4.9920	H	0	0	0	0	0	0	0	0	0	0	0
60.1950	3.9000	6.8700	O	0	0	0	0	0	0	0	0	0	0	0
58.6030	2.8950	3.1330	C	0	0	0	0	0	0	0	0	0	0	0
58.6200	3.8130	2.5320	H	0	0	0	0	0	0	0	0	0	0	0
59.3690	2.2390	2.7010	H	0	0	0	0	0	0	0	0	0	0	0
57.2310	2.2310	3.0550	C	0	0	0	0	0	0	0	0	0	0	0
57.2390	1.3060	3.6450	H	0	0	0	0	0	0	0	0	0	0	0
56.4780	2.8910	3.5010	H	0	0	0	0	0	0	0	0	0	0	0
56.8390	1.9120	1.6110	C	0	0	0	0	0	0	0	0	0	0	0
56.8190	2.8380	1.0240	H	0	0	0	0	0	0	0	0	0	0	0
57.5940	1.2580	1.1580	H	0	0	0	0	0	0	0	0	0	0	0
55.4700	1.2320	1.5530	C	0	0	0	0	0	0	0	0	0	0	0
55.5030	0.2910	2.1140	H	0	0	0	0	0	0	0	0	0	0	0
54.7250	1.8730	2.0420	H	0	0	0	0	0	0	0	0	0	0	0
55.0360	0.9560	0.1130	C	0	0	0	0	0	0	0	0	0	0	0
55.0170	1.8970	-0.4480	H	0	0	0	0	0	0	0	0	0	0	0
55.7680	0.3030	-0.3780	H	0	0	0	0	0	0	0	0	0	0	0
53.6540	0.3000	0.0710	C	0	0	0	0	0	0	0	0	0	0	0
53.6980	-0.6820	0.5560	H	0	0	0	0	0	0	0	0	0	0	0
52.9450	0.9100	0.6440	H	0	0	0	0	0	0	0	0	0	0	0
53.1430	0.1470	-1.3600	C	0	0	0	0	0	0	0	0	0	0	0

53.1220	1.1230	-1.8590	H	0	0	0	0	0	0	0	0	0	0	0	0
53.8300	-0.4730	-1.9480	H	0	0	0	0	0	0	0	0	0	0	0	0
51.7490	-0.4730	-1.3940	C	0	0	0	0	0	0	0	0	0	0	0	0
51.7980	-1.5270	-1.0990	H	0	0	0	0	0	0	0	0	0	0	0	0
51.0790	0.0670	-0.7140	H	0	0	0	0	0	0	0	0	0	0	0	0
51.2420	-0.3660	-2.7310	O	0	0	0	0	0	0	0	0	0	0	0	0
49.9700	-0.8250	-2.8930	C	0	0	0	0	0	0	0	0	0	0	0	0
49.4690	-0.5020	-4.2750	C	0	0	0	0	0	0	0	0	0	0	0	0
50.2160	0.0630	-4.8400	H	0	0	0	0	0	0	0	0	0	0	0	0
49.3630	-1.4580	-4.8010	H	0	0	0	0	0	0	0	0	0	0	0	0
48.1240	0.2260	-4.2630	C	0	0	0	0	0	0	0	0	0	0	0	0
47.7780	0.2740	-5.3050	H	0	0	0	0	0	0	0	0	0	0	0	0
47.3790	-0.4140	-3.7770	H	0	0	0	0	0	0	0	0	0	0	0	0
49.3150	-1.4110	-2.0410	O	0	0	0	0	0	0	0	0	0	0	0	0
46.8350	1.0500	-1.5840	C	0	0	0	0	0	0	0	0	0	0	0	0
45.9010	1.3880	-2.0500	H	0	0	0	0	0	0	0	0	0	0	0	0
46.8900	-0.0360	-1.7110	H	0	0	0	0	0	0	0	0	0	0	0	0
48.0260	1.7390	-2.2670	C	0	0	0	0	0	0	0	0	0	0	0	0
47.9440	2.8070	-2.0280	H	0	0	0	0	0	0	0	0	0	0	0	0
48.9610	1.3900	-1.8200	H	0	0	0	0	0	0	0	0	0	0	0	0
48.0410	1.5850	-3.7200	N	0	0	3	0	0	0	0	0	0	0	0	0
45.5760	0.7670	0.6130	C	0	0	0	0	0	0	0	0	0	0	0	0
44.6850	1.0860	0.0590	H	0	0	0	0	0	0	0	0	0	0	0	0
45.4190	1.2700	1.9440	O	0	0	0	0	0	0	0	0	0	0	0	0
46.4790	0.9390	2.8300	C	0	0	0	0	0	0	0	0	0	0	0	0
47.3900	1.4870	2.5700	H	0	0	0	0	0	0	0	0	0	0	0	0
46.6720	-0.1370	2.8420	H	0	0	0	0	0	0	0	0	0	0	0	0
46.1830	1.2440	3.8380	H	0	0	0	0	0	0	0	0	0	0	0	0
44.4290	-1.2780	0.9180	C	0	0	0	0	0	0	0	0	0	0	0	0
43.6390	-0.9890	0.2180	H	0	0	0	0	0	0	0	0	0	0	0	0
44.1390	-1.0210	1.9410	H	0	0	0	0	0	0	0	0	0	0	0	0
44.5630	-2.3610	0.8590	H	0	0	0	0	0	0	0	0	0	0	0	0
45.6590	-0.6580	0.5680	O	0	0	0	0	0	0	0	0	0	0	0	0
46.8030	1.3730	-0.0850	C	0	0	0	0	0	0	0	0	0	0	0	0
47.7230	0.9820	0.3680	H	0	0	0	0	0	0	0	0	0	0	0	0
46.8080	2.4590	0.0700	H	0	0	0	0	0	0	0	0	0	0	0	0
48.7730	2.6250	-4.4530	C	0	0	0	0	0	0	0	0	0	0	0	0
48.2160	3.5640	-4.3350	H	0	0	0	0	0	0	0	0	0	0	0	0
48.7100	2.4020	-5.5270	H	0	0	0	0	0	0	0	0	0	0	0	0
50.2420	2.8750	-4.1090	C	0	0	0	0	0	0	0	0	0	0	0	0
50.8090	1.9480	-4.0100	H	0	0	0	0	0	0	0	0	0	0	0	0
50.7200	3.4220	-4.9310	H	0	0	0	0	0	0	0	0	0	0	0	0
50.4270	3.7240	-2.8780	C	0	0	0	0	0	0	0	0	0	0	0	0
51.0880	3.0160	-1.9230	O	0	0	0	0	0	0	0	0	0	0	0	0
51.4040	3.6970	-0.6980	C	0	0	0	0	0	0	0	0	0	0	0	0
50.6350	4.4330	-0.4360	H	0	0	0	0	0	0	0	0	0	0	0	0
51.4060	2.9370	0.0890	H	0	0	0	0	0	0	0	0	0	0	0	0
50.0380	4.8780	-2.7710	O	0	0	0	0	0	0	0	0	0	0	0	0
52.7820	4.3370	-0.8260	C	0	0	0	0	0	0	0	0	0	0	0	0
53.4790	3.6130	-1.2650	H	0	0	0	0	0	0	0	0	0	0	0	0
52.7310	5.1690	-1.5390	H	0	0	0	0	0	0	0	0	0	0	0	0
53.3150	4.8250	0.5190	C	0	0	0	0	0	0	0	0	0	0	0	0
52.6280	5.5680	0.9420	H	0	0	0	0	0	0	0	0	0	0	0	0
53.3600	3.9860	1.2230	H	0	0	0	0	0	0	0	0	0	0	0	0
54.7080	5.4380	0.3640	C	0	0	0	0	0	0	0	0	0	0	0	0
55.3810	4.7090	-0.1030	H	0	0	0	0	0	0	0	0	0	0	0	0
54.6510	6.3010	-0.3110	H	0	0	0	0	0	0	0	0	0	0	0	0
55.2890	5.8760	1.7100	C	0	0	0	0	0	0	0	0	0	0	0	0
54.6050	6.5830	2.1940	H	0	0	0	0	0	0	0	0	0	0	0	0
55.3820	5.0070	2.3730	H	0	0	0	0	0	0	0	0	0	0	0	0
56.6590	6.5330	1.5250	C	0	0	0	0	0	0	0	0	0	0	0	0
57.3440	5.8280	1.0380	H	0	0	0	0	0	0	0	0	0	0	0	0
56.5570	7.3960	0.8550	H	0	0	0	0	0	0	0	0	0	0	0	0
57.2570	6.9880	2.8570	C	0	0	0	0	0	0	0	0	0	0	0	0
56.5440	7.6370	3.3790	H	0	0	0	0	0	0	0	0	0	0	0	0
57.4350	6.1180	3.5000	H	0	0	0	0	0	0	0	0	0	0	0	0
58.5650	7.7460	2.6340	C	0	0	0	0	0	0	0	0	0	0	0	0
59.2810	7.1080	2.1010	H	0	0	0	0	0	0	0	0	0	0	0	0
58.3900	8.6090	1.9790	H	0	0	0	0	0	0	0	0	0	0	0	0
59.1850	8.2270	3.9420	C	0	0	0	0	0	0	0	0	0	0	0	0
58.4600	8.8200	4.5100	H	0	0	0	0	0	0	0	0	0	0	0	0
59.4930	7.3910	4.5810	H	0	0	0	0	0	0	0	0	0	0	0	0
60.2940	9.0980	3.6550	O	0	0	0	0	0	0	0	0	0	0	0	0
61.4950	8.4990	3.4260	C	0	0	0	0	0	0	0	0	0	0	0	0
62.5310	9.5250	3.0510	C	0	0	0	0	0	0	0	0	0	0	0	0
62.0700	10.5140	2.9730	H	0	0	0	0	0	0	0	0	0	0	0	0
63.2320	9.5780	3.8930	H	0	0	0	0	0	0	0	0	0	0	0	0
63.2880	9.1430	1.7720	C	0	0	0	0	0	0	0	0	0	0	0	0
64.3010	9.5600	1.8430	H	0	0	0	0	0	0	0	0	0	0	0	0
63.4400	8.0570	1.7270	H	0	0	0	0	0	0	0	0	0	0	0	0
61.7160	7.2980	3.5150	O	0	0	0	0	0	0	0	0	0	0	0	0

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M END
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M17_1
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 32.8660 -9.9140 5.6990 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 31.7170 -10.5760 6.1450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 30.4600 -10.0440 5.8300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 29.5690 -10.5450 6.2020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 30.3400 -8.8930 5.0380 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 31.5000 -8.2770 4.5540 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


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M END
> <NAME>
M17_1

\$\$\$
O24_1
MOE2012 3D

322326 0 0 1 0 0 0 0 0999 V2000
30.4200 -3.9000 -16.2330 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.0400 -4.4750 -16.7150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.1930 -3.1380 -15.3030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.7220 -3.8210 -14.6310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.9150 -2.5510 -15.8780 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.2320 -2.2320 -14.5350 C 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
29.4960 -2.8420 -13.9970 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.9750 -1.2940 -13.5720 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.5460 -1.8840 -12.8490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.6660 -0.6680 -14.1500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.9980 -0.4410 -12.8790 N 0 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0
29.3720 -0.0790 -13.6060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.5020 -1.4490 -15.4940 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.2460 -2.0930 -16.1870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.2100 -5.4660 -7.6710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.5920 -5.1990 -6.8060 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.0210 -4.7340 -7.7650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.7920 -6.7610 -7.4380 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.3650 -6.9260 -6.2120 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.7790 -8.3640 -6.0290 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.1070 -8.7500 -7.0040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
39.6710 -8.4030 -5.3940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.6160 -9.2080 -5.4950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.5850 -10.1090 -6.1230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.6520 -8.7060 -5.6410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.4940 -6.0570 -5.3610 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.9160 -1.5200 -8.3520 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.9970 -2.7420 -8.1230 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.4170 -2.6440 -7.2010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.2730 -2.8940 -8.9320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.7620 -3.9380 -7.9860 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.6010 -4.1500 -9.1210 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.9690 -4.2040 -10.0180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.5340 -3.0850 -9.3330 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.3770 -2.0180 -8.4010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.0540 -1.2120 -8.7070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.7240 -2.3610 -7.4180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.5730 -0.8580 -9.7120 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.1460 0.0690 -9.8380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.8220 -1.5350 -10.5390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.8100 -0.5010 -7.1800 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.0630 -1.0150 -6.2440 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.5730 0.2790 -7.3090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.4680 0.1920 -6.9780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.6380 -0.5170 -6.9390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.2730 0.9220 -7.7690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.4780 0.7450 -6.0320 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.6150 0.6840 -12.1710 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.2950 1.2420 -12.8250 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
29.7970 1.3730 -11.9280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.2670 0.2810 -10.8510 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
31.1960 1.1250 -10.1540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
30.7410 -0.5710 -10.4030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
32.7340 -0.0510 -10.9750 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.1710 -0.5540 -9.7840 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
33.4310 0.1320 -11.9620 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.3470 -5.5000 -8.9540 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.2480 -5.7650 -10.1760 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
38.0400 -5.0130 -10.2630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.6660 -5.7470 -11.1040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
37.7330 -6.7460 -10.1120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.3140 -6.6440 -8.8530 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.7030 -6.5550 -7.9480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.7990 -7.6270 -8.8270 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
34.6370 -6.6390 -9.7150 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.2160 -13.1200 -0.9360 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
35.7390 -13.9690 -0.9010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.1350 -12.6510 -2.2850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
36.5640 -13.4030 -2.9540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

54.3730	8.0750	-20.4690	O	0	0	0	0	0	0	0	0	0	0	0	0
51.6410	12.4350	-15.0910	C	0	0	0	0	0	0	0	0	0	0	0	0
53.0060	12.9470	-14.5860	C	0	0	0	0	0	0	0	0	0	0	0	0
53.5420	13.4990	-15.3670	H	0	0	0	0	0	0	0	0	0	0	0	0
53.6440	12.1150	-14.2670	H	0	0	0	0	0	0	0	0	0	0	0	0
52.8920	13.6200	-13.7280	H	0	0	0	0	0	0	0	0	0	0	0	0
50.9130	11.7510	-13.9140	C	0	0	0	0	0	0	0	0	0	0	0	0
49.9010	11.4380	-14.1960	H	0	0	0	0	0	0	0	0	0	0	0	0
50.8220	12.4200	-13.0510	H	0	0	0	0	0	0	0	0	0	0	0	0
51.4570	10.8600	-13.5800	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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11	12	1	0	0	0	0									
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M END
> <NAME>
O24_1

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U25_1
MOE2012 3D

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22.2060 -26.0620 8.3280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
22.4930 -23.9160 8.6690 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
23.1930 -23.3070 9.2550 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
21.0780 -23.7470 9.2680 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
20.3100 -24.0890 8.5650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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20.8240 -22.3830 9.5990 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
19.9180 -22.3430 9.9520 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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25.8640 -12.0740 14.5360 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
26.2580 -11.4130 13.7540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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27.9140 -11.7070 15.6680 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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28.8700 -12.2110 17.4700 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
28.9420 -13.5020 16.2720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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21.1890 -21.9550 7.1710 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
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23.7250	-10.8630	14.5720	O	0	0	0	0	0	0	0	0	0	0	0	0	0
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24.4050	-12.0350	16.1520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
25.2380	-10.5210	15.8930	H	0	0	0	0	0	0	0	0	0	0	0	0	0
29.8740	-14.1720	11.6410	O	0	0	0	0	0	0	0	0	0	0	0	0	0
30.2550	-14.9000	11.1220	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.8200	-13.8260	12.6480	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.0400	-14.7410	13.2090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.7350	-13.4940	12.1470	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.2620	-12.7360	13.6020	C	0	0	0	0	0	0	0	0	0	0	0	0	0
29.2490	-13.0860	13.8350	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.1090	-11.3870	12.8610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.0290	-10.5520	13.5610	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.9590	-11.1990	12.1970	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.9180	-11.3630	12.0770	O	0	0	0	0	0	0	0	0	0	0	0	0	0
28.8760	-10.4860	11.6590	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.0260	-12.6900	14.8750	N	0	0	3	0	0	0	0	0	0	0	0	0	0
36.4550	0.2370	8.9430	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.3790	0.3930	9.5130	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.9570	-0.6230	9.4020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.5570	1.3510	9.0780	O	0	0	0	0	0	0	0	0	0	0	0	0	0
36.1390	2.5820	9.1180	C	0	0	0	0	0	0	0	0	0	0	0	0	0
35.0930	3.6570	9.2600	C	0	0	0	0	0	0	0	0	0	0	0	0	0
35.1310	4.2570	8.3430	H	0	0	0	0	0	0	0	0	0	0	0	0	0
34.0960	3.2080	9.2890	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.3510	4.5490	10.4750	C	0	0	0	0	0	0	0	0	0	0	0	0	0
34.7880	5.4810	10.3500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.4050	4.8560	10.4710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.3380	2.8040	9.0190	O	0	0	0	0	0	0	0	0	0	0	0	0	0
36.1210	-9.4970	13.5710	C	0	0	0	0	0	0	0	0	0	0	0	0	0
36.7490	-9.6460	14.4570	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.4230	-10.2240	12.8070	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.4770	-12.4520	14.7660	C	0	0	0	0	0	0	0	0	0	0	0	0	0
32.9410	-12.8630	15.6740	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.9060	-13.0620	13.9630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.9400	-11.0000	14.6190	C	0	0	0	0	0	0	0	0	0	0	0	0	0
32.4400	-10.5200	13.7750	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.7320	-10.4270	15.5290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
34.4260	-10.9290	14.3600	C	0	0	0	0	0	0	0	0	0	0	0	0	0
34.7410	-9.6820	13.9090	O	0	0	0	0	0	0	0	0	0	0	0	0	0
35.2190	-11.8430	14.5330	O	0	0	0	0	0	0	0	0	0	0	0	0	0
36.3030	-8.0820	13.0370	C	0	0	0	0	0	0	0	0	0	0	0	0	0
35.6360	-7.9230	12.1830	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.0320	-7.3570	13.8150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.6610	-7.9120	12.6440	O	0	0	0	0	0	0	0	0	0	0	0	0	0
38.0020	-6.5660	12.3160	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.6770	-5.8890	13.1150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
39.0970	-6.5230	12.2830	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.4380	-6.1440	10.9610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.7030	-6.8930	10.2040	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.3430	-6.1270	11.0020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.9570	-4.7670	10.5490	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.7230	-4.0390	11.3360	H	0	0	0	0	0	0	0	0	0	0	0	0	0
39.0500	-4.7990	10.4550	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.3410	-4.3050	9.2280	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.5740	-5.0260	8.4360	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.2490	-4.2730	9.3270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.8600	-2.9230	8.8350	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.7020	-2.2170	9.6580	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.9450	-2.9560	8.6790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.1860	-2.4010	7.5690	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.4450	-3.0470	6.7230	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.0940	-2.4050	7.6640	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.6860	-1.0970	7.2730	O	0	0	0	0	0	0	0	0	0	0	0	0	0
36.7450	-0.0430	7.4700	C	0	0	0	0	0	0	0	0	0	0	0	0	0
35.8200	-0.2500	6.9180	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.1710	0.8540	7.0070	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.2570	4.0610	12.0960	O	0	0	0	0	0	0	0	0	0	0	0	0	0
30.5720	3.6580	11.5370	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.5020	3.8680	11.4330	C	0	0	0	0	0	0	0	0	0	0	0	0	0
32.5880	2.8000	11.2000	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.4710	4.4300	10.4950	H	0	0	0	0	0	0	0	0	0	0	0	0	0
33.6880	4.3120	12.3210	C	0	0	0	0	0	0	0	0	0	0	0	0	0
33.5480	3.7600	13.2620	H	0	0	0	0	0	0	0	0	0	0	0	0	0
33.5870	5.8240	12.6570	C	0	0	0	0	0	0	0	0	0	0	0	0	0
34.5720	6.2780	12.8000	H	0	0	0	0	0	0	0	0	0	0	0	0	0
33.0780	6.3770	11.8610	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.8800	6.0160	13.8790	O	0	0	0	0	0	0	0	0	0	0	0	0	0
32.6740	6.9630	13.9500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
34.9930	3.8760	11.7400	N	0	0	3	0	0	0	0	0	0	0	0	0	0
49.2280	8.4740	9.1350	C	0	0	0	0	0	0	0	0	0	0	0	0	0

50.1810	13.0820	8.3060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.9160	12.8910	8.0670	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.2110	14.8590	7.7540	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0320	15.5000	7.5230	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.2840	15.4010	7.9800	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0620	17.5280	8.8780	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.1810	17.1580	9.4140	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.9510	17.2200	9.4400	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0110	18.9460	8.7630	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.2070	19.6250	10.0030	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.0980	19.2360	10.5100	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.4100	20.6720	9.7560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.9740	19.5480	10.9010	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.0930	19.8850	10.3410	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.7770	18.5060	11.1780	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.1540	20.3870	12.1650	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0550	20.0560	12.6970	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.3090	21.4380	11.8920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.9430	20.2720	13.0930	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.0440	20.6280	12.5760	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7760	19.2170	13.3450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.1520	21.0750	14.3750	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.0840	20.7640	14.8620	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.2830	22.1390	14.1400	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.9830	20.9140	15.3420	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.0820	21.3540	14.9040	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.7690	19.8570	15.5400	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2640	21.6310	16.5440	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.4860	20.8060	17.6860	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.6510	20.1070	17.8210	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.4680	21.4620	18.5620	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.8920	15.3820	23.6990	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.8300	14.5420	23.2060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.9910	16.2930	23.0590	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2550	16.3190	21.9990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.9770	15.8890	23.1590	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.0900	17.6990	23.7140	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1130	18.0610	23.5520	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.9440	17.5230	25.2530	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.0220	18.4750	25.7830	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.9820	17.0660	25.5080	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.9840	16.6980	25.7840	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1140	15.9690	25.1260	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.1110	18.6310	23.1110	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0
35.9340	24.8300	22.0710	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35.5980	24.1930	22.8990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.7810	24.3070	21.6180	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34.9240	24.9440	21.0560	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33.6390	25.0610	21.4990	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32.7100	25.1470	20.3120	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32.9930	26.0180	19.7120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32.8340	24.2410	19.7090	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31.2570	25.2760	20.7320	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30.9420	24.4150	21.3320	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30.6090	25.3360	19.8520	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31.1000	26.1780	21.3340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33.2960	25.0960	22.6720	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7940	24.2810	24.3410	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.3880	24.5730	25.2160	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.9720	25.0560	23.5880	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.8670	19.8890	23.8340	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.0370	20.4200	23.3470	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.4580	19.6650	24.8270	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.0520	20.8400	23.9670	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.8820	20.3970	24.5270	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.4490	21.1430	22.9950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.6040	22.0790	24.6910	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.2510	23.0370	23.7910	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.5320	22.1750	25.9070	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.3080	24.2160	24.6720	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.7480	23.9190	23.7800	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.1260	23.4640	25.4480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8870	25.5000	25.1240	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.5310	25.5340	25.5700	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.3260	24.6820	26.2290	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.4240	26.4420	26.1740	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.5500	25.5880	24.3990	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.8220	26.4190	23.7370	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.6370	24.6780	23.7940	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.1060	25.7440	24.8810	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.8490	24.9070	25.5420	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0

42.0140	26.6630	25.4730	H	0	0	0	0	0	0	0	0	0	0	0	0
41.1230	25.7900	23.7080	C	0	0	0	0	0	0	0	0	0	0	0	0
41.3770	26.6300	23.0500	H	0	0	0	0	0	0	0	0	0	0	0	0
41.2180	24.8740	23.1130	H	0	0	0	0	0	0	0	0	0	0	0	0
39.6810	25.9360	24.1920	C	0	0	0	0	0	0	0	0	0	0	0	0
39.4180	25.1040	24.8570	H	0	0	0	0	0	0	0	0	0	0	0	0
39.5740	26.8470	24.7960	H	0	0	0	0	0	0	0	0	0	0	0	0
38.6920	25.9830	23.0310	C	0	0	0	0	0	0	0	0	0	0	0	0
38.9130	26.8400	22.3830	H	0	0	0	0	0	0	0	0	0	0	0	0
38.7620	25.0630	22.4420	H	0	0	0	0	0	0	0	0	0	0	0	0
37.3760	26.1210	23.5690	O	0	0	0	0	0	0	0	0	0	0	0	0
36.3620	26.2080	22.5690	C	0	0	0	0	0	0	0	0	0	0	0	0
36.6810	26.8490	21.7380	H	0	0	0	0	0	0	0	0	0	0	0	0
35.5040	26.7130	23.0250	H	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	30	1	0	0	0	0
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15	18	1	0	0	0	0
15	62	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	77	1	0	0	0	0
27	28	1	0	0	0	0
27	29	1	0	0	0	0
27	37	1	0	0	0	0
27	39	1	0	0	0	0
30	31	1	0	0	0	0
30	32	1	0	0	0	0
30	33	1	0	0	0	0
33	34	1	0	0	0	0
33	35	1	0	0	0	0
33	36	1	0	0	0	0
36	37	1	0	0	0	0
36	38	2	0	0	0	0
39	40	1	0	0	0	0
39	41	1	0	0	0	0
39	42	1	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	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	52	1	0	0	0	0
52	53	1	0	0	0	0
52	54	1	0	0	0	0
52	55	1	0	0	0	0
55	56	1	0	0	0	0
55	57	1	0	0	0	0
55	58	1	0	0	0	0
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58	60	1	0	0	0	0
58	61	1	0	0	0	0
61	62	1	0	0	0	0
62	63	1	0	0	0	0
62	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	77	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
75	76	1	0	0	0	0
77	93	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
78	125	1	0	0	0	0
81	82	1	0	0	0	0
82	83	1	0	0	0	0
82	89	2	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
86	87	1	0	0	0	0
86	88	1	0	0	0	0
86	140	1	0	0	0	0
90	91	1	0	0	0	0
90	92	1	0	0	0	0
90	100	1	0	0	0	0
90	102	1	0	0	0	0
93	94	1	0	0	0	0
93	95	1	0	0	0	0
93	96	1	0	0	0	0
96	97	1	0	0	0	0
96	98	1	0	0	0	0
96	99	1	0	0	0	0
99	100	1	0	0	0	0
99	101	2	0	0	0	0
102	103	1	0	0	0	0
102	104	1	0	0	0	0
102	105	1	0	0	0	0
105	106	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
112	114	1	0	0	0	0
112	115	1	0	0	0	0
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115	117	1	0	0	0	0
115	118	1	0	0	0	0
118	119	1	0	0	0	0
118	120	1	0	0	0	0
118	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
125	126	1	0	0	0	0
125	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	140	1	0	0	0	0
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135	137	1	0	0	0	0
135	138	1	0	0	0	0
138	139	1	0	0	0	0
140	156	1	0	0	0	0
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141	144	1	0	0	0	0
141	188	1	0	0	0	0
144	145	1	0	0	0	0
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M END
> <NAME>
U25_1

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U28_1
MOE2012 3D

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12.9260 6.7500 -17.6330 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.3450 6.9830 -18.3760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.3910 5.4280 -17.8650 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
12.5270 4.7590 -17.9240 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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14.3080 5.0330 -16.7200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.1300 5.7570 -16.6490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13.7610 5.1090 -15.7720 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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15.3960 3.5580 -17.8560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.8030 3.2610 -15.7520 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.6070 4.0040 -15.7140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15.2550 3.3030 -14.8030 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16.3500 1.9210 -15.9640 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0
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20.6930 10.7460 -4.2640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.8550 10.3950 -3.6500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.3750 10.6250 -5.3040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.9460 12.1430 -4.0640 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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21.4180 13.9910 -2.6860 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.3690 14.4800 -3.6650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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22.7630 13.5800 -1.0960 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.1810 15.0260 -1.9840 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.5340 11.9200 -1.8100 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.5040 2.0540 -12.6580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.5810 0.9640 -12.5560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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18.4240 3.2870 -14.7110 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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19.1100 0.8190 -12.9470 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.1170 2.7130 -11.3380 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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20.1270 2.3730 -11.0180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.0930 2.3780 -10.3560 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.7520 2.8220 -9.0420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.7170 2.5500 -8.8050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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21.3080 6.8190 -7.9170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.7670 6.7180 -5.8100 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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22.4430 6.1750 -5.1380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.9850 8.2190 -5.6410 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
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21.2850 8.7730 -6.2740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.7740 8.5520 -4.2690 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.9620 9.9390 -3.9930 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.8180 10.3410 -4.5500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22.2250 10.0240 -2.9340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

27.9500	16.8160	-4.0320	O	0	0	0	0	0	0	0	0	0	0	0	0	0
28.2770	17.6760	-4.3470	H	0	0	0	0	0	0	0	0	0	0	0	0	0
26.5920	16.7090	-4.4390	C	0	0	0	0	0	0	0	0	0	0	0	0	0
26.0260	17.5320	-3.9920	H	0	0	0	0	0	0	0	0	0	0	0	0	0
26.5500	16.7980	-5.5300	H	0	0	0	0	0	0	0	0	0	0	0	0	0
26.0470	15.3620	-3.9800	C	0	0	0	0	0	0	0	0	0	0	0	0	0
26.6840	14.5630	-4.3790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
26.1320	15.3080	-2.8910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.5990	15.1570	-4.4220	C	0	0	0	0	0	0	0	0	0	0	0	0	0
23.9470	15.8790	-3.9180	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.5290	15.3930	-5.4920	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.0690	13.7240	-4.2450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
23.1400	13.6510	-4.8230	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.7460	13.0300	-4.7610	H	0	0	0	0	0	0	0	0	0	0	0	0	0
23.8000	13.2070	-2.8950	N	0	0	3	0	0	0	0	0	0	0	0	0	0
32.4790	0.3430	0.5870	C	0	0	0	0	0	0	0	0	0	0	0	0	0
33.1810	0.5310	-0.2330	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.6980	-0.3540	0.2660	H	0	0	0	0	0	0	0	0	0	0	0	0	0
33.1940	-0.2280	1.6960	O	0	0	0	0	0	0	0	0	0	0	0	0	0
33.8970	-1.3570	1.4120	C	0	0	0	0	0	0	0	0	0	0	0	0	0
34.7560	-1.7380	2.5920	C	0	0	0	0	0	0	0	0	0	0	0	0	0
34.4650	-1.1170	3.4450	H	0	0	0	0	0	0	0	0	0	0	0	0	0
34.5360	-2.7740	2.8710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.2290	-1.5560	2.2180	C	0	0	0	0	0	0	0	0	0	0	0	0	0
36.3440	-0.7610	1.4700	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.5610	-2.4530	1.6780	H	0	0	0	0	0	0	0	0	0	0	0	0	0
33.8810	-1.9550	0.3460	O	0	0	0	0	0	0	0	0	0	0	0	0	0
28.0090	10.0280	-0.5300	C	0	0	0	0	0	0	0	0	0	0	0	0	0
27.9790	10.0650	0.5660	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.2040	8.9830	-0.7900	H	0	0	0	0	0	0	0	0	0	0	0	0	0
25.0110	12.8840	-2.1330	C	0	0	0	0	0	0	0	0	0	0	0	0	0
25.8360	12.6310	-2.8120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
25.3500	13.7430	-1.5410	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.7830	11.6750	-1.2280	C	0	0	0	0	0	0	0	0	0	0	0	0	0
24.0000	11.8450	-0.4810	H	0	0	0	0	0	0	0	0	0	0	0	0	0
24.4770	10.7970	-1.8080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
26.0560	11.3720	-0.4890	C	0	0	0	0	0	0	0	0	0	0	0	0	0
26.7370	10.3680	-1.1050	O	0	0	0	0	0	0	0	0	0	0	0	0	0
26.4340	11.9890	0.4980	O	0	0	0	0	0	0	0	0	0	0	0	0	0
29.1040	10.9320	-1.0910	C	0	0	0	0	0	0	0	0	0	0	0	0	0
29.1440	10.8730	-2.1860	H	0	0	0	0	0	0	0	0	0	0	0	0	0
28.8690	11.9770	-0.8590	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.3860	10.6590	-0.5320	O	0	0	0	0	0	0	0	0	0	0	0	0	0
30.9690	9.4340	-0.9750	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.3990	8.9830	-1.7950	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.9680	9.6660	-1.3580	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.0840	8.4810	0.2110	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.7360	8.9290	0.9710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.1050	8.3650	0.6910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.6210	7.1150	-0.2100	C	0	0	0	0	0	0	0	0	0	0	0	0	0
30.9500	6.6730	-0.9580	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.6020	7.2330	-0.6850	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.7420	6.1730	0.9890	C	0	0	0	0	0	0	0	0	0	0	0	0	0
32.4430	6.5990	1.7170	H	0	0	0	0	0	0	0	0	0	0	0	0	0
30.7690	6.0860	1.4890	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.2190	4.7860	0.5640	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.5110	4.3480	-0.1490	H	0	0	0	0	0	0	0	0	0	0	0	0	0
33.1760	4.8590	0.0320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.3850	3.8610	1.7670	C	0	0	0	0	0	0	0	0	0	0	0	0	0
33.1260	4.2860	2.4520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.4490	3.7510	2.3280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
32.8860	2.5920	1.3500	O	0	0	0	0	0	0	0	0	0	0	0	0	0
31.8480	1.6560	1.0430	C	0	0	0	0	0	0	0	0	0	0	0	0	0
31.2120	2.0550	0.2460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
31.2470	1.4870	1.9440	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.2570	4.8190	3.9790	O	0	0	0	0	0	0	0	0	0	0	0	0	0
36.0810	5.5750	3.3920	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.4480	3.6860	3.1450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
35.5770	3.5840	2.4910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.3370	3.8520	2.5280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.6150	2.4560	4.0220	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.4860	2.5890	4.6760	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.7490	2.3640	4.6900	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.7670	1.1930	3.1770	C	0	0	0	0	0	0	0	0	0	0	0	0	0
35.8850	1.1060	2.5320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.6460	1.2880	2.5280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.9080	-0.0510	4.0650	C	0	0	0	0	0	0	0	0	0	0	0	0	0
37.7490	0.1410	4.7410	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.0170	-0.1480	4.6970	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.1670	-1.3030	3.3280	N	0	0	3	0	0	0	0	0	0	0	0	0	0
49.7040	-2.2360	11.1040	C	0	0	0	0	0	0	0	0	0	0	0	0	0

49.4890	-1.5880	11.9620	H	0	0	0	0	0	0	0	0	0	0	0
49.0500	-1.9410	10.2760	H	0	0	0	0	0	0	0	0	0	0	0
51.0710	-2.0980	10.6990	O	0	0	0	0	0	0	0	0	0	0	0
51.4790	-0.8160	10.4870	C	0	0	0	0	0	0	0	0	0	0	0
52.9460	-0.7830	10.1590	C	0	0	0	0	0	0	0	0	0	0	0
53.2900	-1.7830	9.8690	H	0	0	0	0	0	0	0	0	0	0	0
53.0700	-0.1500	9.2720	H	0	0	0	0	0	0	0	0	0	0	0
53.7680	-0.2330	11.3210	C	0	0	0	0	0	0	0	0	0	0	0
53.4260	0.7750	11.5890	H	0	0	0	0	0	0	0	0	0	0	0
54.7960	-0.1000	10.9600	H	0	0	0	0	0	0	0	0	0	0	0
50.7720	0.1790	10.5710	O	0	0	0	0	0	0	0	0	0	0	0
40.1260	-4.8470	7.3680	C	0	0	0	0	0	0	0	0	0	0	0
39.6900	-5.7660	6.9560	H	0	0	0	0	0	0	0	0	0	0	0
41.2080	-5.0120	7.3750	H	0	0	0	0	0	0	0	0	0	0	0
37.2650	-2.4630	4.2330	C	0	0	0	0	0	0	0	0	0	0	0
36.3700	-2.5430	4.8630	H	0	0	0	0	0	0	0	0	0	0	0
37.3070	-3.3850	3.6370	H	0	0	0	0	0	0	0	0	0	0	0
38.5280	-2.4220	5.1000	C	0	0	0	0	0	0	0	0	0	0	0
39.4130	-2.3580	4.4570	H	0	0	0	0	0	0	0	0	0	0	0
38.5170	-1.5700	5.7860	H	0	0	0	0	0	0	0	0	0	0	0
38.6380	-3.6640	5.9440	C	0	0	0	0	0	0	0	0	0	0	0
39.8760	-3.7190	6.5160	O	0	0	0	0	0	0	0	0	0	0	0
37.7430	-4.4790	6.1140	O	0	0	0	0	0	0	0	0	0	0	0
39.6170	-4.5770	8.7800	C	0	0	0	0	0	0	0	0	0	0	0
39.9770	-3.6080	9.1490	H	0	0	0	0	0	0	0	0	0	0	0
38.5240	-4.5100	8.7700	H	0	0	0	0	0	0	0	0	0	0	0
39.9720	-5.6550	9.6410	O	0	0	0	0	0	0	0	0	0	0	0
40.9310	-5.3130	10.6420	C	0	0	0	0	0	0	0	0	0	0	0
40.5870	-4.4360	11.2040	H	0	0	0	0	0	0	0	0	0	0	0
40.9650	-6.1530	11.3430	H	0	0	0	0	0	0	0	0	0	0	0
42.3220	-5.0900	10.0480	C	0	0	0	0	0	0	0	0	0	0	0
42.5960	-5.9570	9.4350	H	0	0	0	0	0	0	0	0	0	0	0
42.3010	-4.2310	9.3680	H	0	0	0	0	0	0	0	0	0	0	0
43.3780	-4.8520	11.1270	C	0	0	0	0	0	0	0	0	0	0	0
43.0900	-3.9920	11.7420	H	0	0	0	0	0	0	0	0	0	0	0
43.4300	-5.7240	11.7910	H	0	0	0	0	0	0	0	0	0	0	0
44.7510	-4.5990	10.4990	C	0	0	0	0	0	0	0	0	0	0	0
45.0340	-5.4580	9.8790	H	0	0	0	0	0	0	0	0	0	0	0
44.6930	-3.7280	9.8340	H	0	0	0	0	0	0	0	0	0	0	0
45.8240	-4.3600	11.5590	C	0	0	0	0	0	0	0	0	0	0	0
45.5490	-3.5080	12.1940	H	0	0	0	0	0	0	0	0	0	0	0
45.8950	-5.2250	12.2290	H	0	0	0	0	0	0	0	0	0	0	0
47.1860	-4.0970	10.9240	C	0	0	0	0	0	0	0	0	0	0	0
47.4860	-4.9540	10.3100	H	0	0	0	0	0	0	0	0	0	0	0
47.1400	-3.2040	10.2930	H	0	0	0	0	0	0	0	0	0	0	0
48.1390	-3.9060	11.9690	O	0	0	0	0	0	0	0	0	0	0	0
49.4650	-3.6920	11.4900	C	0	0	0	0	0	0	0	0	0	0	0
49.7000	-4.3690	10.6600	H	0	0	0	0	0	0	0	0	0	0	0
50.1510	-3.9600	12.3010	H	0	0	0	0	0	0	0	0	0	0	0
50.2660	-1.5830	17.5920	O	0	0	0	0	0	0	0	0	0	0	0
49.8630	-2.2940	18.1200	H	0	0	0	0	0	0	0	0	0	0	0
50.9590	-2.1960	16.5150	C	0	0	0	0	0	0	0	0	0	0	0
51.7520	-2.8270	16.9270	H	0	0	0	0	0	0	0	0	0	0	0
50.2570	-2.8240	15.9570	H	0	0	0	0	0	0	0	0	0	0	0
51.5350	-1.1040	15.6250	C	0	0	0	0	0	0	0	0	0	0	0
50.7180	-0.4850	15.2340	H	0	0	0	0	0	0	0	0	0	0	0
52.1580	-0.4330	16.2290	H	0	0	0	0	0	0	0	0	0	0	0
52.3530	-1.6920	14.4780	C	0	0	0	0	0	0	0	0	0	0	0
53.1540	-2.3100	14.8980	H	0	0	0	0	0	0	0	0	0	0	0
51.7180	-2.3570	13.8790	H	0	0	0	0	0	0	0	0	0	0	0
52.9230	-0.5850	13.5790	C	0	0	0	0	0	0	0	0	0	0	0
52.0640	-0.0290	13.1820	H	0	0	0	0	0	0	0	0	0	0	0
53.5180	0.1300	14.1610	H	0	0	0	0	0	0	0	0	0	0	0
53.7150	-1.1540	12.4740	N	0	0	3	0	0	0	0	0	0	0	0
58.3790	-14.0060	11.3330	C	0	0	0	0	0	0	0	0	0	0	0
59.1890	-13.8920	10.6030	H	0	0	0	0	0	0	0	0	0	0	0
58.0860	-13.0110	11.6850	H	0	0	0	0	0	0	0	0	0	0	0
57.2420	-14.6390	10.7290	O	0	0	0	0	0	0	0	0	0	0	0
56.7710	-14.0310	9.6030	C	0	0	0	0	0	0	0	0	0	0	0
55.5390	-14.7380	9.1020	C	0	0	0	0	0	0	0	0	0	0	0
55.0740	-15.3040	9.9150	H	0	0	0	0	0	0	0	0	0	0	0
54.8080	-13.9640	8.8380	H	0	0	0	0	0	0	0	0	0	0	0
55.8270	-15.6110	7.8810	C	0	0	0	0	0	0	0	0	0	0	0
56.1360	-14.9370	7.0700	H	0	0	0	0	0	0	0	0	0	0	0
54.8850	-16.0750	7.5650	H	0	0	0	0	0	0	0	0	0	0	0
57.2500	-13.0320	9.0830	O	0	0	0	0	0	0	0	0	0	0	0
58.2300	-4.0470	14.2130	C	0	0	0	0	0	0	0	0	0	0	0
58.9670	-3.2400	14.1160	H	0	0	0	0	0	0	0	0	0	0	0
58.0840	-4.1920	15.2890	H	0	0	0	0	0	0	0	0	0	0	0
55.0620	-1.5430	12.9220	C	0	0	0	0	0	0	0	0	0	0	0
55.7320	-0.6730	12.9760	H	0	0	0	0	0	0	0	0	0	0	0

55.0320	-1.9470	13.9400	H	0	0	0	0	0	0	0	0	0	0	0	0
55.6330	-2.6260	12.0130	C	0	0	0	0	0	0	0	0	0	0	0	0
55.0080	-3.5260	12.0100	H	0	0	0	0	0	0	0	0	0	0	0	0
55.7070	-2.2860	10.9730	H	0	0	0	0	0	0	0	0	0	0	0	0
57.0130	-2.9980	12.4700	C	0	0	0	0	0	0	0	0	0	0	0	0
56.9640	-3.6620	13.6570	O	0	0	0	0	0	0	0	0	0	0	0	0
58.0300	-2.7320	11.8450	O	0	0	0	0	0	0	0	0	0	0	0	0
58.7310	-5.3410	13.5820	C	0	0	0	0	0	0	0	0	0	0	0	0
57.9700	-6.1210	13.6970	H	0	0	0	0	0	0	0	0	0	0	0	0
58.9020	-5.1990	12.5090	H	0	0	0	0	0	0	0	0	0	0	0	0
59.9450	-5.7220	14.2230	O	0	0	0	0	0	0	0	0	0	0	0	0
60.5280	-6.8980	13.6600	C	0	0	0	0	0	0	0	0	0	0	0	0
60.4570	-6.8740	12.5660	H	0	0	0	0	0	0	0	0	0	0	0	0
61.5930	-6.8770	13.9150	H	0	0	0	0	0	0	0	0	0	0	0	0
59.8990	-8.1640	14.2390	C	0	0	0	0	0	0	0	0	0	0	0	0
60.0470	-8.1760	15.3260	H	0	0	0	0	0	0	0	0	0	0	0	0
58.8140	-8.1510	14.0850	H	0	0	0	0	0	0	0	0	0	0	0	0
60.4880	-9.4260	13.6070	C	0	0	0	0	0	0	0	0	0	0	0	0
60.3240	-9.3960	12.5230	H	0	0	0	0	0	0	0	0	0	0	0	0
61.5730	-9.4530	13.7680	H	0	0	0	0	0	0	0	0	0	0	0	0
59.8520	-10.6910	14.1880	C	0	0	0	0	0	0	0	0	0	0	0	0
60.1020	-10.7730	15.2520	H	0	0	0	0	0	0	0	0	0	0	0	0
58.7600	-10.6150	14.1170	H	0	0	0	0	0	0	0	0	0	0	0	0
60.3170	-11.9450	13.4480	C	0	0	0	0	0	0	0	0	0	0	0	0
60.0880	-11.8540	12.3790	H	0	0	0	0	0	0	0	0	0	0	0	0
61.4070	-12.0450	13.5110	H	0	0	0	0	0	0	0	0	0	0	0	0
59.6620	-13.2030	14.0120	C	0	0	0	0	0	0	0	0	0	0	0	0
60.0670	-13.4110	15.0090	H	0	0	0	0	0	0	0	0	0	0	0	0
58.5780	-13.0740	14.1200	H	0	0	0	0	0	0	0	0	0	0	0	0
59.9780	-14.3220	13.1810	O	0	0	0	0	0	0	0	0	0	0	0	0
58.8520	-14.8710	12.4980	C	0	0	0	0	0	0	0	0	0	0	0	0
58.0370	-15.0750	13.2040	H	0	0	0	0	0	0	0	0	0	0	0	0
59.1550	-15.8500	12.1070	H	0	0	0	0	0	0	0	0	0	0	0	0
56.4110	-19.3830	2.4620	O	0	0	0	0	0	0	0	0	0	0	0	0
55.7230	-19.8050	1.9200	H	0	0	0	0	0	0	0	0	0	0	0	0
55.8270	-19.0710	3.7210	C	0	0	0	0	0	0	0	0	0	0	0	0
54.9650	-18.4190	3.5490	H	0	0	0	0	0	0	0	0	0	0	0	0
55.4850	-20.0000	4.1870	H	0	0	0	0	0	0	0	0	0	0	0	0
56.8670	-18.3770	4.5940	C	0	0	0	0	0	0	0	0	0	0	0	0
57.7260	-19.0440	4.7390	H	0	0	0	0	0	0	0	0	0	0	0	0
57.2550	-17.5010	4.0600	H	0	0	0	0	0	0	0	0	0	0	0	0
56.2880	-17.9560	5.9480	C	0	0	0	0	0	0	0	0	0	0	0	0
55.4080	-17.3290	5.7690	H	0	0	0	0	0	0	0	0	0	0	0	0
55.9520	-18.8460	6.4910	H	0	0	0	0	0	0	0	0	0	0	0	0
57.3300	-17.1880	6.7800	C	0	0	0	0	0	0	0	0	0	0	0	0
58.2010	-17.8320	6.9480	H	0	0	0	0	0	0	0	0	0	0	0	0
57.7200	-16.3570	6.1770	H	0	0	0	0	0	0	0	0	0	0	0	0
56.8700	-16.6350	8.0680	N	0	0	3	0	0	0	0	0	0	0	0	0
66.4440	-12.6110	17.7460	C	0	0	0	0	0	0	0	0	0	0	0	0
66.0070	-11.8120	17.1340	H	0	0	0	0	0	0	0	0	0	0	0	0
66.5740	-13.4660	17.0740	H	0	0	0	0	0	0	0	0	0	0	0	0
67.7530	-12.2570	18.2200	O	0	0	0	0	0	0	0	0	0	0	0	0
67.9180	-10.9560	18.5960	C	0	0	0	0	0	0	0	0	0	0	0	0
69.3440	-10.7460	19.0470	C	0	0	0	0	0	0	0	0	0	0	0	0
69.5430	-11.4160	19.8900	H	0	0	0	0	0	0	0	0	0	0	0	0
70.0110	-11.0030	18.2180	H	0	0	0	0	0	0	0	0	0	0	0	0
69.6020	-9.3110	19.4730	C	0	0	0	0	0	0	0	0	0	0	0	0
69.4140	-8.6160	18.6480	H	0	0	0	0	0	0	0	0	0	0	0	0
70.6410	-9.1890	19.7930	H	0	0	0	0	0	0	0	0	0	0	0	0
68.9510	-9.0250	20.3060	H	0	0	0	0	0	0	0	0	0	0	0	0
67.0460	-10.0990	18.5760	O	0	0	0	0	0	0	0	0	0	0	0	0
58.6860	-19.9940	12.7030	C	0	0	0	0	0	0	0	0	0	0	0	0
57.7950	-20.5840	12.9490	H	0	0	0	0	0	0	0	0	0	0	0	0
59.5420	-20.6630	12.8420	H	0	0	0	0	0	0	0	0	0	0	0	0
56.5110	-17.6480	9.0740	C	0	0	0	0	0	0	0	0	0	0	0	0
56.1670	-17.1430	9.9820	H	0	0	0	0	0	0	0	0	0	0	0	0
55.6710	-18.2670	8.7370	H	0	0	0	0	0	0	0	0	0	0	0	0
57.6950	-18.5370	9.4700	C	0	0	0	0	0	0	0	0	0	0	0	0
57.8400	-19.3470	8.7470	H	0	0	0	0	0	0	0	0	0	0	0	0
58.6070	-17.9290	9.5160	H	0	0	0	0	0	0	0	0	0	0	0	0
57.4870	-19.1390	10.8400	C	0	0	0	0	0	0	0	0	0	0	0	0
58.6840	-19.5740	11.3290	O	0	0	0	0	0	0	0	0	0	0	0	0
56.4190	-19.2030	11.4310	O	0	0	0	0	0	0	0	0	0	0	0	0
58.8260	-18.7760	13.6090	C	0	0	0	0	0	0	0	0	0	0	0	0
59.7020	-18.1970	13.2980	H	0	0	0	0	0	0	0	0	0	0	0	0
57.9490	-18.1270	13.5030	H	0	0	0	0	0	0	0	0	0	0	0	0
58.9500	-19.1930	14.9660	O	0	0	0	0	0	0	0	0	0	0	0	0
59.1520	-18.0920	15.8550	C	0	0	0	0	0	0	0	0	0	0	0	0
58.5260	-17.2400	15.5610	H	0	0	0	0	0	0	0	0	0	0	0	0
58.8160	-18.4150	16.8460	H	0	0	0	0	0	0	0	0	0	0	0	0
60.6310	-17.7100	15.9240	C	0	0	0	0	0	0	0	0	0	0	0	0

61.2030	-18.5660	16.3010	H	0	0	0	0	0	0	0	0	0	0	0	0
61.0200	-17.5110	14.9200	H	0	0	0	0	0	0	0	0	0	0	0	0
60.8610	-16.4840	16.8080	C	0	0	0	0	0	0	0	0	0	0	0	0
60.3050	-15.6320	16.3990	H	0	0	0	0	0	0	0	0	0	0	0	0
60.4700	-16.6730	17.8150	H	0	0	0	0	0	0	0	0	0	0	0	0
62.3490	-16.1350	16.8940	C	0	0	0	0	0	0	0	0	0	0	0	0
62.8890	-16.9620	17.3720	H	0	0	0	0	0	0	0	0	0	0	0	0
62.7610	-16.0220	15.8840	H	0	0	0	0	0	0	0	0	0	0	0	0
62.5800	-14.8450	17.6790	C	0	0	0	0	0	0	0	0	0	0	0	0
62.0810	-14.0050	17.1790	H	0	0	0	0	0	0	0	0	0	0	0	0
62.1240	-14.9160	18.6740	H	0	0	0	0	0	0	0	0	0	0	0	0
64.0670	-14.5360	17.8310	C	0	0	0	0	0	0	0	0	0	0	0	0
64.5550	-15.3240	18.4160	H	0	0	0	0	0	0	0	0	0	0	0	0
64.5390	-14.4760	16.8450	H	0	0	0	0	0	0	0	0	0	0	0	0
64.1960	-13.2800	18.4960	O	0	0	0	0	0	0	0	0	0	0	0	0
65.5300	-12.9850	18.9100	C	0	0	0	0	0	0	0	0	0	0	0	0
65.9480	-13.8210	19.4850	H	0	0	0	0	0	0	0	0	0	0	0	0
65.4680	-12.1440	19.6100	H	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	9	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									
12	13	1	0	0	0	0									
12	14	1	0	0	0	0									
12	15	1	0	0	0	0									
15	16	1	0	0	0	0									
15	32	1	0	0	0	0									
17	18	1	0	0	0	0									
17	19	1	0	0	0	0									
17	20	1	0	0	0	0									
17	64	1	0	0	0	0									
20	21	1	0	0	0	0									
21	22	1	0	0	0	0									
21	28	2	0	0	0	0									
22	23	1	0	0	0	0									
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25	27	1	0	0	0	0									
25	81	1	0	0	0	0									
29	30	1	0	0	0	0									
29	31	1	0	0	0	0									
29	39	1	0	0	0	0									
29	41	1	0	0	0	0									
32	33	1	0	0	0	0									
32	34	1	0	0	0	0									
32	35	1	0	0	0	0									
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35	37	1	0	0	0	0									
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38	39	1	0	0	0	0									
38	40	2	0	0	0	0									
41	42	1	0	0	0	0									
41	43	1	0	0	0	0									
41	44	1	0	0	0	0									
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60	63	1	0	0	0	0									

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67	69	1	0	0	0	0
69	70	1	0	0	0	0
69	71	1	0	0	0	0
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72	73	1	0	0	0	0
72	74	1	0	0	0	0
72	75	1	0	0	0	0
75	76	1	0	0	0	0
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78	80	1	0	0	0	0
78	81	1	0	0	0	0
81	97	1	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
82	129	1	0	0	0	0
85	86	1	0	0	0	0
86	87	1	0	0	0	0
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90	91	1	0	0	0	0
90	92	1	0	0	0	0
90	146	1	0	0	0	0
94	95	1	0	0	0	0
94	96	1	0	0	0	0
94	104	1	0	0	0	0
94	106	1	0	0	0	0
97	98	1	0	0	0	0
97	99	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	1	0	0	0	0
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122	123	1	0	0	0	0
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122	125	1	0	0	0	0
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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	131	1	0	0	0	0
132	133	1	0	0	0	0
132	134	1	0	0	0	0
134	135	1	0	0	0	0
134	136	1	0	0	0	0
134	137	1	0	0	0	0
137	138	1	0	0	0	0
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137	140	1	0	0	0	0
140	141	1	0	0	0	0
140	142	1	0	0	0	0
140	143	1	0	0	0	0
143	144	1	0	0	0	0
143	145	1	0	0	0	0

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147150	1	0	0	0	0
147194	1	0	0	0	0
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162164	1	0	0	0	0
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165168	1	0	0	0	0
168169	1	0	0	0	0
168170	2	0	0	0	0
171172	1	0	0	0	0
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171174	1	0	0	0	0
174175	1	0	0	0	0
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178180	1	0	0	0	0
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199202	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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220276	1	0	0	0	0
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224236	1	0	0	0	0
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227230	1	0	0	0	0
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230233	1	0	0	0	0
233234	1	0	0	0	0
233235	2	0	0	0	0
236237	1	0	0	0	0
236238	1	0	0	0	0
236239	1	0	0	0	0
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240243	1	0	0	0	0
243244	1	0	0	0	0
243245	1	0	0	0	0
243246	1	0	0	0	0
246247	1	0	0	0	0
246248	1	0	0	0	0
246249	1	0	0	0	0
249250	1	0	0	0	0
249251	1	0	0	0	0
249252	1	0	0	0	0
252253	1	0	0	0	0
252254	1	0	0	0	0
252255	1	0	0	0	0
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259261	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
273274	1	0	0	0	0
273275	1	0	0	0	0
273276	1	0	0	0	0
276293	1	0	0	0	0
277278	1	0	0	0	0
277279	1	0	0	0	0
277280	1	0	0	0	0
277325	1	0	0	0	0
280281	1	0	0	0	0
281282	1	0	0	0	0
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282283	1	0	0	0	0
282284	1	0	0	0	0
282285	1	0	0	0	0
285286	1	0	0	0	0
285287	1	0	0	0	0
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290291	1	0	0	0	0
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290302	1	0	0	0	0
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293295	1	0	0	0	0
293296	1	0	0	0	0
296297	1	0	0	0	0
296298	1	0	0	0	0
296299	1	0	0	0	0
299300	1	0	0	0	0
299301	2	0	0	0	0
302303	1	0	0	0	0
302304	1	0	0	0	0
302305	1	0	0	0	0
305306	1	0	0	0	0
306307	1	0	0	0	0

28.0270	2.8940	6.4010	O	0	0	0	0	0	0	0	0	0	0	0	0
29.3220	2.4550	5.9910	C	0	0	0	0	0	0	0	0	0	0	0	0
29.2630	1.5030	5.4490	H	0	0	0	0	0	0	0	0	0	0	0	0
29.9020	2.2540	6.8980	H	0	0	0	0	0	0	0	0	0	0	0	0
29.1090	5.3890	-2.2710	O	0	0	0	0	0	0	0	0	0	0	0	0
28.9190	5.0150	-3.1490	H	0	0	0	0	0	0	0	0	0	0	0	0
30.2310	4.6930	-1.7490	C	0	0	0	0	0	0	0	0	0	0	0	0
29.9460	3.6490	-1.5850	H	0	0	0	0	0	0	0	0	0	0	0	0
31.0400	4.7300	-2.4860	H	0	0	0	0	0	0	0	0	0	0	0	0
30.6560	5.3560	-0.4480	C	0	0	0	0	0	0	0	0	0	0	0	0
30.9020	6.4080	-0.6390	H	0	0	0	0	0	0	0	0	0	0	0	0
29.8070	5.3690	0.2470	H	0	0	0	0	0	0	0	0	0	0	0	0
31.8460	4.6390	0.1840	C	0	0	0	0	0	0	0	0	0	0	0	0
31.5810	3.5900	0.3650	H	0	0	0	0	0	0	0	0	0	0	0	0
32.6950	4.6440	-0.5100	H	0	0	0	0	0	0	0	0	0	0	0	0
32.2550	5.3020	1.5010	C	0	0	0	0	0	0	0	0	0	0	0	0
32.5630	6.3340	1.2980	H	0	0	0	0	0	0	0	0	0	0	0	0
31.3860	5.3440	2.1700	H	0	0	0	0	0	0	0	0	0	0	0	0
33.3890	4.5250	2.1820	C	0	0	0	0	0	0	0	0	0	0	0	0
33.0720	3.4770	2.2190	H	0	0	0	0	0	0	0	0	0	0	0	0
34.2940	4.5430	1.5640	H	0	0	0	0	0	0	0	0	0	0	0	0
33.6520	5.0090	3.5440	N	0	0	3	0	0	0	0	0	0	0	0	0
48.9300	9.6600	5.4160	C	0	0	0	0	0	0	0	0	0	0	0	0
49.1280	9.8860	4.3610	H	0	0	0	0	0	0	0	0	0	0	0	0
48.1900	8.8520	5.4140	H	0	0	0	0	0	0	0	0	0	0	0	0
50.1030	9.1490	6.0690	O	0	0	0	0	0	0	0	0	0	0	0	0
51.2750	9.7830	5.7660	C	0	0	0	0	0	0	0	0	0	0	0	0
52.4050	9.1460	6.5390	C	0	0	0	0	0	0	0	0	0	0	0	0
52.2160	9.2780	7.6100	H	0	0	0	0	0	0	0	0	0	0	0	0
52.3770	8.0700	6.3240	H	0	0	0	0	0	0	0	0	0	0	0	0
53.7880	9.6840	6.1370	C	0	0	0	0	0	0	0	0	0	0	0	0
53.7690	10.2480	5.1970	H	0	0	0	0	0	0	0	0	0	0	0	0
54.4020	8.7980	5.9410	H	0	0	0	0	0	0	0	0	0	0	0	0
51.3850	10.7310	5.0020	O	0	0	0	0	0	0	0	0	0	0	0	0
36.7740	9.5110	4.8460	C	0	0	0	0	0	0	0	0	0	0	0	0
36.0980	10.2540	4.4030	H	0	0	0	0	0	0	0	0	0	0	0	0
36.6500	9.6060	5.9310	H	0	0	0	0	0	0	0	0	0	0	0	0
34.2040	6.3710	3.6120	C	0	0	0	0	0	0	0	0	0	0	0	0
33.4890	7.0790	3.1750	H	0	0	0	0	0	0	0	0	0	0	0	0
34.2440	6.6700	4.6690	H	0	0	0	0	0	0	0	0	0	0	0	0
35.5730	6.5760	2.9690	C	0	0	0	0	0	0	0	0	0	0	0	0
36.3350	5.9060	3.3810	H	0	0	0	0	0	0	0	0	0	0	0	0
35.5390	6.4000	1.8880	H	0	0	0	0	0	0	0	0	0	0	0	0
36.0240	7.9950	3.1850	C	0	0	0	0	0	0	0	0	0	0	0	0
36.3800	8.1790	4.4870	O	0	0	0	0	0	0	0	0	0	0	0	0
36.0590	8.8490	2.3100	O	0	0	0	0	0	0	0	0	0	0	0	0
38.2250	9.7820	4.4690	C	0	0	0	0	0	0	0	0	0	0	0	0
38.8700	9.0290	4.9350	H	0	0	0	0	0	0	0	0	0	0	0	0
38.3560	9.7100	3.3830	H	0	0	0	0	0	0	0	0	0	0	0	0
38.5750	11.0860	4.9240	O	0	0	0	0	0	0	0	0	0	0	0	0
39.8500	11.5290	4.4600	C	0	0	0	0	0	0	0	0	0	0	0	0
39.9360	11.3710	3.3780	H	0	0	0	0	0	0	0	0	0	0	0	0
39.8840	12.6100	4.6310	H	0	0	0	0	0	0	0	0	0	0	0	0
40.9990	10.8620	5.2170	C	0	0	0	0	0	0	0	0	0	0	0	0
40.8350	10.9720	6.2960	H	0	0	0	0	0	0	0	0	0	0	0	0
41.0030	9.7850	5.0180	H	0	0	0	0	0	0	0	0	0	0	0	0
42.3510	11.4600	4.8230	C	0	0	0	0	0	0	0	0	0	0	0	0
42.5000	11.3480	3.7420	H	0	0	0	0	0	0	0	0	0	0	0	0
42.3530	12.5350	5.0390	H	0	0	0	0	0	0	0	0	0	0	0	0
43.5060	10.7870	5.5700	C	0	0	0	0	0	0	0	0	0	0	0	0
43.3530	10.8880	6.6510	H	0	0	0	0	0	0	0	0	0	0	0	0
43.5150	9.7140	5.3430	H	0	0	0	0	0	0	0	0	0	0	0	0
44.8510	11.4030	5.1850	C	0	0	0	0	0	0	0	0	0	0	0	0
45.0110	11.3180	4.1020	H	0	0	0	0	0	0	0	0	0	0	0	0
44.8500	12.4790	5.4030	H	0	0	0	0	0	0	0	0	0	0	0	0
46.0160	10.7430	5.9170	C	0	0	0	0	0	0	0	0	0	0	0	0
45.8860	10.8460	7.0010	H	0	0	0	0	0	0	0	0	0	0	0	0
46.0650	9.6790	5.6630	H	0	0	0	0	0	0	0	0	0	0	0	0
47.2190	11.3990	5.5190	O	0	0	0	0	0	0	0	0	0	0	0	0
48.3840	10.8790	6.1550	C	0	0	0	0	0	0	0	0	0	0	0	0
48.1930	10.6520	7.2100	H	0	0	0	0	0	0	0	0	0	0	0	0
49.1350	11.6760	6.1500	H	0	0	0	0	0	0	0	0	0	0	0	0
54.1090	17.2700	7.8690	O	0	0	0	0	0	0	0	0	0	0	0	0
53.7090	18.1180	8.1340	H	0	0	0	0	0	0	0	0	0	0	0	0
53.4030	16.2420	8.5530	C	0	0	0	0	0	0	0	0	0	0	0	0
53.4690	16.4350	9.6280	H	0	0	0	0	0	0	0	0	0	0	0	0
52.3520	16.2790	8.2480	H	0	0	0	0	0	0	0	0	0	0	0	0
54.0210	14.8920	8.2050	C	0	0	0	0	0	0	0	0	0	0	0	0
53.9570	14.7370	7.1220	H	0	0	0	0	0	0	0	0	0	0	0	0
55.0920	14.9150	8.4430	H	0	0	0	0	0	0	0	0	0	0	0	0
53.3370	13.7500	8.9580	C	0	0	0	0	0	0	0	0	0	0	0	0

53.3550	13.9750	10.0320	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.2810	13.6870	8.6670	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.0200	12.3930	8.7490	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.0870	12.4960	8.9710	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.6150	11.6910	9.4910	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.7890	11.8040	7.3470	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.7040	11.7160	7.2250	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.1360	12.4860	6.5620	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.4350	10.4780	7.2100	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4540	22.2160	3.8790	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.7850	22.7120	4.8000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.6880	21.4960	4.1840	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8200	23.1510	2.9890	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4510	24.3480	2.8110	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.6590	25.2020	1.8500	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.0950	24.5640	1.1600	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.9250	25.7460	2.4580	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.5070	26.2120	1.0640	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.3490	26.5980	1.6520	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8420	27.0680	0.8850	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.4800	24.6900	3.3740	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8730	10.1880	5.5810	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.5270	9.5020	6.1340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0430	9.9730	4.5200	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.8820	10.6420	6.9320	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.0420	10.9270	5.8840	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.2960	11.4670	7.5250	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.6910	9.3930	7.2880	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.4980	9.1010	8.3280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.4430	8.5320	6.6590	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.1700	9.6580	7.1520	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.4880	9.9200	5.8530	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.9650	9.6220	8.0810	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.2150	11.6450	5.8730	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5210	12.2940	5.3290	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.1000	11.8530	6.9430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5570	11.8960	5.4630	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.0250	13.1990	5.8180	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.8170	13.4010	6.8750	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1150	13.1800	5.7020	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.4400	14.2860	4.9150	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5970	14.0080	3.8660	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.3550	14.3430	5.0550	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.0620	15.6540	5.2000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.9120	15.9130	6.2560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1440	15.6080	5.0280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.4470	16.7410	4.3150	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5830	16.4740	3.2600	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.3670	16.7940	4.4980	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.0770	18.1080	4.5800	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.9590	18.3850	5.6350	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1580	18.0690	4.3990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.4570	19.1920	3.7030	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5830	18.9320	2.6450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.3880	19.2880	3.9210	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.1220	20.4290	3.9670	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.6110	21.5040	3.1830	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.3180	21.1620	2.1840	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.4330	22.2110	3.0320	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.7870	18.6060	-0.9930	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.4760	17.9450	-0.8030	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.3180	19.8790	-0.6560	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.6500	19.8510	0.3870	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.1790	20.0820	-1.3000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.2310	20.9260	-0.8500	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.8970	20.9170	-1.8950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.3520	20.6470	-0.2540	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.7160	22.3190	-0.4610	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1020	22.3030	0.5650	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.5490	22.6130	-1.1120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5890	23.3490	-0.5680	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.2360	23.3930	-1.6060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.7420	23.0240	0.0470	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.0640	24.7330	-0.1170	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.4440	24.6800	0.9090	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.9370	25.0210	-0.7170	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9610	25.7030	-0.2510	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.6500	31.6320	-9.4490	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.3650	32.2240	-8.5700	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.0860	30.7080	-9.0560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.4990	31.2520	-10.2210	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

48.5280	32.2000	-10.3530	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.3890	31.6340	-11.1680	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7780	31.3420	-12.1500	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.0040	30.7460	-10.6560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2640	32.6370	-11.3500	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8520	32.9460	-10.3840	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4550	32.1990	-11.9430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.6170	33.5360	-11.8660	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.5750	33.3300	-9.8900	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.6560	28.2910	-5.7550	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.5770	28.8530	-5.5550	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.7980	27.8200	-6.7340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.3330	26.8240	-1.1400	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.5570	27.5990	-1.0950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.2630	27.2980	-0.7990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.4460	26.3860	-2.6060	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.2540	25.6630	-2.7540	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4990	25.9300	-2.9200	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.7240	27.5700	-3.4970	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.4690	27.2400	-4.7950	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.1240	28.6590	-3.1100	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4380	29.2060	-5.7940	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5450	28.6120	-6.0140	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.2890	29.6830	-4.8190	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.6390	30.1980	-6.7960	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5880	31.1630	-6.8540	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.3170	31.4970	-5.8450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.9910	32.0320	-7.3850	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3740	30.6280	-7.6140	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.6970	30.2570	-8.5950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.9530	29.7640	-7.0880	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.2940	31.6990	-7.7820	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.9790	32.0580	-6.7950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.7100	32.5580	-8.3210	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.0800	31.1570	-8.5420	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.3960	30.8020	-9.5300	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6670	30.2940	-8.0060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.9970	32.2230	-8.7040	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.6740	32.5870	-7.7200	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.4010	33.0980	-9.2290	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.7870	31.6920	-9.4670	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.0890	31.3680	-10.4700	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.3510	30.8410	-8.9330	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.8270	32.7440	-9.5750	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.6640	32.3750	-10.3140	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.9310	31.7900	-11.2030	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.2140	33.3010	-10.6880	H	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
1	3	1	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
3	5	1	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
6	7	1	0	0	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	0	0
6	9	1	0	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	0
9	11	1	0	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	0
12	13	1	0	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	0
12	15	1	0	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	0
15	17	1	0	0	0	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	0	0	0
18	19	1	0	0	0	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	0	0	0
20	21	1	0	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	0
20	23	1	0	0	0	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	0	0	0
23	24	1	0	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	0
24	31	2	0	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	0
25	27	1	0	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	0
28	29	1	0	0	0	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	0	0	0
28	87	1	0	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	0
32	34	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

32	42	1	0	0	0	0
32	44	1	0	0	0	0
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
38	41	1	0	0	0	0
41	42	1	0	0	0	0
41	43	2	0	0	0	0
44	45	1	0	0	0	0
44	46	1	0	0	0	0
44	47	1	0	0	0	0
47	48	1	0	0	0	0
48	49	1	0	0	0	0
48	50	1	0	0	0	0
48	51	1	0	0	0	0
51	52	1	0	0	0	0
51	53	1	0	0	0	0
51	54	1	0	0	0	0
54	55	1	0	0	0	0
54	56	1	0	0	0	0
54	57	1	0	0	0	0
57	58	1	0	0	0	0
57	59	1	0	0	0	0
57	60	1	0	0	0	0
60	61	1	0	0	0	0
60	62	1	0	0	0	0
60	63	1	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
67	68	1	0	0	0	0
67	69	1	0	0	0	0
70	71	1	0	0	0	0
70	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
75	76	1	0	0	0	0
75	77	1	0	0	0	0
75	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	84	1	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	103	1	0	0	0	0
88	89	1	0	0	0	0
88	90	1	0	0	0	0
88	91	1	0	0	0	0
88	135	1	0	0	0	0
91	92	1	0	0	0	0
92	93	1	0	0	0	0
92	99	2	0	0	0	0
93	94	1	0	0	0	0
93	95	1	0	0	0	0
93	96	1	0	0	0	0
96	97	1	0	0	0	0
96	98	1	0	0	0	0
96	155	1	0	0	0	0
100	101	1	0	0	0	0
100	102	1	0	0	0	0
100	110	1	0	0	0	0
100	112	1	0	0	0	0
103	104	1	0	0	0	0
103	105	1	0	0	0	0
103	106	1	0	0	0	0
106	107	1	0	0	0	0
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106	109	1	0	0	0	0
109	110	1	0	0	0	0
109	111	2	0	0	0	0
112	113	1	0	0	0	0
112	114	1	0	0	0	0
112	115	1	0	0	0	0

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125127	1	0	0	0	0
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128131	1	0	0	0	0
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161164	1	0	0	0	0
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180183	1	0	0	0	0
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211214	1	0	0	0	0
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214217	1	0	0	0	0
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236248	1	0	0	0	0
239240	1	0	0	0	0
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271273	1	0	0	0	0
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274276	1	0	0	0	0
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276278	1	0	0	0	0

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292295 1 0 0 0 0
292340 1 0 0 0 0
295296 1 0 0 0 0
296297 1 0 0 0 0
296304 2 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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311313 1 0 0 0 0
311314 1 0 0 0 0
314315 1 0 0 0 0
314316 2 0 0 0 0
317318 1 0 0 0 0
317319 1 0 0 0 0
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327329 1 0 0 0 0
327330 1 0 0 0 0
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330332 1 0 0 0 0
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333334 1 0 0 0 0
333335 1 0 0 0 0
333336 1 0 0 0 0
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339340 1 0 0 0 0
340341 1 0 0 0 0
340342 1 0 0 0 0

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```

M END
> <NAME>
U32_1

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$$$$
U36_1
MOE2012 3D

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```

357356 0 0 1 0 0 0 0 0999 V2000
19.7990 14.0460 -5.4030 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.0780 14.9660 -5.5470 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.9830 13.2670 -5.2900 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.5620 13.3790 -6.2120 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21.5710 13.6510 -4.4510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20.6010 11.8100 -5.0640 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.9750 11.7350 -4.1650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19.9740 11.4650 -5.8950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```

21.8340	10.9190	-4.9250	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22.4440	10.9930	-5.8340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22.4520	11.2770	-4.0920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21.4480	9.4580	-4.6850	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20.8290	9.3860	-3.7820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20.8410	9.0950	-5.5230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22.6890	8.5730	-4.5260	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23.2980	8.6310	-5.4360	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23.2960	8.9640	-3.7020	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22.3000	7.1150	-4.2570	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21.7000	7.0370	-3.3410	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21.6580	6.7710	-5.0770	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23.4510	6.2070	-4.1920	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0
23.1010	5.2480	-4.2000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37.8150	10.0230	-6.0140	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37.0130	10.6600	-6.4060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37.4390	8.9960	-6.0810	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.9900	10.0840	-6.8370	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.2700	11.3080	-7.3700	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.4710	11.2250	-8.2760	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.9380	10.2380	-8.1920	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.1060	11.3120	-9.3060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.4660	12.3470	-7.9770	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.9240	13.2990	-8.0450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.2380	12.3760	-8.7570	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.6200	12.3270	-7.1800	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28.4280	5.1420	-0.8850	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27.9640	5.1400	0.1100	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29.1000	4.2770	-0.9030	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24.2600	6.4120	-2.9890	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24.7020	7.4140	-2.9880	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23.6370	6.3200	-2.0900	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25.3830	5.3790	-2.9410	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24.9780	4.3640	-2.8550	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25.9850	5.4480	-3.8550	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26.2810	5.6340	-1.7590	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27.4510	4.9510	-1.9190	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26.0010	6.3400	-0.8010	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29.2240	6.4190	-1.1310	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29.7080	6.3630	-2.1120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28.5560	7.2880	-1.1420	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30.1910	6.5700	-0.0960	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31.0170	7.7230	-0.2710	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30.4300	8.5650	-0.6580	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31.3780	8.0080	0.7230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32.2130	7.4070	-1.1690	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32.7870	6.5830	-0.7270	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31.8670	7.0420	-2.1430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33.1090	8.6300	-1.3680	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32.5220	9.4370	-1.8240	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33.4590	8.9960	-0.3950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34.3150	8.3090	-2.2570	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34.9410	7.5530	-1.7680	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33.9670	7.8790	-3.2040	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35.1450	9.5600	-2.5430	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34.5180	10.3230	-3.0240	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35.4950	10.0090	-1.6050	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.3460	9.2620	-3.4380	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37.0540	8.6070	-2.9180	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.0080	8.7710	-4.3560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.9770	10.5020	-3.7540	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.1450	10.3690	-4.5640	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.8320	9.6330	-4.1310	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.6710	11.3300	-4.5270	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8380	17.5890	-0.8400	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.1360	17.5640	0.0850	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.2960	16.3080	-1.1360	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.0770	15.5570	-0.9820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.4710	16.1110	-0.4430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.8060	16.2940	-2.5790	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.0570	17.0840	-2.7170	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.6380	16.5500	-3.2460	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2200	14.9360	-2.9610	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.9790	14.1570	-2.8150	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.3820	14.6970	-2.2950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.7400	14.9150	-4.4150	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.9690	15.6820	-4.5580	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.5750	15.1650	-5.0810	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1780	13.5400	-4.7930	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9530	12.7880	-4.6150	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.3320	13.3000	-4.1360	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0

42.7180	13.5030	-6.2590	C	0	0	0	0	0	0	0	0	0	0	0
41.9860	14.3110	-6.3860	H	0	0	0	0	0	0	0	0	0	0	0
43.5610	13.7310	-6.9230	H	0	0	0	0	0	0	0	0	0	0	0
42.0880	12.2230	-6.6430	N	0	0	3	0	0	0	0	0	0	0	0
40.7360	2.7650	3.6530	C	0	0	0	0	0	0	0	0	0	0	0
40.4920	1.7800	3.2380	H	0	0	0	0	0	0	0	0	0	0	0
40.8330	3.4740	2.8230	H	0	0	0	0	0	0	0	0	0	0	0
39.6890	3.1960	4.5330	O	0	0	0	0	0	0	0	0	0	0	0
38.4850	3.3920	3.9230	C	0	0	0	0	0	0	0	0	0	0	0
37.4670	3.8950	4.9140	C	0	0	0	0	0	0	0	0	0	0	0
37.8980	3.9300	5.9190	H	0	0	0	0	0	0	0	0	0	0	0
37.2440	4.9340	4.6420	H	0	0	0	0	0	0	0	0	0	0	0
36.1870	3.0600	4.8710	C	0	0	0	0	0	0	0	0	0	0	0
35.8340	3.0500	3.8310	H	0	0	0	0	0	0	0	0	0	0	0
35.4080	3.5660	5.4560	H	0	0	0	0	0	0	0	0	0	0	0
38.2660	3.2330	2.7290	O	0	0	0	0	0	0	0	0	0	0	0
44.1910	7.1110	-4.0920	C	0	0	0	0	0	0	0	0	0	0	0
45.1780	7.1950	-4.5630	H	0	0	0	0	0	0	0	0	0	0	0
44.3880	6.9600	-3.0260	H	0	0	0	0	0	0	0	0	0	0	0
43.0400	11.0990	-6.5880	C	0	0	0	0	0	0	0	0	0	0	0
43.0340	10.5210	-7.5210	H	0	0	0	0	0	0	0	0	0	0	0
44.0790	11.4410	-6.4900	H	0	0	0	0	0	0	0	0	0	0	0
42.6720	10.1780	-5.4270	C	0	0	0	0	0	0	0	0	0	0	0
42.7700	10.7060	-4.4730	H	0	0	0	0	0	0	0	0	0	0	0
41.6410	9.8200	-5.5280	H	0	0	0	0	0	0	0	0	0	0	0
43.5750	8.9760	-5.4060	C	0	0	0	0	0	0	0	0	0	0	0
43.4390	8.3260	-4.2150	O	0	0	0	0	0	0	0	0	0	0	0
44.2910	8.6190	-6.3300	O	0	0	0	0	0	0	0	0	0	0	0
43.3960	5.9420	-4.6650	C	0	0	0	0	0	0	0	0	0	0	0
42.4210	5.8500	-4.1720	H	0	0	0	0	0	0	0	0	0	0	0
43.1830	6.1270	-5.7230	H	0	0	0	0	0	0	0	0	0	0	0
44.1610	4.7440	-4.5920	O	0	0	0	0	0	0	0	0	0	0	0
43.6860	3.7960	-3.6360	C	0	0	0	0	0	0	0	0	0	0	0
42.6220	3.5940	-3.8070	H	0	0	0	0	0	0	0	0	0	0	0
44.2270	2.8620	-3.8260	H	0	0	0	0	0	0	0	0	0	0	0
43.9490	4.2510	-2.2030	C	0	0	0	0	0	0	0	0	0	0	0
45.0070	4.5190	-2.0960	H	0	0	0	0	0	0	0	0	0	0	0
43.3800	5.1650	-1.9960	H	0	0	0	0	0	0	0	0	0	0	0
43.5660	3.1840	-1.1800	C	0	0	0	0	0	0	0	0	0	0	0
42.5060	2.9290	-1.2960	H	0	0	0	0	0	0	0	0	0	0	0
44.1430	2.2700	-1.3600	H	0	0	0	0	0	0	0	0	0	0	0
43.8240	3.6840	0.2430	C	0	0	0	0	0	0	0	0	0	0	0
44.8920	3.9010	0.3680	H	0	0	0	0	0	0	0	0	0	0	0
43.2830	4.6260	0.4020	H	0	0	0	0	0	0	0	0	0	0	0
43.3810	2.6650	1.2880	C	0	0	0	0	0	0	0	0	0	0	0
42.3190	2.4270	1.1550	H	0	0	0	0	0	0	0	0	0	0	0
43.9190	1.7190	1.1530	H	0	0	0	0	0	0	0	0	0	0	0
43.6200	3.1850	2.7030	C	0	0	0	0	0	0	0	0	0	0	0
44.6950	3.2970	2.8790	H	0	0	0	0	0	0	0	0	0	0	0
43.1580	4.1690	2.8490	H	0	0	0	0	0	0	0	0	0	0	0
43.1340	2.2250	3.6420	O	0	0	0	0	0	0	0	0	0	0	0
42.0430	2.6870	4.4360	C	0	0	0	0	0	0	0	0	0	0	0
42.2880	3.6490	4.9020	H	0	0	0	0	0	0	0	0	0	0	0
41.9190	1.9780	5.2640	H	0	0	0	0	0	0	0	0	0	0	0
28.2100	-1.3770	4.2980	O	0	0	0	0	0	0	0	0	0	0	0
27.2950	-1.0830	4.4480	H	0	0	0	0	0	0	0	0	0	0	0
29.0580	-0.3530	4.8010	C	0	0	0	0	0	0	0	0	0	0	0
28.7600	0.6000	4.3510	H	0	0	0	0	0	0	0	0	0	0	0
28.9210	-0.2920	5.8850	H	0	0	0	0	0	0	0	0	0	0	0
30.5020	-0.6850	4.4500	C	0	0	0	0	0	0	0	0	0	0	0
30.7510	-1.6830	4.8320	H	0	0	0	0	0	0	0	0	0	0	0
30.6040	-0.7480	3.3590	H	0	0	0	0	0	0	0	0	0	0	0
31.4720	0.3520	5.0150	C	0	0	0	0	0	0	0	0	0	0	0
31.1950	1.3500	4.6540	H	0	0	0	0	0	0	0	0	0	0	0
31.3880	0.3700	6.1090	H	0	0	0	0	0	0	0	0	0	0	0
32.9180	0.0490	4.6140	C	0	0	0	0	0	0	0	0	0	0	0
33.1850	-0.9650	4.9360	H	0	0	0	0	0	0	0	0	0	0	0
33.0070	0.0770	3.5220	H	0	0	0	0	0	0	0	0	0	0	0
33.8910	1.0550	5.2390	C	0	0	0	0	0	0	0	0	0	0	0
33.5930	2.0690	4.9480	H	0	0	0	0	0	0	0	0	0	0	0
33.8080	0.9900	6.3290	H	0	0	0	0	0	0	0	0	0	0	0
35.3360	0.7810	4.7940	C	0	0	0	0	0	0	0	0	0	0	0
35.5970	-0.2600	5.0200	H	0	0	0	0	0	0	0	0	0	0	0
35.3860	0.8340	3.6970	H	0	0	0	0	0	0	0	0	0	0	0
36.3740	1.6750	5.3480	N	0	0	3	0	0	0	0	0	0	0	0
49.4590	0.3650	9.7330	C	0	0	0	0	0	0	0	0	0	0	0
49.7230	1.3530	9.3370	H	0	0	0	0	0	0	0	0	0	0	0
48.5830	0.0380	9.1650	H	0	0	0	0	0	0	0	0	0	0	0
50.4990	-0.5970	9.4860	O	0	0	0	0	0	0	0	0	0	0	0
51.7820	-0.1590	9.6410	C	0	0	0	0	0	0	0	0	0	0	0
52.7460	-1.2770	9.3240	C	0	0	0	0	0	0	0	0	0	0	0

52.2660	-2.2500	9.4770	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.9600	-1.1960	8.2500	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.0620	-1.1940	10.1080	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.3400	-0.1600	10.3470	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.8310	-1.5650	9.4180	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.1060	0.9800	9.9470	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.8270	0.3530	10.4350	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.1320	-0.1760	11.1000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.7850	-0.1690	10.5350	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.4890	1.6110	6.8170	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37.3020	2.2710	7.1430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35.5830	1.9970	7.3020	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.8100	0.2150	7.3490	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35.9780	-0.4850	7.2160	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37.6780	-0.2150	6.8370	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37.0870	0.3060	8.8250	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.4270	0.2450	9.0610	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.2180	0.4560	9.6720	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.9760	1.8160	10.8360	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.6290	2.3500	10.1340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.0020	2.3130	10.7840	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.4300	1.9040	12.1840	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.7320	2.4750	12.3280	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.7790	3.4350	11.8010	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.8680	2.6850	13.3950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.8260	1.5180	11.8570	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.7170	0.5600	12.3800	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.6940	1.2960	10.7910	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.2240	2.0910	12.0830	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.3210	3.0440	11.5480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.3710	2.3000	13.1490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.3000	1.1170	11.5980	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2140	0.1730	12.1500	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.1370	0.8860	10.5380	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.7040	1.6900	11.7810	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8080	2.6290	11.2230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8770	1.9440	12.8340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.7740	0.7050	11.3180	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.7090	-0.2180	11.9040	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.6320	0.4670	10.2590	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.0530	1.3090	11.5110	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.1380	0.4300	11.2240	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.9490	-0.5710	11.6300	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0120	0.8120	11.7630	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.8090	-2.5330	16.0630	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.0060	-3.0810	16.0980	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.6500	-3.0900	15.0610	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.9030	-4.1150	15.3490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.0950	-3.1120	14.1170	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.9060	-2.2360	14.9290	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48.6180	-1.2030	14.6960	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.4200	-2.1930	15.8970	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.8480	-2.7770	13.8530	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1400	-3.8040	14.1010	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.3190	-2.8160	12.8930	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.1030	-1.9100	13.7110	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.8120	-0.8740	13.5060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.6560	-1.9070	14.6580	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.0110	-2.4200	12.5870	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.3390	-3.4410	12.8220	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.4330	-2.4750	11.6580	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.2350	-1.5150	12.3970	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.9150	-0.4860	12.1930	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.7690	-1.4530	13.3540	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.1000	-2.0440	11.3220	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0
56.2690	-15.2180	16.4810	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.9200	-15.4740	15.4730	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.8860	-14.2120	16.6830	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.7010	-16.0830	17.4770	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.5360	-17.3870	17.1130	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.9170	-18.1560	18.2520	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.9260	-17.5510	19.1650	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.8610	-18.2970	17.9910	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.5680	-19.5220	18.4910	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6360	-20.0770	17.5490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.8570	-20.1130	19.0860	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.8250	-17.8630	16.0250	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.5890	-5.2130	14.0240	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.1720	-4.3770	14.4280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.5280	-5.9510	14.8310	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.4980	-2.2050	11.7790	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0

56.1380	-2.4300	10.9150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.8790	-1.2700	12.2100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6570	-3.3660	12.7670	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.1430	-3.1660	13.7120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.2430	-4.2790	12.3220	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.1140	-3.6140	13.0770	C	0	0	0	0	0	0	0	0	0	0	0	0	0
57.2460	-4.8120	13.7150	O	0	0	0	0	0	0	0	0	0	0	0	0	0
58.0330	-2.8560	12.7990	O	0	0	0	0	0	0	0	0	0	0	0	0	0
59.2600	-5.8220	12.7980	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.6000	-6.5550	12.3170	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.4450	-5.0440	12.0500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.5210	-6.3750	13.1620	O	0	0	0	0	0	0	0	0	0	0	0	0	0
60.6030	-7.7890	12.9780	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.2790	-8.0550	11.9650	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.6630	-8.0570	13.0590	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8080	-8.5420	14.0450	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.1610	-8.2380	15.0380	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.7520	-8.2520	13.9990	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.9230	-10.0570	13.8810	C	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5620	-10.3460	12.8870	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9750	-10.3590	13.9460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.1120	-10.7880	14.9540	C	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5020	-10.5310	15.9460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.0690	-10.4490	14.9200	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.1570	-12.3030	14.7610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.7650	-12.5700	13.7710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.1950	-12.6580	14.7790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3550	-13.0300	15.8350	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.7840	-12.8320	16.8240	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.3150	-12.6870	15.8200	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.4050	-14.4290	15.5590	O	0	0	0	0	0	0	0	0	0	0	0	0	0
57.7920	-15.2340	16.5630	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.1380	-14.9410	17.5620	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.1490	-16.2570	16.4110	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.3400	-19.7960	12.4070	O	0	0	0	0	0	0	0	0	0	0	0	0	0
62.5000	-20.3310	11.6100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.2500	-20.3930	13.0970	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.3710	-20.3650	12.4460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5020	-21.4370	13.3100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9980	-19.6230	14.3870	C	0	0	0	0	0	0	0	0	0	0	0	0	0
61.9040	-19.6430	15.0060	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.8210	-18.5660	14.1490	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8130	-20.1940	15.1640	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.9180	-20.1690	14.5300	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.0040	-21.2450	15.4110	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5520	-19.4050	16.4490	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4280	-19.4680	17.1060	H	0	0	0	0	0	0	0	0	0	0	0	0	0
59.4080	-18.3460	16.2030	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3140	-19.9300	17.1860	C	0	0	0	0	0	0	0	0	0	0	0	0	0
57.4700	-19.9130	16.4900	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.4750	-20.9760	17.4740	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.0110	-19.0910	18.4380	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.9110	-19.1340	19.0610	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.8870	-18.0370	18.1680	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.8550	-19.5730	19.2130	N	0	0	3	0	0	0	0	0	0	0	0	0	0
67.8470	-14.8620	26.9870	C	0	0	0	0	0	0	0	0	0	0	0	0	0
67.3760	-13.8850	27.1500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
67.0830	-15.4880	26.5150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.9350	-14.7710	26.0540	O	0	0	0	0	0	0	0	0	0	0	0	0	0
69.7320	-13.6700	26.1690	C	0	0	0	0	0	0	0	0	0	0	0	0	0
70.8050	-13.7210	25.1090	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.3860	-14.6390	25.2470	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.3210	-13.7460	24.1270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
71.7360	-12.5220	25.1810	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.1840	-11.5870	25.0420	H	0	0	0	0	0	0	0	0	0	0	0	0	0
72.5010	-12.5870	24.4010	H	0	0	0	0	0	0	0	0	0	0	0	0	0
72.2390	-12.4730	26.1520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.5990	-12.7860	27.0030	O	0	0	0	0	0	0	0	0	0	0	0	0	0
58.2080	-19.1400	25.1650	C	0	0	0	0	0	0	0	0	0	0	0	0	0
57.2110	-18.7510	25.4070	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3640	-19.9970	25.8310	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.7700	-18.9290	20.5360	C	0	0	0	0	0	0	0	0	0	0	0	0	0
56.8980	-17.8420	20.4500	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.7700	-19.0900	20.9630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.7780	-19.5150	21.5270	C	0	0	0	0	0	0	0	0	0	0	0	0	0
57.6120	-20.5940	21.6210	H	0	0	0	0	0	0	0	0	0	0	0	0	0
58.8100	-19.3390	21.2100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
57.6110	-18.8820	22.8840	C	0	0	0	0	0	0	0	0	0	0	0	0	0
58.2680	-19.6280	23.8160	O	0	0	0	0	0	0	0	0	0	0	0	0	0
57.0070	-17.8420	23.1070	O	0	0	0	0	0	0	0	0	0	0	0	0	0
59.2910	-18.0960	25.4090	C	0	0	0	0	0	0	0	0	0	0	0	0	0

60.2720	-18.5290	25.1860	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.1470	-17.2380	24.7430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.2230	-17.6700	26.7670	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.2070	-16.6910	27.0980	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.3260	-15.9680	26.2820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8260	-16.1430	27.9660	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5340	-17.3540	27.4630	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.3640	-18.0890	28.2600	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.9170	-17.9220	26.6080	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.5720	-16.3240	27.9050	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.7290	-15.5960	27.0990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.1970	-15.7700	28.7740	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.9030	-16.9910	28.2580	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.7550	-17.6990	29.0820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.2620	-17.5680	27.3970	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.9550	-15.9560	28.6510	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.0780	-15.2220	27.8470	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.6190	-15.3840	29.5250	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.2990	-16.6090	28.9640	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.2030	-17.2360	29.8570	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.6290	-17.2550	28.1430	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.2560	-15.5920	29.2600	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.3080	-15.4850	28.3020	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.7750	-16.4640	28.1350	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69.0860	-14.8580	28.7500	H	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
1	3	1	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
3	5	1	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
6	7	1	0	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	0
6	9	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
15	18	1	0	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	0
18	20	1	0	0	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	0	0
21	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	38	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	25	1	0	0	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	0	0
23	70	1	0	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	0
27	28	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	34	2	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	30	1	0	0	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	0	0
31	32	1	0	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	0
31	93	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	36	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	37	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	45	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	47	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	39	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	40	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	41	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	42	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	43	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	44	1	0	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	0
44	46	2	0	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	0
47	49	1	0	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	0
50	51	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	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51	54	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54	55	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54	56	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

54	57	1	0	0	0	0
57	58	1	0	0	0	0
57	59	1	0	0	0	0
57	60	1	0	0	0	0
60	61	1	0	0	0	0
60	62	1	0	0	0	0
60	63	1	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	69	1	0	0	0	0
69	70	1	0	0	0	0
70	71	1	0	0	0	0
70	72	1	0	0	0	0
73	74	1	0	0	0	0
73	75	1	0	0	0	0
75	76	1	0	0	0	0
75	77	1	0	0	0	0
75	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	84	1	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
87	89	1	0	0	0	0
87	90	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
93	109	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
94	141	1	0	0	0	0
97	98	1	0	0	0	0
98	99	1	0	0	0	0
98	105	2	0	0	0	0
99	100	1	0	0	0	0
99	101	1	0	0	0	0
99	102	1	0	0	0	0
102	103	1	0	0	0	0
102	104	1	0	0	0	0
102	164	1	0	0	0	0
106	107	1	0	0	0	0
106	108	1	0	0	0	0
106	116	1	0	0	0	0
106	118	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
112	114	1	0	0	0	0
112	115	1	0	0	0	0
115	116	1	0	0	0	0
115	117	2	0	0	0	0
118	119	1	0	0	0	0
118	120	1	0	0	0	0
118	121	1	0	0	0	0
121	122	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
125	127	1	0	0	0	0
125	128	1	0	0	0	0
128	129	1	0	0	0	0
128	130	1	0	0	0	0
128	131	1	0	0	0	0
131	132	1	0	0	0	0
131	133	1	0	0	0	0
131	134	1	0	0	0	0
134	135	1	0	0	0	0
134	136	1	0	0	0	0
134	137	1	0	0	0	0

137138	1	0	0	0	0
137139	1	0	0	0	0
137140	1	0	0	0	0
140141	1	0	0	0	0
141142	1	0	0	0	0
141143	1	0	0	0	0
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146147	1	0	0	0	0
146148	1	0	0	0	0
146149	1	0	0	0	0
149150	1	0	0	0	0
149151	1	0	0	0	0
149152	1	0	0	0	0
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152154	1	0	0	0	0
152155	1	0	0	0	0
155156	1	0	0	0	0
155157	1	0	0	0	0
155158	1	0	0	0	0
158159	1	0	0	0	0
158160	1	0	0	0	0
158161	1	0	0	0	0
161162	1	0	0	0	0
161163	1	0	0	0	0
161164	1	0	0	0	0
164180	1	0	0	0	0
165166	1	0	0	0	0
165167	1	0	0	0	0
165168	1	0	0	0	0
165212	1	0	0	0	0
168169	1	0	0	0	0
169170	1	0	0	0	0
169176	2	0	0	0	0
170171	1	0	0	0	0
170172	1	0	0	0	0
170173	1	0	0	0	0
173174	1	0	0	0	0
173175	1	0	0	0	0
173235	1	0	0	0	0
177178	1	0	0	0	0
177179	1	0	0	0	0
177187	1	0	0	0	0
177189	1	0	0	0	0
180181	1	0	0	0	0
180182	1	0	0	0	0
180183	1	0	0	0	0
183184	1	0	0	0	0
183185	1	0	0	0	0
183186	1	0	0	0	0
186187	1	0	0	0	0
186188	2	0	0	0	0
189190	1	0	0	0	0
189191	1	0	0	0	0
189192	1	0	0	0	0
192193	1	0	0	0	0
193194	1	0	0	0	0
193195	1	0	0	0	0
193196	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
199202	1	0	0	0	0
202203	1	0	0	0	0
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
208211	1	0	0	0	0
211212	1	0	0	0	0
212213	1	0	0	0	0
212214	1	0	0	0	0
215216	1	0	0	0	0
215217	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
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
232234	1	0	0	0	0
232235	1	0	0	0	0
235251	1	0	0	0	0
236237	1	0	0	0	0
236238	1	0	0	0	0
236239	1	0	0	0	0
236283	1	0	0	0	0
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
244306	1	0	0	0	0
248249	1	0	0	0	0
248250	1	0	0	0	0
248258	1	0	0	0	0
248260	1	0	0	0	0
251252	1	0	0	0	0
251253	1	0	0	0	0
251254	1	0	0	0	0
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254256	1	0	0	0	0
254257	1	0	0	0	0
257258	1	0	0	0	0
257259	2	0	0	0	0
260261	1	0	0	0	0
260262	1	0	0	0	0
260263	1	0	0	0	0
263264	1	0	0	0	0
264265	1	0	0	0	0
264266	1	0	0	0	0
264267	1	0	0	0	0
267268	1	0	0	0	0
267269	1	0	0	0	0
267270	1	0	0	0	0
270271	1	0	0	0	0
270272	1	0	0	0	0
270273	1	0	0	0	0
273274	1	0	0	0	0
273275	1	0	0	0	0
273276	1	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
279282	1	0	0	0	0
282283	1	0	0	0	0
283284	1	0	0	0	0
283285	1	0	0	0	0
286287	1	0	0	0	0
286288	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
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

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300301 1 0 0 0 0
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311319 2 0 0 0 0
312313 1 0 0 0 0
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312315 1 0 0 0 0
315316 1 0 0 0 0
315317 1 0 0 0 0
315318 1 0 0 0 0
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320330 1 0 0 0 0
320332 1 0 0 0 0
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323325 1 0 0 0 0
323326 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 2 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
336337 1 0 0 0 0
336338 1 0 0 0 0
336339 1 0 0 0 0
339340 1 0 0 0 0
339341 1 0 0 0 0
339342 1 0 0 0 0
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342344 1 0 0 0 0
342345 1 0 0 0 0
345346 1 0 0 0 0
345347 1 0 0 0 0
345348 1 0 0 0 0
348349 1 0 0 0 0
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348351 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
355356 1 0 0 0 0
355357 1 0 0 0 0

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M END
> <NAME>
U36_1

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U75_1
MOE2012 3D

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362361 0 0 1 0 0 0 0 0 0999 V2000
43.4270 9.0650 -26.3390 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.8830 8.8770 -25.3610 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
44.2230 9.2870 -27.0560 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.9420 8.1380 -26.6650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.3980 10.1880 -26.2580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.9630 10.3670 -27.2490 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.5870 9.8170 -25.6170 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.9400 11.4330 -25.6850 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.8370 12.3750 -25.4000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.4510 12.8180 -26.3280 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.0010 11.8300 -24.9400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.2600 13.4680 -24.4000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
42.6210 12.9770 -23.4900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
43.0840 14.0660 -24.8040 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
41.1240 14.3540 -24.0970 N 0 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0

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40.8860	14.8700	-24.9450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9650	12.0420	-26.5520	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.0040	11.5720	-27.5420	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.7600	13.1010	-26.7490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3300	11.9430	-25.8830	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.6240	10.9030	-25.7120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3370	12.4640	-24.9200	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.0930	12.4060	-26.5180	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.8110	7.7500	-11.6690	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8150	7.4160	-11.9580	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2680	7.9080	-12.6060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.1080	6.7250	-10.9480	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.8360	6.0340	-10.0220	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9570	4.9960	-9.3640	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.0110	5.4570	-9.0570	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.7330	4.2460	-10.1320	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.6290	4.2930	-8.1750	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.7180	4.2370	-8.2970	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2590	3.2590	-8.1980	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.0190	6.2210	-9.7750	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.4400	15.7740	-18.3250	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.9570	16.7580	-18.2750	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.1590	15.2590	-17.4010	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.4470	15.3150	-23.0400	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.4410	15.7530	-23.1980	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.7350	16.1470	-23.1120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.3190	14.6900	-21.6540	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.2800	14.4100	-21.4520	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.9490	13.7980	-21.5720	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.7680	15.6610	-20.5950	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.9290	14.9950	-19.4160	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.9680	16.8530	-20.7690	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9560	15.9000	-18.4230	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.4200	14.9210	-18.5960	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2230	16.5180	-19.2870	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.4620	16.5490	-17.2600	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3080	15.7250	-16.4570	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.1010	15.2890	-17.0750	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.7910	16.3860	-15.7290	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.5140	14.6490	-15.7170	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.7000	15.1230	-15.1540	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.0310	13.9790	-16.4380	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3980	13.8290	-14.7780	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2160	13.3730	-15.3480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8510	14.4880	-14.0290	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.5880	12.7330	-14.0800	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.7680	13.1900	-13.5110	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.1320	12.0790	-14.8330	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4580	11.9000	-13.1410	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2900	11.4470	-13.6950	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.9180	12.5430	-12.3800	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.6520	10.8020	-12.4550	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.8340	11.2430	-11.8740	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2310	10.1220	-13.2030	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.5230	10.0860	-11.5810	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.8670	9.0440	-10.8610	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.8660	9.3550	-10.5370	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4410	8.8760	-9.9440	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9150	10.5330	-4.3200	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.4170	10.8300	-5.2490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.9070	10.9940	-4.3000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.3410	10.9490	-3.4860	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9780	9.0130	-4.1980	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.4680	8.7250	-3.2590	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.9400	8.6640	-4.1340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.6410	8.3900	-5.3580	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.3260	6.9410	-5.3910	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.7600	6.4480	-4.5120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.2370	6.8210	-5.3250	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.7760	6.2370	-6.6930	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.3810	6.8450	-7.5140	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.8690	6.2460	-6.7760	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2790	4.8480	-6.8450	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0
46.0940	8.6400	-5.3590	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.3920	9.3390	-4.5680	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.6700	7.7280	-5.1600	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.5170	9.2370	-6.6950	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.9960	10.1810	-6.8890	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.3130	8.5570	-7.5270	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.5920	9.4430	-6.6890	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35.4970	0.3900	5.7430	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0

35.1730	-0.6150	5.4480	H	0	0	0	0	0	0	0	0	0	0	0	0
35.6760	0.9320	4.8090	H	0	0	0	0	0	0	0	0	0	0	0	0
34.4570	1.0930	6.4390	O	0	0	0	0	0	0	0	0	0	0	0	0
33.7410	0.3670	7.3420	C	0	0	0	0	0	0	0	0	0	0	0	0
32.7300	1.2460	8.0300	C	0	0	0	0	0	0	0	0	0	0	0	0
32.7300	2.2390	7.5710	H	0	0	0	0	0	0	0	0	0	0	0	0
31.7380	0.8210	7.8410	H	0	0	0	0	0	0	0	0	0	0	0	0
33.0020	1.3170	9.5310	C	0	0	0	0	0	0	0	0	0	0	0	0
32.8780	0.3030	9.9330	H	0	0	0	0	0	0	0	0	0	0	0	0
32.2240	1.9150	10.0220	H	0	0	0	0	0	0	0	0	0	0	0	0
33.8930	-0.8240	7.5800	O	0	0	0	0	0	0	0	0	0	0	0	0
44.9370	2.6220	-1.4870	C	0	0	0	0	0	0	0	0	0	0	0	0
45.7450	1.9600	-1.8220	H	0	0	0	0	0	0	0	0	0	0	0	0
45.4010	3.3320	-0.7920	H	0	0	0	0	0	0	0	0	0	0	0	0
44.7880	3.9590	-5.7790	C	0	0	0	0	0	0	0	0	0	0	0	0
45.1790	3.0200	-6.1940	H	0	0	0	0	0	0	0	0	0	0	0	0
45.6410	4.4000	-5.2470	H	0	0	0	0	0	0	0	0	0	0	0	0
43.6650	3.6090	-4.8080	C	0	0	0	0	0	0	0	0	0	0	0	0
43.2300	4.5010	-4.3440	H	0	0	0	0	0	0	0	0	0	0	0	0
42.8420	3.0930	-5.3180	H	0	0	0	0	0	0	0	0	0	0	0	0
44.1890	2.6920	-3.7360	C	0	0	0	0	0	0	0	0	0	0	0	0
44.4040	3.3830	-2.5820	O	0	0	0	0	0	0	0	0	0	0	0	0
44.4060	1.4990	-3.8990	O	0	0	0	0	0	0	0	0	0	0	0	0
43.8380	1.8450	-0.7700	C	0	0	0	0	0	0	0	0	0	0	0	0
43.0490	2.5390	-0.4590	H	0	0	0	0	0	0	0	0	0	0	0	0
43.3880	1.1100	-1.4460	H	0	0	0	0	0	0	0	0	0	0	0	0
44.4030	1.1920	0.3630	O	0	0	0	0	0	0	0	0	0	0	0	0
43.4960	0.3060	1.0200	C	0	0	0	0	0	0	0	0	0	0	0	0
43.0280	-0.3660	0.2920	H	0	0	0	0	0	0	0	0	0	0	0	0
44.1000	-0.3150	1.6910	H	0	0	0	0	0	0	0	0	0	0	0	0
42.4470	1.0610	1.8380	C	0	0	0	0	0	0	0	0	0	0	0	0
42.9490	1.7890	2.4880	H	0	0	0	0	0	0	0	0	0	0	0	0
41.8030	1.6440	1.1710	H	0	0	0	0	0	0	0	0	0	0	0	0
41.5870	0.1110	2.6740	C	0	0	0	0	0	0	0	0	0	0	0	0
41.1080	-0.6240	2.0160	H	0	0	0	0	0	0	0	0	0	0	0	0
42.2260	-0.4450	3.3710	H	0	0	0	0	0	0	0	0	0	0	0	0
40.5130	0.8720	3.4560	C	0	0	0	0	0	0	0	0	0	0	0	0
40.9900	1.6200	4.1020	H	0	0	0	0	0	0	0	0	0	0	0	0
39.8670	1.4160	2.7560	H	0	0	0	0	0	0	0	0	0	0	0	0
39.6640	-0.0700	4.3100	C	0	0	0	0	0	0	0	0	0	0	0	0
39.2010	-0.8400	3.6800	H	0	0	0	0	0	0	0	0	0	0	0	0
40.2990	-0.6080	5.0250	H	0	0	0	0	0	0	0	0	0	0	0	0
38.5730	0.6820	5.0680	C	0	0	0	0	0	0	0	0	0	0	0	0
39.0220	1.4380	5.7220	H	0	0	0	0	0	0	0	0	0	0	0	0
37.9000	1.1780	4.3600	H	0	0	0	0	0	0	0	0	0	0	0	0
37.8470	-0.2550	5.8630	O	0	0	0	0	0	0	0	0	0	0	0	0
36.7700	0.3390	6.5850	C	0	0	0	0	0	0	0	0	0	0	0	0
37.0420	1.3340	6.9590	H	0	0	0	0	0	0	0	0	0	0	0	0
36.5930	-0.2800	7.4720	H	0	0	0	0	0	0	0	0	0	0	0	0
34.5660	7.9430	8.6360	C	0	0	0	0	0	0	0	0	0	0	0	0
35.5580	7.9340	9.1000	H	0	0	0	0	0	0	0	0	0	0	0	0
33.8800	8.4840	9.2950	H	0	0	0	0	0	0	0	0	0	0	0	0
34.6390	8.5090	7.7020	H	0	0	0	0	0	0	0	0	0	0	0	0
34.0850	6.5240	8.3460	C	0	0	0	0	0	0	0	0	0	0	0	0
33.0880	6.5530	7.8880	H	0	0	0	0	0	0	0	0	0	0	0	0
34.7690	6.1140	7.5910	H	0	0	0	0	0	0	0	0	0	0	0	0
34.0960	5.6570	9.5370	N	0	0	0	0	0	0	0	0	0	0	0	0
33.8940	4.2480	9.1360	C	0	0	0	0	0	0	0	0	0	0	0	0
32.8520	4.0900	8.8370	H	0	0	0	0	0	0	0	0	0	0	0	0
34.5220	4.0260	8.2620	H	0	0	0	0	0	0	0	0	0	0	0	0
34.3140	3.2630	10.2500	C	0	0	0	0	0	0	0	0	0	0	0	0
35.3130	3.5750	10.5710	H	0	0	0	0	0	0	0	0	0	0	0	0
33.6630	3.3670	11.1280	H	0	0	0	0	0	0	0	0	0	0	0	0
34.3540	1.8450	9.8170	N	0	0	3	0	0	0	0	0	0	0	0	0
33.1080	6.0850	10.5440	C	0	0	0	0	0	0	0	0	0	0	0	0
32.4430	6.8710	10.1650	H	0	0	0	0	0	0	0	0	0	0	0	0
32.4390	5.2680	10.8390	H	0	0	0	0	0	0	0	0	0	0	0	0
33.8290	6.5850	11.7890	C	0	0	0	0	0	0	0	0	0	0	0	0
34.4700	7.4430	11.5680	H	0	0	0	0	0	0	0	0	0	0	0	0
34.4500	5.7980	12.2300	H	0	0	0	0	0	0	0	0	0	0	0	0
33.1000	6.8970	12.5440	H	0	0	0	0	0	0	0	0	0	0	0	0
48.7720	4.1270	10.9990	C	0	0	0	0	0	0	0	0	0	0	0	0
48.4710	5.1610	11.2070	H	0	0	0	0	0	0	0	0	0	0	0	0
47.9430	3.6820	10.4400	H	0	0	0	0	0	0	0	0	0	0	0	0
49.9230	4.0770	10.1380	O	0	0	0	0	0	0	0	0	0	0	0	0
50.8880	5.0090	10.3800	C	0	0	0	0	0	0	0	0	0	0	0	0
52.0060	4.8670	9.3790	C	0	0	0	0	0	0	0	0	0	0	0	0
51.9890	3.8660	8.9380	H	0	0	0	0	0	0	0	0	0	0	0	0
51.7810	5.5710	8.5680	H	0	0	0	0	0	0	0	0	0	0	0	0
53.3830	5.2010	9.9670	C	0	0	0	0	0	0	0	0	0	0	0	0
53.3100	6.0370	10.6750	H	0	0	0	0	0	0	0	0	0	0	0	0

54.0040	5.5930	9.1490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.8430	5.8600	11.2580	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.2970	-0.1650	12.8480	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.9230	-1.1820	13.0190	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.3190	-0.2840	12.4740	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35.0280	1.0090	10.8330	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34.6170	1.2050	11.8320	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34.8400	-0.0520	10.6230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.5490	1.1840	10.8130	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.9470	0.8800	9.8380	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.8390	2.2210	11.0080	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37.1940	0.3390	11.8790	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.5460	0.5070	11.8270	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.5980	-0.3590	12.6860	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.2950	0.6540	14.1350	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.5590	1.6990	13.9310	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.2860	0.6740	14.5600	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.1530	0.0490	15.0980	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.2790	0.8530	15.4530	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.9490	1.8610	15.7280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.7190	0.4020	16.3490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.3230	0.8820	14.3370	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.6090	-0.1470	14.0840	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.8850	1.3050	13.4260	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.5570	1.6960	14.7260	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43.2580	2.7250	14.9590	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.0090	1.2750	15.6320	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.5860	1.7030	13.5940	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.9130	0.6750	13.3910	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.1200	2.0790	12.6750	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.7980	2.5680	13.9360	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4840	3.6020	14.1240	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2640	2.2200	14.8660	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.8330	2.5480	12.8150	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.2040	1.5280	12.6660	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.3810	2.9040	11.8830	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.9110	3.4070	13.1840	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.0210	3.3490	12.2890	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2960	2.3090	12.0770	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.8790	3.7820	12.8160	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.0550	-0.1550	8.3270	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.2080	0.5360	7.4910	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.4920	-1.0180	7.9610	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.0380	-0.5150	8.6480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.3530	0.5410	9.4900	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.2090	-0.1610	10.3210	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.0420	1.3180	9.8470	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.0780	1.1600	9.0910	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6140	2.0960	10.1390	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.3020	1.5320	11.0260	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.4530	2.7390	10.4390	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.4820	3.0310	9.6530	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.8220	3.4840	8.7120	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.5880	2.4430	9.4180	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.1470	4.1110	10.6020	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
55.0530	0.1540	8.7580	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.4170	-0.8710	8.8990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.1710	0.2310	9.4060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.6210	0.3260	7.3080	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.4640	0.1930	6.6220	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.1900	1.3170	7.1330	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.8610	-0.4200	7.0520	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.2120	11.0850	20.7490	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.3180	11.3680	21.3170	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.9100	10.4260	19.9280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.8490	12.2490	20.2050	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.0240	13.0820	19.5140	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.7590	14.3200	19.0810	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8420	14.1530	19.1140	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.5150	14.4780	18.0230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3550	15.5480	19.8960	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.2670	15.6170	20.0210	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.6400	16.4190	19.2930	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.8390	12.8790	19.2850	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.2640	3.3400	16.6240	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.8870	2.3110	16.6880	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.1200	3.3860	17.3060	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.5520	3.6330	11.8550	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.7320	4.2830	12.1790	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53.1060	2.6370	11.7380	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54.5930	3.6490	12.9740	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

57.8450	12.5720	28.5600	O	0	0	0	0	0	0	0	0	0	0	0	0
57.5250	13.4170	29.6650	C	0	0	0	0	0	0	0	0	0	0	0	0
57.0380	14.3360	29.3180	H	0	0	0	0	0	0	0	0	0	0	0	0
56.7950	12.8730	30.2740	H	0	0	0	0	0	0	0	0	0	0	0	0
58.7620	13.7170	30.5090	C	0	0	0	0	0	0	0	0	0	0	0	0
59.2400	12.7740	30.8010	H	0	0	0	0	0	0	0	0	0	0	0	0
59.5030	14.2580	29.9100	H	0	0	0	0	0	0	0	0	0	0	0	0
58.4060	14.5370	31.7480	C	0	0	0	0	0	0	0	0	0	0	0	0
57.9210	15.4710	31.4400	H	0	0	0	0	0	0	0	0	0	0	0	0
57.6850	13.9850	32.3630	H	0	0	0	0	0	0	0	0	0	0	0	0
59.6490	14.8570	32.5810	C	0	0	0	0	0	0	0	0	0	0	0	0
60.1200	13.9250	32.9160	H	0	0	0	0	0	0	0	0	0	0	0	0
60.3810	15.3840	31.9570	H	0	0	0	0	0	0	0	0	0	0	0	0
59.2980	15.7200	33.7910	C	0	0	0	0	0	0	0	0	0	0	0	0
58.7860	16.6320	33.4650	H	0	0	0	0	0	0	0	0	0	0	0	0
58.5840	15.1950	34.4380	H	0	0	0	0	0	0	0	0	0	0	0	0
60.5380	16.0850	34.6030	C	0	0	0	0	0	0	0	0	0	0	0	0
60.9640	15.1800	35.0500	H	0	0	0	0	0	0	0	0	0	0	0	0
61.3120	16.5340	33.9700	H	0	0	0	0	0	0	0	0	0	0	0	0
60.1590	16.9490	35.6740	O	0	0	0	0	0	0	0	0	0	0	0	0
60.6750	18.2740	35.5660	C	0	0	0	0	0	0	0	0	0	0	0	0
61.7620	18.2500	35.4150	H	0	0	0	0	0	0	0	0	0	0	0	0
60.5200	18.7590	36.5360	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
5	8	1	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
8	17	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	39	1	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
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
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
24	25	1	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
24	27	1	0	0	0	0	0	0	0	0	0	0	0	0	0
24	71	1	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
28	29	1	0	0	0	0	0	0	0	0	0	0	0	0	0
28	35	2	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
29	31	1	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
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	88	1	0	0	0	0	0	0	0	0	0	0	0	0	0
36	37	1	0	0	0	0	0	0	0	0	0	0	0	0	0
36	38	1	0	0	0	0	0	0	0	0	0	0	0	0	0
36	46	1	0	0	0	0	0	0	0	0	0	0	0	0	0
36	48	1	0	0	0	0	0	0	0	0	0	0	0	0	0
39	40	1	0	0	0	0	0	0	0	0	0	0	0	0	0
39	41	1	0	0	0	0	0	0	0	0	0	0	0	0	0
39	42	1	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
42	44	1	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
45	46	1	0	0	0	0	0	0	0	0	0	0	0	0	0
45	47	2	0	0	0	0	0	0	0	0	0	0	0	0	0
48	49	1	0	0	0	0	0	0	0	0	0	0	0	0	0
48	50	1	0	0	0	0	0	0	0	0	0	0	0	0	0
48	51	1	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
52	53	1	0	0	0	0	0	0	0	0	0	0	0	0	0
52	54	1	0	0	0	0	0	0	0	0	0	0	0	0	0
52	55	1	0	0	0	0	0	0	0	0	0	0	0	0	0
55	56	1	0	0	0	0	0	0	0	0	0	0	0	0	0
55	57	1	0	0	0	0	0	0	0	0	0	0	0	0	0
55	58	1	0	0	0	0	0	0	0	0	0	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
61	62	1	0	0	0	0
61	63	1	0	0	0	0
61	64	1	0	0	0	0
64	65	1	0	0	0	0
64	66	1	0	0	0	0
64	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
71	72	1	0	0	0	0
71	73	1	0	0	0	0
74	75	1	0	0	0	0
74	76	1	0	0	0	0
74	77	1	0	0	0	0
74	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
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82	83	1	0	0	0	0
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82	85	1	0	0	0	0
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85	87	1	0	0	0	0
85	88	1	0	0	0	0
88	111	1	0	0	0	0
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89	91	1	0	0	0	0
89	92	1	0	0	0	0
92	93	1	0	0	0	0
92	94	1	0	0	0	0
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96	98	1	0	0	0	0
96	99	1	0	0	0	0
96	143	1	0	0	0	0
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100	107	2	0	0	0	0
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111	114	1	0	0	0	0
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359360 1 0 0 0 0
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360362 1 0 0 0 0

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M END
> <NAME>
U75_1

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$$$$
U80_1
MOE2012 3D

```

```

347346 0 0 1 0 0 0 0 0999 V2000
24.5790 -16.9610 -17.4080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.3270 -17.3050 -18.1330 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.8440 -16.3440 -17.9370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.0740 -17.8590 -17.0350 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.2220 -16.2350 -16.3090 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.2120 -15.8330 -15.3150 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.5270 -15.0820 -15.7310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.6040 -16.7110 -15.0580 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
24.8400 -15.3120 -14.0160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.5900 -16.0300 -13.6650 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
25.3620 -14.3650 -14.1980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
23.7690 -15.0900 -12.9420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

```


40.1080	5.0460	-0.2900	C	0	0	0	0	0	0	0	0	0	0	0	0	0
38.9580	5.9930	-0.0890	C	0	0	0	0	0	0	0	0	0	0	0	0	0
39.1470	6.8880	-0.6890	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.0340	5.5310	-0.4580	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.8300	6.3030	1.3990	C	0	0	0	0	0	0	0	0	0	0	0	0	0
39.7190	6.8340	1.7580	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.8400	5.3480	1.9400	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.2370	5.2330	0.1430	O	0	0	0	0	0	0	0	0	0	0	0	0	0
43.2850	-7.3630	-7.0950	C	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2550	-7.8070	-7.3520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.8730	-6.9810	-8.0360	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.3620	-11.2720	-4.3230	C	0	0	0	0	0	0	0	0	0	0	0	0	0
42.8130	-10.7590	-3.4640	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.2100	-11.7990	-4.7800	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.8210	-10.2380	-5.3160	C	0	0	0	0	0	0	0	0	0	0	0	0	0
41.4570	-10.7330	-6.2230	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.0070	-9.6600	-4.8670	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.8980	-9.2610	-5.7240	C	0	0	0	0	0	0	0	0	0	0	0	0	0
42.3740	-8.3570	-6.6010	O	0	0	0	0	0	0	0	0	0	0	0	0	0
44.0540	-9.2700	-5.3250	O	0	0	0	0	0	0	0	0	0	0	0	0	0
43.4400	-6.2200	-6.0990	C	0	0	0	0	0	0	0	0	0	0	0	0	0
42.4550	-5.7980	-5.8740	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.8660	-6.5900	-5.1600	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2890	-5.2290	-6.6690	O	0	0	0	0	0	0	0	0	0	0	0	0	0
44.6320	-4.1850	-5.7560	C	0	0	0	0	0	0	0	0	0	0	0	0	0
44.9620	-4.6080	-4.8000	H	0	0	0	0	0	0	0	0	0	0	0	0	0
45.4910	-3.6630	-6.1910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.4830	-3.1940	-5.5650	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1320	-2.8540	-6.5470	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.6300	-3.6950	-5.0950	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.9070	-1.9980	-4.7100	C	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2590	-2.3520	-3.7340	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.7490	-1.4840	-5.1910	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.7530	-1.0120	-4.5110	C	0	0	0	0	0	0	0	0	0	0	0	0	0
42.3940	-0.6650	-5.4880	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.9150	-1.5220	-4.0210	H	0	0	0	0	0	0	0	0	0	0	0	0	0
43.1830	0.1900	-3.6700	C	0	0	0	0	0	0	0	0	0	0	0	0	0
43.5530	-0.1440	-2.6930	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.0260	0.7040	-4.1490	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.0410	1.1810	-3.4630	C	0	0	0	0	0	0	0	0	0	0	0	0	0
41.6820	1.5480	-4.4320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
41.2130	0.6940	-2.9360	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.5350	2.2760	-2.6940	O	0	0	0	0	0	0	0	0	0	0	0	0	0
41.5570	3.2850	-2.4560	C	0	0	0	0	0	0	0	0	0	0	0	0	0
40.9390	3.4590	-3.3460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
42.0950	4.2210	-2.2750	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.9170	2.5990	1.8940	C	0	0	0	0	0	0	0	0	0	0	0	0	0
36.1540	1.9600	2.3520	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.8550	2.4710	2.4470	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.1060	2.2380	0.8770	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.5190	4.0080	1.8740	N	0	0	0	0	0	0	0	0	0	0	0	0	0
36.3490	4.5110	3.2470	C	0	0	0	0	0	0	0	0	0	0	0	0	0
35.5270	3.9670	3.7320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.2520	4.2810	3.8270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
36.0790	6.0190	3.4120	C	0	0	0	0	0	0	0	0	0	0	0	0	0
35.2060	6.3290	2.8270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.7890	6.1740	4.4600	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.2600	6.9640	3.1350	C	0	0	0	0	0	0	0	0	0	0	0	0	0
36.9610	7.9490	3.5150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
38.1230	6.6730	3.7490	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.3140	4.1770	1.0640	C	0	0	0	0	0	0	0	0	0	0	0	0	0
34.4440	3.6820	1.5090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.4650	3.7640	0.0590	H	0	0	0	0	0	0	0	0	0	0	0	0	0
35.0770	5.2350	0.9170	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.6030	7.0410	1.7130	N	0	0	3	0	0	0	0	0	0	0	0	0	0
51.9560	11.5170	4.3740	C	0	0	0	0	0	0	0	0	0	0	0	0	0
51.8670	12.4570	3.8150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
51.2880	10.8080	3.8750	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.2820	10.9720	4.2830	O	0	0	0	0	0	0	0	0	0	0	0	0	0
54.3030	11.8740	4.2960	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6320	11.1660	4.2130	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.5030	10.2180	3.6770	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.3030	11.7810	3.6040	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.1720	10.9370	5.6230	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.3800	10.4370	6.1930	H	0	0	0	0	0	0	0	0	0	0	0	0	0
56.3350	11.8940	6.1380	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.1820	13.0860	4.4060	O	0	0	0	0	0	0	0	0	0	0	0	0	0
40.1930	9.3770	4.6700	C	0	0	0	0	0	0	0	0	0	0	0	0	0
39.3210	9.7280	5.2350	H	0	0	0	0	0	0	0	0	0	0	0	0	0
40.5180	8.4530	5.1620	H	0	0	0	0	0	0	0	0	0	0	0	0	0
37.5000	8.3860	1.1360	C	0	0	0	0	0	0	0	0	0	0	0	0	0

37.3290	8.2670	0.0580	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36.5820	8.8680	1.5000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.6790	9.3430	1.3050	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.6120	8.9300	0.9050	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.4970	10.2510	0.7160	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.8780	9.7840	2.7290	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39.8610	9.0470	3.3140	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38.2390	10.6770	3.2650	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.3200	10.3990	4.6880	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.1540	10.0320	4.0800	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40.9780	11.3420	4.2480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41.7330	10.6140	6.0350	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.8210	11.5320	6.1480	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.6820	12.3800	5.4680	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42.7950	11.9260	7.1690	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.1600	10.8330	5.9110	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.2450	9.9780	6.5930	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44.1920	10.4130	4.9000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3410	11.7850	6.1070	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.2450	12.6330	5.4190	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45.3230	12.1900	7.1260	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.6760	11.0750	5.8620	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.7760	10.2340	6.5590	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46.6880	10.6570	4.8480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.8610	12.0250	6.0350	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.7710	12.8730	5.3450	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47.8580	12.4570	7.0440	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.1920	11.3170	5.7930	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.3160	10.4980	6.5100	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2170	10.9100	4.7770	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50.2460	12.2650	5.9640	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.5480	11.6980	5.8340	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51.6210	10.7530	6.3860	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52.2480	12.3860	6.3230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1460	11.4510	3.5090	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.0000	10.9650	3.0230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.5210	12.0660	4.3350	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.6990	12.1140	2.7590	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.1720	10.4530	3.9610	N	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9970	11.1240	4.5550	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.2820	11.6590	5.4710	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.6370	11.8820	3.8460	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8150	10.1810	4.8550	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5480	9.6270	3.9460	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.1130	9.4460	5.6080	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.5890	10.9770	5.3460	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.8490	11.5670	6.2350	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.3460	11.6980	4.5560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.8110	9.5290	4.9010	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1160	10.0280	5.8280	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.7000	9.0750	4.4490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.1470	8.6970	5.1540	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.4100	10.1210	5.6190	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0
63.8650	-4.1320	8.9180	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.7640	-3.6990	8.4620	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.0180	-3.6870	8.3870	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.7940	-5.5490	8.6980	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.9730	-6.2260	8.8080	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.7320	-7.6890	8.5340	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.9760	-8.0430	9.2390	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.3350	-7.7670	7.5170	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.0330	-8.4860	8.6750	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.4820	-8.2860	9.6580	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.7630	-8.0800	7.9630	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66.0540	-5.7260	9.0820	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.0460	6.3440	9.8470	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.0280	7.1330	10.6080	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.2220	5.6490	10.0520	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.5510	9.4160	6.9120	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58.5860	9.0900	7.0660	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.3270	10.0890	7.7510	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.6750	8.1630	6.9630	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6250	8.3740	6.7320	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.0070	7.4120	6.2370	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56.7120	7.5640	8.3430	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57.8960	6.9220	8.5440	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55.8060	7.6630	9.1600	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.3720	5.5990	9.9010	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.3770	4.8040	9.1480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.1940	6.2860	9.6670	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5440	5.0630	11.2090	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

60.7500	4.3140	11.3540	C	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5780	4.8070	10.8300	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.9950	4.3150	12.4220	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.5620	2.8720	10.8830	C	0	0	0	0	0	0	0	0	0	0	0	0	0
59.7090	2.4300	11.4120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
60.2960	2.8560	9.8200	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.8190	2.0320	11.1110	C	0	0	0	0	0	0	0	0	0	0	0	0	0
62.6600	2.4750	10.5620	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.0830	2.0470	12.1750	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.6160	0.5840	10.6560	C	0	0	0	0	0	0	0	0	0	0	0	0	0
60.7810	0.1400	11.2120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.3420	0.5680	9.5940	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.8760	-0.2550	10.8700	C	0	0	0	0	0	0	0	0	0	0	0	0	0
63.7160	0.1750	10.3100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1740	-0.2290	11.9250	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.6720	-1.7050	10.4410	C	0	0	0	0	0	0	0	0	0	0	0	0	0
61.8650	-2.1590	11.0280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.4090	-1.7460	9.3790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.8890	-2.4160	10.6670	O	0	0	0	0	0	0	0	0	0	0	0	0	0
63.7870	-3.8140	10.4090	C	0	0	0	0	0	0	0	0	0	0	0	0	0
62.8750	-4.2290	10.8550	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.6210	-4.2970	10.9290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.9520	-12.2880	11.4130	C	0	0	0	0	0	0	0	0	0	0	0	0	0
61.6550	-11.6200	10.5960	H	0	0	0	0	0	0	0	0	0	0	0	0	0
61.0660	-12.4830	12.0270	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.2510	-13.2500	10.9830	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.0240	-11.7310	12.2340	N	0	0	0	0	0	0	0	0	0	0	0	0	0
64.3030	-11.6420	11.5150	C	0	0	0	0	0	0	0	0	0	0	0	0	0
65.0820	-11.3600	12.2370	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.5790	-12.6510	11.1810	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.3680	-10.6790	10.3140	C	0	0	0	0	0	0	0	0	0	0	0	0	0
63.6000	-10.9410	9.5790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.1730	-9.6610	10.6610	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.7550	-10.7400	9.6580	C	0	0	0	0	0	0	0	0	0	0	0	0	0
66.5140	-10.4610	10.4020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.9850	-11.7850	9.4120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.6200	-10.4650	12.8390	C	0	0	0	0	0	0	0	0	0	0	0	0	0
61.7540	-10.6160	13.4920	H	0	0	0	0	0	0	0	0	0	0	0	0	0
62.3520	-9.7080	12.0940	H	0	0	0	0	0	0	0	0	0	0	0	0	0
63.4210	-10.0630	13.4700	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.9630	-9.9340	8.4510	N	0	0	3	0	0	0	0	0	0	0	0	0	0
69.0580	-20.6220	1.1200	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.0280	-20.9850	1.0230	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.9840	-19.6120	1.5350	H	0	0	0	0	0	0	0	0	0	0	0	0	0
69.8030	-21.4000	2.0690	O	0	0	0	0	0	0	0	0	0	0	0	0	0
69.5770	-22.7450	2.0490	C	0	0	0	0	0	0	0	0	0	0	0	0	0
70.4180	-23.4060	3.1150	C	0	0	0	0	0	0	0	0	0	0	0	0	0
71.4720	-23.1900	2.9080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.1470	-22.9770	4.0860	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.2110	-24.9100	3.1540	C	0	0	0	0	0	0	0	0	0	0	0	0	0
69.1650	-25.1580	3.3630	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.8330	-25.3600	3.9350	H	0	0	0	0	0	0	0	0	0	0	0	0	0
70.4790	-25.3690	2.1970	H	0	0	0	0	0	0	0	0	0	0	0	0	0
68.8170	-23.3230	1.2860	O	0	0	0	0	0	0	0	0	0	0	0	0	0
65.1490	-10.6880	2.4380	C	0	0	0	0	0	0	0	0	0	0	0	0	0
64.0770	-10.4530	2.4060	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.6010	-10.1360	1.6070	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.1940	-10.3820	7.2890	C	0	0	0	0	0	0	0	0	0	0	0	0	0
65.1980	-11.4800	7.2550	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.1400	-10.0900	7.3710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.7960	-9.8820	5.9720	C	0	0	0	0	0	0	0	0	0	0	0	0	0
65.7690	-8.7900	5.9050	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.8370	-10.2180	5.8980	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.0360	-10.4290	4.7920	C	0	0	0	0	0	0	0	0	0	0	0	0	0
65.7480	-10.2070	3.6510	O	0	0	0	0	0	0	0	0	0	0	0	0	0
63.9420	-10.9730	4.8520	O	0	0	0	0	0	0	0	0	0	0	0	0	0
65.4010	-12.1810	2.2640	C	0	0	0	0	0	0	0	0	0	0	0	0	0
66.4790	-12.3710	2.2710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.9580	-12.7410	3.0950	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.8280	-12.6020	1.0300	O	0	0	0	0	0	0	0	0	0	0	0	0	0
64.8790	-14.0150	0.8340	C	0	0	0	0	0	0	0	0	0	0	0	0	0
64.5530	-14.5390	1.7400	H	0	0	0	0	0	0	0	0	0	0	0	0	0
64.1520	-14.2460	0.0480	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.2660	-14.4730	0.3870	C	0	0	0	0	0	0	0	0	0	0	0	0	0
66.5810	-13.8850	-0.4840	H	0	0	0	0	0	0	0	0	0	0	0	0	0
67.0000	-14.2650	1.1740	H	0	0	0	0	0	0	0	0	0	0	0	0	0
66.2800	-15.9640	0.0550	C	0	0	0	0	0	0	0	0	0	0	0	0	0
65.9450	-16.5360	0.9290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
65.5690	-16.1680	-0.7560	H	0	0	0	0	0	0	0	0	0	0	0	0	0
67.6760	-16.4330	-0.3580	C	0	0	0	0	0	0	0	0	0	0	0	0	0
68.0050	-15.8800	-1.2450	H	0	0	0	0	0	0	0	0	0	0	0	0	0

68.3880	-16.2100	0.4460	H	0	0	0	0	0	0	0	0	0	0	0	0
67.6910	-17.9320	-0.6510	C	0	0	0	0	0	0	0	0	0	0	0	0
67.3120	-18.4860	0.2160	H	0	0	0	0	0	0	0	0	0	0	0	0
67.0050	-18.1660	-1.4740	H	0	0	0	0	0	0	0	0	0	0	0	0
69.0910	-18.4240	-1.0070	C	0	0	0	0	0	0	0	0	0	0	0	0
69.4120	-17.9670	-1.9490	H	0	0	0	0	0	0	0	0	0	0	0	0
69.8220	-18.1430	-0.2390	H	0	0	0	0	0	0	0	0	0	0	0	0
69.0540	-19.8360	-1.2120	O	0	0	0	0	0	0	0	0	0	0	0	0
69.7670	-20.5890	-0.2330	C	0	0	0	0	0	0	0	0	0	0	0	0
70.7930	-20.2140	-0.1330	H	0	0	0	0	0	0	0	0	0	0	0	0
69.8610	-21.6100	-0.6200	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	15	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
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	19	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
19	20	1	0	0	0	0	0	0	0	0	0	0	0	0	0
19	36	1	0	0	0	0	0	0	0	0	0	0	0	0	0
21	22	1	0	0	0	0	0	0	0	0	0	0	0	0	0
21	23	1	0	0	0	0	0	0	0	0	0	0	0	0	0
21	24	1	0	0	0	0	0	0	0	0	0	0	0	0	0
21	68	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
25	26	1	0	0	0	0	0	0	0	0	0	0	0	0	0
25	32	2	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	28	1	0	0	0	0	0	0	0	0	0	0	0	0	0
26	29	1	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
29	31	1	0	0	0	0	0	0	0	0	0	0	0	0	0
29	89	1	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
33	35	1	0	0	0	0	0	0	0	0	0	0	0	0	0
33	43	1	0	0	0	0	0	0	0	0	0	0	0	0	0
33	45	1	0	0	0	0	0	0	0	0	0	0	0	0	0
36	37	1	0	0	0	0	0	0	0	0	0	0	0	0	0
36	38	1	0	0	0	0	0	0	0	0	0	0	0	0	0
36	39	1	0	0	0	0	0	0	0	0	0	0	0	0	0
39	40	1	0	0	0	0	0	0	0	0	0	0	0	0	0
39	41	1	0	0	0	0	0	0	0	0	0	0	0	0	0
39	42	1	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
42	44	2	0	0	0	0	0	0	0	0	0	0	0	0	0
45	46	1	0	0	0	0	0	0	0	0	0	0	0	0	0
45	47	1	0	0	0	0	0	0	0	0	0	0	0	0	0
45	48	1	0	0	0	0	0	0	0	0	0	0	0	0	0
48	49	1	0	0	0	0	0	0	0	0	0	0	0	0	0
49	50	1	0	0	0	0	0	0	0	0	0	0	0	0	0
49	51	1	0	0	0	0	0	0	0	0	0	0	0	0	0
49	52	1	0	0	0	0	0	0	0	0	0	0	0	0	0
52	53	1	0	0	0	0	0	0	0	0	0	0	0	0	0
52	54	1	0	0	0	0	0	0	0	0	0	0	0	0	0
52	55	1	0	0	0	0	0	0	0	0	0	0	0	0	0
55	56	1	0	0	0	0	0	0	0	0	0	0	0	0	0
55	57	1	0	0	0	0	0	0	0	0	0	0	0	0	0
55	58	1	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
58	60	1	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
61	62	1	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
61	64	1	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
64	66	1	0	0	0	0	0	0	0	0	0	0	0	0	0
64	67	1	0	0	0	0	0	0	0	0	0	0	0	0	0
67	68	1	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
68	70	1	0	0	0	0	0	0	0	0	0	0	0	0	0

71	72	1	0	0	0	0
71	73	1	0	0	0	0
71	74	1	0	0	0	0
71	75	1	0	0	0	0
75	76	1	0	0	0	0
75	85	1	0	0	0	0
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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
82	83	1	0	0	0	0
82	84	1	0	0	0	0
82	89	1	0	0	0	0
85	86	1	0	0	0	0
85	87	1	0	0	0	0
85	88	1	0	0	0	0
89	105	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	137	1	0	0	0	0
93	94	1	0	0	0	0
94	95	1	0	0	0	0
94	101	2	0	0	0	0
95	96	1	0	0	0	0
95	97	1	0	0	0	0
95	98	1	0	0	0	0
98	99	1	0	0	0	0
98	100	1	0	0	0	0
98	158	1	0	0	0	0
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102	114	1	0	0	0	0
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108	110	1	0	0	0	0
108	111	1	0	0	0	0
111	112	1	0	0	0	0
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114	117	1	0	0	0	0
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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	126	1	0	0	0	0
124	127	1	0	0	0	0
127	128	1	0	0	0	0
127	129	1	0	0	0	0
127	130	1	0	0	0	0
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133	135	1	0	0	0	0
133	136	1	0	0	0	0
136	137	1	0	0	0	0
137	138	1	0	0	0	0
137	139	1	0	0	0	0
140	141	1	0	0	0	0
140	142	1	0	0	0	0
140	143	1	0	0	0	0
140	144	1	0	0	0	0
144	145	1	0	0	0	0
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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
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151152	1	0	0	0	0
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151158	1	0	0	0	0
154155	1	0	0	0	0
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154157	1	0	0	0	0
158174	1	0	0	0	0
159160	1	0	0	0	0
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159206	1	0	0	0	0
162163	1	0	0	0	0
163164	1	0	0	0	0
163170	2	0	0	0	0
164165	1	0	0	0	0
164166	1	0	0	0	0
164167	1	0	0	0	0
167168	1	0	0	0	0
167169	1	0	0	0	0
167227	1	0	0	0	0
171172	1	0	0	0	0
171173	1	0	0	0	0
171181	1	0	0	0	0
171183	1	0	0	0	0
174175	1	0	0	0	0
174176	1	0	0	0	0
174177	1	0	0	0	0
177178	1	0	0	0	0
177179	1	0	0	0	0
177180	1	0	0	0	0
180181	1	0	0	0	0
180182	2	0	0	0	0
183184	1	0	0	0	0
183185	1	0	0	0	0
183186	1	0	0	0	0
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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
193194	1	0	0	0	0
193195	1	0	0	0	0
193196	1	0	0	0	0
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199200	1	0	0	0	0
199201	1	0	0	0	0
199202	1	0	0	0	0
202203	1	0	0	0	0
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202205	1	0	0	0	0
205206	1	0	0	0	0
206207	1	0	0	0	0
206208	1	0	0	0	0
209210	1	0	0	0	0
209211	1	0	0	0	0
209212	1	0	0	0	0
209213	1	0	0	0	0
213214	1	0	0	0	0
213223	1	0	0	0	0
214215	1	0	0	0	0
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214217	1	0	0	0	0
217218	1	0	0	0	0
217219	1	0	0	0	0
217220	1	0	0	0	0
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220227	1	0	0	0	0
223224	1	0	0	0	0
223225	1	0	0	0	0
223226	1	0	0	0	0
227243	1	0	0	0	0
228229	1	0	0	0	0
228230	1	0	0	0	0
228231	1	0	0	0	0
228275	1	0	0	0	0
231232	1	0	0	0	0

232233	1	0	0	0	0
232239	2	0	0	0	0
233234	1	0	0	0	0
233235	1	0	0	0	0
233236	1	0	0	0	0
236237	1	0	0	0	0
236238	1	0	0	0	0
236296	1	0	0	0	0
240241	1	0	0	0	0
240242	1	0	0	0	0
240250	1	0	0	0	0
240252	1	0	0	0	0
243244	1	0	0	0	0
243245	1	0	0	0	0
243246	1	0	0	0	0
246247	1	0	0	0	0
246248	1	0	0	0	0
246249	1	0	0	0	0
249250	1	0	0	0	0
249251	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
256257	1	0	0	0	0
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
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
275276	1	0	0	0	0
275277	1	0	0	0	0
278279	1	0	0	0	0
278280	1	0	0	0	0
278281	1	0	0	0	0
278282	1	0	0	0	0
282283	1	0	0	0	0
282292	1	0	0	0	0
283284	1	0	0	0	0
283285	1	0	0	0	0
283286	1	0	0	0	0
286287	1	0	0	0	0
286288	1	0	0	0	0
286289	1	0	0	0	0
289290	1	0	0	0	0
289291	1	0	0	0	0
289296	1	0	0	0	0
292293	1	0	0	0	0
292294	1	0	0	0	0
292295	1	0	0	0	0
296313	1	0	0	0	0
297298	1	0	0	0	0
297299	1	0	0	0	0
297300	1	0	0	0	0
297345	1	0	0	0	0
300301	1	0	0	0	0
301302	1	0	0	0	0
301309	2	0	0	0	0
302303	1	0	0	0	0
302304	1	0	0	0	0
302305	1	0	0	0	0
305306	1	0	0	0	0
305307	1	0	0	0	0
305308	1	0	0	0	0
310311	1	0	0	0	0
310312	1	0	0	0	0
310320	1	0	0	0	0
310322	1	0	0	0	0

48.2210	26.6400	6.5000	H	0	0	0	0	0	0	0	0	0	0	0
48.4320	30.8910	2.7210	C	0	0	0	0	0	0	0	0	0	0	0
48.3770	30.2160	1.8570	H	0	0	0	0	0	0	0	0	0	0	0
49.4930	31.1370	2.8480	H	0	0	0	0	0	0	0	0	0	0	0
47.9340	30.2150	3.9960	C	0	0	0	0	0	0	0	0	0	0	0
48.0850	30.8690	4.8620	H	0	0	0	0	0	0	0	0	0	0	0
46.8690	29.9760	3.9130	H	0	0	0	0	0	0	0	0	0	0	0
48.6760	28.9280	4.2410	C	0	0	0	0	0	0	0	0	0	0	0
48.0200	28.2090	5.1970	O	0	0	0	0	0	0	0	0	0	0	0
49.7000	28.5810	3.6710	O	0	0	0	0	0	0	0	0	0	0	0
48.1470	25.8860	4.4800	C	0	0	0	0	0	0	0	0	0	0	0
47.0540	25.8520	4.4390	H	0	0	0	0	0	0	0	0	0	0	0
48.5100	26.1600	3.4830	H	0	0	0	0	0	0	0	0	0	0	0
48.6730	24.6180	4.8600	O	0	0	0	0	0	0	0	0	0	0	0
48.4330	23.5920	3.8950	C	0	0	0	0	0	0	0	0	0	0	0
48.6850	23.9500	2.8900	H	0	0	0	0	0	0	0	0	0	0	0
49.1250	22.7760	4.1300	H	0	0	0	0	0	0	0	0	0	0	0
46.9980	23.0690	3.9620	C	0	0	0	0	0	0	0	0	0	0	0
46.7710	22.7620	4.9900	H	0	0	0	0	0	0	0	0	0	0	0
46.2930	23.8740	3.7240	H	0	0	0	0	0	0	0	0	0	0	0
46.7800	21.9010	2.9980	C	0	0	0	0	0	0	0	0	0	0	0
47.0140	22.2220	1.9760	H	0	0	0	0	0	0	0	0	0	0	0
47.4710	21.0860	3.2470	H	0	0	0	0	0	0	0	0	0	0	0
45.3400	21.3840	3.0540	C	0	0	0	0	0	0	0	0	0	0	0
45.1100	21.0450	4.0720	H	0	0	0	0	0	0	0	0	0	0	0
44.6470	22.2020	2.8220	H	0	0	0	0	0	0	0	0	0	0	0
45.1200	20.2350	2.0700	C	0	0	0	0	0	0	0	0	0	0	0
45.3550	20.5610	1.0490	H	0	0	0	0	0	0	0	0	0	0	0
45.8120	19.4110	2.2880	H	0	0	0	0	0	0	0	0	0	0	0
43.6870	19.7120	2.1120	C	0	0	0	0	0	0	0	0	0	0	0
43.4570	19.3250	3.1110	H	0	0	0	0	0	0	0	0	0	0	0
42.9850	20.5170	1.8710	H	0	0	0	0	0	0	0	0	0	0	0
43.5680	18.6560	1.1560	O	0	0	0	0	0	0	0	0	0	0	0
42.2460	18.1220	1.0900	C	0	0	0	0	0	0	0	0	0	0	0
41.7700	18.1160	2.0770	H	0	0	0	0	0	0	0	0	0	0	0
42.3330	17.0720	0.7890	H	0	0	0	0	0	0	0	0	0	0	0
38.7530	16.6180	6.4410	C	0	0	0	0	0	0	0	0	0	0	0
38.0250	15.7990	6.5140	H	0	0	0	0	0	0	0	0	0	0	0
39.7240	16.1680	6.6890	H	0	0	0	0	0	0	0	0	0	0	0
38.7520	17.1730	5.0720	N	0	0	0	0	0	0	0	0	0	0	0
38.7820	16.0460	4.1080	C	0	0	0	0	0	0	0	0	0	0	0
39.7190	15.4880	4.2280	H	0	0	0	0	0	0	0	0	0	0	0
37.9670	15.3500	4.3490	H	0	0	0	0	0	0	0	0	0	0	0
38.5760	16.4790	2.6400	C	0	0	0	0	0	0	0	0	0	0	0
37.6070	16.9910	2.5890	H	0	0	0	0	0	0	0	0	0	0	0
39.3440	17.2010	2.3510	H	0	0	0	0	0	0	0	0	0	0	0
38.5780	15.3540	1.6940	N	0	0	3	0	0	0	0	0	0	0	0
39.8920	18.0920	4.8690	C	0	0	0	0	0	0	0	0	0	0	0
40.4440	18.2810	5.7990	H	0	0	0	0	0	0	0	0	0	0	0
40.6550	17.6700	4.2030	H	0	0	0	0	0	0	0	0	0	0	0
38.3580	17.6430	7.5070	C	0	0	0	0	0	0	0	0	0	0	0
39.0560	18.4830	7.5510	H	0	0	0	0	0	0	0	0	0	0	0
37.3510	18.0290	7.3170	H	0	0	0	0	0	0	0	0	0	0	0
38.3630	17.0000	8.7770	O	0	0	0	0	0	0	0	0	0	0	0
38.0660	17.6560	9.4320	H	0	0	0	0	0	0	0	0	0	0	0
39.4140	19.4430	4.3270	C	0	0	0	0	0	0	0	0	0	0	0
38.8990	19.3330	3.3680	H	0	0	0	0	0	0	0	0	0	0	0
38.7340	19.9240	5.0390	H	0	0	0	0	0	0	0	0	0	0	0
40.5350	20.3010	4.1310	O	0	0	0	0	0	0	0	0	0	0	0
40.1830	21.1760	3.8890	H	0	0	0	0	0	0	0	0	0	0	0
39.0860	4.2360	9.3020	C	0	0	0	0	0	0	0	0	0	0	0
39.3380	3.5420	8.4910	H	0	0	0	0	0	0	0	0	0	0	0
39.2370	5.2590	8.9450	H	0	0	0	0	0	0	0	0	0	0	0
37.7170	4.0800	9.6980	O	0	0	0	0	0	0	0	0	0	0	0
36.8110	4.0670	8.6800	C	0	0	0	0	0	0	0	0	0	0	0
35.4260	3.8220	9.2200	C	0	0	0	0	0	0	0	0	0	0	0
35.4100	3.9720	10.3050	H	0	0	0	0	0	0	0	0	0	0	0
34.7710	4.5990	8.8070	H	0	0	0	0	0	0	0	0	0	0	0
34.9050	2.4370	8.8330	C	0	0	0	0	0	0	0	0	0	0	0
34.7740	2.4350	7.7430	H	0	0	0	0	0	0	0	0	0	0	0
33.9070	2.3100	9.2710	H	0	0	0	0	0	0	0	0	0	0	0
37.0680	4.2260	7.4940	O	0	0	0	0	0	0	0	0	0	0	0
42.7480	12.0460	3.6170	C	0	0	0	0	0	0	0	0	0	0	0
43.3860	12.0240	2.7250	H	0	0	0	0	0	0	0	0	0	0	0
43.2980	12.6290	4.3650	H	0	0	0	0	0	0	0	0	0	0	0
39.8520	14.6290	1.6130	C	0	0	0	0	0	0	0	0	0	0	0
40.2680	14.6290	0.5980	H	0	0	0	0	0	0	0	0	0	0	0
40.6290	15.0970	2.2290	H	0	0	0	0	0	0	0	0	0	0	0
39.6120	13.1910	2.0560	C	0	0	0	0	0	0	0	0	0	0	0
39.1010	13.1380	3.0250	H	0	0	0	0	0	0	0	0	0	0	0
38.9720	12.6600	1.3400	H	0	0	0	0	0	0	0	0	0	0	0

56.5280	-3.0270	35.0840	H	0	0	0	0	0	0	0	0	0	0	0	0
56.6080	-4.0140	36.5280	H	0	0	0	0	0	0	0	0	0	0	0	0
57.7330	-2.1820	36.6560	C	0	0	0	0	0	0	0	0	0	0	0	0
58.3820	-2.5240	37.4710	H	0	0	0	0	0	0	0	0	0	0	0	0
58.3060	-1.5210	35.9970	H	0	0	0	0	0	0	0	0	0	0	0	0
56.6150	-1.4810	37.1990	O	0	0	0	0	0	0	0	0	0	0	0	0
56.9840	-0.3600	38.0010	C	0	0	0	0	0	0	0	0	0	0	0	0
57.8400	-0.6010	38.6440	H	0	0	0	0	0	0	0	0	0	0	0	0
56.1470	-0.1590	38.6780	H	0	0	0	0	0	0	0	0	0	0	0	0
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M END
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U86_1

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$$$$
U87_1
MOE2012 3D

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50.4510 9.5420 -29.9490 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51.3910 9.0940 -30.2940 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50.5440 10.6110 -30.1830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
49.2940 8.9380 -30.6440 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.1020 9.8020 -30.5140 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.0550 10.2400 -29.5100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.1540 10.6470 -31.2140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
46.8000 9.0110 -30.7130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
46.7640 8.5640 -31.7130 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
46.7630 8.1850 -29.9900 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
45.5790 9.9170 -30.5230 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
45.6060 10.3560 -29.5180 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
45.6120 10.7330 -31.2540 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
49.6140 8.7070 -32.0690 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
48.7000 8.5720 -32.6600 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50.1100 9.5800 -32.5140 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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44.3550	9.1340	-30.6910	N	0	0	3	0	0	0	0	0	0	0	0	0
44.3480	8.7050	-31.6170	H	0	0	0	0	0	0	0	0	0	0	0	0
50.4070	9.3310	-28.4300	C	0	0	0	0	0	0	0	0	0	0	0	0
49.5420	9.8200	-27.9720	H	0	0	0	0	0	0	0	0	0	0	0	0
50.3780	8.2630	-28.1910	H	0	0	0	0	0	0	0	0	0	0	0	0
51.5820	9.8890	-27.8490	O	0	0	0	0	0	0	0	0	0	0	0	0
51.5490	9.6970	-26.8950	H	0	0	0	0	0	0	0	0	0	0	0	0
50.4590	7.4470	-32.2900	C	0	0	0	0	0	0	0	0	0	0	0	0
51.4480	7.5320	-31.8310	H	0	0	0	0	0	0	0	0	0	0	0	0
49.9530	6.5670	-31.8810	H	0	0	0	0	0	0	0	0	0	0	0	0
50.6420	7.2470	-33.6890	O	0	0	0	0	0	0	0	0	0	0	0	0
51.1740	6.4390	-33.7920	H	0	0	0	0	0	0	0	0	0	0	0	0
37.1360	9.2660	-17.7270	C	0	0	0	0	0	0	0	0	0	0	0	0
37.5820	10.2130	-17.4000	H	0	0	0	0	0	0	0	0	0	0	0	0
37.8110	8.8020	-18.4550	H	0	0	0	0	0	0	0	0	0	0	0	0
36.9640	8.3850	-16.6100	O	0	0	0	0	0	0	0	0	0	0	0	0
38.1030	8.1170	-15.9110	C	0	0	0	0	0	0	0	0	0	0	0	0
37.8060	7.1440	-14.8010	C	0	0	0	0	0	0	0	0	0	0	0	0
36.7400	7.1540	-14.5540	H	0	0	0	0	0	0	0	0	0	0	0	0
38.0170	6.1430	-15.1990	H	0	0	0	0	0	0	0	0	0	0	0	0
38.6510	7.3740	-13.5490	C	0	0	0	0	0	0	0	0	0	0	0	0
39.7140	7.2840	-13.8070	H	0	0	0	0	0	0	0	0	0	0	0	0
38.4690	6.5210	-12.8810	H	0	0	0	0	0	0	0	0	0	0	0	0
39.2140	8.5540	-16.1790	O	0	0	0	0	0	0	0	0	0	0	0	0
38.3890	9.7090	-29.7820	C	0	0	0	0	0	0	0	0	0	0	0	0
38.1730	10.5130	-30.4970	H	0	0	0	0	0	0	0	0	0	0	0	0
37.6020	8.9600	-29.9270	H	0	0	0	0	0	0	0	0	0	0	0	0
43.1650	9.9690	-30.5230	C	0	0	0	0	0	0	0	0	0	0	0	0
43.1780	10.4500	-29.5370	H	0	0	0	0	0	0	0	0	0	0	0	0
43.1460	10.7630	-31.2800	H	0	0	0	0	0	0	0	0	0	0	0	0
41.9160	9.1030	-30.6470	C	0	0	0	0	0	0	0	0	0	0	0	0
41.8380	8.6680	-31.6500	H	0	0	0	0	0	0	0	0	0	0	0	0
41.9610	8.2900	-29.9110	H	0	0	0	0	0	0	0	0	0	0	0	0
40.6740	9.9130	-30.3850	C	0	0	0	0	0	0	0	0	0	0	0	0
39.6430	9.0760	-30.0770	O	0	0	0	0	0	0	0	0	0	0	0	0
40.5960	11.1320	-30.4510	O	0	0	0	0	0	0	0	0	0	0	0	0
38.3600	10.2160	-28.3440	C	0	0	0	0	0	0	0	0	0	0	0	0
38.5750	9.3850	-27.6640	H	0	0	0	0	0	0	0	0	0	0	0	0
39.1310	10.9790	-28.1940	H	0	0	0	0	0	0	0	0	0	0	0	0
37.0710	10.7600	-28.0760	O	0	0	0	0	0	0	0	0	0	0	0	0
36.9750	11.3930	-26.7990	C	0	0	0	0	0	0	0	0	0	0	0	0
37.8200	12.0760	-26.6490	H	0	0	0	0	0	0	0	0	0	0	0	0
36.0660	12.0030	-26.8230	H	0	0	0	0	0	0	0	0	0	0	0	0
36.8700	10.3740	-25.6630	C	0	0	0	0	0	0	0	0	0	0	0	0
36.0710	9.6590	-25.8910	H	0	0	0	0	0	0	0	0	0	0	0	0
37.7930	9.7880	-25.6010	H	0	0	0	0	0	0	0	0	0	0	0	0
36.6050	11.0530	-24.3180	C	0	0	0	0	0	0	0	0	0	0	0	0
37.4050	11.7730	-24.1060	H	0	0	0	0	0	0	0	0	0	0	0	0
35.6670	11.6180	-24.3700	H	0	0	0	0	0	0	0	0	0	0	0	0
36.5250	10.0300	-23.1810	C	0	0	0	0	0	0	0	0	0	0	0	0
35.7350	9.3010	-23.3990	H	0	0	0	0	0	0	0	0	0	0	0	0
37.4690	9.4750	-23.1200	H	0	0	0	0	0	0	0	0	0	0	0	0
36.2400	10.7040	-21.8380	C	0	0	0	0	0	0	0	0	0	0	0	0
37.0150	11.4470	-21.6140	H	0	0	0	0	0	0	0	0	0	0	0	0
35.2960	11.2600	-21.8870	H	0	0	0	0	0	0	0	0	0	0	0	0
36.1700	9.6900	-20.6990	C	0	0	0	0	0	0	0	0	0	0	0	0
35.3810	8.9550	-20.8980	H	0	0	0	0	0	0	0	0	0	0	0	0
37.1280	9.1680	-20.6030	H	0	0	0	0	0	0	0	0	0	0	0	0
35.8700	10.3910	-19.4910	O	0	0	0	0	0	0	0	0	0	0	0	0
35.7720	9.5330	-18.3550	C	0	0	0	0	0	0	0	0	0	0	0	0
35.2550	8.5990	-18.6060	H	0	0	0	0	0	0	0	0	0	0	0	0
35.1410	10.0400	-17.6180	H	0	0	0	0	0	0	0	0	0	0	0	0
32.6790	10.9480	-12.6090	C	0	0	0	0	0	0	0	0	0	0	0	0
31.8550	11.2850	-13.2480	H	0	0	0	0	0	0	0	0	0	0	0	0
32.2400	10.1760	-11.9620	H	0	0	0	0	0	0	0	0	0	0	0	0
33.7890	10.4060	-13.4160	N	0	0	0	0	0	0	0	0	0	0	0	0
34.7020	9.6060	-12.5720	C	0	0	0	0	0	0	0	0	0	0	0	0
34.7750	10.0270	-11.5630	H	0	0	0	0	0	0	0	0	0	0	0	0
34.3240	8.5830	-12.4470	H	0	0	0	0	0	0	0	0	0	0	0	0
36.1210	9.6010	-13.1550	C	0	0	0	0	0	0	0	0	0	0	0	0
36.1060	9.1980	-14.1680	H	0	0	0	0	0	0	0	0	0	0	0	0
36.4680	10.6350	-13.2390	H	0	0	0	0	0	0	0	0	0	0	0	0
37.0730	8.7880	-12.2630	C	0	0	0	0	0	0	0	0	0	0	0	0
37.1320	9.2790	-11.2840	H	0	0	0	0	0	0	0	0	0	0	0	0
36.6210	7.8100	-12.0470	H	0	0	0	0	0	0	0	0	0	0	0	0
33.2790	9.5900	-14.5390	C	0	0	0	0	0	0	0	0	0	0	0	0
34.0830	8.9810	-14.9700	H	0	0	0	0	0	0	0	0	0	0	0	0
32.5270	8.8670	-14.1950	H	0	0	0	0	0	0	0	0	0	0	0	0
38.4400	8.5880	-12.7500	N	0	0	3	0	0	0	0	0	0	0	0	0
33.1050	12.1630	-11.7780	C	0	0	0	0	0	0	0	0	0	0	0	0
33.8800	11.9120	-11.0500	H	0	0	0	0	0	0	0	0	0	0	0	0

54.8920	9.2780	21.7990	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.1090	8.6430	22.6650	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6040	9.0110	21.0100	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.5740	8.9970	21.2900	O	0	0	0	0	0	0	0	0	0	0	0	0	0
52.6430	8.6480	22.2240	C	0	0	0	0	0	0	0	0	0	0	0	0	0
51.3050	8.4530	21.5610	C	0	0	0	0	0	0	0	0	0	0	0	0	0
51.2940	8.9570	20.5890	H	0	0	0	0	0	0	0	0	0	0	0	0	0
51.1850	7.3810	21.3680	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1620	8.9570	22.4440	C	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1680	8.3460	23.3570	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2070	8.7510	21.9460	H	0	0	0	0	0	0	0	0	0	0	0	0	0
52.8600	8.4950	23.4180	O	0	0	0	0	0	0	0	0	0	0	0	0	0
53.0480	14.6540	11.1930	C	0	0	0	0	0	0	0	0	0	0	0	0	0
53.6430	15.4490	10.7280	H	0	0	0	0	0	0	0	0	0	0	0	0	0
52.0870	15.1110	11.4530	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.5580	11.2360	8.1260	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.1780	11.0480	9.0090	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.1940	11.7940	7.4260	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.3670	12.0830	8.5770	C	0	0	0	0	0	0	0	0	0	0	0	0	0
52.8240	12.5110	7.7290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
52.6760	11.4540	9.1540	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.8190	13.2150	9.4630	C	0	0	0	0	0	0	0	0	0	0	0	0	0
52.7820	13.5950	10.2620	O	0	0	0	0	0	0	0	0	0	0	0	0	0
54.9330	13.7180	9.4580	O	0	0	0	0	0	0	0	0	0	0	0	0	0
53.7200	14.1180	12.4520	C	0	0	0	0	0	0	0	0	0	0	0	0	0
53.0910	13.3440	12.9050	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.6820	13.6600	12.1970	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.9070	15.1970	13.3640	O	0	0	0	0	0	0	0	0	0	0	0	0	0
54.7500	14.8660	14.4680	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.6560	14.3580	14.1170	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.0670	15.8160	14.9120	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.0180	14.0390	15.5260	C	0	0	0	0	0	0	0	0	0	0	0	0	0
53.1040	14.5640	15.8290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.6950	13.0840	15.0980	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.9100	13.7820	16.7420	C	0	0	0	0	0	0	0	0	0	0	0	0	0
55.8220	13.2670	16.4190	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.2190	14.7400	17.1790	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.2020	12.9410	17.8100	C	0	0	0	0	0	0	0	0	0	0	0	0	0
53.3070	13.4670	18.1620	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.8720	11.9920	17.3710	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.1340	12.6640	18.9890	C	0	0	0	0	0	0	0	0	0	0	0	0	0
56.0500	12.1740	18.6340	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.4600	13.6080	19.4440	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.4870	11.7880	20.0600	C	0	0	0	0	0	0	0	0	0	0	0	0	0
53.6250	12.2980	20.5030	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.1620	10.8430	19.6150	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.4730	11.5460	21.0620	O	0	0	0	0	0	0	0	0	0	0	0	0	0
55.0140	10.7570	22.1650	C	0	0	0	0	0	0	0	0	0	0	0	0	0
54.0790	11.1730	22.5570	H	0	0	0	0	0	0	0	0	0	0	0	0	0
55.7810	10.8610	22.9390	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.0620	12.8350	17.2240	C	0	0	0	0	0	0	0	0	0	0	0	0	0
48.2940	12.8850	16.4420	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2460	13.8800	17.5080	H	0	0	0	0	0	0	0	0	0	0	0	0	0
48.5900	12.0400	18.3750	N	0	0	0	0	0	0	0	0	0	0	0	0	0
49.4250	12.2990	19.5640	C	0	0	0	0	0	0	0	0	0	0	0	0	0
50.4830	12.3010	19.2830	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2120	13.2890	19.9860	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2470	11.2110	20.6350	C	0	0	0	0	0	0	0	0	0	0	0	0	0
48.2610	11.2990	21.1020	H	0	0	0	0	0	0	0	0	0	0	0	0	0
49.2930	10.2280	20.1530	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.3400	11.3220	21.7080	C	0	0	0	0	0	0	0	0	0	0	0	0	0
51.3180	11.1890	21.2290	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.3710	12.3510	22.0850	H	0	0	0	0	0	0	0	0	0	0	0	0	0
47.1650	12.3140	18.6460	C	0	0	0	0	0	0	0	0	0	0	0	0	0
46.8850	12.0090	19.6610	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.9470	13.3900	18.6060	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.2480	10.3780	22.8330	N	0	0	3	0	0	0	0	0	0	0	0	0	0
50.3110	12.2380	16.5630	C	0	0	0	0	0	0	0	0	0	0	0	0	0
51.1650	12.2240	17.2440	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.1300	11.2120	16.2250	H	0	0	0	0	0	0	0	0	0	0	0	0	0
50.6900	13.0230	15.4370	O	0	0	0	0	0	0	0	0	0	0	0	0	0
50.0350	12.8750	14.7320	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.2410	11.5430	17.6970	C	0	0	0	0	0	0	0	0	0	0	0	0	0
46.3390	11.8850	16.6640	H	0	0	0	0	0	0	0	0	0	0	0	0	0
46.4550	10.4690	17.7370	H	0	0	0	0	0	0	0	0	0	0	0	0	0
44.8900	11.7390	18.1010	O	0	0	0	0	0	0	0	0	0	0	0	0	0
44.3350	11.2410	17.4750	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.7360	11.8080	38.3630	C	0	0	0	0	0	0	0	0	0	0	0	0	0
54.3390	12.7240	38.3160	H	0	0	0	0	0	0	0	0	0	0	0	0	0
53.8250	11.3430	37.3760	H	0	0	0	0	0	0	0	0	0	0	0	0	0
54.2730	10.8740	39.3130	O	0	0	0	0	0	0	0	0	0	0	0	0	0

54.7490	11.4080	40.4750	C	0	0	0	0	0	0	0	0	0	0	0	0
55.2920	10.3000	41.3450	C	0	0	0	0	0	0	0	0	0	0	0	0
54.4840	9.5880	41.5440	H	0	0	0	0	0	0	0	0	0	0	0	0
56.0930	9.7910	40.7980	H	0	0	0	0	0	0	0	0	0	0	0	0
55.8370	10.8240	42.6620	C	0	0	0	0	0	0	0	0	0	0	0	0
56.6510	11.5370	42.4960	H	0	0	0	0	0	0	0	0	0	0	0	0
56.2240	10.0000	43.2700	H	0	0	0	0	0	0	0	0	0	0	0	0
55.0560	11.3350	43.2360	H	0	0	0	0	0	0	0	0	0	0	0	0
54.7320	12.5950	40.7670	O	0	0	0	0	0	0	0	0	0	0	0	0
47.9840	13.0070	27.8200	C	0	0	0	0	0	0	0	0	0	0	0	0
47.2430	13.7300	27.4590	H	0	0	0	0	0	0	0	0	0	0	0	0
47.4590	12.0860	28.1000	H	0	0	0	0	0	0	0	0	0	0	0	0
49.1760	10.7120	23.7890	C	0	0	0	0	0	0	0	0	0	0	0	0
48.2140	10.8410	23.2790	H	0	0	0	0	0	0	0	0	0	0	0	0
49.0320	9.8730	24.4840	H	0	0	0	0	0	0	0	0	0	0	0	0
49.5110	11.9360	24.6460	C	0	0	0	0	0	0	0	0	0	0	0	0
50.4630	11.7660	25.1650	H	0	0	0	0	0	0	0	0	0	0	0	0
49.5930	12.8510	24.0530	H	0	0	0	0	0	0	0	0	0	0	0	0
48.4260	12.1580	25.6690	C	0	0	0	0	0	0	0	0	0	0	0	0
48.9430	12.7370	26.7890	O	0	0	0	0	0	0	0	0	0	0	0	0
47.2470	11.8840	25.4920	O	0	0	0	0	0	0	0	0	0	0	0	0
48.7130	13.5730	29.0320	C	0	0	0	0	0	0	0	0	0	0	0	0
49.4590	12.8500	29.3800	H	0	0	0	0	0	0	0	0	0	0	0	0
49.2430	14.4900	28.7500	H	0	0	0	0	0	0	0	0	0	0	0	0
47.7620	13.8500	30.0560	O	0	0	0	0	0	0	0	0	0	0	0	0
48.3450	14.4230	31.2280	C	0	0	0	0	0	0	0	0	0	0	0	0
49.0760	15.1930	30.9560	H	0	0	0	0	0	0	0	0	0	0	0	0
47.5330	14.9220	31.7680	H	0	0	0	0	0	0	0	0	0	0	0	0
48.9630	13.3510	32.1260	C	0	0	0	0	0	0	0	0	0	0	0	0
48.2130	12.5780	32.3340	H	0	0	0	0	0	0	0	0	0	0	0	0
49.7790	12.8450	31.6000	H	0	0	0	0	0	0	0	0	0	0	0	0
49.4880	13.9450	33.4350	C	0	0	0	0	0	0	0	0	0	0	0	0
50.2390	14.7130	33.2120	H	0	0	0	0	0	0	0	0	0	0	0	0
48.6680	14.4400	33.9680	H	0	0	0	0	0	0	0	0	0	0	0	0
50.1060	12.8690	34.3310	C	0	0	0	0	0	0	0	0	0	0	0	0
49.3540	12.1030	34.5560	H	0	0	0	0	0	0	0	0	0	0	0	0
50.9250	12.3720	33.7970	H	0	0	0	0	0	0	0	0	0	0	0	0
50.6360	13.4630	35.6370	C	0	0	0	0	0	0	0	0	0	0	0	0
51.3880	14.2340	35.4250	H	0	0	0	0	0	0	0	0	0	0	0	0
49.8280	13.9740	36.1760	H	0	0	0	0	0	0	0	0	0	0	0	0
51.2490	12.3970	36.5400	C	0	0	0	0	0	0	0	0	0	0	0	0
50.4950	11.6430	36.7960	H	0	0	0	0	0	0	0	0	0	0	0	0
52.0830	11.9070	36.0270	H	0	0	0	0	0	0	0	0	0	0	0	0
51.7130	13.0310	37.7320	O	0	0	0	0	0	0	0	0	0	0	0	0
52.2750	12.1210	38.6750	C	0	0	0	0	0	0	0	0	0	0	0	0
51.6780	11.2030	38.7420	H	0	0	0	0	0	0	0	0	0	0	0	0
52.2080	12.5960	39.6600	H	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									
5	7	1	0	0	0	0									
5	8	1	0	0	0	0									
8	9	1	0	0	0	0									
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8	11	1	0	0	0	0									
11	12	1	0	0	0	0									
11	13	1	0	0	0	0									
11	17	1	0	0	0	0									
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14	24	1	0	0	0	0									
17	18	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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33	34	1	0	0	0	0									

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37	95	1	0	0	0	0
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41	53	1	0	0	0	0
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75	76	1	0	0	0	0
76	77	1	0	0	0	0
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337340	1	0	0	0	0
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342343	1	0	0	0	0
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342345	1	0	0	0	0
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350362	1	0	0	0	0
353354	1	0	0	0	0
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356357	1	0	0	0	0
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59.6440	-18.8570	12.8000	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8690	-19.6470	13.5290	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.7870	-19.3420	11.8250	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.6480	-17.8050	12.9810	N	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72.4790	-11.7740	19.5780	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72.4260	-11.0730	18.7360	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72.0390	-12.7090	19.2160	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
73.8400	-12.0670	19.9330	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
74.7080	-11.0150	19.8950	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
76.0890	-11.4980	20.2720	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
76.0460	-11.9180	21.2820	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
76.3860	-12.2830	19.5690	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
77.1150	-10.3780	20.2360	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
77.1820	-9.9380	19.2350	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
78.1040	-10.7580	20.5090	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
76.8490	-9.5790	20.9360	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
74.4130	-9.8650	19.6080	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.3060	-16.2320	18.7830	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.3110	-15.8310	19.0170	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5930	-16.8410	19.6480	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.4820	-16.9160	14.1270	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.2850	-16.1670	14.1230	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.5430	-16.3540	14.0560	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.5670	-17.6550	15.4640	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.7490	-18.3690	15.5990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.5170	-18.2010	15.5150	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60.5070	-16.6650	16.5960	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61.2610	-17.1030	17.6420	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59.8610	-15.6260	16.5750	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.3260	-15.1180	18.5770	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.3080	-15.5570	18.3720	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.0490	-14.5030	17.7130	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.3680	-14.3120	19.7510	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.2710	-13.2110	19.6480	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63.1810	-12.7290	18.6670	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62.9590	-12.4780	20.3990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.7100	-13.6430	19.9320	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64.7470	-14.1560	20.9010	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.0350	-14.3800	19.1900	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.6710	-12.4530	19.9260	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.6310	-11.9550	18.9490	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65.3520	-11.7190	20.6760	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.1080	-12.8920	20.2190	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.1480	-13.3830	21.1990	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.4250	-13.6320	19.4740	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.0730	-11.7060	20.2020	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68.0430	-11.2080	19.2250	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67.7590	-10.9510	20.9340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69.5060	-12.1370	20.5040	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69.5580	-12.5920	21.5000	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69.8420	-12.8650	19.7600	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70.3400	-10.9790	20.4660	O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71.7040	-11.2530	20.7850	C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71.7780	-11.9430	21.6340	H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72.1500	-10.3110	21.1240	H	0	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	0
1	7	1	0	0	0	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	0	0	0
2	3	1	0	0	0	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	0	0	0
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9	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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12	13	1	0	0	0	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	0	0	0
12	15	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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M END
> <NAME>
U93_1

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