

## Electronic Supporting Information

Title: Lanthanide-induced conformational change of methanol dehydrogenase involving coordination change of cofactor pyrroloquinoline quinone

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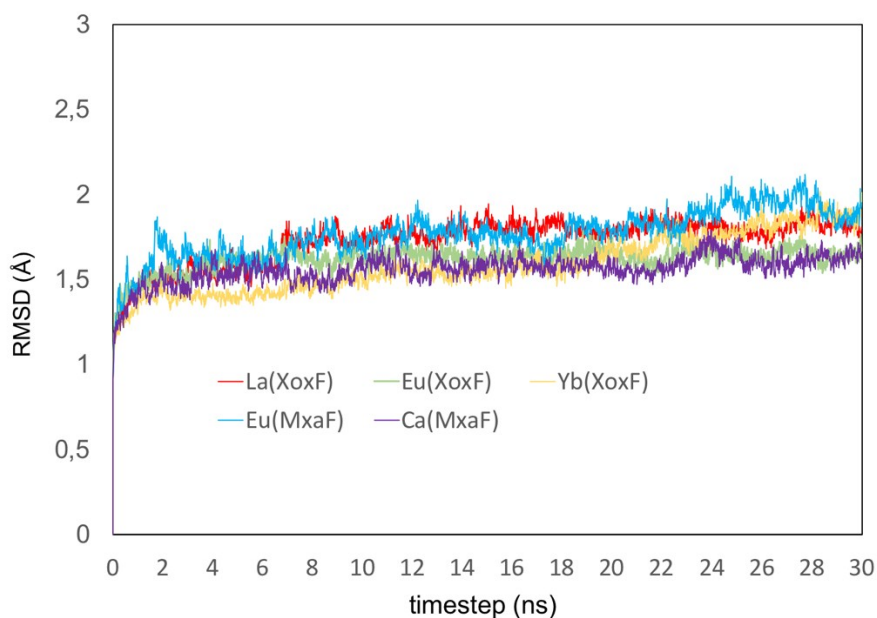
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**Fig.S1:** Time evolution of RMSD (excluding waters and counterions) in all MD simulations

**Fig.S2:** Radial distribution functions around central metal ion in all MD simulations (X-axis in Å)

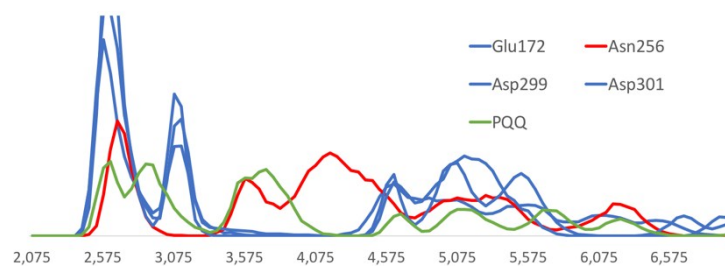
**Fig.S3** Coordination sphere around  $\text{Eu}^{3+}$  in  $\text{XoxF}^-$  and  $\text{MxaF}^-$ -type Eu-MDH obtained by MD simulation.

XYZ coordinates all atoms excluding waters and counterions of MD simulations of Eu-MDH and Yb-MDH of  $\text{XoxF}^-$ -type at  $t = 50$  ns

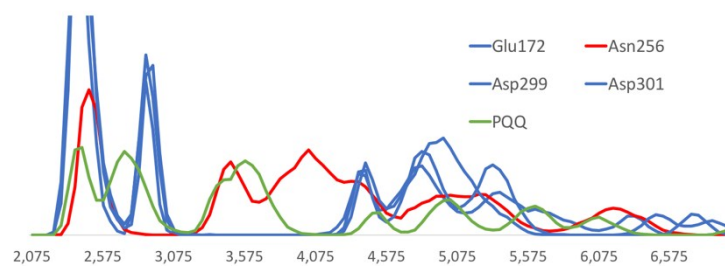


**Fig.S1** Time evolution of RMSD (excluding waters and counterions) of all MD simulations

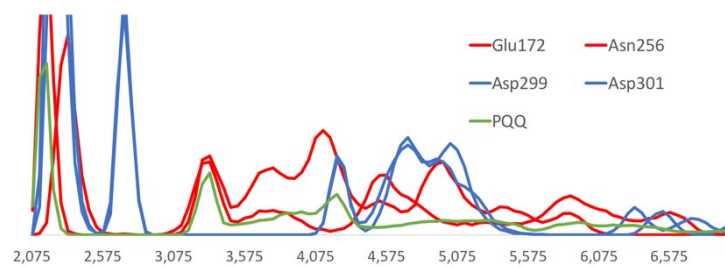
### La-MDH of XoxF type



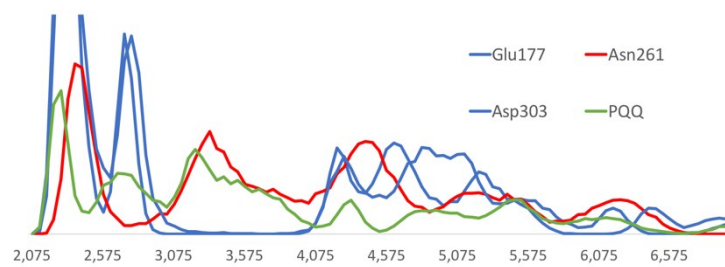
### Eu-MDH of XoxF type



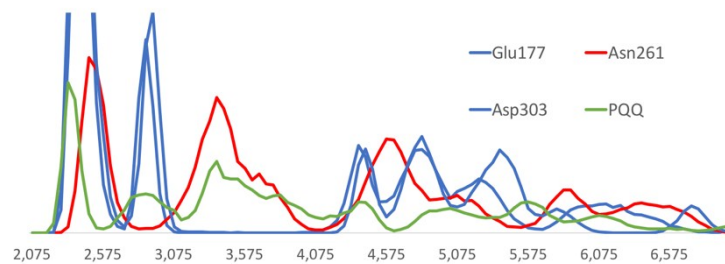
### Yb-MDH of XoxF type



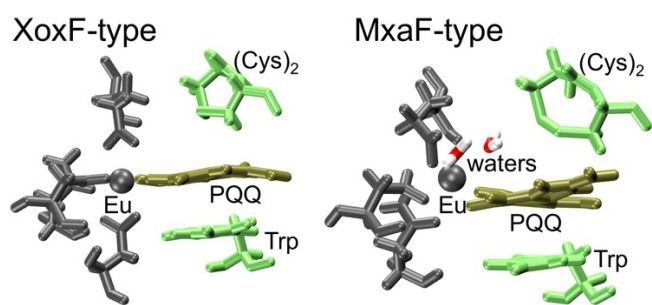
### Ca-MDH of MxaF type



### Eu-MDH of MxaF type



**Fig.S2** Radial distribution functions around central metal ion in all MD simulations (X-axis in Å)



**Fig.S3** Coordination sphere around  $\text{Eu}^{3+}$  in XoxF- and MxaF-type Eu-MDH obtained from MD simulation.

## Eu-MDH (XoxF type)

				-3.9070	7.5360	24.8780	C	0	0.9970	-1.4860	30.6660	H	0	
				-3.6060	8.3740	24.2490	H	0	2.6740	-0.4120	29.8170	N	0	
-10.4320	8.1090	23.1150	N	0	-4.9920	7.4340	24.9170	H	0	2.8780	0.4500	29.3320	H	0
-11.0670	8.6590	22.5540	H	0	-3.3930	7.7070	25.8240	H	0	3.3380	-0.3710	30.5770	H	0
-10.5680	8.3200	24.0930	H	0	-3.3610	2.3780	25.1180	C	0	2.8730	-1.1180	29.1220	H	0
-10.8900	7.2180	22.9860	H	0	-2.2440	1.7080	25.1100	O	0	-0.3690	-2.7360	25.8350	C	0
-9.0400	7.9830	22.6730	C	0	-4.4840	1.8550	25.6030	N	0	0.4540	-3.5050	26.2550	O	0
-9.0590	7.5360	21.6790	H	0	-5.2730	2.4860	25.5790	H	0	-1.5750	-3.2560	25.3970	N	0
-8.4470	9.3490	22.2860	C	0	-4.7200	0.4700	26.1160	C	0	-2.3000	-2.6570	25.0290	H	0
-8.3890	9.8980	23.2250	H	0	-4.0140	0.2220	26.9080	H	0	-1.8780	-4.7010	25.5360	C	0
-7.4260	9.2840	21.9100	H	0	-6.1770	0.3530	26.7990	C	0	-1.8870	-4.9290	26.6020	H	0
-9.3580	10.0440	21.3200	C	0	-6.8400	0.9610	26.1830	H	0	-3.3750	-4.8520	25.1900	C	0
-10.0590	9.4630	20.5420	O	0	-6.5750	-0.6620	26.8150	H	0	-3.9980	-4.3320	25.9180	H	0
-9.4420	11.3880	21.3900	N	0	-6.2820	0.9600	28.1820	C	0	-3.5250	-4.5460	24.1550	H	0
-10.1830	11.6700	20.7650	H	0	-5.7260	0.3080	28.8560	H	0	-3.8380	-6.2960	25.2920	C	0
-8.9820	11.9010	22.1290	H	0	-5.7430	1.9040	28.1040	H	0	-4.8690	-6.2940	24.9370	H	0
-8.1720	7.1340	23.5550	C	0	-7.7040	1.2050	28.5980	C	0	-3.1810	-6.9060	24.6730	H	0
-7.2050	6.6370	23.0760	O	0	-8.2010	1.7810	27.8170	H	0	-3.8800	-6.9490	26.7280	C	0
-8.4670	6.9930	24.8660	N	0	-8.1030	0.2030	28.7540	H	0	-3.4140	-6.3170	27.6940	O	0
-9.1090	7.6420	25.2990	H	0	-7.8250	1.8800	29.9580	C	0	-4.4180	-8.0930	26.9910	O	0
-7.6280	6.0610	25.6830	C	0	-8.7870	1.6680	30.4250	H	0	-0.9880	-5.5740	24.7170	C	0
-6.6090	6.4370	25.5890	H	0	-7.0690	1.4280	30.6010	H	0	-0.7280	-5.2750	23.5060	O	0
-7.8830	6.3460	27.2210	C	0	-7.5700	3.3400	29.8940	N	0	-0.4490	-6.6460	25.2840	N	0
-7.2240	5.7250	27.8270	H	0	-6.7120	3.6510	29.4610	H	0	-0.5110	-6.9500	26.7800	C	0
-7.6720	7.3940	27.4350	H	0	-8.3050	3.8030	29.3790	H	0	-1.4230	-7.5260	26.9380	H	0
-9.2620	5.8610	27.6800	C	0	-7.6670	3.8710	30.7480	H	0	-0.3890	-6.0980	27.4490	H	0
-9.4030	4.8350	28.3660	O	0	-4.5570	-0.6540	25.0900	C	0	0.6750	-7.8720	27.0540	C	0
-10.1970	6.5700	27.3640	O	0	-4.0100	-1.6320	25.4830	O	0	0.5110	-8.5060	27.9260	H	0
-7.5760	4.5850	25.2860	C	0	-4.9100	-0.4620	23.8160	N	0	1.5120	-7.2140	27.2890	H	0
-6.6590	3.8620	25.7310	O	0	-5.4140	0.3660	23.5320	H	0	0.8240	-8.5970	25.7190	C	0
-8.5250	4.1730	24.4680	N	0	-4.7400	-1.5970	22.8090	C	0	0.2330	-9.5120	25.6770	H	0
-9.1030	4.8170	23.9480	H	0	-4.7550	-2.5560	23.3280	H	0	1.8520	-8.9600	25.7050	H	0
-8.6950	2.7220	24.1290	C	0	-5.9750	-1.4660	21.8520	C	0	0.4770	-7.6160	24.5880	C	0
-8.6220	2.1620	25.0610	H	0	-6.1230	-0.4050	21.6510	H	0	1.3840	-7.1410	24.2140	H	0
-10.0450	2.4270	23.3780	C	0	-5.6770	-1.9570	20.9260	H	0	-0.1720	-8.2100	23.3770	C	0
-10.0080	2.5130	22.2920	H	0	-7.3520	-2.0340	22.2970	C	0	-1.2580	-8.7610	23.4960	O	0
-10.3240	1.4060	23.6370	H	0	-7.6150	-1.6930	23.2980	H	0	0.4850	-8.1860	22.1990	N	0
-11.2560	3.3010	23.8520	C	0	-8.4870	-1.4710	21.4080	C	0	1.1980	-7.4870	22.0410	H	0
-12.1380	2.6610	23.8060	H	0	-8.3830	-0.4200	21.1400	H	0	0.1510	-9.0150	21.0230	C	0
-11.0490	3.6110	24.8760	H	0	-8.6860	-1.9850	20.4670	H	0	0.9740	-8.7650	20.3530	H	0
-11.3820	4.5260	22.9380	C	0	-9.4250	-1.4950	21.9630	H	0	0.1670	-10.0710	21.2930	H	0
-12.1990	4.6310	21.9860	O	0	-7.4050	-3.5470	22.1780	C	0	-1.1290	-8.6210	20.2560	C	0
-10.6640	5.4510	23.2030	O	0	-8.4280	-3.8870	22.3410	H	0	-1.5650	-9.4980	19.5480	O	0
-7.5820	2.2930	23.2250	C	0	-7.0570	-3.8030	21.1770	H	0	-1.6870	-7.4080	20.3380	N	0
-7.1140	1.1900	23.3040	O	0	-6.7830	-3.9580	22.9740	H	0	-1.2000	-6.7510	20.9310	H	0
-7.0770	3.1860	22.3430	N	0	-3.4040	-1.6970	22.0910	C	0	-2.9000	-7.0850	19.6330	C	0
-7.5530	4.0730	22.2620	H	0	-3.0220	-2.7710	21.7340	O	0	-3.5960	-7.9180	19.5360	H	0
-5.9260	2.8510	21.4620	C	0	-2.5010	-0.7190	22.2170	N	0	-3.7650	-5.9910	20.4120	C	0
-6.0770	1.8880	20.9750	H	0	-2.8470	0.1360	22.6300	H	0	-3.1700	-5.0930	20.5760	H	0
-5.8800	3.9330	20.3250	C	0	-1.0890	-0.7500	21.9530	C	0	-4.7120	-5.7730	19.9180	H	0
-6.2930	4.8210	20.8030	H	0	-0.8790	-1.5920	21.3230	H	0	-3.9780	-6.4450	21.8700	C	0
-4.8680	4.2290	20.0490	H	0	-0.7010	0.5130	21.2010	C	0	-3.0350	-6.5240	22.4120	H	0
-6.6830	3.7610	19.0510	C	0	-1.4950	0.6780	20.4730	H	0	-4.4450	-5.6560	22.4600	H	0
-6.6420	4.7010	18.4990	H	0	-0.8200	1.4540	21.7380	H	0	-4.7900	-7.7310	22.0960	C	0
-6.0370	2.8200	18.0230	C	0	0.6970	0.6430	20.4440	C	0	-6.0110	-7.7070	21.9320	O	0
-6.0540	1.8180	18.4500	H	0	0.7500	1.5920	19.9090	H	0	-4.3740	-8.8470	22.7100	N	0
-6.5930	3.0010	17.1020	H	0	1.5470	0.7810	21.1120	H	0	-4.9800	-9.6430	22.5710	H	0
-4.9870	3.0880	17.9080	H	0	0.7940	-0.4350	19.4320	C	0	-3.4440	-8.9400	23.0930	H	0
-8.0850	3.3360	19.3250	C	0	-0.2060	-1.1590	19.0840	O	0	-2.3910	-6.5740	18.2130	C	0
-8.1380	2.3730	19.8320	H	0	1.8860	-0.6710	18.8430	O	0	-1.1630	-6.4940	17.9420	O	0
-8.6610	4.1530	19.7600	H	0	-0.2660	-0.9180	23.2110	C	0	-3.2990	-6.3710	17.2330	N	0
-8.5730	3.1110	18.3770	H	0	0.9390	-1.1970	23.0570	O	0	-4.2720	-6.2530	17.4790	H	0
-4.6110	2.8690	22.2230	C	0	-0.7560	-0.7200	24.4240	N	0	-3.0700	-5.9990	15.8740	C	0
-3.6290	2.1700	21.8350	O	0	-1.6770	-0.3090	24.4780	H	0	-2.3010	-5.2390	15.7340	H	0
-4.5940	3.5930	23.3660	N	0	-0.0800	-1.2760	25.6760	C	0	-2.7770	-7.2870	15.0670	C	0
-5.3840	4.1680	23.6230	H	0	1.0010	-1.1940	25.5560	H	0	-2.0540	-7.8130	15.6890	H	0
-3.5180	3.6810	24.3050	C	0	-0.5190	-0.4630	26.8920	C	0	-3.6650	-7.9190	15.0860	H	0
-2.5650	3.7430	23.7800	H	0	-0.1900	0.5620	26.7230	H	0	-2.1210	-7.1270	13.7110	C	0
-3.5160	4.9970	25.1240	C	0	-1.5890	-0.4220	27.0930	H	0	-2.6960	-6.7750	12.5310	C	0
-4.5150	5.1320	25.5390	H	0	0.2460	-0.9760	28.1010	C	0	-3.7260	-6.4600	12.4470	H	0
-2.5590	5.0190	26.3650	C	0	-0.2310	-1.8560	28.5330	H	0	-1.8060	-6.7950	11.5090	N	0
-2.6680	4.1270	26.9820	H	0	1.2590	-1.2230	27.7840	H	0	-2.0290	-6.7120	10.5270	H	0
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-2.8170	5.8870	26.9720	H	0	0.7530	1.0270	29.0480	H	0	0.6410	-7.1040	11.3470	C	0
-3.3560	6.2600	24.2340	C	0	-0.6320	0.0950	29.7870	H	0	0.6220	-6.6260	10.3780	H	0
-2.3020	6.4040	23.9990	H	0	1.3180	-0.4840	30.3790	C	0	1.7790	-7.5180	10.0240	C	0
-3.9070	6.0240	23.3240	H	0	1.3770	0.0790	31.3100	H	0	2.7090	-7.4760	11.4750	H	0

1.6280	-7.8720	13.4120	C	0	1.9790	-3.3470	13.9370	H	0	5.2340	0.0130	11.6350	C	0
2.4280	-8.0850	14.1070	H	0	1.3200	-4.8410	15.4030	C	0	5.9740	0.6070	11.1000	H	0
0.3240	-7.7940	14.0140	C	0	0.6290	-5.6830	15.3590	H	0	5.4820	0.0330	13.2100	C	0
0.1650	-7.9150	15.0750	H	0	2.3540	-5.1640	15.5240	H	0	6.4620	-0.4140	13.3820	H	0
-0.7640	-7.3530	13.3580	C	0	1.0170	-3.7130	16.4710	C	0	5.4310	1.4380	13.7020	C	0
-4.3260	-5.2860	15.3030	C	0	1.7090	-2.8750	16.3920	H	0	6.3480	1.8810	13.3150	H	0
-5.2800	-5.9560	14.8940	O	0	0.0050	-3.3090	16.4400	H	0	4.6410	1.9630	13.1650	H	0
-4.5350	-3.9850	15.5140	N	0	1.1530	-4.4230	17.8060	C	0	5.3710	1.6160	14.7760	H	0
-3.8020	-3.5830	16.0810	H	0	0.2000	-4.8590	18.1040	H	0	4.5880	-0.7150	13.9440	O	0
-5.7450	-3.1580	15.3800	C	0	1.8610	-5.2460	17.7140	H	0	3.6990	-0.3690	13.8380	H	0
-6.6310	-3.7930	15.3780	H	0	1.5500	-3.4590	18.8360	N	0	5.4570	-1.4330	11.2840	C	0
-5.9440	-2.2890	16.6620	C	0	2.3250	-2.9380	18.4520	H	0	6.5870	-1.6980	10.9550	O	0
-6.9150	-1.7970	16.6170	H	0	0.8880	-2.7000	18.9000	H	0	4.4480	-2.2980	11.3450	N	0
-5.9860	-3.1350	17.9790	C	0	1.7880	-3.8900	19.7180	H	0	3.6180	-1.9680	11.8160	H	0
-6.5450	-4.0560	17.8140	H	0	-0.8590	-2.6330	14.0540	C	0	4.3960	-3.7940	11.1480	C	0
-4.9690	-3.4560	18.2070	H	0	-1.8510	-2.8350	14.7940	O	0	3.3500	-4.0390	11.3300	H	0
-6.3480	-2.5090	18.7940	H	0	-0.4170	-1.4370	13.6460	N	0	4.7720	-4.0860	9.6610	C	0
-4.8800	-1.1690	16.7200	C	0	0.2970	-1.4860	12.9340	H	0	5.7400	-3.7350	9.3040	H	0
-3.8520	-1.5280	16.6780	H	0	-0.7460	-0.1420	14.3190	C	0	4.7830	-5.1710	9.5520	H	0
-5.0500	-0.3320	13.2890	H	0	-1.7210	-0.2850	14.8750	H	0	3.8100	-3.5190	8.6560	C	0
-4.8740	-0.6790	17.6940	H	0	0.2160	-0.1010	15.4700	C	0	2.7930	-3.5950	9.0420	H	0
-5.8910	-2.2800	14.0550	C	0	-0.1290	0.8040	15.9690	H	0	3.9830	-2.4460	8.5650	H	0
-6.9360	-1.8050	13.6940	O	0	0.0020	-0.9720	16.0890	H	0	3.9730	-4.1460	7.2810	C	0
-4.7890	-2.3280	13.2890	N	0	1.7590	0.1050	15.1760	C	0	3.2030	-3.7650	6.6110	H	0
-3.9520	-2.7910	13.6140	H	0	2.2110	0.4890	14.1190	O	0	4.9440	-3.7630	6.9670	H	0
-4.6720	-1.8850	11.8580	C	0	2.5580	-0.3680	16.0780	N	0	3.8340	-5.5770	7.3580	N	0
-5.6920	-1.7930	11.4850	H	0	3.5410	-0.5630	15.9540	H	0	4.7030	-6.0690	7.2080	H	0
-3.9960	-0.5130	11.7430	C	0	2.2780	-0.6400	17.0100	H	0	2.7300	-6.2720	7.5220	C	0
-4.4420	0.0890	12.5340	H	0	-0.7810	0.9870	13.3800	C	0	1.5900	-5.6530	7.6590	N	0
-2.9530	-0.5870	12.0530	H	0	-0.1590	0.9400	12.2950	O	0	1.5980	-4.6560	7.4980	H	0
-4.0020	0.2380	10.4400	C	0	-1.4340	2.0720	13.6450	N	0	0.6780	-6.0830	7.6110	H	0
-5.0370	0.1580	10.1080	H	0	-1.8800	2.1080	14.5500	H	0	2.7170	-7.5140	7.4300	N	0
-3.7160	1.2600	10.6870	H	0	-1.8080	3.1860	12.6840	C	0	3.4280	-7.9810	6.8870	H	0
-2.8060	-0.2510	9.1600	S	0	-2.1640	2.6510	11.8040	H	0	1.9100	-8.0370	7.7380	H	0
-3.2190	0.8940	7.8640	C	0	-3.0290	3.8970	13.3420	C	0	5.2000	-4.6260	12.1400	C	0
-3.4380	1.8570	8.3250	H	0	-2.7800	4.2370	14.3480	H	0	5.1690	-5.8990	12.0510	O	0
-2.4470	0.9520	7.0970	H	0	-3.2480	4.8660	12.8940	H	0	6.0110	-3.9660	12.9570	N	0
-4.0650	0.4900	7.3070	H	0	-4.3870	3.1890	13.2650	C	0	6.0500	-2.9730	12.7740	H	0
-3.9310	-3.0430	11.1900	C	0	-5.0530	3.0270	12.0280	C	0	6.6810	-4.5860	14.0900	C	0
-3.1890	-3.7280	11.8990	O	0	-4.6260	3.5000	11.1560	H	0	7.2160	-5.4630	13.7230	H	0
-4.0600	-3.3030	9.8210	N	0	-6.3510	2.4660	12.0610	C	0	7.6310	-3.5700	14.7250	C	0
-4.7680	-2.8830	9.2360	H	0	-6.8830	2.3580	11.1270	H	0	8.2920	-3.1570	13.9640	H	0
-3.3570	-4.3340	9.0210	C	0	-6.9360	1.9850	13.2400	C	0	6.9990	-2.7390	15.0400	H	0
-3.6800	-5.3010	9.4060	H	0	-8.1550	1.4400	13.2600	O	0	8.4220	-4.0970	15.9490	C	0
-3.7040	-4.1950	7.5120	C	0	-8.5690	1.4060	14.1250	H	0	9.4120	-5.1350	15.8280	C	0
-3.3280	-3.2110	7.2310	H	0	-6.2020	2.0870	14.4540	C	0	9.4970	-5.5730	14.8440	H	0
-3.1260	-4.9200	6.9400	H	0	-6.7100	1.6630	15.3080	H	0	10.2280	-5.4640	16.9200	C	0
-5.2920	-4.3210	7.2670	C	0	-4.9200	2.6820	14.4930	C	0	10.9910	-6.2280	16.9310	H	0
-5.8040	-3.9380	8.1500	H	0	-4.3100	2.6890	15.3840	H	0	9.9250	-4.8810	18.1340	C	0
-5.7010	-3.7020	6.4700	H	0	-0.6050	4.0910	12.2750	C	0	10.7150	-5.3100	19.1870	O	0
-5.8170	-5.7350	6.9520	C	0	-0.8010	4.8590	11.3570	O	0	10.3630	-5.1550	20.0670	H	0
-5.3410	-6.4400	6.0550	O	0	0.5270	3.9810	13.0040	N	0	8.8950	-3.9420	18.2860	C	0
-6.8920	-6.1720	7.6130	N	0	0.4660	3.3450	13.7870	H	0	8.6550	-3.4110	19.1950	H	0
-7.2270	-7.1050	7.4220	H	0	1.8190	4.3500	12.5330	C	0	8.1390	-3.6060	17.1840	C	0
-7.2610	-5.5250	8.2950	H	0	1.7920	5.3850	12.1920	H	0	7.4170	-2.8050	17.2420	H	0
-1.8660	-4.2390	9.1370	C	0	2.7560	4.3940	13.7040	C	0	5.7090	-5.1290	15.1240	C	0
-1.2680	-5.3290	9.1120	O	0	3.6870	4.7890	13.2970	H	0	4.5910	-4.6340	15.2230	O	0
-1.2670	-3.0930	9.4590	N	0	2.4180	5.2740	14.2510	H	0	6.1640	-6.0490	15.9650	N	0
-1.8540	-2.2800	9.5830	H	0	2.9020	3.4820	14.2820	H	0	7.0690	-6.4850	15.8620	H	0
0.1770	-2.9840	9.7460	C	0	2.4510	3.4760	11.3680	C	0	5.5090	-6.3490	17.1990	C	0
0.5760	-3.8560	9.2290	H	0	3.5850	3.6400	10.8750	O	0	5.0670	-5.4220	17.5630	H	0
0.6350	-1.7570	8.8870	C	0	1.7190	2.4060	10.8900	N	0	4.3350	-7.3110	17.0070	C	0
-0.0960	-1.0310	9.2430	H	0	0.8010	2.2440	11.2800	H	0	3.7910	-6.7830	16.2250	H	0
1.6620	-1.4270	9.0400	H	0	1.9930	1.3450	9.8800	C	0	4.8630	-8.2320	16.7600	H	0
0.3800	-1.9230	7.4060	C	0	1.3400	0.4720	9.9130	H	0	3.4930	-7.4720	18.2100	O	0
0.4430	-2.9950	6.9210	O	0	1.9120	2.0570	8.3810	C	0	2.8400	-8.1220	17.9410	H	0
-0.0740	-0.8780	6.7070	N	0	2.6460	2.8620	8.3510	H	0	6.4630	-6.8470	18.2480	C	0
-0.5120	-1.0450	5.8120	H	0	2.2920	1.4400	7.5670	H	0	7.4590	-7.5700	18.0900	O	0
-0.0570	0.0860	7.0050	H	0	0.5360	2.5170	8.0750	C	0	6.1380	-6.5300	19.5340	N	0
0.5570	-3.0380	11.2030	C	0	-0.4230	2.2440	8.7950	O	0	5.3930	-5.8710	19.7110	H	0
1.4810	-2.3510	11.6120	O	0	0.3780	3.0480	6.8910	N	0	7.0350	-6.6620	20.7240	C	0
-0.1430	-3.7350	12.0420	N	0	-0.5150	3.4790	6.6980	H	0	8.0270	-6.6790	20.2730	H	0
-0.9110	-4.2580	11.6490	H	0	1.1990	3.2870	6.3530	H	0	6.8810	-5.4840	21.6720	C	0
-0.1010	-3.7970	13.4700	C	0	3.4140	0.6430	10.0390	C	0	6.8510	-4.5560	21.1000	H	0
-0.7510	-4.6500	13.6610	H	0	4.0730	0.2570	9.0610	O	0	5.8870	-5.5400	22.1160	H	0
1.2990	-4.1970	13.9960	C	0	3.8440	0.4750	11.2950	N	0	7.7890	-5.3580	22.8410	C	0
1.7530	-4.9360	13.3350	H	0	3.1720	0.7730	11.9870	H	0	7.7850	-4.3420	23.2370	H	0

7.3980	-5.9670	23.6550	H	0	12.1700	-16.3250	17.2150	C	0	10.3060	-23.0180	12.9440	O	0
9.2850	-5.5410	22.4730	C	0	11.8940	-15.3430	16.8310	H	0	12.4450	-23.1750	13.6050	N	0
10.0390	-6.4390	22.9870	O	0	12.6660	-16.0360	18.6520	C	0	13.2140	-22.8080	14.1470	H	0
9.7820	-4.8450	21.5960	O	0	13.6890	-15.6730	18.5540	H	0	12.6390	-24.5500	13.0950	C	0
6.8350	-8.0270	21.3610	C	0	12.0160	-15.3330	19.1720	H	0	12.8590	-24.6260	12.0300	H	0
6.5810	-8.1520	22.5570	O	0	12.8290	-17.3020	19.4510	C	0	13.9510	-24.8990	13.8060	C	0
7.0390	-9.0590	20.5640	N	0	13.8180	-17.9800	19.2610	O	0	14.1810	-25.9620	13.7440	H	0
7.2750	-8.8580	19.6030	H	0	11.9180	-17.5950	20.3670	N	0	14.8170	-24.4160	13.3530	H	0
6.8960	-10.4190	20.9630	C	0	11.7760	-18.4830	20.8270	H	0	13.9140	-24.6530	15.2570	O	0
6.6650	-10.5000	22.0250	H	0	11.2120	-16.8950	20.5470	H	0	14.3660	-25.3930	15.6690	H	0
5.7330	-10.8990	20.1780	C	0	13.2390	-17.0280	16.3940	C	0	11.5830	-25.5500	13.5970	C	0
6.0810	-10.9080	19.1450	H	0	13.0860	-18.1450	16.0110	O	0	11.3960	-26.5520	12.9140	O	0
5.6030	-11.9180	20.5430	H	0	14.4680	-16.4370	16.1690	N	0	10.9610	-25.2880	14.7280	N	0
4.4030	-10.1490	20.4420	C	0	14.7380	-15.5650	16.5990	H	0	11.0830	-24.3460	15.0730	H	0
4.4300	-9.0650	20.3330	H	0	15.5360	-17.1460	15.3590	C	0	10.0040	-26.1390	15.4410	C	0
3.4560	-10.6300	19.4490	C	0	15.0070	-17.4500	14.4560	H	0	10.1390	-27.1340	15.0170	H	0
3.7310	-10.5360	18.3990	H	0	16.7190	-16.1200	15.1080	C	0	10.2810	-26.0510	16.9450	C	0
3.2230	-11.6550	19.7350	H	0	17.5520	-16.6830	14.6870	H	0	9.9540	-25.0580	17.2510	H	0
2.4880	-10.1820	19.6750	H	0	16.3230	-14.9330	14.2220	C	0	9.8000	-26.9770	17.2600	H	0
3.8380	-10.4450	21.8610	C	0	15.4630	-14.4460	14.6810	H	0	11.8120	-26.2130	17.3280	C	0
3.9870	-11.4940	22.1180	H	0	17.1520	-14.2270	14.2830	H	0	12.3030	-26.8700	16.6100	H	0
4.4870	-9.9260	22.5670	H	0	16.0040	-15.2660	13.2350	H	0	12.3690	-25.2770	17.2810	H	0
2.8540	-10.0710	22.1450	H	0	17.1770	-15.7090	16.3920	O	0	12.0390	-26.7870	18.7440	C	0
8.1270	-11.2870	20.6860	C	0	17.8500	-16.3180	16.7060	H	0	11.7920	-27.8480	17.7380	H	0
8.9310	-11.0470	19.7690	O	0	16.1360	-18.4470	15.9360	C	0	13.0960	-26.5540	18.8720	H	0
8.3140	-12.2830	21.5350	N	0	17.0290	-19.0200	15.1970	O	0	11.3380	-26.0600	19.7710	N	0
7.6270	-12.3540	22.2730	H	0	15.8740	-18.8910	17.1400	N	0	11.7410	-25.1890	20.0860	H	0
9.5590	-13.0880	21.6480	C	0	15.1920	-18.2990	17.5930	H	0	10.1840	-26.4050	20.3050	C	0
10.3350	-12.7070	20.9840	H	0	16.3220	-20.1640	17.7180	C	0	9.4380	-27.2800	19.8020	N	0
10.1450	-12.7640	23.0790	C	0	17.2460	-20.5220	17.2640	H	0	9.8630	-27.9080	19.1350	H	0
9.3970	-12.7070	23.8690	H	0	16.6180	-19.8110	19.2030	C	0	8.5760	-27.5770	20.2370	H	0
10.8010	-13.6040	23.3090	H	0	15.6990	-19.5310	19.7180	H	0	9.7820	-25.7770	21.3310	N	0
10.9000	-11.4360	23.1600	C	0	17.0370	-20.6750	19.7170	H	0	10.3270	-25.0110	21.7000	H	0
11.8380	-11.2160	22.4820	O	0	17.5710	-18.5970	19.4720	C	0	8.8090	-25.9180	21.5630	H	0
10.4640	-10.5670	24.0510	N	0	18.4610	-18.7100	18.8520	H	0	8.5390	-25.8730	14.9960	C	0
10.8290	-9.6260	24.0160	H	0	17.0410	-17.6660	19.2730	H	0	7.7260	-26.7290	15.2630	O	0
9.7440	-10.8990	24.6770	H	0	17.8460	-18.5630	21.0400	C	0	8.3380	-24.7490	14.2810	N	0
9.3070	-14.6120	21.4290	C	0	18.0610	-17.5250	21.2960	H	0	9.1790	-24.3110	13.9350	H	0
10.2550	-15.3230	21.1570	O	0	16.9280	-18.8230	21.5670	H	0	7.0190	-24.2120	13.8930	C	0
8.0900	-15.0890	21.6310	N	0	18.9790	-19.4600	21.5390	C	0	6.4260	-23.9480	14.7690	H	0
7.3570	-14.3970	21.6950	H	0	18.9090	-19.5450	22.6240	H	0	7.0360	-22.8730	13.0640	C	0
7.8960	-16.5070	21.8370	C	0	18.8080	-20.4920	21.2350	H	0	7.9020	-22.3190	13.4260	H	0
8.6170	-16.8120	22.5960	H	0	20.2850	-19.0910	20.8950	N	0	7.1920	-23.1080	12.0110	H	0
6.5140	-16.9470	22.3500	C	0	20.5690	-18.1760	21.2140	H	0	5.7730	-22.0190	13.1370	C	0
5.8620	-17.0900	21.4880	H	0	21.0230	-19.7300	21.1520	H	0	4.8480	-22.5940	13.1850	H	0
6.7100	-17.8980	22.8440	H	0	20.3900	-19.1340	19.8910	H	0	5.7730	-21.0770	14.3530	C	0
5.7590	-16.0610	23.3720	C	0	15.2650	-21.2730	17.7600	C	0	4.7590	-20.6830	14.4250	H	0
6.3450	-15.9680	24.2860	H	0	15.7170	-22.3800	17.7210	O	0	5.9670	-21.6300	15.2710	H	0
5.5380	-15.0750	22.9630	H	0	13.9080	-21.0150	17.8160	N	0	6.5460	-20.3300	14.1730	H	0
4.4940	-16.8330	23.8450	C	0	13.5660	-20.0780	17.9740	H	0	5.8050	-21.1090	11.8300	C	0
4.0290	-17.9020	23.3710	O	0	12.8600	-22.0550	17.7620	C	0	4.9300	-20.4590	11.8180	H	0
3.7610	-16.2620	24.7490	N	0	13.3080	-23.0480	17.8090	H	0	6.7620	-20.5870	11.8320	H	0
2.9340	-16.7220	25.1010	H	0	11.9780	-22.0180	19.1040	C	0	5.7700	-21.6970	10.9130	H	0
4.0810	-15.4220	25.2080	H	0	11.3310	-22.8930	19.0450	H	0	6.1770	-25.2690	13.2020	C	0
8.2720	-17.4130	20.5600	C	0	12.6080	-21.9800	19.9930	H	0	6.5860	-25.7930	12.1660	O	0
8.7060	-18.5870	20.7170	O	0	11.1820	-20.7210	19.2180	C	0	4.8490	-25.4390	13.5800	N	0
8.1030	-16.8730	19.3760	N	0	11.0490	-19.8850	18.2820	O	0	4.5240	-24.8180	14.3070	H	0
7.6990	-15.9480	19.4050	H	0	10.6550	-20.4870	20.3810	N	0	3.8560	-26.2560	12.7700	C	0
8.5990	-17.3640	18.0820	C	0	10.1110	-19.6380	20.3370	H	0	4.3430	-26.6500	11.8770	H	0
8.9960	-18.3750	18.1700	H	0	10.6380	-21.1750	21.1210	H	0	3.3010	-27.4500	13.6270	C	0
7.4200	-17.5410	17.1500	C	0	12.0250	-22.1050	16.4740	C	0	2.5950	-28.0360	13.0400	H	0
7.0510	-16.5240	17.0220	H	0	11.2060	-23.0170	16.3920	O	0	4.1750	-28.0700	13.8240	H	0
7.8480	-18.1150	15.7340	C	0	12.0560	-21.2300	15.5040	N	0	2.6440	-27.0130	14.8750	C	0
8.0740	-19.1730	15.8700	H	0	12.6090	-20.4120	15.7200	H	0	3.3250	-26.2780	15.3050	H	0
7.1830	-18.1450	14.8700	H	0	11.2030	-21.2570	14.3410	C	0	1.7640	-26.4020	14.6750	H	0
8.7620	-17.6010	15.4370	H	0	10.1640	-21.2320	14.6700	H	0	2.2550	-28.0400	15.8750	C	0
6.2690	-18.4100	17.6970	C	0	11.3670	-19.9970	13.4360	C	0	1.4030	-28.6460	15.5630	H	0
6.6530	-19.4180	17.8510	H	0	11.2730	-19.0740	14.0070	H	0	3.0580	-28.7740	15.9480	H	0
5.9240	-18.1040	18.6840	H	0	12.7570	-19.8260	12.7770	C	0	2.0050	-27.2980	17.1540	N	0
5.0270	-18.5210	16.7420	C	0	13.0290	-20.6800	12.1570	H	0	2.8170	-27.1350	17.7320	H	0
4.3200	-19.2330	17.1680	H	0	12.9220	-18.9460	12.1540	H	0	0.8280	-26.9210	17.6740	C	0
4.6350	-17.5080	16.6490	H	0	13.4460	-19.7320	13.6160	H	0	-0.3160	-27.2860	17.1660	N	0
5.3380	-18.9350	15.7830	H	0	10.2760	-19.8810	12.3470	C	0	-0.3290	-27.8050	16.2990	H	0
9.7020	-16.5020	17.4720	C	0	10.2860	-18.9340	11.8080	H	0	-1.0880	-26.7300	17.5040	H	0
9.4530	-15.3110	17.3000	O	0	10.4280	-20.6490	11.5880	H	0	0.8040	-26.1700	18.7760	N	0
10.9290	-17.0800	17.2870	N	0	9.2980	-20.0880	12.7800	H	0	1.6980	-25.7780	19.0360	H	0
11.0210	-18.0710	17.4560	H	0	11.3050	-22.5480	13.4520	C	0	-0.0480	-25.9100	19.2520	H	0

2.6380	-25.4020	12.3640	C	0	-14.8620	-20.2340	7.8610	H	0	-8.1530	-14.3120	-7.9990	C	0
2.4280	-24.3110	12.8860	O	0	-13.9360	-18.2650	7.6400	C	0	-9.0240	-13.7540	-7.6550	H	0
1.9300	-25.8510	11.3090	N	0	-14.8010	-17.6770	7.3710	H	0	-7.3180	-13.6120	-8.0160	H	0
2.2420	-26.7010	10.8630	H	0	-12.6710	-17.6210	7.6060	C	0	-8.3960	-14.7720	-9.4390	C	0
0.5790	-25.4230	11.1330	C	0	-12.5760	-16.6040	7.2540	H	0	-7.4990	-15.2210	-9.8670	H	0
0.5380	-24.3410	11.0090	H	0	-11.5120	-18.3400	7.9570	C	0	-9.2690	-15.4170	-9.5350	H	0
0.0750	-26.0090	9.8130	C	0	-10.5930	-17.8040	7.7720	H	0	-8.6260	-13.6470	-10.2600	N	0
0.7400	-25.7430	8.9910	H	0	-9.8730	-20.6820	5.9200	C	0	-8.2180	-12.7730	-9.9600	H	0
0.0100	-27.0860	9.9650	H	0	-8.8430	-20.3050	5.3810	O	0	-9.4410	-13.5850	-11.3480	C	0
-1.2930	-25.5170	9.4020	C	0	-11.0210	-20.5360	5.4040	N	0	-10.1090	-14.6040	-11.8420	N	0
-1.9070	-25.4330	10.2990	H	0	-11.8070	-20.7190	6.0110	H	0	-9.8450	-15.5240	-11.5210	H	0
-1.1600	-24.1690	8.6940	C	0	-11.2160	-19.7450	4.1590	C	0	-10.9710	-14.4450	-12.3430	H	0
-0.8950	-24.3180	7.6480	H	0	-10.3990	-19.0290	4.0640	H	0	-9.5760	-12.4180	-11.8680	N	0
-2.1320	-23.6850	8.7790	H	0	-11.2750	-20.6630	2.9820	C	0	-9.1770	-11.5870	-11.4570	H	0
-0.4290	-23.5460	9.2110	H	0	-10.3400	-21.2120	2.8750	H	0	-10.3850	-12.2200	-12.4390	H	0
-2.0900	-26.3920	8.4590	C	0	-12.0270	-21.4140	3.2240	H	0	-8.1740	-13.7540	-5.2330	C	0
-2.0880	-27.3520	8.9750	H	0	-11.6670	-19.9340	1.8250	O	0	-9.1680	-13.4360	-4.6100	O	0
-3.1390	-26.1500	8.2910	H	0	-10.9160	-19.3930	1.5700	H	0	-7.1730	-12.8410	-5.3640	N	0
-1.5820	-26.4660	7.4970	H	0	-12.5660	-18.9200	4.2400	C	0	-6.2940	-13.1730	-5.7360	H	0
-0.3210	-25.8630	12.2550	C	0	-13.6260	-19.4360	4.6170	O	0	-7.2300	-11.4370	-4.8970	C	0
-0.3620	-27.0720	12.6670	O	0	-12.5030	-17.6900	3.8270	N	0	-6.4300	-10.8930	-5.3990	H	0
-0.9610	-24.8090	12.8060	N	0	-11.6800	-17.2670	3.4230	H	0	-8.1660	-10.9650	-5.1960	H	0
-0.8530	-23.9000	12.3780	H	0	-13.7070	-16.9330	3.6040	C	0	-7.1200	-11.3070	-3.3480	C	0
-1.9820	-24.9190	13.7930	C	0	-14.3110	-16.7890	4.4990	H	0	-7.5980	-10.3270	-2.8560	O	0
-1.6200	-25.7700	14.3710	H	0	-13.2610	-15.4630	3.1380	C	0	-6.5110	-12.3030	-2.6670	N	0
-1.9810	-23.6770	14.6140	C	0	-14.1740	-14.9690	2.8050	H	0	-5.9610	-12.9670	-3.1930	H	0
-1.1360	-23.6840	15.3020	H	0	-12.6750	-14.6990	4.3060	C	0	-6.6050	-12.5200	-1.2450	C	0
-1.8520	-22.7940	13.9870	H	0	-12.7130	-13.6190	4.1660	H	0	-7.6060	-12.2510	-0.9090	H	0
-2.9030	-23.6080	15.1910	H	0	-13.3330	-14.8520	5.1620	H	0	-6.5000	-13.9620	-0.9000	C	0
-3.3550	-25.1800	13.2260	C	0	-11.7290	-15.1260	4.6380	H	0	-7.3350	-14.4640	-1.3890	H	0
-3.8670	-26.2460	13.3920	O	0	-12.2460	-15.5880	2.1490	O	0	-5.5800	-14.4320	-1.2460	H	0
-3.9170	-24.3110	12.4320	N	0	-11.6650	-14.8250	2.1110	H	0	-6.6820	-14.2910	0.6150	C	0
-3.4470	-23.4370	12.2440	H	0	-14.6630	-17.4550	2.4280	C	0	-7.5330	-13.5820	1.4110	N	0
-5.1680	-24.5360	11.6650	C	0	-15.8040	-17.0990	2.3750	O	0	-7.5660	-14.2570	2.5800	C	0
-5.1910	-25.5250	11.2070	H	0	-14.1140	-18.2640	1.5260	N	0	-7.9590	-13.9210	3.5280	H	0
-6.3590	-24.3330	12.6400	C	0	-13.1170	-18.4250	1.5190	H	0	-6.8590	-15.3570	2.4380	N	0
-7.2800	-24.2780	12.0610	H	0	-14.7390	-18.9450	0.4190	C	0	-6.8010	-15.9840	3.2280	H	0
-6.4250	-25.1520	13.3560	H	0	-14.0960	-19.7900	0.1690	H	0	-6.3430	-15.4570	1.2230	C	0
-6.2560	-23.0420	13.3860	C	0	-15.7260	-19.2990	0.7160	H	0	-5.7350	-16.2170	0.7550	H	0
-5.6380	-22.8710	14.5840	C	0	-14.7360	-18.1280	-0.9210	C	0	-5.6570	-11.5420	-0.5030	C	0
-5.2230	-23.6900	15.1520	H	0	-15.1220	-18.7060	-1.9460	O	0	-4.7750	-11.9720	0.2240	O	0
-5.8640	-21.5210	14.9950	N	0	-14.1870	-16.9390	-0.8430	N	0	-5.6840	-10.3040	-0.8650	N	0
-5.5350	-21.1460	15.8730	H	0	-14.1370	-16.4390	0.0330	H	0	-6.5050	-10.1180	-1.4230	H	0
-6.5370	-20.7960	14.0320	C	0	-13.5040	-16.2090	-1.9210	C	0	-4.9380	-9.1630	-0.3810	C	0
-7.0740	-19.4970	14.0070	C	0	-14.1580	-16.2100	-2.7930	H	0	-3.8920	-9.4630	-0.4400	H	0
-7.0840	-18.8860	14.8970	H	0	-13.2420	-14.7400	-1.5750	C	0	-5.1650	-7.9520	-1.2110	C	0
-7.6220	-19.0510	12.8050	C	0	-12.8880	-14.1640	-2.4300	H	0	-4.9880	-8.1930	-2.2590	H	0
-8.1690	-18.1220	12.8720	H	0	-14.2110	-14.3180	-1.3090	H	0	-6.2500	-7.8510	-1.2000	H	0
-7.7350	-19.9000	11.6750	C	0	-12.6000	-14.5930	-0.7060	H	0	-4.4880	-6.6450	-0.8490	C	0
-8.1780	-19.5030	10.7730	H	0	-12.3210	-16.9670	-2.4610	C	0	-4.9100	-5.8490	-1.4630	H	0
-7.3660	-21.2970	11.8230	C	0	-11.5950	-17.5610	-1.6720	O	0	-4.7360	-6.3180	0.1610	H	0
-7.5330	-22.0280	11.0450	H	0	-12.0810	-16.9040	-3.7490	N	0	-2.9960	-6.7200	-0.9120	C	0
-6.7630	-21.7210	12.9450	C	0	-12.8070	-16.4670	-4.2980	H	0	-2.3510	-7.0930	0.1440	O	0
-5.1380	-23.5860	10.4600	C	0	-10.8960	-17.4180	-4.4740	C	0	-2.4460	-6.3460	-1.9980	O	0
-4.3510	-22.6460	10.2850	O	0	-10.1220	-17.8540	-3.8430	H	0	-5.3230	-8.7820	1.0910	C	0
-6.0700	-23.8180	9.5010	N	0	-11.4050	-18.3820	-5.5340	C	0	-6.3910	-9.0620	1.5130	O	0
-6.7220	-24.5800	9.6160	H	0	-12.2210	-17.9490	-6.1120	H	0	-4.4150	-8.1740	1.8910	N	0
-6.4830	-23.0110	8.2730	C	0	-10.5430	-18.4530	-6.1980	H	0	-3.5770	-7.9330	1.3820	H	0
-5.9860	-22.0410	8.2820	H	0	-11.8790	-19.7610	-5.0380	C	0	-4.5090	-7.8250	3.2930	C	0
-5.9690	-23.8140	7.0580	C	0	-12.6350	-19.6270	-4.2640	H	0	-3.8730	-6.9930	3.5970	H	0
-5.8850	-23.2060	6.1570	H	0	-12.4660	-20.5890	-6.2020	C	0	-5.5420	-7.5610	3.5180	H	0
-4.9450	-24.0710	7.3300	H	0	-12.8530	-21.4610	-5.6770	H	0	-4.0300	-8.9780	4.1660	C	0
-6.8830	-24.9240	6.8620	O	0	-13.2450	-19.9970	-6.6820	H	0	-3.1790	-9.7610	3.7180	O	0
-6.4610	-25.5830	6.3060	H	0	-11.6820	-20.8250	-6.9220	H	0	-4.2740	-8.9500	5.4660	N	0
-7.9680	-22.6910	8.4090	C	0	-10.7200	-20.6150	-4.4610	C	0	-4.9420	-8.2440	5.7400	H	0
-8.7160	-23.3460	9.1500	O	0	-10.3690	-20.0210	-3.6170	H	0	-4.1460	-10.0580	6.3910	C	0
-8.3980	-21.7130	7.5950	N	0	-11.1970	-21.4660	-3.9750	H	0	-4.1380	-11.0450	5.9290	H	0
-7.6360	-21.3610	7.0320	H	0	-9.8640	-20.8300	-5.1010	H	0	-3.1550	-10.0140	6.8430	H	0
-9.7720	-21.2830	7.3980	C	0	-10.1680	-16.3000	-5.1850	C	0	-5.2850	-10.0900	7.4010	C	0
-10.4350	-22.1470	7.4340	H	0	-10.8070	-15.5700	-5.9690	O	0	-6.1260	-9.1990	7.4110	O	0
-10.2760	-20.4110	8.6010	C	0	-8.8570	-16.1880	-4.9940	N	0	-5.2090	-10.8540	8.5340	N	0
-10.3690	-21.0150	9.5040	H	0	-8.4430	-16.8550	-4.3590	H	0	-4.2960	-12.0140	8.7170	C	0
-9.5060	-19.6500	8.7310	H	0	-7.9430	-15.1800	-5.6320	C	0	-3.3950	-11.6450	9.2070	H	0
-11.5890	-19.6780	8.3410	C	0	-6.9210	-15.3500	-5.2950	H	0	-3.9860	-12.4740	7.7790	H	0
-12.8180	-20.3470	8.3120	C	0	-7.8820	-15.5160	-7.1310	C	0	-5.2650	-12.8850	9.6180	C	0
-12.9180	-21.3770	8.6210	H	0	-6.8580	-15.7190	-7.4440	H	0	-4.5930	-13.4060	10.3000	H	0
-13.9680	-19.6390	7.9720	C	0	-8.5000	-16.3490	-7.4650	H	0	-5.8490	-13.6300	9.0780	H	0

-6.2270	-11.9630	10.4280	C	0	-11.1910	-13.6640	20.3140	C	0	-10.0380	-8.2130	4.5230	C	0
-5.9060	-11.8120	11.4580	H	0	-11.5630	-14.7840	19.9050	O	0	-8.9710	-8.2340	5.4500	N	0
-7.2660	-12.2740	10.5370	H	0	-11.0860	-12.6580	19.3550	N	0	-7.8630	-8.0180	4.6920	C	0
-6.2710	-10.7290	9.5340	C	0	-10.4980	-11.8710	19.5910	H	0	-6.8970	-8.1170	5.1650	H	0
-7.2290	-10.6060	9.0300	H	0	-11.6780	-12.8100	18.0230	C	0	-8.1320	-8.0080	3.3650	N	0
-6.1240	-9.4890	10.3900	C	0	-11.9610	-13.8570	17.9160	H	0	-7.4680	-7.8240	2.6270	H	0
-5.0430	-8.9460	10.4780	O	0	-12.8360	-11.8750	17.7890	C	0	-9.5180	-8.1850	3.2950	C	0
-7.1510	-9.1900	11.1680	N	0	-12.5460	-10.8260	17.8440	H	0	-9.9960	-8.2930	2.3330	H	0
-7.9890	-9.7330	11.0110	H	0	-13.6830	-12.1590	16.5280	C	0	-11.4290	-10.6400	3.4740	C	0
-6.9600	-8.5180	12.4960	C	0	-13.6310	-13.1940	16.1930	H	0	-10.4280	-11.3480	3.4380	O	0
-5.9520	-8.1030	12.5100	H	0	-14.7480	-12.0010	16.6940	H	0	-12.1850	-10.2500	2.3870	N	0
-7.9730	-7.3080	12.7360	C	0	-13.3650	-11.4440	15.7690	H	0	-13.0080	-9.6670	2.4540	H	0
-8.9170	-7.8450	12.8270	H	0	-13.6760	-12.1230	18.8970	O	0	-11.8350	-10.5930	0.9930	C	0
-7.8800	-6.7700	13.6790	H	0	-13.1260	-12.0310	19.6780	H	0	-10.7800	-10.8610	0.9330	H	0
-7.9280	-6.3060	11.5260	C	0	-10.5950	-12.5100	16.9600	C	0	-12.7130	-11.7970	0.5450	C	0
-8.4900	-6.7490	10.7040	H	0	-9.7630	-11.6630	17.1330	O	0	-12.5570	-12.0220	-0.5100	H	0
-8.7490	-5.0610	11.9920	C	0	-10.5690	-13.2590	15.8440	N	0	-12.3190	-12.6630	1.0760	H	0
-8.2330	-4.5110	12.7780	H	0	-11.2970	-13.9470	15.7130	H	0	-14.0960	-11.5990	0.8820	O	0
-8.6210	-4.3420	11.1830	H	0	-9.8140	-12.9430	14.6330	C	0	-14.1990	-11.6140	1.8360	H	0
-9.8200	-5.2620	12.0240	H	0	-9.2080	-12.0470	14.7720	H	0	-12.1460	-9.5370	0.0070	C	0
-6.4920	-5.8400	11.1410	C	0	-8.8140	-14.0500	14.3050	C	0	-12.7760	-8.5910	0.2670	O	0
-6.5350	-4.9720	10.4830	H	0	-8.0950	-14.0960	15.1220	H	0	-11.6180	-9.7150	-1.1650	N	0
-5.8950	-5.6420	12.0310	H	0	-9.3980	-14.9660	14.2120	H	0	-10.9530	-10.4720	-1.2410	H	0
-6.1170	-6.6880	10.5680	H	0	-8.1140	-13.9450	12.9110	C	0	-11.9160	-9.0080	-2.3530	C	0
-7.1980	-9.4320	13.6940	C	0	-8.8180	-13.6080	12.1500	H	0	-11.5690	-7.9800	-2.2480	H	0
-8.1680	-10.2060	13.6440	O	0	-7.4260	-13.1060	13.0150	H	0	-11.1610	-9.6580	-3.5270	C	0
-6.4230	-9.3280	14.7570	N	0	-7.2420	-15.5060	12.3730	S	0	-11.4620	-9.3390	-4.5250	H	0
-5.6870	-8.6370	14.7330	H	0	-5.7890	-15.7740	13.3810	C	0	-10.1040	-9.6880	-3.2600	H	0
-6.5810	-10.0990	16.0270	C	0	-4.9810	-16.1420	12.7490	H	0	-11.3390	-10.7330	-3.5080	H	0
-7.5210	-10.6450	15.9470	H	0	-5.4910	-14.7770	13.7040	H	0	-13.5210	-9.0530	-2.7690	C	0
-5.4370	-11.1470	16.2510	C	0	-5.9710	-16.3530	14.2870	H	0	-14.2890	-9.6630	-2.0760	O	0
-4.5150	-10.5680	16.2000	H	0	-10.8220	-12.6010	13.5040	C	0	-13.9180	-8.4650	-3.9890	N	0
-5.6460	-11.8900	17.5470	C	0	-11.7840	-13.3920	13.3670	O	0	-13.2320	-7.9510	-4.5240	H	0
-4.9490	-12.7200	17.6660	H	0	-10.6270	-11.5670	12.7390	N	0	-15.3410	-8.5010	-4.3540	C	0
-5.4130	-11.2440	18.3940	H	0	-9.7660	-11.0820	12.9490	H	0	-15.9000	-8.0310	-3.5450	H	0
-6.6860	-12.1680	17.7140	H	0	-11.4950	-10.9830	11.6790	C	0	-15.4090	-7.8170	-5.6940	C	0
-5.3670	-12.2180	15.1130	C	0	-12.4510	-11.5040	11.7140	H	0	-15.1580	-6.7750	-5.4950	H	0
-4.8910	-11.9730	14.1630	H	0	-11.8910	-9.4980	11.8490	C	0	-14.7170	-8.3050	-6.3800	H	0
-4.8950	-13.1560	15.4080	H	0	-11.0990	-8.7690	11.6790	H	0	-16.8260	-7.8400	-6.3440	C	0
-6.4330	-12.3160	14.9090	H	0	-12.5280	-9.3250	10.9820	H	0	-17.1610	-8.9440	-7.0400	C	0
-6.6110	-9.1880	17.2440	C	0	-12.5600	-9.1360	13.1940	C	0	-16.3870	-9.6950	-7.1030	H	0
-5.8080	-8.2960	17.3940	O	0	-13.9340	-9.5000	13.4310	C	0	-18.4140	-9.0780	-7.5720	C	0
-7.6420	-9.3950	18.0160	N	0	-14.5310	-9.8780	12.6140	H	0	-18.6820	-9.9450	-8.1570	H	0
-8.3660	-10.0380	17.7300	H	0	-14.4830	-9.3570	14.6720	C	0	-19.4450	-8.1730	-7.3470	C	0
-7.8670	-8.6250	19.2010	C	0	-15.5070	-9.6270	14.8840	H	0	-20.7780	-8.3320	-7.7060	O	0
-6.8950	-8.3800	19.6310	H	0	-13.7490	-8.8820	15.7740	C	0	-21.3060	-7.5330	-7.6440	H	0
-8.3830	-7.1870	18.8660	C	0	-14.2730	-8.7230	17.0040	O	0	-19.0970	-6.9610	-6.7150	C	0
-7.6210	-6.7500	18.2200	H	0	-15.2230	-8.8580	16.9530	H	0	-19.8190	-6.1660	-6.6030	H	0
-9.8220	-7.3090	18.3390	C	0	-12.3640	-8.5740	15.5830	C	0	-17.7740	-6.8020	-6.1510	C	0
-9.8730	-8.1240	17.6170	H	0	-11.7460	-8.3140	16.4290	H	0	-17.5090	-5.8670	-5.6800	H	0
-10.6100	-7.4100	19.0850	H	0	-11.8040	-8.7020	14.2780	C	0	-15.9520	-9.9580	-4.2910	C	0
-9.9000	-6.3820	17.7710	H	0	-10.7550	-8.4810	14.1510	H	0	-15.3450	-10.9320	-4.7450	O	0
-8.5380	-6.3530	20.0860	C	0	-10.9080	-11.2090	10.2610	C	0	-17.2010	-10.0550	-3.8300	N	0
-9.0120	-5.4330	19.7460	H	0	-9.7330	-10.8940	10.0530	O	0	-17.8810	-11.3470	-3.9050	C	0
-9.2480	-6.7600	20.8050	H	0	-11.6630	-11.8630	9.3100	N	0	-17.3600	-12.1520	-3.3860	H	0
-7.5790	-6.1030	20.5390	H	0	-12.6510	-11.9980	9.4710	H	0	-18.1440	-11.6210	-4.9270	H	0
-8.6410	-9.4060	20.3150	C	0	-11.1010	-12.1500	7.9890	C	0	-19.1690	-11.1410	-3.1870	C	0
-9.6580	-9.9700	20.0450	O	0	-10.1250	-11.6700	7.9160	H	0	-18.9370	-11.2370	-2.1260	H	0
-8.1600	-9.5320	21.5250	N	0	-11.0320	-13.6840	7.7470	C	0	-19.8720	-11.9090	-3.5100	H	0
-7.2180	-9.2470	21.7510	H	0	-12.0550	-14.0120	7.5620	H	0	-19.5310	-9.7650	-3.5240	C	0
-8.8620	-10.2090	22.6600	C	0	-10.0740	-13.9280	6.5740	C	0	-20.3550	-9.4130	-2.9030	H	0
-8.2490	-10.0600	23.5490	H	0	-10.0140	-14.9940	6.3530	H	0	-19.7610	-9.7630	-4.5890	H	0
-9.7880	-9.6830	22.8920	H	0	-10.2960	-13.5250	5.5860	H	0	-18.1630	-9.0780	-3.1890	C	0
-9.1210	-11.6720	22.2970	C	0	-9.0770	-13.5580	6.8140	H	0	-18.1850	-8.1320	-3.7300	H	0
-8.1070	-12.4160	22.1680	O	0	-10.5320	-14.5280	8.9240	C	0	-17.9290	-8.7110	-1.6990	C	0
-10.3530	-12.0570	22.1560	N	0	-9.5180	-14.2090	9.1640	H	0	-18.8760	-8.4250	-1.0020	O	0
-11.0630	-11.3470	22.0420	H	0	-11.1650	-14.3890	9.8010	H	0	-16.6970	-8.7940	-1.2300	N	0
-10.6890	-13.4600	21.7710	C	0	-10.5240	-15.5510	8.5490	H	0	-15.9520	-9.0390	-1.8660	H	0
-9.8590	-14.1370	21.9760	H	0	-11.9620	-11.4450	6.9690	C	0	-16.2570	-8.4240	0.0830	C	0
-11.8390	-13.9330	22.7510	C	0	-13.1860	-11.5180	7.0520	O	0	-15.2100	-8.7170	0.1540	H	0
-11.9910	-14.9670	22.4410	H	0	-11.2940	-10.7580	5.9810	N	0	-16.2290	-6.9550	0.1670	C	0
-11.3230	-13.9810	24.1680	C	0	-10.2850	-10.7560	6.0350	H	0	-17.2630	-6.6180	0.2400	H	0
-10.2580	-14.1800	24.2920	H	0	-11.8840	-10.0200	4.7890	C	0	-15.7150	-6.6600	1.0810	H	0
-11.5240	-13.0770	24.7420	H	0	-12.9680	-10.1350	4.8000	H	0	-15.5470	-6.2520	-0.9330	C	0
-11.9030	-14.7470	24.6820	H	0	-11.5020	-8.5020	4.8560	C	0	-16.1260	-5.3680	-1.6070	O	0
-12.9930	-13.1840	22.6590	O	0	-12.0460	-7.8460	4.1770	H	0	-14.3140	-6.5040	-1.2390	N	0
-13.5870	-13.6280	22.0500	H	0	-11.6260	-8.0750	5.8520	H	0	-13.8900	-5.9650	-1.9800	H	0



-13.7530	-7.2260	-0.8100	H	0	-10.5850	-16.4230	11.8250	H	0	-8.3990	-26.2750	20.5470	H	0
-17.0760	-9.1660	1.1990	C	0	-10.2710	-18.1490	12.2610	H	0	-7.8920	-24.1240	21.0640	C	0
-17.8980	-8.5530	1.8970	O	0	-10.9290	-17.5710	10.6200	H	0	-7.4410	-23.8240	20.1180	H	0
-16.9260	-10.4710	1.2840	N	0	-12.8830	-18.8760	11.8900	C	0	-8.4460	-23.3090	21.5280	H	0
-16.6550	-10.8290	0.3800	H	0	-12.7680	-19.0140	10.8150	H	0	-6.7810	-24.8010	21.9250	C	0
-17.5190	-11.2400	2.3770	C	0	-12.2570	-19.5200	12.5070	H	0	-7.1870	-25.0310	22.9100	H	0
-18.5280	-10.9180	2.6310	H	0	-13.9090	-18.6820	12.2030	H	0	-6.3820	-25.6730	21.4080	H	0
-17.6420	-12.7210	1.8030	C	0	-13.3770	-16.1550	15.8130	C	0	-5.7200	-23.6710	21.9650	C	0
-17.9970	-12.5740	0.7830	H	0	-12.5190	-15.3530	16.2040	O	0	-5.2840	-23.6390	20.9670	H	0
-16.6500	-13.1590	1.6920	H	0	-14.0360	-16.9270	16.6050	N	0	-6.1450	-22.7120	22.2640	H	0
-18.6230	-13.5920	2.4240	C	0	-14.7030	-17.5860	16.2270	H	0	-4.6720	-24.1270	22.9190	N	0
-19.1140	-14.6910	1.8070	N	0	-13.8350	-16.9170	18.0850	C	0	-4.3820	-25.0900	22.8280	H	0
-19.9440	-15.3160	2.6880	C	0	-13.5850	-15.9320	18.4800	H	0	-3.8900	-23.4890	22.8780	H	0
-20.3180	-16.3010	2.4530	H	0	-15.1720	-17.3520	18.7300	C	0	-4.9970	-24.1300	23.8750	H	0
-20.0070	-14.6630	3.8460	N	0	-15.9250	-16.6150	18.4500	H	0	-10.3220	-26.3620	18.9990	C	0
-20.4800	-15.1780	4.5750	H	0	-15.4850	-18.2490	18.1950	H	0	-10.5630	-27.3230	19.6940	O	0
-19.1230	-13.6210	3.7520	C	0	-15.1930	-17.5420	20.2500	C	0	-10.5010	-26.4450	17.6800	N	0
-18.8750	-12.9900	4.5930	H	0	-16.2130	-17.9590	20.8110	O	0	-10.5850	-27.7400	16.9710	C	0
-16.5230	-11.2100	3.5400	C	0	-14.2010	-17.0960	20.8900	O	0	-11.5040	-28.2240	17.3030	H	0
-15.3650	-11.3940	3.3620	O	0	-12.6670	-18.8240	18.4360	C	0	-9.7370	-28.4090	17.1230	H	0
-17.0650	-10.9220	4.8060	N	0	-12.8370	-19.0850	18.4870	O	0	-10.5780	-27.5340	15.4870	C	0
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-16.2780	-10.7370	5.9860	C	0	-11.5480	-16.3220	18.9100	H	0	-9.9590	-28.2390	14.9330	H	0
-15.2260	-10.9500	5.7980	H	0	-10.2590	-18.0240	19.2090	C	0	-10.2470	-26.0760	15.2670	C	0
-16.3230	-9.2090	6.4890	C	0	-9.9880	-18.7560	18.4480	H	0	-10.8680	-25.7240	14.4430	H	0
-17.3310	-8.9390	6.8030	H	0	-9.0510	-17.0750	19.2540	C	0	-9.1830	-25.9320	15.0790	H	0
-15.3840	-8.9660	7.6170	C	0	-9.2590	-16.4020	20.0850	H	0	-10.4720	-25.3880	16.7080	C	0
-14.3350	-9.2030	7.4390	H	0	-8.1730	-17.7210	19.2530	H	0	-9.4860	-24.9310	16.7980	H	0
-15.3490	-7.9300	7.9550	H	0	-8.7820	-16.1940	18.0170	C	0	-11.6630	-24.4020	16.8040	C	0
-15.7340	-9.2790	8.6010	H	0	-9.6220	-15.5070	17.9210	H	0	-12.5520	-24.5940	17.6450	O	0
-15.9550	-8.3060	5.3210	C	0	-7.5650	-15.3840	18.2670	C	0	-11.4720	-23.3010	16.0150	N	0
-14.9950	-8.5620	4.8730	H	0	-7.6290	-14.8280	19.2030	H	0	-10.6660	-23.2090	15.4140	H	0
-16.7520	-8.1910	4.5870	H	0	-6.6230	-15.9320	18.2310	H	0	-12.2580	-22.0380	15.9750	C	0
-15.8060	-7.3120	5.7430	H	0	-7.5050	-14.6110	17.5010	H	0	-12.1110	-21.4170	16.8590	H	0
-16.6980	-11.6350	7.1330	C	0	-8.6110	-16.9950	16.7230	C	0	-11.8530	-21.1650	14.7420	C	0
-17.8600	-11.8160	7.2540	O	0	-8.1780	-16.3810	15.9330	H	0	-12.6050	-20.4130	14.5040	H	0
-15.7880	-12.2120	7.8820	N	0	-7.7700	-17.6860	16.7860	H	0	-10.9200	-20.6110	14.8440	H	0
-14.8300	-12.1100	7.5770	H	0	-9.5440	-17.4280	16.3630	H	0	-11.7130	-21.9780	13.4950	C	0
-16.0380	-13.2080	8.9030	C	0	-10.4120	-18.7120	20.4870	C	0	-12.8140	-22.1780	12.6570	C	0
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-14.4670	-14.3660	8.0950	H	0	-12.2400	-17.9510	20.9420	H	0	-13.5560	-23.1390	10.8550	H	0
-15.4730	-15.1870	9.2330	H	0	-11.7410	-19.2940	22.5420	C	0	-11.4730	-23.5050	11.1940	C	0
-16.2730	-15.3440	7.3530	C	0	-10.8810	-19.2340	23.2090	H	0	-11.4310	-24.2840	10.0610	O	0
-16.9300	-16.5000	7.7050	C	0	-12.9480	-18.7590	23.3340	C	0	-12.2740	-24.2210	9.6060	H	0
-17.0560	-16.8300	8.7250	H	0	-13.9120	-19.0090	22.8930	H	0	-10.3610	-23.4100	12.0670	C	0
-17.5940	-17.2030	6.6390	C	0	-13.0390	-19.2620	24.8210	C	0	-9.4010	-23.8600	11.8600	H	0
-18.1750	-18.0660	6.9290	H	0	-13.3890	-20.2940	24.8170	H	0	-10.5110	-22.6640	13.2260	C	0
-17.6240	-16.7790	5.2730	C	0	-12.0150	-19.1280	25.1720	H	0	-9.6920	-22.5950	13.9270	H	0
-18.3450	-17.4110	4.2870	O	0	-13.7210	-18.5510	25.2860	H	0	-13.8130	-22.3180	15.9090	C	0
-17.7520	-17.6050	3.5570	H	0	-12.9380	-17.3520	23.4380	O	0	-14.1790	-23.2690	15.2360	O	0
-16.8200	-15.6660	4.9810	C	0	-13.1990	-17.0530	22.5630	H	0	-14.7170	-21.4880	16.4560	N	0
-16.6520	-15.4020	3.9480	H	0	-11.9260	-20.8020	22.2230	C	0	-14.3680	-20.7590	17.0620	H	0
-16.1480	-14.9340	5.9820	C	0	-11.7100	-21.5820	23.1310	O	0	-16.0940	-21.4050	16.0550	C	0
-15.5210	-14.1100	5.6770	H	0	-12.3600	-21.1970	21.0340	N	0	-16.3270	-22.1960	15.3410	H	0
-15.4030	-12.8880	10.2770	C	0	-12.4150	-20.5200	20.2860	H	0	-16.9840	-21.5280	17.3070	C	0
-14.3240	-12.3590	10.3420	O	0	-12.7020	-22.4880	20.5800	C	0	-16.5810	-20.7920	18.0030	H	0
-15.8810	-13.5060	11.3400	N	0	-12.8900	-23.0610	21.4870	H	0	-17.9970	-21.2080	17.0660	H	0
-16.6680	-14.1200	11.1910	H	0	-14.0120	-22.5750	19.7660	C	0	-17.0840	-22.5470	17.6800	H	0
-15.3400	-13.4240	12.6970	C	0	-13.6910	-22.2870	18.7650	H	0	-16.2780	-20.0730	15.2640	C	0
-14.4190	-12.8420	12.6590	H	0	-14.4530	-23.5550	19.9500	H	0	-15.6150	-19.1220	15.6370	O	0
-16.3420	-12.5860	13.4970	C	0	-15.0660	-21.5660	20.3220	C	0	-17.2150	-19.9780	14.2840	N	0
-17.2200	-13.2250	13.6000	H	0	-14.9540	-20.5910	19.8480	H	0	-17.8470	-20.7610	14.1990	H	0
-16.0740	-12.4540	14.5460	H	0	-16.0540	-21.8260	19.9430	H	0	-17.5090	-18.6340	13.6630	C	0
-16.6990	-11.6820	13.0050	H	0	-15.3490	-21.5530	21.8010	C	0	-16.5820	-18.0650	13.5950	H	0
-15.1140	-14.8630	13.2010	C	0	-15.3030	-22.5490	22.4530	O	0	-17.9920	-18.8500	12.1910	C	0
-16.0860	-15.6620	13.2260	O	0	-15.6810	-20.4680	22.4140	N	0	-18.8940	-19.4610	12.2210	H	0
-13.9250	-15.1750	13.5760	N	0	-15.9150	-20.5220	23.3950	H	0	-18.4460	-17.5500	11.5050	C	0
-13.1930	-14.4790	13.5740	H	0	-15.9150	-19.6070	21.9410	H	0	-19.2440	-17.1560	12.1350	H	0
-13.6370	-16.4150	14.3030	C	0	-11.4680	-23.0870	19.9430	C	0	-17.5490	-16.9300	11.5010	H	0
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-12.3730	-16.9490	13.6600	C	0	-11.1880	-24.3450	20.2240	N	0	-16.8690	-19.6220	11.4020	C	0
-11.6680	-16.1280	13.7840	H	0	-11.4960	-24.6240	21.1450	H	0	-16.0790	-18.9090	11.1640	H	0
-11.9490	-17.7850	14.2160	H	0	-9.9590	-24.9640	19.6200	C	0	-16.4510	-20.4870	11.9160	H	0
-12.3620	-17.4670	12.1930	C	0	-9.4160	-24.3090	18.9380	H	0	-17.4620	-20.0570	10.0730	C	0
-12.9190	-16.8010	11.5340	H	0	-8.8730	-25.3030	20.6870	C	0	-18.3320	-20.6920	10.2360	H	0
-10.9040	-17.4580	11.7040	C	0	-9.4300	-25.5730	21.5840	H	0	-17.7390	-19.1730	9.4970	H	0

-16.7050	-20.5700	9.4790	H	0	-24.5320	-5.9610	6.9910	H	0	-22.7210	-0.2970	-8.2590	H	0
-18.5440	-17.8700	14.4100	C	0	-22.9370	-5.5310	5.5780	C	0	-24.3360	-0.3740	-9.4720	C	0
-19.6230	-18.3890	14.7400	O	0	-23.4200	-4.3630	5.0680	O	0	-23.8890	-0.8780	-10.5040	O	0
-18.1620	-16.6800	14.8530	N	0	-24.0680	-3.8920	5.5970	H	0	-25.4910	0.3350	-9.5210	N	0
-17.3150	-16.3120	14.4430	H	0	-21.7150	-5.9700	5.0650	C	0	-25.9270	0.5360	-10.4100	H	0
-19.0130	-15.9090	15.6760	C	0	-21.2100	-5.4050	4.2950	H	0	-25.9900	0.5630	-8.6730	H	0
-19.5560	-16.5370	16.3820	H	0	-21.0810	-7.1280	5.6370	C	0	-22.8870	-3.0080	-8.5450	C	0
-18.1000	-15.0320	16.4990	C	0	-20.1150	-7.5200	5.3570	H	0	-21.6710	-2.8850	-8.3740	O	0
-17.4100	-15.7510	16.9400	H	0	-21.1140	-10.2660	5.1310	C	0	-23.3870	-3.6930	-9.5600	N	0
-17.4180	-14.3730	15.9610	H	0	-20.0150	-10.6200	4.7230	O	0	-24.3890	-3.6920	-9.6870	H	0
-18.9160	-14.2690	17.5840	C	0	-22.0090	-9.7610	4.2700	N	0	-22.6790	-4.6500	-10.4270	C	0
-19.6620	-13.5390	17.2710	H	0	-22.9430	-9.7070	4.6510	H	0	-22.0590	-5.2260	-9.7390	H	0
-19.3500	-15.0340	18.2280	H	0	-21.8940	-9.5190	2.7890	C	0	-23.8540	-5.5370	-11.0330	C	0
-17.9300	-13.4410	18.4310	C	0	-20.8470	-9.3550	2.5360	H	0	-23.4850	-6.4350	-11.5280	H	0
-17.1440	-14.1100	18.7810	H	0	-22.3510	-10.7970	1.9640	C	0	-24.4240	-5.9160	-10.1840	H	0
-17.4850	-12.7290	17.7370	H	0	-23.4250	-10.9140	2.1080	H	0	-24.7200	-4.8120	-11.9340	O	0
-18.4940	-12.5450	19.5050	C	0	-21.8700	-10.6160	0.4590	C	0	-25.4890	-5.3790	-12.0210	H	0
-17.6320	-11.9370	19.7820	H	0	-22.0600	-9.5620	0.2580	H	0	-21.8490	-3.9670	-11.4710	C	0
-19.2540	-11.9650	18.9830	H	0	-20.8080	-10.8420	0.3690	H	0	-21.0480	-4.5830	-12.0890	O	0
-19.1380	-13.2800	20.5720	N	0	-22.4920	-11.2340	-0.1900	H	0	-21.9380	-2.6630	-12.9570	N	0
-19.9380	-13.8060	20.2500	H	0	-21.7420	-11.9460	2.5520	O	0	-22.6290	-2.1100	-11.1880	H	0
-18.5900	-13.9680	21.0670	H	0	-21.3640	-11.6350	3.3780	H	0	-21.1040	-1.9290	-12.6250	C	0
-19.5490	-12.6460	21.2430	H	0	-22.8260	-8.2700	2.4480	C	0	-20.9980	-2.5400	-13.5220	H	0
-20.0510	-15.1350	14.8390	C	0	-24.0410	-8.3020	2.6430	O	0	-21.8980	-0.6330	-12.9570	C	0
-21.2320	-15.1110	15.2600	O	0	-22.2390	-7.2610	1.7940	N	0	-22.9150	-0.8490	-13.2840	H	0
-19.6520	-14.6990	13.5990	N	0	-20.8330	-7.1000	1.4310	C	0	-22.0420	-0.0480	-12.0480	H	0
-18.7270	-14.8870	13.2400	H	0	-20.3680	-7.8670	0.8110	H	0	-21.2010	0.1530	-14.0400	C	0
-20.5800	-14.1510	12.6380	C	0	-20.2500	-7.0320	2.3500	H	0	-20.1530	0.2960	-13.7740	H	0
-21.4640	-14.7880	12.6350	H	0	-20.5970	-5.6170	0.9680	C	0	-21.1100	-0.4590	-14.9370	H	0
-21.0580	-12.7180	13.0230	C	0	-20.4880	-5.5740	-0.1160	H	0	-21.9140	1.5310	-14.3390	C	0
-21.5700	-12.2250	12.1970	H	0	-19.7240	-5.1020	1.3690	H	0	-23.1590	1.7060	-14.1350	O	0
-21.8970	-12.9110	13.6920	H	0	-21.8770	-4.9120	1.3060	C	0	-21.3220	2.4540	-15.0550	N	0
-20.1890	-11.6990	13.5510	C	0	-22.1050	-4.1480	0.5630	H	0	-21.8740	3.1410	-15.5470	H	0
-20.0800	-11.4620	14.8390	C	0	-21.6780	-4.3720	2.2310	H	0	-20.4120	2.1490	-15.3710	H	0
-20.5930	-11.9270	15.6680	H	0	-22.9750	-6.0600	1.4340	C	0	-19.6360	-1.7350	-12.0940	C	0
-19.1660	-10.4640	15.0250	N	0	-23.5080	-5.7390	2.3290	H	0	-18.6920	-1.4760	-12.8430	O	0
-18.9640	-10.0980	15.9440	H	0	-23.7030	-6.0590	0.0720	C	0	-19.5000	-1.8080	-10.7710	N	0
-18.6730	-9.9260	13.8630	C	0	-23.1190	-6.5630	-0.8680	O	0	-20.3450	-1.8480	-10.2210	H	0
-17.7640	-8.9090	13.5780	C	0	-24.8480	-5.3970	-0.0830	N	0	-18.2070	-1.7500	-10.0930	C	0
-17.3220	-8.2770	14.3350	H	0	-25.3560	-4.9470	0.6640	H	0	-17.7930	-0.7430	-10.0320	H	0
-17.5400	-8.7400	12.1950	C	0	-25.3330	-5.2220	-1.4370	C	0	-18.4570	-2.3590	-8.6070	C	0
-17.0120	-7.8560	11.8700	H	0	-25.2890	-6.2020	-1.9130	H	0	-19.3790	-1.9390	-8.2050	H	0
-18.0520	-9.5490	11.1610	C	0	-26.7810	-4.7610	-1.3720	C	0	-18.4910	-3.4440	-8.7060	H	0
-17.8440	-9.2670	10.1390	H	0	-26.6960	-3.7910	-0.8800	H	0	-17.5810	-2.0550	-8.0330	H	0
-18.9200	-10.6460	11.5060	C	0	-27.4140	-4.6410	-2.7430	C	0	-17.1730	-2.6500	-10.6720	C	0
-19.4520	-11.2130	10.7560	H	0	-26.8980	-3.8450	-3.2810	H	0	-15.9920	-2.3270	-10.7540	O	0
-19.2680	-10.8020	12.8610	C	0	-27.3780	-5.5580	-3.3320	H	0	-17.5790	-3.8780	-11.1730	N	0
-19.9850	-14.0280	11.2160	C	0	-28.4370	-4.2880	-2.8720	H	0	-18.5140	-4.1620	-10.9160	H	0
-18.7940	-14.1760	10.9310	O	0	-27.7590	-5.5860	-0.5310	C	0	-16.5490	-4.8700	-11.6800	C	0
-20.8780	-13.6930	10.2640	N	0	-28.0790	-6.4910	-1.0490	H	0	-15.7530	-4.9240	-10.9370	H	0
-21.8330	-13.5270	10.5500	H	0	-27.2210	-5.7760	0.3970	H	0	-17.1100	-6.2850	-11.7900	C	0
-20.6080	-13.4130	8.8160	C	0	-28.6860	-5.0430	-0.3460	H	0	-18.0200	-6.4310	-12.3710	H	0
-19.5450	-13.1760	8.7700	H	0	-24.4430	-4.2460	-2.2560	C	0	-15.9800	-7.2020	-12.2270	C	0
-20.6370	-14.7380	7.9730	C	0	-24.0490	-3.2250	-1.7120	O	0	-15.7690	-7.0460	-13.2850	H	0
-20.2750	-14.4580	6.9830	H	0	-24.0340	-4.5770	-3.4500	N	0	-15.1130	-6.8520	-11.6660	H	0
-19.8850	-15.3900	8.4170	H	0	-24.3770	-5.4780	-3.7500	H	0	-16.2090	-8.2560	-12.0680	H	0
-21.9830	-15.4520	8.0570	C	0	-23.1150	-3.8100	-4.3310	C	0	-17.6060	-6.7870	-10.3750	C	0
-22.0430	-16.0500	8.9670	H	0	-23.0220	-2.7840	-3.9760	H	0	-18.2660	-7.6360	-10.5520	H	0
-22.7590	-14.6880	8.1060	H	0	-21.6780	-4.3690	-4.3630	C	0	-16.8860	-7.1660	-9.6500	H	0
-22.0690	-16.3790	6.8850	C	0	-21.7890	-5.3560	-4.8130	H	0	-18.1710	-5.9460	-9.9730	H	0
-21.4170	-16.2130	5.8350	O	0	-21.0840	-3.7730	-5.0550	H	0	-16.0060	-4.2760	-13.0200	C	0
-22.9230	-17.3330	6.9650	N	0	-20.7850	-4.4940	-3.0900	C	0	-14.8380	-4.4790	-13.3900	O	0
-23.4100	-17.8390	6.2400	H	0	-20.8970	-3.5640	-2.5340	H	0	-16.8510	-3.5730	-13.7520	N	0
-23.3870	-17.4470	7.8540	H	0	-21.1480	-5.3230	-2.4810	H	0	-17.7270	-3.4210	-13.2720	H	0
-21.4520	-12.2710	8.2690	C	0	-19.3080	-4.6900	-3.3460	C	0	-16.5550	-3.0080	-15.1060	C	0
-22.5520	-12.1180	8.6720	O	0	-18.7270	-4.0500	-4.1820	O	0	-16.0820	-3.8490	-15.6130	H	0
-20.8880	-11.4730	7.3550	N	0	-18.6250	-5.4470	-2.5120	N	0	-17.9010	-2.8220	-15.8710	C	0
-19.8900	-11.5970	7.2570	H	0	-17.6160	-5.4410	-2.5500	H	0	-17.7780	-2.4320	-16.8810	H	0
-21.5430	-10.3690	6.6120	C	0	-19.0560	-5.9480	-1.7480	H	0	-18.3770	-3.8010	-15.8100	H	0
-22.6280	-10.4570	6.6650	H	0	-23.5910	-3.6110	-5.7740	C	0	-18.5250	-2.0950	-15.3520	H	0
-21.0680	-9.0490	7.2700	C	0	-23.9100	-4.6450	-6.3840	O	0	-15.6690	-1.7250	-15.1520	C	0
-21.1840	-8.9890	8.3520	H	0	-23.5370	-2.3080	-6.2710	N	0	-15.2330	-1.1890	-16.1350	O	0
-19.9870	-8.9120	7.2520	H	0	-23.2510	-1.4850	-5.7600	H	0	-15.5200	-1.0660	-13.9530	N	0
-21.6950	-7.7770	6.7390	C	0	-23.8700	-2.1210	-7.6850	C	0	-15.8140	-1.6140	-13.1570	H	0
-22.8470	-7.1930	7.3430	C	0	-24.8830	-2.4850	-7.8580	H	0	-14.8600	0.2730	-13.7250	C	0
-23.3280	-7.7080	8.1620	H	0	-23.7580	-0.6030	-8.1200	C	0	-14.3500	0.5350	-14.6520	H	0
-23.5020	-6.1160	6.7060	C	0	-24.2130	0.1090	-7.4310	H	0	-15.8840	1.3190	-13.3730	C	0

-15.2930	2.2020	-13.1260	H	0	-7.3490	-8.6130	-5.4850	H	0	-8.7200	0.1860	9.2320	H	0
-16.7180	1.6790	-14.6560	C	0	-6.8360	-7.0950	-6.2230	H	0	-10.4680	0.4870	9.7970	H	0
-16.1740	1.5430	-15.5910	H	0	-6.7180	-5.5600	-4.1110	C	0	-8.9430	0.7280	10.8540	H	0
-17.5850	1.0240	-14.7310	H	0	-5.6380	-5.6810	-4.0300	H	0	-10.4770	-1.3160	11.9220	C	0
-17.0530	2.7160	-14.6600	H	0	-7.0030	-4.8490	-4.8860	H	0	-11.6650	-1.5770	11.8690	O	0
-16.7740	0.9540	-12.1840	C	0	-6.9020	-4.9280	-3.2420	H	0	-9.8900	-1.1560	13.1120	N	0
-16.4200	0.0520	-11.6850	H	0	-9.5490	-5.7290	-3.4280	C	0	-8.9490	-0.8010	13.2060	H	0
-16.7750	1.7490	-11.4390	H	0	-10.2520	-4.7180	-3.7220	O	0	-10.4710	-1.4690	14.4460	C	0
-17.7770	0.6870	-12.5170	H	0	-9.2910	-6.0440	-2.1890	N	0	-11.4930	-1.8320	14.3360	H	0
-13.7370	0.1940	-12.6820	C	0	-8.6400	-6.7760	-1.9430	H	0	-9.6570	-2.6590	15.0090	C	0
-12.7730	0.9780	-12.7880	O	0	-9.4080	-5.1420	-1.0480	C	0	-9.5530	-3.4710	14.2890	H	0
-13.6620	-0.8720	-11.8880	N	0	-9.5370	-4.1190	-1.4010	H	0	-8.6460	-2.3530	15.2750	H	0
-14.4540	-1.4850	-11.7590	H	0	-10.6450	-5.3310	-0.2940	C	0	-10.3720	-3.1200	16.2300	C	0
-12.4040	-1.2120	-11.2370	C	0	-11.4520	-5.6110	-0.9720	H	0	-11.4660	-3.9900	16.1010	C	0
-11.9330	-0.5010	-10.5580	H	0	-10.5510	-6.2380	0.3030	H	0	-11.7880	-4.3390	15.1310	H	0
-12.7450	-2.4210	-10.3260	C	0	-11.0570	-4.2650	0.7350	C	0	-12.0930	-4.3280	17.2840	C	0
-13.5550	-2.1060	-9.6690	H	0	-10.7910	-4.4010	1.9560	O	0	-12.8930	-5.0480	17.1850	H	0
-13.0740	-3.2050	-11.0080	H	0	-11.6580	-3.1360	0.3850	N	0	-11.6010	-3.9640	18.5040	C	0
-11.8310	-2.7070	-9.8060	H	0	-12.0230	-2.4580	1.0380	H	0	-12.2420	-4.5560	19.5410	O	0
-11.2830	-1.6800	-12.2410	C	0	-12.1560	-3.1670	-0.4930	H	0	-12.6270	-5.3620	19.1890	H	0
-11.4070	-2.3850	-13.2220	O	0	-8.1850	-5.1280	-0.0760	C	0	-10.5210	-3.1280	18.6520	C	0
-10.0780	-1.1330	-12.0200	N	0	-7.5350	-6.1700	0.1910	O	0	-10.3310	-2.7400	19.6420	H	0
-10.0560	-0.5260	-11.2130	H	0	-7.9310	-3.9540	0.5480	N	0	-9.8990	-2.6960	17.4790	C	0
-9.1310	-1.1180	-13.1480	C	0	-8.5330	-3.1740	0.3240	H	0	-9.0630	-2.0120	17.5070	H	0
-9.5820	-0.8060	-14.0900	H	0	-6.7830	-3.6950	1.4220	C	0	-10.5730	-0.2510	15.3630	C	0
-8.1150	0.0200	-12.9550	C	0	-6.0450	-4.4130	1.0630	H	0	-9.7070	0.6180	15.3430	O	0
-7.5090	0.0900	-13.8580	H	0	-6.1660	-2.3070	1.2140	C	0	-11.5970	-0.2330	16.2260	N	0
-8.5430	0.9950	-12.7220	H	0	-6.3730	-2.1180	0.1610	H	0	-12.2370	-1.0140	16.2120	H	0
-6.8500	-0.3420	-11.6400	S	0	-6.6150	-1.6020	1.9140	H	0	-11.7400	0.6470	17.3390	C	0
-8.3580	-2.4360	-13.4420	C	0	-4.6870	-2.2000	1.4850	C	0	-10.7560	0.9460	17.6980	H	0
-7.9310	-2.6630	-14.5260	O	0	-4.5940	-1.7170	2.4580	H	0	-12.5170	1.8710	16.9250	C	0
-8.0980	-3.1650	-12.3600	N	0	-4.3230	-3.2200	1.6130	H	0	-11.9680	2.4960	16.2210	H	0
-8.4920	-2.8420	-11.4610	H	0	-3.9930	-1.4930	0.3060	C	0	-13.4750	1.6160	16.4710	H	0
-6.9160	-3.9740	-12.2360	C	0	-4.5330	-0.5990	-0.0040	H	0	-12.7810	2.4820	17.7890	H	0
-6.6210	-4.1940	-13.2620	H	0	-3.0240	-1.0960	0.6090	H	0	-12.5550	-0.1070	18.4600	C	0
-5.7630	-3.1620	-11.6190	C	0	-3.7640	-2.4200	-0.8230	N	0	-13.0310	-1.2110	18.2310	O	0
-5.9410	-2.8630	-10.5860	H	0	-3.0000	-3.0810	-0.8050	H	0	-12.6770	0.4770	19.6510	N	0
-4.8370	-3.7170	-11.4660	H	0	-4.4030	-2.5700	-1.9770	C	0	-12.3760	1.4410	19.6650	H	0
-5.4870	-1.6150	-12.4480	S	0	-5.2600	-1.6550	-2.4390	N	0	-13.4570	-0.1340	20.7810	C	0
-7.2610	-5.2090	-11.3280	C	0	-5.1260	-0.7180	-2.0850	H	0	-12.9060	-0.9720	21.2080	H	0
-6.8860	-5.3540	-10.1660	O	0	-5.7660	-1.8770	-3.2840	H	0	-13.3400	0.9260	21.9370	C	0
-8.0650	-6.1380	-11.9090	N	0	-4.2520	-3.5520	-2.8050	N	0	-12.2980	1.2220	22.0560	H	0
-8.3340	-6.1060	-12.8820	H	0	-3.5620	-4.2690	-2.6320	H	0	-13.8580	1.8200	21.5900	H	0
-8.8420	-7.0240	-11.1120	C	0	-4.6780	-3.5230	-3.7200	H	0	-14.0460	0.5300	23.1980	C	0
-9.6360	-7.3690	-11.7740	H	0	-6.9610	-3.9720	2.9620	C	0	-13.8240	-0.3880	23.9460	O	0
-7.9830	-8.3530	-10.7600	C	0	-6.0370	-4.0480	3.7450	O	0	-14.7160	1.4970	23.7430	N	0
-7.3280	-8.5520	-11.6090	H	0	-8.2300	-4.2750	3.3640	N	0	-15.1370	1.2570	24.6290	H	0
-7.3560	-8.1360	-9.8950	H	0	-8.9870	-4.1280	2.7120	H	0	-14.6970	2.4260	23.3470	H	0
-8.8290	-9.5590	-10.4440	C	0	-8.6020	-4.8480	4.6570	C	0	-14.8330	-0.5990	20.4790	C	0
-8.3280	-10.6370	-9.9940	O	0	-9.4460	-5.5280	4.5460	H	0	-15.8280	0.2040	20.5430	O	0
-10.0480	-9.4390	-10.6320	O	0	-7.7630	-5.3860	5.0990	H	0	-15.0860	-1.8780	20.1630	N	0
-9.6290	-6.3130	-9.9290	C	0	-9.1250	-3.8990	5.6320	C	0	-14.3150	-2.5260	20.0870	H	0
-10.0260	-5.1700	-10.0240	O	0	-9.5510	-2.7840	5.3130	O	0	-16.3840	-2.3890	19.7890	C	0
-9.9410	-6.9470	-8.7670	N	0	-9.4190	-4.3880	6.8820	N	0	-16.1550	-3.4540	19.7540	H	0
-9.5670	-7.8840	-8.7160	H	0	-9.2770	-5.3870	6.9210	H	0	-17.2320	-2.2190	20.4520	H	0
-11.0250	-6.5920	-7.8290	C	0	-10.2860	-3.8940	7.9880	C	0	-16.8570	-2.0800	18.3740	C	0
-11.3280	-5.5560	-7.9800	H	0	-11.1300	-3.3310	7.5880	H	0	-17.9520	-2.5380	18.1160	O	0
-12.2800	-7.4100	-8.1490	C	0	-10.8290	-5.0520	8.8810	C	0	-16.0900	-1.4320	17.5070	N	0
-13.0700	-6.9490	-7.5560	H	0	-10.0260	-5.5140	9.4550	H	0	-15.1870	-1.1320	17.8460	H	0
-12.8330	-7.2800	-9.5610	C	0	-11.5350	-4.6880	9.6270	H	0	-16.3240	-1.3190	16.0750	C	0
-12.7130	-6.2420	-9.8710	H	0	-11.4760	-6.1490	8.0100	C	0	-17.2010	-1.9290	15.8610	H	0
-12.2100	-7.7640	-10.3130	H	0	-10.9360	-6.4350	7.1070	H	0	-16.7870	0.1060	15.7030	C	0
-13.8380	-7.6990	-9.5010	H	0	-11.7270	-7.4100	8.8310	C	0	-15.9380	0.7810	15.8150	H	0
-12.1350	-8.8990	-7.8970	C	0	-10.8010	-7.9050	9.1250	H	0	-17.0610	0.1580	14.6490	H	0
-11.3150	-9.2860	-8.5020	H	0	-12.3060	-7.2030	9.7300	H	0	-17.8180	0.6940	16.5960	C	0
-11.9210	-8.9500	-6.8290	H	0	-12.1390	-8.1840	8.1820	H	0	-18.7200	0.1800	16.9270	H	0
-13.1200	-9.3650	-7.9270	H	0	-12.7700	-5.6570	7.4510	C	0	-17.1290	0.8310	17.4300	H	0
-10.6780	-6.6870	-6.2860	C	0	-12.6010	-5.0190	6.5830	H	0	-18.1770	2.1310	16.1220	C	0
-11.5320	-7.0180	-5.4830	O	0	-13.4910	-6.4210	7.1610	H	0	-17.3370	2.8070	16.2790	H	0
-9.3870	-6.5800	-5.8090	N	0	-13.3140	-4.9960	8.1260	H	0	-18.5840	2.1090	15.1110	H	0
-8.7380	-6.4250	-6.5670	H	0	-9.4580	-2.9730	8.8800	C	0	-19.2130	2.6840	17.0100	C	0
-8.9780	-6.7680	-4.3980	C	0	-8.2150	-3.0910	8.9750	O	0	-19.4240	3.6520	16.5530	H	0
-9.3990	-7.6880	-3.9920	H	0	-10.1510	-2.1480	9.6550	N	0	-20.1280	2.0920	17.0240	H	0
-7.4960	-6.9010	-4.2000	C	0	-11.1510	-2.1260	9.5160	H	0	-18.7440	2.9190	18.4240	N	0
-7.3600	-7.3590	-3.2200	H	0	-9.6100	-1.2660	10.6630	C	0	-19.1250	3.7980	18.7450	H	0
-6.8210	-7.6780	-5.3020	C	0	-8.6180	-1.6800	10.8410	H	0	-19.1270	2.1830	18.9990	H	0
-5.7550	-7.8440	-5.1500	H	0	-9.4470	0.1980	10.0450	C	0	-17.7380	2.8910	18.5140	H	0

-15.1750	-1.9090	15.2490	C	0	-18.0020	-2.8980	-1.4080	H	0	-15.3320	3.1620	6.1140	C	0
-13.9770	-1.9160	15.5730	O	0	-18.1420	-2.7700	0.6050	C	0	-15.4760	2.1370	5.7720	H	0
-15.6200	-2.2630	14.0260	N	0	-19.2210	-2.9030	0.5380	H	0	-14.6160	3.6510	5.4530	H	0
-16.5980	-2.1270	13.8120	H	0	-17.8230	-3.8110	0.6670	H	0	-14.8560	3.2210	7.0930	H	0
-14.7840	-2.7510	12.9910	C	0	-18.0370	-2.2360	1.5500	H	0	-18.8340	2.2500	5.2090	C	0
-13.7560	-2.3940	13.0450	H	0	-18.2880	-0.9790	-1.0090	O	0	-19.9670	2.7810	5.3370	O	0
-14.7670	-4.3030	12.9290	C	0	-18.8160	-1.1900	-1.7830	H	0	-18.3760	1.1700	5.9020	N	0
-14.3940	-4.6370	13.8970	H	0	-15.8160	-1.5510	-2.2310	C	0	-17.4110	0.8740	5.8700	H	0
-16.1050	-5.0980	12.7740	C	0	-15.6890	-0.3390	-2.3570	O	0	-19.3660	0.3230	6.6580	C	0
-15.9900	-6.1740	12.6430	H	0	-15.6870	-2.4750	-3.2000	N	0	-20.2470	0.9270	6.8750	H	0
-16.7790	-4.8730	13.6010	H	0	-15.8800	-3.4570	-3.0620	H	0	-19.7680	-0.9440	5.9070	C	0
-16.6480	-4.8360	11.8660	H	0	-15.4410	-2.1410	-4.5780	C	0	-18.9010	-1.6040	5.8790	H	0
-13.7610	-4.7760	11.8390	C	0	-14.4520	-1.6950	-4.4700	H	0	-20.9850	-1.6630	6.4920	C	0
-14.3110	-4.8240	10.8990	H	0	-15.2520	-3.4210	-5.3770	C	0	-20.9380	-1.6110	7.5790	H	0
-12.9550	-4.0500	11.7270	H	0	-14.6430	-4.1470	-4.8380	H	0	-21.8540	-1.1010	6.1480	H	0
-13.1200	-6.1470	12.1920	C	0	-16.2000	-3.9240	-5.5670	H	0	-21.0290	-2.6980	6.1530	H	0
-12.1970	-6.2250	11.6170	H	0	-14.5880	-3.2090	-6.7440	C	0	-20.1380	-0.5940	4.4490	C	0
-12.9210	-6.1630	13.2630	H	0	-15.0320	-2.3050	-7.1610	H	0	-20.9910	0.0840	4.4440	H	0
-13.7880	-6.9670	11.9290	H	0	-13.0500	-3.0550	-6.4580	C	0	-19.2890	-0.1140	3.9610	H	0
-15.3410	-2.0350	11.7240	C	0	-12.7530	-3.9090	-8.0630	H	0	-20.5370	-1.8500	3.5590	C	0
-16.5210	-1.7660	11.6140	O	0	-12.5570	-3.0530	-7.4300	H	0	-20.2080	-1.6970	2.5310	H	0
-14.4580	-1.7580	10.7750	N	0	-12.8540	-2.1300	-5.9160	H	0	-20.0090	-2.7750	3.7900	H	0
-13.5140	-1.7700	11.1350	H	0	-14.7630	-4.4190	-7.7290	C	0	-21.6230	-1.9260	3.6010	H	0
-14.7390	-0.9380	9.5800	C	0	-15.7980	-4.4950	-8.0630	H	0	-18.8510	-0.0430	8.0180	C	0
-15.8130	-0.7880	9.6920	H	0	-14.1070	-4.3260	-8.5950	H	0	-17.6510	-0.4280	8.1370	O	0
-14.2220	0.4650	9.6780	C	0	-14.3630	-5.3290	-7.2820	H	0	-19.6270	0.2960	9.0740	N	0
-13.1390	0.5780	9.6450	H	0	-16.3180	-0.9450	-5.1660	C	0	-20.5680	0.6470	8.9670	H	0
-14.5990	1.0970	8.8730	H	0	-15.8760	-0.0210	-5.8100	O	0	-19.2290	-0.0460	10.4410	C	0
-14.6430	1.1400	10.9690	C	0	-17.6370	-1.1770	-4.8340	N	0	-18.1560	-0.1890	10.5720	H	0
-15.8010	1.9070	10.9680	C	0	-17.8800	-1.9960	-4.2950	H	0	-19.4530	1.1550	11.3750	C	0
-16.3050	2.0960	10.0320	H	0	-18.6760	-0.2760	-5.3200	C	0	-19.1390	0.9590	12.4000	H	0
-16.2460	2.6100	12.0760	C	0	-18.3510	0.0900	-6.2940	H	0	-19.0450	2.0790	10.9650	H	0
-17.1460	3.2030	12.0100	H	0	-20.0340	-1.0080	-5.4140	C	0	-20.5120	1.4060	11.4410	H	0
-15.5050	2.5120	13.2880	C	0	-20.6870	-0.5270	-6.1420	H	0	-20.0340	-1.2520	10.9670	C	0
-15.8650	3.1730	14.0630	H	0	-19.8140	-2.0250	-5.7410	H	0	-21.2770	-1.1550	11.2240	O	0
-14.3600	1.7990	13.3550	C	0	-20.7680	-0.9440	-4.0330	C	0	-19.3580	-2.3600	11.3580	N	0
-13.7520	1.6290	14.2310	H	0	-20.1040	-1.1420	-2.9790	O	0	-18.3660	-2.3280	11.5420	H	0
-13.9090	1.0800	12.1910	C	0	-21.9400	-0.5960	-3.9540	O	0	-20.0120	-3.5600	11.8480	C	0
-12.9960	0.5160	12.3130	H	0	-18.7910	1.0570	-4.4840	C	0	-21.0910	-3.4260	11.7690	H	0
-14.2520	-1.6690	8.2980	C	0	-19.6000	1.8870	-4.8400	O	0	-19.6140	-4.8820	11.0930	C	0
-13.1490	-2.3520	8.3730	O	0	-17.8950	1.3130	-3.5430	N	0	-18.5930	-5.0940	11.4110	H	0
-15.0290	-1.5490	7.2240	N	0	-17.2190	0.6040	-3.2990	H	0	-20.1370	-5.7670	11.4570	H	0
-15.9350	-1.1210	7.3530	H	0	-17.6140	2.6600	-3.0500	C	0	-19.8330	-4.7470	9.5630	C	0
-14.6850	-2.0400	5.9200	C	0	-16.5300	2.7190	-2.9450	H	0	-19.3220	-3.8530	9.2080	H	0
-13.6120	-2.2300	5.9220	H	0	-17.9890	3.3980	-3.7600	H	0	-19.1750	-5.9600	8.9890	C	0
-15.3870	-3.3960	5.8240	C	0	-18.1880	3.0720	-1.6900	C	0	-18.0900	-5.8560	8.9890	H	0
-14.9470	-3.9550	4.9980	H	0	-18.3630	4.2530	-1.4730	O	0	-19.4230	-6.8910	9.4990	H	0
-15.1270	-3.9680	6.7140	H	0	-18.3630	2.1370	-0.7350	N	0	-19.4410	-6.0230	7.9330	H	0
-16.8790	-3.2430	5.6070	C	0	-18.2480	1.1930	-1.0760	H	0	-21.3210	-4.6110	9.1790	C	0
-17.3060	-2.8130	6.5130	H	0	-19.0040	2.3170	0.5780	C	0	-21.6910	-5.5720	9.5340	H	0
-17.0400	-2.6150	4.7320	H	0	-19.4500	3.3090	0.5130	H	0	-21.7880	-3.7580	9.6720	H	0
-17.7350	-4.7270	5.1920	S	0	-20.1100	1.2320	0.7950	C	0	-21.4900	-4.5400	8.1040	H	0
-17.0980	-5.3370	3.6190	C	0	-19.6040	0.2860	0.9880	H	0	-19.8350	-3.7020	13.3920	C	0
-17.7290	-6.1400	3.2380	H	0	-20.5570	1.3640	1.7810	H	0	-18.7570	-3.3910	13.9170	O	0
-17.0940	-4.4850	2.9390	H	0	-21.2100	1.1300	-0.2830	C	0	-20.7820	-4.3470	14.0740	N	0
-16.0710	-5.6920	3.7150	H	0	-21.8980	1.9760	-0.2710	H	0	-21.6160	-4.6550	13.5950	H	0
-15.0700	-1.1370	4.7260	C	0	-20.7210	1.0330	-1.2530	H	0	-20.5690	-4.6110	15.5200	C	0
-15.9510	-0.2640	4.8910	O	0	-22.2000	-0.0310	-0.1760	C	0	-20.1880	-3.7410	16.0550	H	0
-14.5250	-1.4580	3.6300	N	0	-23.0130	-0.0960	0.7040	O	0	-21.9660	-4.9930	16.0050	C	0
-13.8330	-2.1930	3.6650	H	0	-22.2180	-0.9530	-1.1400	N	0	-22.6800	-4.1770	15.8880	H	0
-14.7280	-0.7710	2.3860	C	0	-22.9300	-1.6660	-1.0720	H	0	-22.2720	-5.7590	15.2920	H	0
-15.6040	-0.1250	2.4370	H	0	-21.5780	-0.9830	-1.9200	H	0	-22.0980	-5.6190	17.4240	C	0
-13.3940	0.0000	1.9120	C	0	-17.9700	2.3610	1.7210	C	0	-21.0540	-5.5800	18.1120	O	0
-13.5390	0.3010	0.8740	H	0	-16.8540	1.7600	1.6780	O	0	-23.1240	-6.2250	17.6640	O	0
-13.0970	1.3520	2.6890	C	0	-18.3100	3.0530	2.8180	N	0	-19.5500	-5.7700	15.6620	C	0
-12.0880	1.6520	2.4080	H	0	-19.1420	3.6250	2.8410	H	0	-19.9180	-6.8740	15.2850	O	0
-13.9310	2.0310	2.5120	H	0	-17.7830	2.8250	4.1850	C	0	-18.4260	-5.5110	16.3570	N	0
-13.0560	1.2280	3.7710	H	0	-16.9650	2.1210	4.0270	H	0	-18.3110	-4.5550	16.6630	H	0
-12.2120	-0.7190	1.9170	O	0	-17.1050	4.0970	4.6530	C	0	-17.4740	-6.5670	16.7230	C	0
-11.5170	-0.1340	1.6080	H	0	-16.3580	4.4420	3.9390	H	0	-17.0170	-6.9700	15.8190	H	0
-15.0540	-1.7580	1.3050	C	0	-18.0150	5.3940	4.6640	C	0	-16.2630	-5.8680	17.4020	C	0
-15.0150	-2.9930	1.4650	O	0	-18.9700	5.1130	5.1070	H	0	-15.9270	-5.0230	16.8010	H	0
-15.6330	-1.2500	0.2170	N	0	-17.5700	6.2190	5.2210	H	0	-16.3950	-5.4360	18.3940	H	0
-15.6930	-0.2470	0.1180	H	0	-18.1220	5.6970	3.6220	H	0	-15.3640	-6.4840	17.4400	H	0
-16.2230	-2.0590	-0.7810	C	0	-16.5740	4.0560	6.0950	C	0	-18.0900	-7.7900	17.4970	C	0
-15.7420	-3.0350	-0.7130	H	0	-16.2170	5.0380	6.4040	H	0	-17.4100	-8.8630	17.4740	O	0
-17.6620	-2.1690	-0.6720	C	0	-17.3190	3.6610	6.7860	H	0	-19.3350	-7.6780	18.0670	N	0

-19.8440	-6.8110	17.9630	H	0	-22.6520	1.3220	14.5870	H	0	-23.0800	6.5510	1.3640	H	0
-19.9190	-8.7900	18.7960	C	0	-22.0020	-0.5500	15.0500	C	0	-21.6320	5.8500	0.0230	C	0
-19.0660	-9.3990	19.0960	H	0	-22.4140	-1.5470	14.8910	H	0	-20.8150	5.1370	0.1340	H	0
-20.6080	-8.2650	20.0480	C	0	-20.4950	-0.6740	15.0070	C	0	-22.5830	5.3590	-0.9870	C	0
-19.9190	-7.7020	20.6780	H	0	-20.1450	-1.4560	15.6820	H	0	-23.0900	4.4430	-0.6810	H	0
-21.3040	-7.4730	19.7690	H	0	-20.2190	-0.9210	13.9810	H	0	-23.2820	6.1840	-1.1210	H	0
-21.2980	-9.3800	20.7390	C	0	-20.0240	0.2620	15.3040	H	0	-21.9490	5.0850	-2.3800	C	0
-20.8920	-10.4920	20.8650	O	0	-22.5330	-0.2310	16.4540	C	0	-21.6290	6.0520	-2.7660	H	0
-22.4530	-9.0540	21.2690	N	0	-21.8400	0.4660	16.9260	H	0	-21.0010	4.5530	-2.3030	H	0
-22.8490	-9.8200	21.7950	H	0	-23.5200	0.2200	16.3570	H	0	-22.6940	4.2370	-3.4120	C	0
-22.8940	-8.1480	21.2050	H	0	-22.5590	-1.1420	17.0530	H	0	-23.7590	4.4680	-3.3790	H	0
-20.8940	-9.5830	17.8850	C	0	-24.2040	1.3640	12.4690	C	0	-22.2620	4.5840	-4.3500	H	0
-20.8360	-10.8350	17.9840	O	0	-24.8520	2.2630	12.9380	O	0	-22.3330	2.7400	-3.2690	C	0
-21.7840	-9.0630	17.0620	N	0	-23.6330	1.3760	11.2210	N	0	-21.2460	2.6830	-3.3220	H	0
-21.7770	-8.0610	16.9340	H	0	-23.1580	0.5470	10.8930	H	0	-22.6630	2.4010	-2.2870	H	0
-22.8400	-9.8220	16.3580	C	0	-23.9880	2.3690	10.1690	C	0	-22.9790	1.9290	-4.3860	N	0
-22.8240	-10.9050	16.4810	H	0	-25.0520	2.2320	9.9750	H	0	-23.9200	1.6460	-4.1530	H	0
-24.2510	-9.3890	16.8310	C	0	-23.7020	3.7760	10.5950	C	0	-22.9260	2.3840	-5.2870	H	0
-25.0020	-9.9860	16.3140	H	0	-24.0410	4.4170	9.7810	H	0	-22.5220	1.0320	-4.4750	H	0
-24.3050	-9.6700	18.3410	C	0	-24.4410	4.0420	11.3510	H	0	-20.8300	7.1010	-0.3440	C	0
-23.8390	-10.6290	18.5690	H	0	-22.3800	4.1360	11.0800	C	0	-21.2250	8.2270	-0.0850	O	0
-23.9390	-8.9240	19.0460	H	0	-21.8770	4.1360	12.3200	C	0	-19.7220	6.8340	-1.0020	N	0
-25.3340	-9.9120	18.6050	H	0	-22.5600	3.9270	13.1300	H	0	-19.3940	5.8850	-1.1090	H	0
-24.6180	-8.0730	16.6340	O	0	-20.5860	4.4980	12.3560	N	0	-18.6870	7.8310	-1.0600	C	0
-24.0630	-7.4580	17.1190	H	0	-20.0300	4.4730	13.1980	H	0	-19.0880	8.8190	-0.8370	H	0
-22.7720	-9.6280	14.8410	C	0	-20.1510	4.7360	11.1590	C	0	-17.6910	7.6130	0.0110	C	0
-23.5400	-10.2140	14.0370	O	0	-18.9590	5.2540	10.6930	C	0	-18.0280	7.6980	1.0440	H	0
-21.8520	-8.7620	14.4170	N	0	-18.2720	5.5250	11.4820	H	0	-17.3890	6.5740	-0.1190	H	0
-21.2180	-8.3840	15.1070	H	0	-18.7140	5.5100	9.3900	C	0	-16.4010	8.3730	-0.1130	C	0
-21.7620	-8.5060	12.9520	C	0	-17.8020	6.0490	9.1770	H	0	-16.1730	9.7050	0.3720	N	0
-20.9090	-7.9000	12.6490	H	0	-19.7510	5.3590	8.4520	C	0	-14.8630	9.9370	0.1570	C	0
-21.8590	-9.4420	12.4020	H	0	-19.6160	5.6590	7.4230	H	0	-14.3540	10.8530	0.4200	H	0
-22.9190	-7.7380	12.3730	C	0	-21.0010	4.8060	8.8300	C	0	-14.2130	8.8520	-0.2340	N	0
-23.1640	-7.7240	11.1170	O	0	-21.7080	4.6780	8.0240	H	0	-13.2110	8.7230	-0.2440	H	0
-23.8050	-7.1160	13.1570	N	0	-21.2400	4.5670	10.2420	C	0	-15.1320	7.8820	-0.4270	C	0
-23.7630	-7.2040	14.1620	H	0	-23.3380	2.1920	8.8150	C	0	-14.9660	6.8950	-0.8310	H	0
-24.9450	-6.3330	12.5840	C	0	-22.3460	1.4420	8.8070	O	0	-18.1060	8.0420	-2.4710	C	0
-25.2970	-6.7790	11.6530	H	0	-23.8940	2.7350	7.6920	N	0	-17.3320	8.9610	-2.7330	O	0
-26.0790	-6.3120	13.5820	C	0	-24.8190	3.1360	7.7420	H	0	-18.4440	7.1260	-3.3900	N	0
-25.6100	-6.2570	14.5640	H	0	-23.1830	2.6700	6.4050	C	0	-19.2810	6.5880	-3.2130	H	0
-26.8000	-5.5070	13.4420	H	0	-22.1060	2.5650	6.5410	H	0	-17.8050	7.0370	-4.6990	C	0
-26.9080	-7.5750	13.5200	C	0	-23.5820	1.3600	5.7100	C	0	-17.5590	8.0520	-5.0120	H	0
-27.3380	-7.7270	12.5300	H	0	-22.9420	1.3500	4.8270	H	0	-16.5290	6.3100	-4.7000	C	0
-26.2610	-8.4370	13.6800	H	0	-23.3250	0.5440	6.3850	H	0	-15.8430	6.6990	-3.9490	H	0
-28.0450	-7.5390	14.4870	C	0	-24.9980	1.2220	5.1400	C	0	-16.5730	5.2850	-4.3320	H	0
-27.7890	-7.1820	15.4850	H	0	-25.7110	1.5320	5.9040	H	0	-16.1100	6.2890	-5.7070	H	0
-28.7320	-6.8080	14.0590	H	0	-25.0720	1.9660	4.3460	H	0	-18.8460	6.4170	-5.6490	C	0
-28.5810	-8.9680	14.5850	C	0	-25.3490	-0.2260	4.7130	C	0	-19.6120	5.5690	-5.2220	O	0
-28.7920	-9.1860	13.5380	H	0	-24.7970	-0.4180	3.7930	H	0	-18.7050	6.6440	-6.9660	N	0
-27.9000	-9.6910	15.0340	H	0	-25.0370	-0.8590	5.5440	H	0	-18.1840	7.4840	-7.1760	H	0
-29.8370	-8.8470	15.3320	N	0	-26.8470	-0.3850	4.5220	C	0	-19.6640	6.3080	-8.0280	C	0
-30.3450	-8.1140	14.8570	H	0	-27.3110	0.1410	5.3570	H	0	-20.5040	5.7850	-7.5720	H	0
-30.4340	-9.6610	15.3670	H	0	-27.0690	0.0320	3.5400	H	0	-20.4030	7.5070	-8.4710	C	0
-29.5580	-8.5440	16.2540	H	0	-27.2150	-1.8180	4.5620	N	0	-21.0160	7.9020	-7.6610	H	0
-24.4860	-4.9150	12.3200	C	0	-28.2040	-1.9670	4.4280	H	0	-19.6390	8.2320	-8.7510	H	0
-23.5520	-4.4460	12.9050	O	0	-26.8070	-2.3480	3.8050	H	0	-21.3840	7.2070	-9.6140	C	0
-25.0640	-4.1850	11.3900	N	0	-27.0800	-2.2690	5.4560	H	0	-22.0150	6.1370	-9.5060	O	0
-25.9220	-4.6060	11.0640	H	0	-23.4090	3.8440	5.4620	C	0	-21.7120	8.0980	-10.4580	O	0
-24.5540	-2.8550	10.9410	C	0	-24.5160	4.4850	5.5430	O	0	-19.1630	5.4480	-9.1540	C	0
-23.5620	-2.9780	10.5060	H	0	-22.5490	4.1670	4.5180	N	0	-18.3670	5.9420	-10.0080	O	0
-25.4770	-2.4770	9.7390	C	0	-21.6790	3.6550	4.5060	H	0	-19.6880	4.2360	-9.2610	N	0
-26.5110	-2.6910	10.0080	H	0	-22.6460	5.3800	3.6750	C	0	-20.2920	3.8910	-8.5280	H	0
-25.3980	-1.4810	9.3050	H	0	-23.6810	5.6130	3.4250	H	0	-19.2270	3.2980	-10.2840	C	0
-25.2760	-3.4490	8.5160	C	0	-22.1330	6.5970	4.4770	C	0	-18.1390	3.3520	-10.2680	H	0
-24.2130	-3.3770	8.2830	H	0	-22.6370	6.6140	5.4440	H	0	-19.7990	1.8530	-9.9870	C	0
-25.6200	-4.3810	8.9640	H	0	-21.0580	6.4550	4.5940	H	0	-19.5800	1.2270	-10.8520	H	0
-26.1310	-3.1180	7.3190	C	0	-22.4270	7.9620	3.8900	C	0	-19.0190	1.3250	-8.7680	C	0
-25.6610	-3.3200	6.2070	O	0	-21.9050	8.7340	4.4560	H	0	-19.0930	2.0850	-7.9890	H	0
-27.2860	-2.6490	7.4520	O	0	-21.8250	8.0060	2.9820	H	0	-19.4200	0.3970	-8.3600	H	0
-24.8070	-1.8090	12.0240	C	0	-24.0720	8.5030	3.6700	S	0	-17.9320	1.2550	-8.7990	H	0
-25.9660	-1.4970	12.2970	O	0	-24.4640	9.2230	5.2380	C	0	-21.3160	1.8080	-9.7830	C	0
-23.8100	-1.1270	12.6220	N	0	-24.0180	10.2120	5.3470	H	0	-21.7900	2.1430	-10.7060	H	0
-22.9270	-1.5320	12.3440	H	0	-25.5400	9.3910	5.2960	H	0	-21.7630	0.8150	-9.7340	H	0
-23.8670	0.1620	13.3380	C	0	-24.1140	8.6240	6.0780	H	0	-21.7190	2.3660	-8.9380	H	0
-24.6710	0.1040	14.0720	H	0	-21.8530	5.2470	2.4010	C	0	-19.6220	3.8580	-11.6190	C	0
-22.5310	0.4400	13.9580	C	0	-20.7730	4.7030	2.4740	O	0	-18.8640	3.7730	-12.6150	O	0
-21.7410	0.7900	13.2940	H	0	-22.2790	5.9380	1.3080	N	0	-20.7040	4.6550	-11.7340	N	0

-21.1350	4.9670	-10.8760	H	0	-12.0260	2.0640	-1.0020	C	0	-9.1470	4.6770	11.1410	N	0
-21.2690	5.3170	-12.9110	C	0	-12.0840	1.0370	-0.6400	H	0	-8.5390	3.8810	11.2690	H	0
-21.3370	4.5750	-13.7070	H	0	-11.0220	2.3910	-1.2720	H	0	-9.6750	5.2920	12.3500	C	0
-22.6750	5.9620	-12.6600	C	0	-12.3220	2.4670	-0.0340	H	0	-10.6660	5.6740	12.1020	H	0
-22.6030	6.9010	-12.1100	H	0	-13.5470	3.6000	-2.3690	C	0	-10.0220	4.3240	13.4650	C	0
-23.5300	6.2230	-13.9190	C	0	-12.8510	4.2940	-2.8400	H	0	-9.1060	3.8120	13.7590	H	0
-23.0360	6.9260	-14.5890	H	0	-14.3740	3.4880	-3.0690	H	0	-10.6940	5.0560	14.6830	C	0
-23.8810	5.2990	-14.3790	H	0	-14.1830	4.3100	-1.1640	C	0	-11.2990	4.3090	15.1960	H	0
-24.3980	6.7630	-13.5410	H	0	-15.0010	4.9530	-1.4880	H	0	-9.9680	5.4080	15.4170	H	0
-23.4610	5.1330	-11.8850	O	0	-14.6860	3.6370	-0.4710	H	0	-11.3670	5.8670	14.4050	H	0
-23.2170	5.4030	-10.9970	H	0	-13.3910	4.8490	-0.6430	H	0	-10.9290	3.1700	12.9450	C	0
-20.3650	6.3770	-13.4350	C	0	-11.6960	0.2150	-3.3930	C	0	-11.9610	3.5220	12.9330	H	0
-20.1930	6.3760	-14.6690	O	0	-12.4620	-0.7380	-3.1580	O	0	-10.4990	2.7920	12.0180	H	0
-19.6820	7.1960	-12.5980	N	0	-10.4250	0.0990	-3.5200	N	0	-10.7550	2.3490	13.6410	H	0
-19.8650	7.1400	-11.6060	H	0	-9.9200	0.8430	-3.9790	H	0	-8.7010	6.2790	12.8940	C	0
-18.5480	8.0420	-12.9970	C	0	-9.6870	-1.1340	-3.1030	C	0	-7.5610	5.9430	13.0810	O	0
-18.7800	8.4830	-13.9670	H	0	-10.4010	-1.9530	-3.0230	H	0	-9.2720	7.4540	13.1700	N	0
-18.2720	9.1530	-11.9510	C	0	-8.7450	-1.6260	-4.1960	C	0	-10.2730	7.5160	13.0520	H	0
-18.1230	8.7080	-10.9670	H	0	-8.0730	-2.3370	-3.7150	H	0	-8.5340	8.5130	13.8020	C	0
-17.3290	9.6330	-12.2170	H	0	-9.4150	-2.1560	-5.4310	C	0	-7.6040	8.2400	14.2990	H	0
-19.4670	10.1210	-11.8370	C	0	-8.7130	-2.8300	-5.9210	H	0	-8.1230	9.5120	12.6620	C	0
-19.6760	10.6400	-12.7730	H	0	-10.2300	-2.8190	-5.1410	H	0	-9.0230	9.6420	12.0610	H	0
-20.3820	9.6480	-11.4810	H	0	-9.7210	-1.3190	-6.0580	H	0	-7.6500	10.8440	13.1410	C	0
-19.1710	11.3220	-10.9390	C	0	-7.9410	-0.4850	-4.4930	O	0	-8.4560	11.4350	13.5780	H	0
-20.0030	12.0220	-10.8630	H	0	-7.7920	-0.4440	-5.4400	H	0	-6.9060	10.9040	13.9360	H	0
-18.8950	10.9830	-9.9410	H	0	-8.9460	-0.8780	-1.8130	C	0	-7.2010	11.3540	12.2890	H	0
-17.9640	12.1340	-11.5040	C	0	-8.7270	-1.8630	-1.0840	O	0	-7.0820	8.9030	11.8070	C	0
-17.0690	11.5270	-11.3650	H	0	-8.5260	0.3810	-1.5200	N	0	-6.8430	9.6980	11.1010	H	0
-17.9650	12.1780	-12.5930	H	0	-8.8290	1.1390	-2.1160	H	0	-6.2230	8.6420	12.4250	H	0
-17.9210	13.5130	-10.9090	N	0	-7.9260	0.7710	-0.2070	C	0	-7.5180	8.0410	11.3010	H	0
-17.8880	13.5450	-9.9000	H	0	-6.9740	0.3360	0.0960	H	0	-9.4490	9.1310	14.8310	C	0
-17.1750	14.0110	-11.3720	H	0	-7.7350	1.8410	-0.2890	H	0	-10.5150	9.7210	14.4570	O	0
-18.7780	13.9730	-11.1840	H	0	-8.8070	0.5780	1.0260	C	0	-9.1400	9.0470	16.1410	N	0
-17.2450	7.2860	-13.3210	C	0	-10.0260	0.5030	0.9610	O	0	-8.2850	8.5670	16.3840	H	0
-16.3870	7.7800	-14.1590	O	0	-8.1190	0.4980	2.1820	N	0	-9.7860	9.6150	17.2690	C	0
-17.1060	6.1380	-12.6130	N	0	-7.1240	0.6360	2.0820	H	0	-9.3620	9.0800	18.1190	H	0
-17.8020	5.8090	-11.9600	H	0	-8.6230	0.2440	3.5270	C	0	-9.5870	11.1870	17.3400	C	0
-16.0180	5.1920	-12.9280	C	0	-9.3850	-0.5110	3.3350	H	0	-9.9680	11.5460	16.3830	H	0
-16.3150	4.1640	-13.1360	H	0	-7.5400	-0.2850	4.4230	C	0	-10.1350	11.6810	18.1420	H	0
-15.4780	5.4580	-13.8360	H	0	-6.7820	0.4890	4.5430	H	0	-8.0430	11.5440	17.4650	C	0
-15.1240	5.0720	-11.6920	C	0	-8.0550	-0.5190	5.3550	H	0	-7.6450	11.0140	18.3300	H	0
-13.9670	4.7030	-11.8610	O	0	-7.0500	-1.2160	4.1400	H	0	-7.5150	11.1140	16.6140	H	0
-15.6390	5.3830	-10.4880	N	0	-9.2910	1.4720	4.2100	C	0	-7.7860	13.0820	17.6130	C	0
-16.6300	5.5770	-10.4780	H	0	-9.0620	2.5760	3.7020	O	0	-8.4180	13.2550	18.4840	H	0
-14.8030	5.3700	-9.2810	C	0	-10.0680	1.3380	5.3660	N	0	-6.7410	13.1990	17.9000	H	0
-13.7520	5.4530	-9.5590	H	0	-10.6240	0.1050	5.8410	C	0	-8.2940	13.9690	16.3940	C	0
-15.3480	6.4740	-8.3330	C	0	-10.0330	-0.5550	6.4760	H	0	-7.9830	13.5870	15.4220	H	0
-16.2580	6.0910	-7.8730	H	0	-10.9550	-0.5220	5.0130	H	0	-9.3820	13.9410	16.3400	H	0
-14.5890	6.5180	-7.5520	H	0	-11.8640	0.5110	6.6240	C	0	-7.7680	15.3370	16.6300	N	0
-15.5970	7.8890	-9.0050	C	0	-12.1660	-0.2140	7.3800	H	0	-8.3620	15.9400	16.0800	H	0
-14.6750	8.1260	-9.5370	H	0	-12.7220	0.6700	5.9710	H	0	-8.0030	15.6800	17.5510	H	0
-16.4210	7.7240	-9.7000	H	0	-11.4790	1.8600	7.1730	C	0	-6.8060	15.5310	16.3880	H	0
-16.0760	9.0570	-8.0420	C	0	-10.9980	1.6320	8.1250	H	0	-11.2500	9.1250	17.2550	C	0
-16.9040	8.7880	-7.1660	O	0	-12.3290	2.5310	7.3000	H	0	-11.5860	7.9590	17.3540	O	0
-15.7410	10.2460	-8.3270	O	0	-10.4210	2.4260	6.2220	C	0	-12.1510	10.0150	16.9430	N	0
-15.0190	4.0630	-8.5170	C	0	-10.8980	3.1800	5.5960	H	0	-11.8760	10.9810	17.0530	H	0
-16.1600	3.5600	-8.4500	O	0	-9.2280	2.9770	6.9950	C	0	-13.6390	9.7900	16.7640	C	0
-13.9690	3.7040	-7.7180	N	0	-8.1890	2.4180	6.9910	O	0	-13.7900	8.7820	17.1510	H	0
-13.1400	4.2260	-7.9610	H	0	-9.3220	4.1260	7.7050	N	0	-14.4540	10.7310	17.6970	C	0
-14.0410	2.4100	-6.9250	C	0	-10.0560	4.7570	7.4170	H	0	-15.5210	10.6790	17.4790	H	0
-15.0920	2.2050	-6.7220	H	0	-8.4350	4.5870	8.7820	C	0	-14.2340	10.3840	18.7060	H	0
-13.6010	1.1280	-7.6830	C	0	-7.9410	3.6680	9.0970	H	0	-14.0930	12.2650	17.6190	C	0
-13.4340	0.2890	-7.0080	H	0	-7.3440	5.4820	8.1160	C	0	-12.8460	12.6210	17.5600	O	0
-14.6810	0.7470	-8.6020	C	0	-7.1590	5.1970	7.0810	H	0	-14.9780	13.1440	17.5970	O	0
-14.4760	-0.2680	-8.9400	H	0	-7.6200	6.5360	8.1460	H	0	-14.1950	9.7790	15.3640	C	0
-15.6380	0.7230	-8.0800	H	0	-6.0560	5.3700	8.9890	C	0	-15.3560	9.9410	15.1420	O	0
-14.7750	1.3910	-9.4760	H	0	-6.3830	5.3840	10.0290	H	0	-13.3430	9.7610	14.3100	N	0
-12.4930	1.3000	-8.4950	O	0	-5.1190	4.1600	8.5990	C	0	-12.3800	9.5820	14.5600	H	0
-12.7130	1.8980	-9.2130	H	0	-5.6360	3.2380	8.8630	H	0	-13.7380	9.6450	12.9120	C	0
-13.2540	2.5440	-5.6180	C	0	-4.8270	4.2720	7.5550	H	0	-14.7880	9.3880	12.7720	H	0
-12.5060	3.5090	-5.5290	O	0	-4.2200	4.1420	9.2160	H	0	-13.7840	11.0590	12.2520	C	0
-13.1850	1.6430	-4.6090	N	0	-5.2750	6.6960	8.9620	C	0	-14.2190	10.9230	11.2620	H	0
-13.8760	0.9060	-4.6230	H	0	-4.7590	6.9410	8.0340	H	0	-14.5780	11.6850	12.6590	H	0
-12.2440	1.6530	-3.4990	C	0	-5.9680	7.4520	9.3320	H	0	-12.4260	11.8140	12.1460	C	0
-11.4200	2.3140	-3.7700	H	0	-4.4740	6.4870	9.6710	H	0	-11.6540	11.1300	12.4970	H	0
-12.9260	2.2090	-2.1560	C	0	-9.1160	5.3080	9.9740	C	0	-12.1410	12.0260	11.1150	H	0
-13.7840	1.5670	-1.9550	H	0	-9.7100	6.3890	9.8440	O	0	-12.3310	13.1910	12.8370	C	0

-11.3060	13.5610	12.8140	H	0	-10.5990	8.6380	-5.7050	H	0	-11.2150	10.1570	-11.2890	C	0
-13.0190	13.9690	12.5070	H	0	-11.9520	9.6310	-5.0650	H	0	-12.1470	10.5500	-11.6950	H	0
-12.5370	12.9690	14.3630	C	0	-12.8820	6.9650	-5.4680	C	0	-11.5280	8.9640	-10.2730	C	0
-13.5540	12.6690	14.6130	H	0	-12.3400	6.8500	-6.4070	H	0	-10.6410	8.3460	-10.1350	H	0
-11.8980	12.2330	14.8510	H	0	-13.4280	6.0790	-5.1450	H	0	-12.1350	9.2100	-8.8840	C	0
-12.3590	14.1610	15.1860	N	0	-13.6920	7.6460	-5.7280	H	0	-12.3930	8.3550	-8.2590	H	0
-11.4230	14.5270	15.0930	H	0	-9.9010	5.9860	-4.9120	C	0	-11.3490	9.7050	-8.3140	H	0
-12.9880	14.8970	14.8980	H	0	-8.8980	6.7310	-5.0040	O	0	-13.0330	9.8270	-8.8830	H	0
-12.5100	13.9540	16.1630	H	0	-9.9900	4.7900	-5.4890	N	0	-12.5770	8.0720	-10.9360	C	0
-12.8700	8.6560	12.1700	C	0	-10.8630	4.2900	-5.4010	H	0	-12.1560	7.6390	-11.8430	H	0
-11.9900	8.0080	12.6850	O	0	-9.3320	4.3260	-6.6650	C	0	-12.9070	7.3470	-10.1930	H	0
-13.4000	8.2270	11.0290	N	0	-8.2540	4.4770	-6.6130	H	0	-13.4200	8.7170	-11.1860	H	0
-14.3240	8.5940	10.8510	H	0	-9.6730	2.8080	-6.7970	C	0	-10.6280	11.3300	-10.5520	C	0
-12.8290	7.2790	10.1200	C	0	-10.7070	2.5880	-7.0620	H	0	-9.4370	11.5910	-10.6210	O	0
-11.7860	7.1390	10.4030	H	0	-9.1330	2.4630	-7.6780	H	0	-11.4850	12.0260	-9.8020	N	0
-13.5910	5.8910	10.0730	C	0	-9.2680	2.0650	-5.6480	O	0	-12.4800	11.8670	-8.9790	H	0
-13.5710	5.5400	11.1050	H	0	-8.8130	1.3290	-6.0650	H	0	-11.0940	13.1030	-8.8600	C	0
-15.0590	5.8310	9.6250	C	0	-9.8730	5.1240	-7.9290	C	0	-10.2410	13.6440	-9.2720	H	0
-15.5790	6.4840	10.3250	H	0	-10.8820	5.8320	-7.9250	O	0	-12.2100	14.1520	-8.7140	C	0
-15.1830	6.3960	8.7010	H	0	-9.2710	4.8740	-9.1530	N	0	-13.1870	13.6710	-11.8360	H	0
-15.5250	4.8460	9.5910	H	0	-8.4690	4.2660	-9.2410	H	0	-12.1880	14.6050	-7.7220	H	0
-12.7790	4.9530	9.1700	C	0	-9.8650	5.3220	-10.4130	C	0	-12.3370	15.2210	-9.7990	C	0
-11.7500	4.8860	9.5210	H	0	-10.0930	4.4330	-10.9990	H	0	-11.3910	15.2500	-10.3390	H	0
-13.0810	3.9100	9.2600	H	0	-10.8410	5.7530	-10.1880	H	0	-13.0640	14.8790	-10.5360	H	0
-12.8090	5.2930	8.1350	H	0	-9.0040	6.3050	-11.2050	C	0	-12.8580	16.5460	-9.3890	C	0
-12.6980	7.8700	8.7240	C	0	-9.5030	6.8710	-12.1670	O	0	-13.0330	17.0350	-10.3480	H	0
-13.5490	8.5520	8.1130	O	0	-7.7250	6.4160	-10.9100	N	0	-13.7250	16.3950	-8.7470	H	0
-11.5210	7.6830	8.1260	N	0	-7.4430	5.8530	-10.1210	H	0	-11.9040	17.3290	-8.5550	N	0
-10.8470	7.1440	8.6510	H	0	-6.8080	7.2550	-11.6310	C	0	-10.9810	16.9900	-8.3230	H	0
-10.9880	8.1710	6.8890	C	0	-7.2490	8.2500	-11.5810	H	0	-12.1620	18.5650	-8.1500	C	0
-11.5680	9.0150	6.5170	H	0	-5.8690	7.2080	-11.0790	H	0	-13.3160	19.2090	-8.3120	N	0
-9.5670	8.7170	7.0900	C	0	-6.5980	6.9210	-13.0960	C	0	-14.0510	18.8760	-8.9200	H	0
-8.9140	7.8980	7.3890	H	0	-6.3860	7.7440	-14.0260	O	0	-13.3960	20.0890	-7.8230	H	0
-9.1590	9.1710	6.1860	H	0	-6.7460	5.6120	-13.3970	N	0	-11.2080	19.1570	-7.4880	N	0
-9.3360	9.7940	8.1300	C	0	-7.1680	5.0740	-12.6530	H	0	-10.3080	18.7100	-7.3840	H	0
-9.7360	9.3840	9.0570	H	0	-6.7490	5.0280	-14.7380	C	0	-11.4110	20.0530	-7.0690	H	0
-7.9610	10.2090	8.3350	C	0	-6.0250	5.5920	-15.3260	H	0	-10.7180	12.4520	-7.5200	C	0
-7.6780	10.9080	7.5480	H	0	-6.3660	3.5550	-14.8170	C	0	-11.5560	12.1680	-6.6870	O	0
-7.9540	10.7420	9.2860	H	0	-6.7690	3.0580	-13.9350	H	0	-9.4210	12.1230	-7.4210	N	0
-7.2110	9.4190	8.3680	H	0	-6.8860	3.1380	-15.6790	H	0	-8.8480	12.2060	-8.2480	H	0
-10.2680	11.0040	8.1110	C	0	-4.8610	3.2700	-14.9310	C	0	-8.8500	11.4980	-6.2780	C	0
-9.7950	11.7430	8.7580	H	0	-4.7980	2.2010	-15.1380	H	0	-9.2880	10.5060	-6.1780	H	0
-10.2660	11.4100	7.0990	H	0	-4.4260	3.8290	-15.7590	H	0	-7.7860	11.4630	-6.5120	H	0
-11.2790	10.7800	8.4530	H	0	-4.0890	3.5110	-13.6660	C	0	-9.0370	12.4270	-5.0950	C	0
-10.9660	7.1690	5.6560	C	0	-3.6760	4.6110	-13.2880	O	0	-8.8220	13.6080	-5.2140	O	0
-10.7840	6.0020	5.9270	O	0	-3.6700	2.6680	-12.8460	O	0	-9.4410	11.8950	-3.9530	N	0
-11.1940	7.5760	4.4190	N	0	-8.0970	5.2040	-15.4000	C	0	-9.7730	10.9420	-3.9860	H	0
-11.5540	8.5130	4.3080	H	0	-8.1380	5.1630	-16.6440	O	0	-9.8620	12.6300	-2.7370	C	0
-11.4270	6.6580	3.2790	C	0	-9.1490	5.5640	-14.6010	N	0	-9.1330	13.4040	-2.4980	H	0
-10.6880	5.8620	3.3690	H	0	-8.9440	5.8260	-13.6470	H	0	-11.2790	13.2170	-3.0830	C	0
-12.9200	6.1420	3.4390	C	0	-10.3960	6.0400	-15.2060	C	0	-11.6410	14.0050	-2.4240	H	0
-12.9600	5.4370	4.2700	H	0	-10.3680	5.8770	-16.2840	H	0	-11.2200	13.5340	-4.1250	H	0
-13.9270	7.2310	3.7460	C	0	-11.6300	5.3890	-14.5910	C	0	-12.4380	12.2120	-3.1590	C	0
-13.5790	7.7530	4.6380	H	0	-11.4440	5.1720	-13.5400	H	0	-12.1730	11.3510	-3.7720	H	0
-13.8590	7.9270	2.9100	H	0	-12.5060	6.0350	-14.6440	H	0	-12.5910	11.8770	-2.1340	H	0
-14.9880	6.9890	3.8090	H	0	-12.0170	3.9870	-15.2050	C	0	-13.6550	12.8010	-3.8010	C	0
-13.3590	5.2900	2.2340	C	0	-13.2550	3.8530	-15.8930	C	0	-14.1290	13.5370	-3.1530	H	0
-13.5260	5.8910	1.3400	H	0	-13.9630	4.6680	-15.9220	H	0	-13.4000	13.2620	-4.7550	H	0
-12.6690	4.5000	1.9390	H	0	-13.6820	2.6660	-16.4560	C	0	-14.6070	11.7020	-4.0570	N	0
-14.3260	4.8380	2.4550	H	0	-14.5990	2.5070	-17.0040	H	0	-15.2120	11.5250	-3.2670	H	0
-11.0520	7.2580	1.8560	C	0	-12.8600	1.5310	-16.2500	C	0	-14.9930	11.1940	-5.2410	C	0
-11.4970	8.3520	1.5830	O	0	-13.0640	0.5650	-16.6880	H	0	-14.4060	11.5000	-6.3700	N	0
-10.2500	6.5450	1.0550	N	0	-11.5590	1.7010	-15.6270	C	0	-13.5480	12.0310	-6.3420	H	0
-9.7400	5.7210	1.3410	H	0	-10.8320	0.9030	-15.6420	H	0	-14.7450	11.1530	-7.2560	H	0
-9.8700	7.0380	-0.2630	C	0	-11.1460	2.9090	-15.1680	C	0	-16.1320	10.4960	-5.2450	N	0
-9.6230	8.0920	-0.1390	H	0	-10.2170	2.9990	-14.6250	H	0	-16.6350	10.3480	-4.3820	H	0
-8.9440	6.5490	-0.5670	H	0	-10.5660	7.5710	-15.1430	C	0	-16.4990	10.1300	-6.1120	H	0
-10.8200	6.9970	-1.4640	C	0	-11.6170	8.0940	-15.4660	O	0	-9.8480	11.7030	-1.4590	C	0
-12.0470	7.0200	-1.2540	O	0	-9.4720	8.2560	-14.7560	N	0	-9.7210	10.4870	-1.6920	O	0
-10.2440	6.9450	-2.6650	N	0	-8.6930	7.7870	-14.3160	H	0	-10.0500	12.1800	-0.2640	N	0
-9.2380	7.0050	-2.7280	H	0	-9.4800	9.7220	-14.8060	C	0	-10.3930	13.1300	-0.2600	H	0
-10.9820	6.4480	-3.8780	C	0	-8.5110	10.2180	-14.8700	H	0	-10.3330	11.4360	0.9930	C	0
-11.7730	5.7180	-3.7060	H	0	-10.0060	10.1880	-15.6400	H	0	-10.6130	10.4080	0.7620	H	0
-11.9540	7.6030	-4.3970	H	0	-10.1640	10.3630	-13.5180	C	0	-9.0280	11.3030	1.9220	C	0
-12.5540	7.7740	-3.5030	H	0	-10.3710	11.5570	-13.5550	O	0	-8.5130	12.2540	2.0580	H	0
-11.2340	8.8410	-4.8420	C	0	-10.4510	9.6480	-12.4180	N	0	-9.4200	10.8460	3.3980	C	0
-10.5510	9.3030	-4.1290	H	0	-10.4810	8.6410	-12.4920	H	0	-8.4990	10.7900	3.9790	H	0

-10.0540	11.5890	3.8820	H	0	-19.3310	6.7740	15.4350	N	0	-16.0780	15.2890	9.7890	C	0
-9.9910	9.9180	3.4050	H	0	-19.1310	7.7580	15.3270	H	0	-15.1370	14.8830	9.4190	H	0
-8.0220	10.2370	1.5080	C	0	-20.5640	6.4860	16.1170	C	0	-15.6670	16.3350	10.8220	C	0
-7.0790	10.5440	1.9590	H	0	-20.5860	5.3980	16.1780	H	0	-15.4860	17.2890	10.3270	H	0
-8.2950	9.2450	1.8700	H	0	-20.4860	7.2510	17.4410	C	0	-16.4580	16.4350	11.5640	H	0
-7.8490	10.1980	0.4330	H	0	-20.1290	8.2660	17.2670	H	0	-14.7480	16.0710	11.3460	H	0
-11.4940	12.1180	1.6530	C	0	-21.5190	7.3230	17.7820	H	0	-16.5900	14.0130	10.5630	C	0
-11.5430	13.3750	1.6370	O	0	-19.6200	6.6770	18.5430	C	0	-17.4910	14.2260	11.1380	H	0
-12.4730	11.4240	2.1800	N	0	-19.8620	5.5560	18.9450	O	0	-16.6230	13.0920	9.9810	H	0
-12.4810	10.4420	1.9440	H	0	-18.6270	7.4000	19.0680	N	0	-15.9120	13.7930	11.3880	H	0
-13.6000	11.8340	3.0270	C	0	-17.9120	6.9160	19.5920	H	0	-16.4350	16.7620	7.6660	C	0
-13.6020	12.9240	3.0400	H	0	-18.4400	8.3440	18.7590	H	0	-16.5280	17.9780	7.7570	O	0
-14.4930	11.3360	2.6510	H	0	-21.8710	6.8340	15.3330	C	0	-15.6980	16.1850	6.6780	N	0
-13.5220	11.2620	4.5050	C	0	-22.8800	6.2440	15.6620	O	0	-15.6930	15.1820	6.5650	H	0
-13.0260	10.1850	4.7980	O	0	-21.8280	7.6220	14.2080	N	0	-15.0590	16.8840	5.5830	C	0
-14.0050	12.0550	5.4700	N	0	-20.9870	8.1640	14.0720	H	0	-15.7410	17.6740	5.2700	H	0
-14.3460	12.9930	5.3130	H	0	-23.1190	8.1450	13.6620	C	0	-13.8560	17.5840	6.0780	C	0
-13.9270	11.7530	6.9060	C	0	-23.9310	7.5040	14.0040	H	0	-13.3340	18.0130	5.2220	H	0
-13.4150	10.7920	6.9580	H	0	-23.4930	9.4960	14.2940	C	0	-14.1350	18.3870	6.7610	H	0
-13.0680	12.8120	7.6290	C	0	-24.5260	9.6560	16.0480	H	0	-12.8840	16.6580	6.8320	C	0
-12.9430	12.5770	8.6860	H	0	-23.4180	9.4500	15.7540	C	0	-12.8510	16.5580	8.1480	C	0
-12.1260	12.9370	7.0960	H	0	-23.7370	10.4550	16.0300	H	0	-13.5120	17.1080	8.8000	H	0
-13.6340	13.7430	7.5890	H	0	-24.1970	8.7640	16.0870	H	0	-11.8010	15.7700	8.5180	N	0
-15.3180	11.5330	7.5320	C	0	-22.3790	9.3000	16.0480	H	0	-11.5510	15.4780	9.4520	H	0
-16.1550	12.4250	7.4050	O	0	-22.5820	10.3820	13.7890	O	0	-11.1620	15.2450	7.3890	C	0
-15.5260	10.4590	8.3620	N	0	-21.9840	10.4460	14.5370	H	0	-10.0630	14.3810	7.2590	C	0
-14.8360	9.7220	8.3460	H	0	-23.2260	8.2450	12.1090	C	0	-9.7120	13.9680	8.1930	H	0
-16.8740	10.1990	8.8280	C	0	-24.3320	8.4430	11.5720	O	0	-9.5880	13.9650	6.0320	C	0
-17.4170	11.1330	8.6810	H	0	-22.0700	8.1550	11.4120	N	0	-8.8650	13.1800	5.8640	H	0
-17.5310	9.0270	7.9780	C	0	-21.1940	8.0100	11.8930	H	0	-10.2130	14.6040	4.9180	C	0
-16.9480	8.1530	8.2680	H	0	-22.0250	8.0410	9.9250	C	0	-9.9290	14.2960	3.9230	H	0
-18.5080	8.7580	8.3810	H	0	-21.0370	7.6660	9.6560	H	0	-11.3060	15.5110	5.0490	C	0
-17.7010	9.2130	6.4490	C	0	-22.6670	7.2280	9.5840	H	0	-11.7750	15.9930	4.2030	H	0
-16.6220	8.9320	5.5500	C	0	-22.1550	9.4610	9.2070	C	0	-11.8450	15.8000	6.3160	C	0
-15.7420	8.4770	5.9800	H	0	-22.0420	9.6470	7.9900	O	0	-14.7740	15.9780	4.3930	C	0
-16.7650	9.2080	4.1540	C	0	-22.2110	10.5350	9.9960	N	0	-14.9070	14.7610	4.4750	O	0
-15.9700	9.0800	3.4340	H	0	-22.4790	10.3570	10.9540	H	0	-14.4660	16.5630	3.2210	N	0
-17.9800	9.6750	3.7080	C	0	-22.0560	11.9870	9.6410	C	0	-14.4320	17.5730	3.1960	H	0
-18.2210	9.8310	2.3910	O	0	-22.8440	12.2610	8.9400	H	0	-13.9410	15.9140	2.0270	C	0
-17.4560	9.7020	1.8240	H	0	-22.3340	12.6520	11.0150	C	0	-13.4770	14.9540	2.2520	H	0
-19.0860	9.8520	4.5870	C	0	-21.8110	12.1070	11.8010	H	0	-15.1310	15.6830	1.0040	C	0
-20.0790	10.0370	4.2040	H	0	-21.8370	13.6170	11.1120	H	0	-16.0260	15.2470	1.4460	H	0
-18.9020	9.6860	5.9770	C	0	-23.7450	12.8180	11.3620	C	0	-15.3740	16.7300	0.8220	H	0
-19.8090	9.8260	6.5460	H	0	-24.6100	13.1150	10.5730	O	0	-14.7360	15.1000	-0.3890	C	0
-16.9120	9.7920	10.3280	C	0	-24.0870	12.8380	12.6620	N	0	-13.7220	15.3650	-0.6900	H	0
-16.0630	9.0630	10.8110	O	0	-25.0730	12.9590	12.8450	H	0	-14.8270	13.6100	-0.1970	C	0
-17.8840	10.2740	11.1530	N	0	-23.3540	12.9350	13.3500	H	0	-14.8290	13.1710	-1.1950	H	0
-18.6920	10.6940	10.7160	H	0	-20.6580	12.2830	9.1070	C	0	-13.9930	13.2870	0.4270	H	0
-17.9600	10.0850	12.6200	C	0	-19.7100	11.8580	9.6980	O	0	-15.7540	13.3460	0.3120	H	0
-17.0190	10.3890	13.0790	H	0	-20.6150	12.9330	7.8940	N	0	-15.6430	15.6560	-1.4420	C	0
-19.1350	10.9020	13.1160	C	0	-21.4230	13.3100	7.4190	H	0	-15.5680	16.7420	-1.4050	H	0
-18.8170	11.9390	13.0130	H	0	-19.3740	13.3200	7.1720	C	0	-15.3100	15.2950	-2.4160	H	0
-20.0080	10.7310	12.4860	H	0	-18.6430	12.5640	7.4600	H	0	-16.6380	15.2510	-1.2570	H	0
-19.4870	10.6590	14.6370	C	0	-19.5390	13.2680	5.6110	C	0	-12.8430	16.7080	1.4110	C	0
-19.2710	9.6000	15.2370	O	0	-20.1070	12.4160	5.2370	H	0	-12.9090	17.9430	1.4080	O	0
-20.2790	11.4920	15.1240	O	0	-19.9970	14.1740	5.2160	H	0	-11.6810	16.0600	1.0520	N	0
-18.1950	8.5710	13.0060	C	0	-18.1480	13.1390	4.9660	C	0	-11.7650	15.0580	0.9660	H	0
-19.1750	7.8970	12.6870	O	0	-17.5600	13.7680	5.6340	H	0	-10.5600	16.6930	0.5430	C	0
-17.2580	8.0180	13.8270	N	0	-17.7890	12.1200	5.1100	H	0	-10.8770	17.7310	0.4450	H	0
-16.5780	8.6680	14.1950	H	0	-17.9540	13.4650	3.5050	C	0	-9.5050	16.5800	1.6590	C	0
-17.2980	6.5550	14.0670	C	0	-16.9510	13.2100	3.1630	H	0	-9.0220	15.6130	1.7960	H	0
-17.2950	6.0020	13.1270	H	0	-18.5450	12.7940	2.8820	H	0	-8.8100	17.3760	1.3910	H	0
-16.1080	5.9950	14.8710	C	0	-18.2660	14.8650	3.2870	N	0	-9.8690	17.0080	2.5930	H	0
-16.3330	4.9420	15.0410	H	0	-18.3600	15.4310	4.1190	H	0	-10.0250	16.2160	-0.8340	C	0
-14.8560	6.2720	13.9740	C	0	-18.5830	15.3640	2.1120	C	0	-9.5350	15.1040	-0.9770	O	0
-13.9780	5.7370	14.3380	H	0	-18.8340	14.6400	1.0330	N	0	-9.9040	17.0310	-1.8840	N	0
-15.0120	5.7570	13.0260	H	0	-18.8220	13.6330	1.1170	H	0	-10.1850	17.9770	-1.6680	H	0
-14.7790	7.3530	13.8590	H	0	-19.3190	15.0340	0.2400	H	0	-9.3880	16.5870	-3.2090	C	0
-15.8730	6.6490	16.2020	C	0	-18.7200	16.6460	2.0520	N	0	-9.7360	15.5540	-3.2290	H	0
-15.4920	7.6680	16.1330	H	0	-18.6390	17.1940	2.8970	H	0	-10.1530	17.3790	-4.2770	C	0
-16.8100	6.6070	16.7570	H	0	-18.8200	17.1280	1.1710	H	0	-9.8800	18.4200	-4.1060	H	0
-14.9260	5.9450	17.0940	C	0	-18.9070	14.6890	7.6700	C	0	-9.6920	17.1430	-5.2360	H	0
-15.0920	6.2930	18.1140	H	0	-19.6690	15.6600	7.7890	O	0	-11.6510	17.1860	-4.3160	C	0
-15.0740	4.8650	17.0920	H	0	-17.6160	14.7230	8.0630	N	0	-12.5800	18.0270	-3.6450	C	0
-13.8960	6.2010	16.8480	H	0	-17.0170	13.9120	8.0080	H	0	-12.2390	18.7250	-2.8960	H	0
-18.5850	5.9870	14.7010	C	0	-17.0690	15.9110	8.7550	C	0	-13.9530	17.8920	-3.9100	C	0
-18.7930	4.7360	14.6310	O	0	-17.8730	16.3950	9.3090	H	0	-14.7440	18.4530	-3.4360	H	0



-14.4450	17.0900	-4.8940	C	0	-13.7890	25.8520	-1.3370	C	0	-3.9580	24.5560	4.8240	N	0
-15.7970	16.9300	-5.1190	O	0	-14.4890	25.8260	-2.1730	H	0	-3.1530	23.9610	4.6910	H	0
-16.0240	16.1640	-5.6510	H	0	-13.7950	24.8690	-0.8660	H	0	-3.9970	25.4110	6.0150	C	0
-13.5520	16.3070	-5.6510	C	0	-14.1580	26.7750	-0.2210	C	0	-5.0010	25.7620	6.2530	H	0
-13.9220	15.7660	-6.5100	H	0	-13.3720	27.3090	0.6050	O	0	-3.3440	24.7110	7.2460	C	0
-12.1970	16.3640	-5.3850	C	0	-15.3810	27.0470	-0.1360	O	0	-3.7010	23.6810	7.2300	H	0
-11.4810	15.7740	-5.9380	H	0	-11.5210	23.8950	-1.1400	C	0	-2.2570	24.6900	7.3270	H	0
-7.8800	16.8120	-3.4200	C	0	-11.9920	23.3530	-0.1720	O	0	-3.8980	25.3680	8.5270	C	0
-7.2960	17.8510	-3.0100	O	0	-11.2890	23.3030	-2.3150	N	0	-5.1330	25.2620	8.6640	O	0
-7.3230	15.9190	-4.1690	N	0	-10.9460	23.7900	-3.1310	H	0	-3.2460	26.2000	9.1880	O	0
-7.9660	15.2250	-4.5220	H	0	-11.6230	21.9230	-2.5290	C	0	-3.3920	26.7880	5.9350	C	0
-5.9050	15.8160	-4.4450	C	0	-12.5640	21.6340	-2.0610	H	0	-2.5500	27.0370	5.0370	O	0
-5.4330	16.1070	-3.5060	H	0	-11.7800	21.7710	-4.0250	C	0	-3.6140	27.7270	6.8500	N	0
-5.5960	14.3720	-4.7120	C	0	-11.0970	22.4750	-4.5000	H	0	-4.3410	27.4830	7.5080	H	0
-6.1400	14.1110	-5.6200	H	0	-11.5320	20.7410	-4.2830	H	0	-2.6960	28.7620	7.2190	C	0
-4.5410	14.2100	-4.9310	H	0	-13.2320	21.9150	-4.4470	C	0	-2.6380	29.4220	6.3530	H	0
-5.9690	13.4380	-3.8020	O	0	-13.9240	21.2720	-3.9030	H	0	-2.9680	29.5310	8.5560	C	0
-5.8280	12.5720	-4.1910	H	0	-13.6450	22.8850	-4.1730	H	0	-4.0300	29.7470	8.4440	H	0
-5.3600	16.7290	-5.6270	C	0	-13.4480	21.7300	-5.9110	C	0	-2.8730	28.9080	9.4460	H	0
-4.1930	16.6770	-6.0550	O	0	-14.5020	22.0820	-6.4800	O	0	-2.2340	30.6530	8.7800	O	0
-6.2980	17.5720	-6.1380	N	0	-12.4810	21.2950	-6.5520	O	0	-2.6460	31.4090	8.3570	H	0
-7.1490	17.6760	-5.6040	H	0	-10.4900	21.0350	-1.9590	C	0	-1.2260	28.3190	7.2850	C	0
-6.1110	18.3550	-7.4640	C	0	-10.7330	20.0610	-1.2510	O	0	-0.3500	28.9040	6.6550	O	0
-5.0930	18.7410	-7.3990	H	0	-9.3190	21.3830	-2.3130	N	0	-0.9620	27.2860	8.0600	N	0
-6.2030	17.3260	-8.6020	C	0	-9.2180	22.1880	-2.9160	H	0	-1.7090	26.8850	8.6080	H	0
-5.7760	17.7540	-9.5080	H	0	-8.0420	20.6770	-1.8750	C	0	0.3630	26.7280	8.1210	C	0
-5.5390	16.4890	-8.3850	H	0	-8.2680	19.6560	-2.1840	H	0	1.0240	27.5380	8.4280	H	0
-7.4390	16.6300	-9.1410	C	0	-6.8430	21.2370	-2.7390	C	0	0.3330	25.7150	9.2550	C	0
-7.9990	17.4890	-9.5100	H	0	-6.8410	22.3150	-2.5750	H	0	-0.3400	24.8770	9.0740	H	0
-7.3080	15.9380	-9.9730	H	0	-5.5050	20.6370	-2.2190	C	0	1.3730	25.4090	9.3670	H	0
-8.2310	15.8580	-8.0760	C	0	-4.6870	21.0690	-2.7950	H	0	-0.1290	26.3010	10.6190	C	0
-9.3020	16.3840	-7.7600	O	0	-5.3740	21.0040	-1.2010	H	0	-0.4190	25.4440	11.4510	O	0
-7.7810	14.7280	-7.5910	N	0	-5.5370	19.5480	-2.2730	H	0	-0.1560	27.5630	10.8290	O	0
-8.3320	14.2960	-6.8640	H	0	-6.8950	20.8080	-4.2310	C	0	0.8740	26.0860	6.8460	C	0
-7.0400	14.1930	-8.0200	H	0	-6.8550	19.7390	-4.4390	H	0	1.9550	25.5060	6.9320	O	0
-7.1360	19.4730	-7.5600	C	0	-7.8340	21.1360	-4.6780	H	0	0.1920	26.0790	5.7130	N	0
-8.2620	19.2470	-7.2080	O	0	-6.0860	21.2870	-4.7830	H	0	-0.7470	26.4260	5.5810	H	0
-6.7970	20.6350	-8.1590	N	0	-7.8590	20.7790	-0.3140	C	0	0.6200	25.1570	4.6660	C	0
-5.8850	20.8440	-8.5380	H	0	-7.2200	19.9070	0.2450	O	0	0.6210	24.1600	5.1070	H	0
-7.7140	21.7250	-8.4790	C	0	-8.3450	21.8190	0.3640	N	0	-0.5010	25.1520	3.5950	C	0
-7.3110	22.2060	-9.3700	H	0	-8.7540	22.5340	-0.2200	H	0	-1.4590	24.8550	4.0220	H	0
-8.7200	21.3940	-8.7340	H	0	-8.2260	22.2160	1.7430	C	0	-0.6810	26.1320	3.1530	H	0
-7.7440	22.8580	-7.4000	C	0	-8.6290	23.2240	1.8380	H	0	-0.2990	24.0970	2.5270	C	0
-6.8270	23.0180	-6.5940	O	0	-9.0170	21.1250	2.6090	C	0	-0.0460	22.7560	2.8430	C	0
-8.8550	23.6440	-7.2810	N	0	-8.7640	20.1310	2.2420	H	0	-0.1180	22.4400	3.8740	H	0
-10.0560	23.4890	-8.0530	C	0	-8.7460	21.2360	3.6590	H	0	0.2570	21.8070	1.8200	C	0
-10.5490	22.5840	-7.6980	H	0	-10.5800	21.2930	2.3960	C	0	0.3190	20.7340	1.9290	H	0
-9.8210	23.3830	-9.1120	H	0	-10.7390	21.2200	1.3200	H	0	0.3000	22.2470	0.4820	C	0
-11.0640	24.6410	-7.7970	C	0	-11.3460	20.1020	2.9950	C	0	0.5000	21.4920	-0.2630	H	0
-12.1100	24.3460	-7.8740	H	0	-12.3070	20.1310	2.4820	H	0	0.1390	23.6160	0.1840	C	0
-10.8750	25.4000	-8.5560	H	0	-10.8670	19.1360	2.8370	H	0	0.3100	23.9800	-0.8190	H	0
-10.6020	25.1140	-6.4740	C	0	-11.5090	20.2840	4.0570	H	0	-0.1950	24.5250	1.1690	C	0
-11.1040	24.6140	-5.6460	H	0	-11.0610	22.5800	2.9750	C	0	-0.3900	25.5520	0.8970	H	0
-10.7860	26.1870	-6.4410	H	0	-10.5980	22.5570	3.9620	H	0	1.8820	25.4640	3.8870	C	0
-9.0960	24.8010	-6.3360	C	0	-10.7240	23.4390	2.3940	H	0	1.9210	26.5030	3.2980	O	0
-8.5950	25.6460	-6.8070	H	0	-12.1490	22.5360	3.0100	H	0	2.9010	24.5160	3.9550	N	0
-8.5540	24.4890	-4.9170	C	0	-6.7360	22.3070	2.1990	C	0	2.7980	23.8070	4.6660	H	0
-8.6780	23.4160	-4.3780	O	0	-6.0450	21.3660	2.5930	O	0	4.1320	24.6280	3.2350	C	0
-8.0620	25.5270	-4.1490	N	0	-6.2000	23.5400	2.1180	N	0	4.7600	23.8460	3.6630	H	0
-8.0560	26.4150	-4.6310	H	0	-6.7770	24.3470	1.9290	H	0	3.9040	24.2330	1.7890	C	0
-7.6980	25.3900	-2.7110	C	0	-4.8430	23.9640	2.5980	C	0	2.8750	24.4540	1.5030	H	0
-6.9470	24.6020	-2.6640	H	0	-4.2830	23.0350	2.7100	H	0	4.4880	24.9830	1.2560	H	0
-7.0250	26.7260	-2.4420	C	0	-4.1700	24.7710	1.4810	C	0	4.2460	22.8240	1.3830	C	0
-7.6980	27.5820	-2.3890	H	0	-4.6670	25.7400	1.4480	H	0	4.5320	21.8730	2.1510	O	0
-6.5860	26.6000	-1.4520	H	0	-3.1100	24.9330	1.6730	H	0	3.9610	22.5660	0.1180	N	0
-5.8630	27.0550	-3.3540	C	0	-4.1610	24.1290	0.0590	C	0	3.9640	21.5890	-0.1380	H	0
-5.0230	26.1420	-3.5170	O	0	-5.1620	23.9800	-0.3440	H	0	3.6210	23.2570	-0.5360	H	0
-5.9100	28.0770	-4.0730	O	0	-3.4540	25.1910	-0.8550	C	0	5.0400	25.8600	3.4260	C	0
-8.7740	25.1170	-1.6980	C	0	-4.1660	25.9830	-1.0860	H	0	6.0170	25.9730	2.6520	O	0
-8.6030	24.3440	-0.7590	O	0	-2.5470	25.6140	-0.4250	H	0	4.7490	26.6870	4.4330	N	0
-9.9980	25.6690	-1.9570	N	0	-3.2380	24.7460	-1.8260	H	0	3.9740	26.3960	5.0110	H	0
-10.1120	26.3790	-2.6660	H	0	-3.4450	22.8080	0.0690	C	0	5.3090	27.9980	4.5960	C	0
-11.1940	25.3910	-1.1120	C	0	-4.1440	22.0040	0.2970	H	0	5.2420	28.5400	3.6530	H	0
-11.0480	25.7260	-0.0850	H	0	-2.9240	22.5690	-0.8570	H	0	4.5820	28.7640	5.6940	C	0
-12.3610	26.1520	-1.7650	C	0	-2.7170	22.8500	0.8790	H	0	4.6240	28.2470	6.6530	H	0
-12.1390	27.1960	-1.5440	H	0	-5.0230	24.6610	3.9740	C	0	5.0420	29.7510	5.7490	H	0
-12.4030	25.8960	-2.8240	H	0	-6.0710	25.2260	4.1400	O	0	3.0630	28.8410	5.3990	C	0

2.5790	27.8640	5.3940	H	0	13.2300	22.7490	-0.8350	H	0	-5.3590	23.6890	-11.2810	H	0
2.5250	29.3400	6.2040	H	0	8.9760	24.0630	-3.6390	C	0	-6.0930	25.6860	-10.9750	C	0
2.6370	29.5720	4.1160	C	0	9.0850	23.6550	-4.8020	O	0	-6.2730	26.0050	-12.0020	H	0
2.9980	30.5970	4.2000	H	0	8.1990	23.5930	-2.6600	N	0	-7.3970	25.0000	-10.4820	C	0
2.9610	29.0870	3.1950	H	0	8.4400	23.8570	-1.7150	H	0	-7.7420	24.1040	-10.9980	H	0
1.0970	29.3350	4.2090	C	0	7.2010	22.5550	-2.8260	C	0	-7.3070	24.6460	-9.4550	H	0
0.8640	28.2730	4.2900	H	0	7.6320	21.8000	-3.4830	H	0	-8.2200	25.7140	-10.5050	H	0
0.7980	29.7860	5.1560	H	0	7.0260	21.9870	-1.3420	C	0	-5.9080	26.9150	-10.2800	O	0
0.4150	30.0350	3.1050	N	0	6.6770	22.8610	-0.7930	H	0	-5.8440	27.5600	-10.9880	H	0
0.8420	29.7450	2.2360	H	0	6.2330	21.2430	-1.4280	H	0	-3.7810	25.0180	-11.7670	C	0
-0.5060	29.6210	3.1050	H	0	8.2530	21.3520	-0.6550	C	0	-3.6780	24.6310	-12.9390	O	0
0.2060	31.0220	3.1370	H	0	9.5870	21.3480	-1.1590	N	0	-2.7780	25.8480	-11.3130	N	0
6.8230	28.0170	4.8290	C	0	10.3460	20.6950	-0.2820	C	0	-2.8840	26.3170	-10.4250	H	0
7.5060	29.0630	4.6000	O	0	11.3270	20.3900	-0.6150	H	0	-1.8960	26.5710	-12.2680	C	0
7.4070	26.9180	5.2350	N	0	9.5620	20.3680	0.8080	N	0	-2.4690	27.1630	-12.9820	H	0
6.7400	26.1670	5.3450	H	0	9.8410	19.8840	1.6500	H	0	-0.9880	27.5740	-11.4950	C	0
8.8930	26.8010	5.5480	C	0	8.3110	20.6760	0.5890	C	0	-0.6420	27.0940	-10.5800	H	0
9.3390	27.7640	5.7960	H	0	7.4330	20.3790	1.1430	H	0	-0.1570	27.8470	-12.1450	H	0
9.0650	25.9460	6.8340	C	0	5.7840	22.9280	-3.2960	C	0	-1.8030	28.8100	-11.0230	C	0
10.1370	25.7540	6.8810	H	0	4.9000	21.9960	-3.2850	O	0	-2.1310	29.3490	-11.9120	H	0
8.7000	26.4710	7.7160	H	0	5.4520	24.1890	-3.5310	N	0	-2.7230	28.5860	-10.4840	H	0
8.3240	24.6010	6.8150	C	0	6.1880	24.8780	-3.4710	H	0	-0.9810	29.7460	-10.1310	C	0
8.2580	24.1600	5.8200	H	0	4.1760	24.7150	-3.9400	C	0	-1.6260	30.5910	-9.8910	H	0
8.8830	23.9560	7.4930	H	0	4.3020	25.5600	-4.6170	H	0	-0.6560	29.2500	-9.2170	H	0
6.9370	24.6990	7.4580	C	0	3.7370	23.9840	-4.6200	H	0	0.3150	30.2880	-10.8100	C	0
6.8420	24.7000	8.6700	O	0	3.2410	25.1370	-2.8080	C	0	0.8760	30.9710	-10.1720	H	0
5.9570	24.7510	6.7410	O	0	3.4420	24.7320	-1.6630	O	0	1.0550	29.5150	-11.0150	H	0
9.7870	26.1760	4.4050	C	0	2.1580	25.8520	-3.1950	N	0	-0.0080	31.1910	-11.9360	N	0
10.9790	26.3710	4.3870	O	0	1.9320	25.9980	-4.1680	H	0	-0.5400	32.0130	-11.6880	H	0
9.2330	25.5620	3.4130	N	0	1.1660	26.4450	-2.3100	C	0	0.8340	31.5260	-12.3820	H	0
8.2510	25.3370	3.4880	H	0	1.1250	25.7310	-1.4860	H	0	-0.3970	30.5820	-12.6420	H	0
9.9470	25.0200	2.2000	C	0	1.6240	27.3650	-1.9470	H	0	-0.9340	25.6490	-13.0670	C	0
10.9350	25.4670	2.0900	H	0	-0.2720	26.6110	-2.9070	C	0	-0.4170	25.9180	-14.1680	O	0
10.1570	23.4910	2.5810	C	0	-0.6320	25.9290	-3.8110	O	0	-0.6190	24.4490	-12.4310	N	0
9.1760	23.0520	2.7610	H	0	-1.0740	27.5850	-2.4540	N	0	-1.0660	24.3520	-11.5310	H	0
10.4380	22.9200	1.6960	H	0	-0.7340	28.6080	-1.4760	C	0	0.3570	23.5390	-12.9300	C	0
11.0220	23.2050	3.7830	C	0	0.2450	28.9310	-1.8320	H	0	1.0590	24.1580	-13.4890	H	0
12.3840	23.5480	3.8630	C	0	-0.7110	28.1790	-0.4740	H	0	1.1520	22.8950	-11.7820	C	0
12.8540	23.9890	2.9950	H	0	-1.7180	29.8400	-1.6090	C	0	1.9130	22.2750	-12.2560	H	0
13.2250	23.2480	4.9780	C	0	-1.3310	30.6500	-2.2270	H	0	1.9460	23.9060	-10.9130	C	0
14.2510	23.5820	5.0340	H	0	-2.0650	30.2240	-0.6490	H	0	2.3940	23.3390	-10.0970	H	0
12.5960	22.6940	6.1200	C	0	-2.8720	29.0760	-2.1990	C	0	2.7860	24.3320	-11.4620	H	0
13.2670	22.4440	6.9280	H	0	-3.4740	29.7920	-2.7580	H	0	1.3230	24.7760	-10.7060	H	0
11.2400	22.2360	6.0150	C	0	-3.5390	28.7170	-1.4150	H	0	0.2600	22.1160	-11.0510	O	0
10.8660	21.7240	6.8890	H	0	-2.3120	27.9670	-3.0980	C	0	-0.3520	22.6380	-10.5270	H	0
10.4360	22.5460	4.8560	C	0	-3.0000	27.1220	-3.0570	H	0	-0.2690	22.5090	-13.9040	C	0
9.4070	22.2170	4.8290	H	0	-2.1940	28.3620	-4.5860	C	0	0.3500	21.4710	-14.3080	O	0
9.1360	25.2720	0.9030	C	0	-1.1530	28.8410	-5.0580	O	0	-1.4880	22.7430	-14.3440	N	0
8.8130	24.3420	0.1560	O	0	-3.3180	28.1910	-5.2990	N	0	-1.9640	23.5180	-13.9040	H	0
8.6750	26.4840	0.5720	N	0	-4.1740	27.8420	-4.8920	H	0	-2.2090	21.9100	-15.3220	C	0
8.8600	27.7110	1.3790	C	0	-3.3610	28.2150	-6.7440	C	0	-1.6150	21.0610	-15.6600	H	0
9.9100	27.9300	1.5750	H	0	-4.3690	28.3270	-7.1440	H	0	-3.5430	21.4630	-14.7180	C	0
8.3600	27.6130	2.3430	H	0	-2.8160	29.1330	-6.9640	H	0	-4.1160	22.3650	-14.5030	H	0
8.2650	28.8410	0.5390	C	0	-2.6530	27.1060	-7.5480	C	0	-3.9220	20.9250	-15.5870	H	0
8.9510	29.3700	-0.1220	H	0	-3.1830	26.8270	-8.6420	O	0	-3.5680	20.5280	-13.5290	C	0
7.8100	29.6220	1.1490	H	0	-1.5850	26.4330	-7.0730	N	0	-3.4880	20.8290	-12.2160	C	0
7.1240	28.1540	-0.2290	C	0	-1.4250	26.4250	-6.0760	H	0	-3.3730	21.8450	-11.8670	H	0
7.0080	28.6380	-1.1980	H	0	-0.8150	25.5170	-7.8860	C	0	-3.5310	19.6420	-11.4650	N	0
6.2070	28.1180	0.3590	H	0	-0.4720	26.1270	-8.7220	H	0	-3.3840	19.6940	-10.4670	H	0
7.6460	26.7780	-0.4370	C	0	0.4150	25.0110	-7.1300	C	0	-3.5030	18.5170	-12.2390	C	0
6.9370	25.9510	-0.3930	H	0	0.1240	24.5820	-6.1710	H	0	-3.4030	17.1580	-11.9610	C	0
8.0790	26.4720	-1.8730	C	0	0.8430	24.3370	-7.8720	H	0	-3.3440	16.8380	-10.9310	H	0
7.3140	26.5480	-2.8340	O	0	1.4750	26.0980	-6.9490	C	0	-3.5010	16.2820	-12.9930	C	0
9.3440	26.0690	-2.0830	N	0	2.3890	25.8430	-6.1830	O	0	-3.3850	15.2160	-12.8690	H	0
9.7860	25.8040	-1.2140	H	0	1.4270	27.1090	-7.6350	O	0	-3.6110	16.7630	-14.3670	C	0
9.7370	25.3490	-3.2500	C	0	-1.6040	24.3150	-8.2710	C	0	-3.7770	16.0660	-15.1750	H	0
9.5300	25.9310	-4.1490	H	0	-1.4110	23.8170	-9.3720	O	0	-3.8410	18.1340	-14.5520	C	0
11.2600	25.0800	-3.3240	C	0	-2.5640	23.8430	-7.4400	N	0	-4.0110	18.3750	-15.5910	H	0
11.5890	24.7800	-4.3200	H	0	-2.7570	24.2990	-6.5600	H	0	-3.6310	19.0620	-13.5580	C	0
11.8040	26.0220	-3.2600	H	0	-3.4160	22.7820	-7.9060	C	0	-2.5110	22.7060	-16.5810	C	0
11.9040	24.1120	-2.4350	C	0	-2.8540	21.8860	-8.1710	H	0	-2.8820	23.8780	-16.5090	O	0
11.3070	23.2010	-2.3970	H	0	-4.0330	22.3930	-7.0950	H	0	-2.3440	22.0940	-17.7730	N	0
12.8100	23.7970	-2.9530	H	0	-4.2910	23.1380	-9.1140	C	0	-1.6890	20.7490	-18.0190	C	0
12.2900	24.5380	-1.0370	C	0	-4.6780	22.1230	-9.6850	O	0	-2.1690	19.9970	-17.3930	H	0
11.9150	25.4620	-0.4050	O	0	-4.5720	24.3980	-9.4670	N	0	-0.6110	20.8660	-17.9100	H	0
13.0890	23.6740	-0.4530	N	0	-4.2160	25.1710	-8.9230	H	0	-2.0780	20.4090	-19.5000	C	0
13.4220	23.8160	0.4890	H	0	-4.9640	24.6150	-10.8620	C	0	-3.0350	19.8880	-19.5080	H	0

-1.2730	19.8490	-19.9760	H	0	-12.9060	17.9160	-13.5290	H	0	-5.4650	6.5110	-0.0860	H	0
-2.3090	21.7160	-20.1580	C	0	-12.2870	19.9980	-13.4120	C	0	-3.9530	6.9400	-0.8280	H	0
-3.0090	21.6830	-20.9930	H	0	-12.6250	20.0370	-12.3770	H	0	-4.8620	8.0960	0.1710	H	0
-1.3340	22.1120	-20.4400	H	0	-11.3120	20.4850	-13.4290	H	0	-4.9860	9.0720	-2.0200	O	0
-2.8000	22.6560	-19.0380	C	0	-13.2660	20.6510	-14.2980	C	0	-4.0810	8.7640	-1.9400	H	0
-2.3250	23.6340	-19.1130	H	0	-12.8970	20.5250	-15.3160	H	0	-6.2860	5.5990	-2.6750	C	0
-4.3890	22.8510	-19.0200	C	0	-14.2760	20.2780	-14.1290	H	0	-7.4410	5.4530	-2.2330	O	0
-5.1420	21.8800	-18.7730	O	0	-13.2530	22.1440	-13.9790	C	0	-5.5390	4.5950	-2.8280	N	0
-4.8580	24.1090	-19.2780	N	0	-13.0440	22.2320	-12.9130	H	0	-4.6770	4.7140	-3.3400	H	0
-4.2020	24.8040	-19.6070	H	0	-12.5600	22.6990	-14.6120	H	0	-6.0400	3.1960	-2.8930	C	0
-6.3080	24.3820	-19.1760	C	0	-14.6130	22.7050	-14.1600	N	0	-6.8450	3.0710	-2.1690	H	0
-6.5550	25.4440	-19.1830	H	0	-15.2470	22.2100	-13.5490	H	0	-6.2930	2.6790	-4.3360	C	0
-6.6230	24.0840	-20.1750	H	0	-14.6700	23.6880	-13.9330	H	0	-6.6370	1.6450	-4.3440	H	0
-7.0600	23.7440	-17.9630	C	0	-14.9590	22.7160	-15.1090	H	0	-7.1400	3.2400	-4.7310	H	0
-6.5030	23.6910	-16.8690	O	0	-10.7260	16.3020	-13.3900	C	0	-5.0660	2.7600	-5.2360	C	0
-8.2410	23.2280	-18.1360	N	0	-11.4930	15.4600	-12.9930	O	0	-4.6320	3.8930	-5.7840	C	0
-8.6670	23.3120	-19.0480	H	0	-9.8110	16.0230	-14.3100	N	0	-5.1120	4.8600	-5.7520	H	0
-9.0190	22.6730	-17.0960	C	0	-9.3250	16.8680	-14.5750	H	0	-3.4180	3.5920	-6.4480	N	0
-8.7290	23.0750	-16.1250	H	0	-9.4800	14.6920	-14.8480	C	0	-2.9150	4.3630	-6.8660	H	0
-10.4680	23.0750	-17.3530	C	0	-10.2940	13.9770	-14.7290	H	0	-2.9880	2.2910	-6.2220	C	0
-10.9050	22.5070	-18.1740	H	0	-9.2880	14.9170	-16.4110	C	0	-1.9480	1.5340	-6.7720	C	0
-11.0570	22.6740	-16.5280	H	0	-8.2580	15.1120	-16.7120	H	0	-1.2100	1.9590	-7.4360	H	0
-10.8940	24.5820	-17.3670	C	0	-9.4200	13.9370	-16.8710	H	0	-1.8270	0.1330	-6.4040	C	0
-10.7800	24.9760	-18.3770	H	0	-10.2550	15.7440	-17.2080	C	0	-1.1330	-0.5060	-6.9290	H	0
-11.9230	24.7280	-17.0400	H	0	-10.0650	16.7640	-16.8720	H	0	-2.9070	-0.4680	-5.7290	C	0
-10.0690	25.5400	-16.4200	C	0	-9.9600	15.7820	-18.7280	C	0	-3.0130	-1.5380	-5.6310	H	0
-9.9810	25.1280	-15.2160	O	0	-9.6020	14.7870	-18.9960	H	0	-3.9300	0.3230	-5.1840	C	0
-9.6020	26.5970	-16.8790	O	0	-10.9280	15.8960	-19.2150	H	0	-4.6570	-0.0500	-4.4780	H	0
-8.7750	21.1730	-16.8330	C	0	-9.2120	16.5480	-18.9330	H	0	-4.0810	1.7090	-5.4740	C	0
-9.5540	20.4480	-16.2660	O	0	-11.7470	15.4440	-16.9600	C	0	-5.0000	2.2100	-2.3290	C	0
-7.6210	20.6370	-17.2320	N	0	-12.3460	16.1590	-17.5260	H	0	-5.3640	1.0600	-2.0430	O	0
-6.9880	21.2700	-17.7000	H	0	-11.9770	14.4190	-17.2490	H	0	-3.7040	2.6380	-2.1410	N	0
-7.2450	19.1440	-17.1870	C	0	-11.9690	15.5240	-15.8960	H	0	-3.4350	3.5830	-5.3780	H	0
-8.0020	18.4890	-17.6180	H	0	-8.2410	14.0840	-14.1570	C	0	-2.7550	2.1250	-1.1330	C	0
-5.9350	18.9100	-17.8880	C	0	-7.7390	13.1030	-14.6110	O	0	-2.5200	1.0740	-1.2980	H	0
-6.0790	19.1350	-18.9450	H	0	-7.7380	14.7090	-13.0350	N	0	-1.8100	2.5970	-1.4050	H	0
-5.2350	19.6520	-17.5030	H	0	-8.2080	15.5360	-12.6960	H	0	-3.1310	2.3700	0.3460	C	0
-5.2780	17.5400	-17.9760	C	0	-6.2780	14.6750	-12.8330	C	0	-4.0500	1.7590	0.8650	O	0
-4.2130	17.6710	-18.1690	H	0	-5.6770	14.5890	-13.7380	H	0	-2.2770	3.1780	0.9740	N	0
-5.2900	17.0230	-17.0160	H	0	-5.9060	15.6330	-12.4700	H	0	-1.5280	3.5720	0.4230	H	0
-5.7950	16.5650	-19.0070	C	0	-5.7800	13.5530	-11.9060	C	0	-2.2630	3.3430	2.3670	C	0
-6.1840	16.9730	-20.1140	O	0	-4.7430	13.7550	-11.2880	O	0	-3.1230	2.7710	2.7150	H	0
-6.1180	15.3440	-18.6680	N	0	-6.4660	12.3880	-11.8340	N	0	-1.0100	2.6780	2.9760	C	0
-6.6100	14.7660	-19.3340	H	0	-7.4560	12.3470	-12.0310	H	0	-0.1190	3.1290	2.5380	H	0
-5.8030	14.9210	-17.8060	H	0	-6.0050	11.3160	-10.8920	C	0	-1.0620	2.6680	4.0640	H	0
-7.3100	18.6310	-15.7100	C	0	-6.7770	10.5470	-10.8800	H	0	-0.8660	1.2810	2.5810	C	0
-7.5300	17.4800	-15.5170	O	0	-5.0590	10.8930	-11.2300	H	0	-0.0270	0.8330	1.6510	C	0
-7.1830	19.5230	-14.7100	N	0	-5.9960	11.7610	-9.4180	C	0	0.5600	1.4990	1.0350	H	0
-7.1950	20.4870	-15.0140	H	0	-6.8990	12.2610	-8.7920	O	0	-0.0840	-0.5510	1.5330	N	0
-7.1990	19.1330	-13.2780	C	0	-4.7730	11.5750	-8.9090	N	0	0.5790	-1.0800	0.9840	H	0
-6.3910	18.4220	-13.1080	H	0	-4.0470	11.1840	-9.4910	H	0	-0.9540	-1.0440	2.4410	C	0
-7.0960	20.3520	-12.3720	C	0	-4.4560	11.8140	-7.5010	C	0	-1.2800	-2.4130	2.7420	C	0
-7.1130	19.9680	-11.3520	H	0	-3.3930	11.6690	-7.3070	H	0	-0.7710	-3.1690	2.1620	H	0
-6.1140	20.7990	-12.5270	H	0	-4.7990	12.8300	-7.3040	H	0	-2.0880	-2.6170	3.8850	C	0
-8.0510	21.4600	-12.5050	C	0	-5.1260	10.9410	-6.5690	C	0	-2.3330	-3.6240	4.1870	H	0
-7.9580	22.4400	-13.4130	C	0	-5.2160	11.1980	-5.3290	O	0	-2.5500	-1.5540	4.6350	C	0
-7.1610	22.5610	-14.1320	H	0	-5.6860	9.8610	-7.0920	N	0	-3.1380	-1.7250	5.5250	H	0
-9.1450	23.1880	-13.3790	N	0	-5.5980	9.8140	-8.0970	H	0	-2.2550	-0.2170	4.2430	C	0
-9.4200	23.9610	-13.9690	H	0	-6.5040	8.8520	-6.4370	C	0	-2.6700	0.5990	4.8160	H	0
-9.8640	22.8450	-12.2710	C	0	-7.3090	9.3570	-5.9040	H	0	-1.4330	0.0530	3.1140	C	0
-11.0910	23.3640	-11.8910	C	0	-7.1150	7.9110	-7.4880	C	0	-2.1810	4.7740	2.8390	C	0
-11.5350	24.2580	-12.3040	H	0	-7.6390	7.0640	-7.0460	H	0	-1.7720	5.7040	2.1400	O	0
-11.7880	22.6510	-10.9530	C	0	-8.2760	8.7630	-8.1000	C	0	-2.4550	4.8860	4.1220	N	0
-12.7550	22.9180	-10.5510	H	0	-7.9020	9.7660	-8.3030	H	0	-2.4570	4.0970	4.7520	H	0
-11.3980	21.4080	-10.5050	C	0	-8.6720	8.2600	-8.9830	H	0	-2.4910	6.1080	4.9760	C	0
-12.1030	20.8780	-9.8830	H	0	-9.0980	8.6900	-7.3880	H	0	-1.6280	6.6430	4.5800	H	0
-10.0350	20.9950	-10.8010	C	0	-6.1720	7.5610	-8.5020	O	0	-3.7730	6.8690	4.8120	C	0
-9.6640	20.0870	-10.3510	H	0	-6.0740	6.6090	-8.5710	H	0	-4.2770	7.0790	5.7550	H	0
-9.2920	21.6330	-11.7780	C	0	-5.7030	8.0560	-5.3480	C	0	-3.4820	7.8130	4.3510	H	0
-8.4620	18.3310	-12.8870	C	0	-4.4610	8.0570	-5.3810	O	0	-4.8620	6.2380	3.9570	C	0
-8.3250	17.4590	-12.0930	O	0	-6.3050	7.5340	-4.3210	N	0	-5.5680	6.9970	3.0000	C	0
-9.6500	18.5440	-13.4240	N	0	-7.3130	7.5820	-4.3340	H	0	-5.3140	8.0070	2.7150	H	0
-9.6050	19.1300	-14.2450	H	0	-5.6440	6.9260	-3.0860	C	0	-6.7740	6.5430	2.4090	C	0
-10.8750	17.8150	-13.1120	C	0	-4.5790	6.8680	-3.3140	H	0	-7.2150	7.1440	1.6270	H	0
-11.0190	17.8530	-12.0320	H	0	-5.7050	7.9230	-1.8100	C	0	-7.2460	5.2820	2.7440	C	0
-12.0590	18.5350	-13.8250	C	0	-6.7700	8.1340	-1.7090	H	0	-8.4590	4.8610	2.2490	O	0
-12.0280	18.4250	-14.9090	H	0	-4.9460	7.3240	-0.5940	C	0	-8.7100	4.1420	2.8330	H	0

-6.6190	4.5320	3.7090	C	0	1.8300	16.2790	16.7860	H	0	1.7330	12.0340	10.0060	C	0
-7.0370	3.6040	4.0700	H	0	2.2070	15.1190	15.0130	C	0	1.5910	11.7230	11.0310	H	0
-5.4030	4.9670	4.2900	C	0	1.8110	14.1830	14.6170	H	0	2.4890	13.2220	9.7610	C	0
-5.0930	4.4170	5.1670	H	0	2.0450	15.9230	14.2950	H	0	2.9960	13.9060	10.8600	O	0
-2.0320	5.7970	6.4310	C	0	3.7190	14.9880	15.3000	C	0	3.3960	14.7230	10.5540	H	0
-2.1110	4.6590	6.7620	O	0	3.8190	14.2850	16.1280	H	0	2.6560	13.5830	8.4180	C	0
-1.6630	6.7930	7.1530	N	0	4.6580	14.4520	14.2070	C	0	3.2720	14.4620	8.2990	H	0
-1.6770	7.7430	6.8100	H	0	4.2350	13.5200	13.8320	H	0	2.1410	12.8580	7.3370	C	0
-1.2200	6.6300	8.5620	C	0	4.8120	15.1740	13.4050	H	0	2.2510	13.1950	6.3170	H	0
-1.8060	5.8570	9.0600	H	0	5.6070	14.2540	14.7060	H	0	-1.1300	10.2080	4.9760	C	0
0.2980	6.3450	8.5500	C	0	4.2730	16.3620	15.7200	C	0	-1.2450	8.9860	5.2710	O	0
0.5660	6.2110	9.5980	H	0	5.3070	16.2800	16.0540	H	0	-1.3150	10.7160	3.7550	N	0
0.6240	5.4840	7.9650	H	0	4.3930	16.9530	14.8120	H	0	-1.2190	11.7140	3.6370	H	0
0.9850	7.5420	8.1370	O	0	3.6550	16.8470	16.4760	H	0	-1.6260	9.8260	2.6210	C	0
1.9220	7.3960	8.2860	H	0	-0.0110	15.8220	15.8360	C	0	-1.3140	8.8110	2.8650	H	0
-1.5400	7.8780	9.4550	C	0	-0.2350	16.9890	15.3860	O	0	-3.2260	9.8420	2.4700	C	0
-1.8480	8.9850	8.9380	O	0	-1.0080	14.9380	16.0200	N	0	-3.5100	8.8730	2.0610	H	0
-1.4300	7.7720	10.7650	N	0	-0.7270	14.0580	16.4270	H	0	-3.6070	9.9280	3.4870	H	0
-1.1630	6.8690	11.1300	H	0	-2.3800	15.0510	15.5650	C	0	-3.8090	11.0060	1.6490	C	0
-1.7240	8.8530	11.7340	C	0	-2.7460	14.0430	15.7560	H	0	-4.3890	12.2070	2.1480	C	0
-1.4970	9.8360	11.3200	H	0	-3.0920	16.0370	16.3670	C	0	-4.4140	12.4870	3.1910	H	0
-3.2330	8.8330	12.0280	C	0	-2.7730	15.9360	17.4040	H	0	-5.0730	13.1120	1.2800	C	0
-3.8050	9.1450	11.1550	H	0	-2.7270	17.0160	16.0560	H	0	-5.4090	14.1020	1.5520	H	0
-3.4920	7.8020	12.2710	H	0	-4.5720	16.8050	16.2160	C	0	-5.1340	12.8580	-0.0560	C	0
-3.6310	9.8350	13.1770	C	0	-5.0950	14.8050	15.7840	O	0	-5.5120	13.7900	-0.9680	O	0
-3.6630	11.2210	12.8940	C	0	-5.1750	16.8670	16.3400	O	0	-5.5670	13.4310	-1.8570	H	0
-3.6020	11.5570	11.8690	H	0	-2.4240	15.3040	14.0690	C	0	-4.6030	11.6130	-0.5080	C	0
-4.2230	12.1060	13.8400	C	0	-3.1000	16.2530	13.5780	O	0	-4.7410	11.3630	-1.5500	H	0
-4.2310	13.1740	13.6800	H	0	-1.6840	14.4530	13.2930	N	0	-3.8910	10.7270	0.2980	C	0
-4.6370	11.5360	15.0970	C	0	-0.9800	13.9520	13.8160	H	0	-3.4970	9.8240	-0.1430	H	0
-4.9470	12.2750	16.2170	O	0	-1.5460	14.5070	11.8400	C	0	-0.8120	10.2290	1.4240	C	0
-4.9960	13.2050	15.9830	H	0	-2.2340	15.2520	11.4410	H	0	-0.2080	11.2920	1.2100	O	0
-4.4450	10.2140	15.3990	C	0	-0.0930	15.0500	11.5910	C	0	-0.6370	9.2430	0.5580	N	0
-4.5750	9.8800	16.4170	H	0	0.6000	14.5960	12.2980	H	0	-1.0040	8.3250	0.7650	H	0
-3.9280	9.3350	14.4700	C	0	0.2730	14.7120	10.6220	H	0	-0.0290	9.4710	-0.7880	C	0
-3.7490	8.2840	14.6400	H	0	0.0640	16.5900	11.4650	C	0	0.4400	10.4420	-0.9450	H	0
-0.8520	8.7770	13.0170	C	0	-0.3840	16.9950	12.3720	H	0	0.6110	8.6060	-0.9590	H	0
-0.6880	7.7040	13.6200	O	0	1.5930	16.9470	11.3610	C	0	-1.0780	9.5170	-1.9170	C	0
-0.3130	9.8810	13.4960	N	0	1.7300	18.0230	11.2540	H	0	-2.0810	8.8190	-1.6840	O	0
-0.2280	10.6680	12.8690	H	0	2.1780	16.5640	12.1960	H	0	-0.7770	10.2240	-2.9590	N	0
0.3200	10.0220	14.7750	C	0	2.1250	16.4950	10.5230	H	0	0.0970	10.7270	-3.0270	H	0
0.3850	9.0610	15.2840	H	0	-0.6360	17.2650	10.2900	C	0	-1.6270	10.2970	-4.2130	C	0
1.8020	10.3840	14.5150	C	0	-1.6900	16.9900	10.2340	H	0	-2.5790	9.8380	-3.9450	H	0
2.2370	9.4990	14.0510	H	0	-0.6780	18.3320	10.5120	H	0	-1.9180	11.7460	-4.5720	C	0
1.9600	11.1410	13.7480	H	0	-0.1840	16.9870	9.3380	H	0	-2.5950	11.8080	-5.4250	H	0
2.5310	10.8340	15.7510	C	0	-1.7390	13.1360	11.1880	C	0	-2.6030	12.4630	-3.4060	C	0
3.5790	11.4700	15.5590	O	0	-1.0300	12.1860	11.5090	O	0	-3.5650	11.9680	-3.2740	H	0
2.0720	10.7000	16.9140	O	0	-2.5020	13.0750	10.1280	N	0	-2.0210	12.4470	-2.4850	H	0
-0.4520	10.9900	15.7160	C	0	-2.9880	13.9000	9.8090	H	0	-2.6710	13.5120	-3.6940	H	0
-0.3350	12.2080	15.5420	O	0	-2.5710	11.8820	9.2520	C	0	-0.8330	12.5520	-4.8340	O	0
-1.1170	10.5050	16.8050	N	0	-1.9300	11.1050	9.6680	H	0	-1.0960	13.4740	-4.7820	H	0
-1.1610	9.1510	17.3230	C	0	-4.0670	11.4260	9.1070	C	0	-1.0920	9.6810	-5.4240	C	0
-0.1540	8.7860	17.5260	H	0	-4.0660	10.3370	9.0790	H	0	0.0910	9.7160	-5.6700	O	0
-1.6580	8.5910	16.5310	H	0	-4.6780	11.7080	9.9650	H	0	-1.9600	9.0360	-6.2180	N	0
-1.9830	9.1130	18.6290	C	0	-4.7980	11.8700	7.8370	C	0	-2.9460	9.1170	-6.0150	H	0
-1.2850	8.9910	19.4570	H	0	-5.7060	12.9470	7.8650	C	0	-1.6700	8.3320	-7.4410	C	0
-2.7150	8.3060	18.6040	H	0	-5.8830	13.4760	8.7900	H	0	-0.8710	7.6290	-7.2040	H	0
-2.6930	10.5140	18.6510	C	0	-6.4150	13.2970	6.6700	C	0	-2.7930	7.4340	-7.8890	C	0
-2.7700	11.0000	19.6240	H	0	-7.0490	14.1710	6.6730	H	0	-3.6810	8.0610	-7.8190	H	0
-3.7140	10.3400	18.3130	H	0	-6.2500	12.4940	5.5370	C	0	-2.7220	6.9560	-8.8660	H	0
-1.9740	11.4010	17.6560	C	0	-6.8170	12.8050	4.6730	H	0	-2.8920	6.3720	-6.9720	O	0
-2.6110	12.0500	17.0540	H	0	-5.4710	11.3610	5.5340	C	0	-3.3640	6.7840	-6.2440	H	0
-1.0680	12.4720	18.4560	C	0	-5.4850	10.7480	4.6450	H	0	-1.2900	9.2910	-8.5800	C	0
-1.5910	13.5300	18.7940	O	0	-4.5940	11.1740	6.6910	C	0	-1.3880	10.4990	-8.4200	O	0
0.1750	12.2130	18.7770	N	0	-3.8880	10.3600	6.7660	H	0	-1.0260	8.6890	-9.7330	N	0
0.5890	11.4440	18.2700	H	0	-1.8920	12.1500	7.8840	C	0	-0.9200	7.6850	-9.7740	H	0
1.1420	13.2160	19.4140	C	0	-1.6640	13.2870	7.4880	O	0	-0.7080	9.2350	-11.0640	C	0
0.6810	13.6370	20.3070	H	0	-1.4910	11.1090	7.1790	N	0	0.3550	9.4500	-10.9580	H	0
2.3130	12.3720	19.9550	C	0	-1.6110	10.2150	7.6340	H	0	-0.8870	8.2260	-12.2450	C	0
2.8040	11.8050	19.1650	H	0	-0.6100	11.1650	6.0130	C	0	-0.5360	8.6540	-13.1830	H	0
3.1950	12.9280	20.2730	H	0	-0.6890	12.2100	5.7130	H	0	-0.1990	7.4050	-12.0450	H	0
2.0570	11.6980	20.7730	H	0	0.8060	10.8130	6.4880	C	0	-2.2350	7.6510	-12.3630	C	0
1.5940	14.4060	18.5270	C	0	0.8350	9.7630	6.7770	H	0	-2.5330	6.8220	-11.5380	O	0
2.0240	15.4280	19.0490	O	0	1.4500	10.8380	5.6100	H	0	-2.8880	7.7880	-13.4820	N	0
1.3500	14.2970	17.1280	N	0	1.4490	11.6140	7.5780	C	0	-3.7480	7.2650	-13.5680	H	0
1.1590	13.3220	16.9440	H	0	1.3160	11.2100	8.9670	C	0	-2.5020	8.3000	-14.2620	H	0
1.3810	15.4240	16.2790	C	0	0.9260	10.2280	9.1900	H	0	-1.5670	10.4920	-11.3760	C	0

-2.6840	10.5980	-10.7870	O	0	1.2300	13.2320	-19.6420	H	0	2.8280	19.9020	-24.6930	H	0
-1.1360	11.3740	-12.2760	N	0	3.2520	12.4310	-19.7580	C	0	4.1040	20.9250	-25.3750	H	0
0.1840	11.4830	-12.8790	C	0	3.8800	12.0910	-20.5820	H	0	3.9280	19.0710	-26.4330	N	0
0.1070	11.3280	-13.9550	H	0	3.7170	13.2690	-19.2390	H	0	3.2120	19.2710	-27.1180	H	0
0.9630	10.8320	-12.4830	H	0	3.1280	11.6020	-19.0610	H	0	4.8790	19.0510	-26.7720	H	0
0.4590	12.9270	-12.6050	C	0	2.0810	14.0610	-21.3440	C	0	3.8180	18.1000	-26.1780	H	0
1.2750	13.3190	-13.2110	H	0	1.9780	15.2380	-20.8900	O	0	1.8650	20.4670	-20.6700	C	0
0.6510	13.0320	-11.5370	H	0	2.1590	13.8740	-22.6450	N	0	0.8340	20.7510	-21.2590	O	0
-0.8060	13.6350	-13.0550	C	0	2.3210	12.9310	-22.9670	H	0	2.5910	21.3330	-19.9780	N	0
-0.7330	13.8620	-14.1190	H	0	1.9970	14.9350	-23.7590	C	0	3.3230	20.8690	-19.4590	H	0
-0.9230	14.5330	-12.4480	H	0	2.8110	15.6560	-23.6870	H	0	1.9480	22.6080	-19.5950	C	0
-1.9210	12.5940	-12.5470	C	0	2.0720	14.0510	-25.0030	C	0	2.3700	23.4150	-20.1930	H	0
-2.2990	12.9140	-11.5760	H	0	3.0420	13.5570	-25.0560	H	0	0.8620	22.6150	-19.6910	H	0
-3.1430	12.3940	-13.5260	C	0	1.2700	13.3130	-24.9710	H	0	2.0470	22.9650	-18.0820	C	0
-3.5320	13.2720	-14.3580	O	0	1.9180	14.7520	-26.4000	C	0	1.4060	23.9160	-17.7180	O	0
-3.8110	11.2150	-13.4960	N	0	2.3370	14.1820	-27.2300	H	0	2.6920	22.1410	-17.2540	N	0
-3.5500	10.5220	-12.8090	H	0	0.8520	14.8380	-26.6090	H	0	2.9240	21.2340	-17.6320	H	0
-4.7740	10.7850	-14.5440	C	0	2.6540	16.1390	-26.4270	C	0	2.9750	22.4020	-15.9030	C	0
-5.3030	9.8810	-14.2440	H	0	3.8710	16.2150	-26.0310	O	0	3.7160	23.1990	-15.8450	H	0
-5.4560	11.5910	-14.8150	H	0	2.0700	17.1500	-26.9310	O	0	2.1030	22.8220	-15.4020	H	0
-3.9980	10.3290	-15.7940	C	0	0.7090	15.6550	-23.7410	C	0	3.2060	21.1020	-15.0660	C	0
-3.1450	9.3660	-15.7280	O	0	0.6230	16.9070	-23.8250	O	0	3.1110	19.9880	-15.5500	O	0
-4.3500	10.8440	-16.9580	N	0	-0.3680	15.0070	-23.3940	N	0	3.6510	21.2580	-13.7680	N	0
-4.8590	11.7160	-16.9410	H	0	-0.3000	14.0210	-23.1870	H	0	3.8570	22.2170	-13.5280	H	0
-3.9370	10.1200	-18.1930	C	0	-1.6780	15.6630	-23.2310	C	0	3.9840	20.2710	-12.7170	C	0
-4.3050	9.0950	-18.1390	H	0	-1.9600	16.3250	-24.0500	H	0	4.8100	19.7260	-13.1760	H	0
-4.4750	10.8190	-19.4930	C	0	-2.6750	14.5630	-23.0740	C	0	4.5910	20.9570	-11.4560	C	0
-5.5530	10.9500	-19.5810	H	0	-2.3730	13.9020	-22.2620	H	0	3.8000	21.5720	-11.0280	H	0
-3.9160	12.2240	-19.6410	C	0	-3.5540	15.0170	-22.6170	H	0	4.8910	20.1300	-10.8130	H	0
-4.5910	12.9800	-20.0420	H	0	-3.0570	13.8270	-24.3500	C	0	5.8540	21.8400	-11.6050	C	0
-3.6650	12.5540	-18.6330	H	0	-3.5080	14.5230	-25.0570	H	0	5.7810	23.0320	-11.2200	O	0
-2.9730	12.0640	-20.1630	H	0	-2.1350	13.4440	-24.7900	H	0	6.8920	21.3790	-12.1100	O	0
-4.1840	10.0280	-20.6200	O	0	-3.9470	12.6220	-24.1730	C	0	2.9000	19.2160	-12.2490	C	0
-4.7690	9.2710	-20.5450	H	0	-3.7620	11.5470	-24.8200	O	0	3.2050	18.2940	-11.5150	O	0
-2.4200	9.7980	-18.2960	C	0	-5.0130	12.6680	-23.3820	N	0	1.6760	19.5300	-12.6890	N	0
-1.5170	10.6470	-18.0580	O	0	-5.6500	11.9570	-23.7120	H	0	1.5280	20.3240	-13.2960	H	0
-2.0100	8.5810	-18.7190	N	0	-5.3260	13.4780	-22.8660	H	0	0.4720	18.7080	-12.4270	C	0
-2.6830	7.8490	-18.8950	H	0	-1.6670	16.5070	-21.9180	C	0	-0.4220	19.2610	-12.7150	H	0
-0.6100	8.1650	-18.7730	C	0	-2.5160	17.3360	-21.7860	O	0	0.4980	17.3720	-13.2720	C	0
-0.0980	8.6090	-17.9190	H	0	-0.7550	16.2460	-20.9070	N	0	1.1750	16.6460	-12.8210	H	0
-0.4910	6.6520	-18.8450	C	0	-0.1120	15.4870	-21.0780	H	0	-0.5170	17.0020	-13.1300	H	0
-0.9180	6.3010	-19.7850	H	0	-0.6650	16.9970	-19.6550	C	0	0.5550	17.4060	-14.7820	C	0
0.5750	6.4410	-18.9320	H	0	-1.5360	17.6400	-19.5330	H	0	0.8720	16.3860	-15.3450	O	0
-0.9950	5.8010	-17.7450	C	0	-0.6100	15.9770	-18.4300	C	0	0.2210	18.4740	-15.4590	N	0
-1.9050	6.1020	-16.7490	C	0	0.2630	15.3240	-18.4520	H	0	0.4330	18.3890	-16.4430	H	0
-2.3820	7.0700	-16.7100	H	0	-0.5780	16.5410	-17.4980	H	0	0.2640	19.3810	-15.0160	H	0
-2.0430	5.0650	-15.9270	N	0	-1.9350	15.1470	-18.2290	C	0	0.2320	18.3440	-10.9500	C	0
-2.3290	5.2890	-14.9850	H	0	-2.6750	15.9070	-17.9780	H	0	0.3170	17.2010	-10.5840	O	0
-1.3820	3.9500	-16.3180	C	0	-2.2330	14.5510	-19.0920	H	0	-0.0260	19.3430	-10.1070	N	0
-1.1180	2.7290	-15.6600	C	0	-1.7170	14.3580	-16.9550	C	0	0.2840	20.2630	-10.3860	H	0
-1.5030	2.4650	-14.6860	H	0	-1.2970	14.9500	-16.1420	H	0	-0.1520	19.0780	-8.6330	C	0
-0.4230	1.7010	-16.4070	C	0	-2.6520	13.9320	-16.5930	H	0	0.4930	18.2330	-8.3940	H	0
-0.2920	0.7140	-15.9900	H	0	-0.8960	13.1730	-17.1730	N	0	0.1730	20.3080	-7.7720	C	0
0.1400	2.0630	-17.6930	C	0	-1.3660	12.3680	-17.5620	H	0	-0.2320	21.1780	-8.2880	H	0
0.6410	1.3220	-18.2980	H	0	0.3530	12.8920	-16.9130	C	0	-0.1970	20.1840	-6.7540	H	0
-0.0270	3.3610	-18.1890	C	0	1.1420	13.7310	-16.2340	N	0	1.7410	20.3570	-7.7260	C	0
0.3140	3.6020	-19.1850	H	0	0.8600	14.6340	-15.8810	H	0	2.0910	19.5040	-7.1440	H	0
-0.7540	4.3600	-17.5420	C	0	2.0580	13.3620	-16.0220	H	0	2.2440	20.2410	-8.6860	H	0
0.1460	8.8530	-19.8800	C	0	0.8400	11.7020	-17.2760	N	0	2.3500	21.6400	-7.0310	C	0
1.3340	9.2110	-19.6880	O	0	0.2020	11.0330	-17.6830	H	0	2.4570	22.3580	-7.8450	H	0
-0.6510	9.2710	-20.9120	N	0	1.7730	11.3970	-17.0390	H	0	1.5910	21.9730	-6.3230	H	0
-1.6200	8.9840	-20.9140	H	0	0.5290	17.9140	-19.5850	C	0	3.6340	21.3520	-6.2010	C	0
-0.1480	10.0090	-22.0560	C	0	0.7000	18.4950	-18.4930	O	0	3.8220	22.2070	-5.5520	H	0
0.8490	9.5880	-22.1870	H	0	1.2320	18.1180	-20.7310	N	0	3.5150	20.5680	-5.4530	H	0
-0.9330	9.7890	-23.3380	C	0	0.9200	17.6790	-21.5860	H	0	4.8010	21.1430	-7.1080	N	0
-0.9610	8.7190	-23.5440	H	0	2.4150	19.0470	-20.8200	C	0	4.6840	20.2480	-7.5620	H	0
-1.8590	10.3480	-23.2010	H	0	3.1150	18.8590	-20.0050	H	0	5.0200	21.9400	-7.6890	H	0
-0.1550	10.4080	-24.5010	C	0	3.0600	18.8650	-22.2140	C	0	5.6400	20.8600	-6.6210	H	0
1.0520	10.3450	-24.5720	O	0	3.3390	17.8230	-22.3720	H	0	-1.6100	18.6950	-8.2690	C	0
-0.8370	11.0020	-25.4510	N	0	2.3200	19.1630	-22.9560	H	0	-2.5710	19.1640	-8.8600	O	0
-0.3400	11.5940	-26.1010	H	0	4.2600	19.7150	-22.6530	C	0	-1.8700	17.9620	-7.1530	N	0
-1.7590	11.3160	-25.1840	H	0	4.0230	20.7790	-22.6470	H	0	-2.8300	17.6510	-7.1160	H	0
0.1290	11.4020	-21.6670	C	0	4.9930	19.6100	-21.8540	H	0	-0.9790	17.3900	-6.1580	C	0
-0.4890	12.3380	-22.1580	O	0	4.7350	19.3160	-24.0930	C	0	0.0510	17.6940	-6.3460	H	0
1.2590	11.5980	-20.9250	N	0	5.7710	19.6490	-24.1480	H	0	-1.4140	18.0330	-4.8100	C	0
1.6590	10.7340	-20.5870	H	0	4.6640	18.2380	-24.2310	H	0	-2.4920	17.8680	-4.8290	H	0
1.9280	12.8710	-20.3980	C	0	3.8050	19.8950	-25.1780	C	0	-1.0960	17.4450	-3.9480	H	0

-1.3340	19.4420	-4.4970	C	0	-1.7000	14.3960	0.7320	H	0	-6.9230	14.7140	12.9660	C	0
-2.3480	20.3430	-4.5480	C	0	-2.0590	15.3770	2.1960	H	0	-7.6490	15.1410	13.6590	H	0
-3.3400	20.1350	-4.9200	H	0	-1.8230	16.4540	0.3330	C	0	-6.3790	13.9630	13.5380	H	0
-1.8160	21.6210	-4.2820	N	0	-1.4700	17.7820	0.6730	C	0	-7.5830	14.0070	11.7790	C	0
-2.3440	22.4680	-4.4330	H	0	-0.8640	18.0270	1.5330	H	0	-8.4460	13.3890	12.0290	H	0
-0.4890	21.5910	-3.9340	C	0	-1.8150	18.8180	-0.2340	C	0	-6.9270	13.3410	11.2180	H	0
0.3510	22.5550	-3.3980	C	0	-1.3340	19.7690	-0.0580	H	0	-7.9760	15.2290	10.8920	C	0
0.0820	23.5960	-3.4900	H	0	-2.5360	18.5360	-1.3850	C	0	-7.9330	14.9370	9.8430	H	0
1.6310	22.0930	-2.9380	C	0	-2.8610	19.2910	-2.0860	H	0	-9.4100	15.7130	11.2460	C	0
2.3590	22.7870	-2.5430	H	0	-2.9240	17.2040	-1.6520	C	0	-10.3420	15.0060	10.9620	O	0
1.9410	20.7340	-3.0320	C	0	-3.7470	17.1350	-2.3480	H	0	-9.5690	16.8270	11.9410	N	0
2.9390	20.4390	-2.7440	H	0	-2.5520	16.1610	-0.8340	C	0	-8.7470	17.3720	12.1590	H	0
1.1080	19.7810	-3.6420	C	0	-2.9700	15.1960	-1.0780	H	0	-10.9380	17.3230	12.4000	C	0
1.4190	18.7550	-3.7710	H	0	0.0290	14.8220	3.2480	C	0	-11.6320	16.4890	12.5100	H	0
-0.2240	20.1410	-3.9960	C	0	-0.4630	13.7510	3.4910	O	0	-10.7600	17.8130	13.8460	C	0
-0.9380	15.9180	-6.2310	C	0	0.3760	15.7120	4.1260	N	0	-10.2180	18.7540	13.7540	H	0
-1.0310	15.2040	-5.2720	O	0	0.7880	16.5800	3.8130	H	0	-11.7530	18.0730	14.2150	H	0
-0.9030	15.3980	-7.4190	N	0	0.1280	15.6340	5.5690	C	0	-10.0040	16.8430	14.7550	C	0
-0.9390	15.9360	-8.2730	H	0	-0.0230	14.5920	5.8490	H	0	-9.0430	17.3820	15.3560	O	0
-0.7970	13.9710	-7.7180	C	0	1.3620	16.1980	6.3320	C	0	-10.3060	15.6210	14.8230	O	0
-1.2110	13.4990	-6.8270	H	0	1.4240	17.2850	6.2750	H	0	-11.5850	18.3480	11.3970	C	0
-1.6570	13.7020	-9.0330	C	0	1.1950	16.0740	7.4020	H	0	-12.8010	18.5660	11.3010	O	0
-0.9580	13.6330	-9.8670	H	0	2.2450	15.6950	5.9380	H	0	-10.7900	18.8560	10.4480	N	0
-2.1490	12.7300	-9.0590	H	0	-1.1150	16.5000	5.9850	C	0	-9.7930	18.7600	10.5730	H	0
-2.6770	14.5650	-9.4390	O	0	-1.2870	17.6400	5.6120	O	0	-11.2640	19.5970	9.2940	C	0
-3.1400	14.2550	-10.2200	H	0	-2.0330	15.9510	6.8330	N	0	-12.3480	19.6840	9.3580	H	0
0.6900	13.5720	-7.7120	C	0	-1.9870	14.9730	7.0810	H	0	-10.8280	21.0290	9.4000	C	0
1.5850	14.4370	-7.8630	O	0	-3.3720	16.6200	6.9790	C	0	-11.0700	21.7050	8.5800	H	0
1.0000	12.2700	-7.4800	N	0	-3.3120	17.7020	6.8610	H	0	-11.4110	21.7230	10.6160	C	0
0.1950	11.6700	-7.3700	H	0	-4.3840	15.9620	5.9590	C	0	-10.8110	22.6170	10.7850	H	0
2.2790	11.6570	-7.2060	C	0	-4.1810	14.9030	5.7980	H	0	-12.4860	21.8340	10.4750	H	0
2.1810	10.6290	-6.8560	H	0	-5.3580	15.9910	6.4460	H	0	-11.1760	21.0960	11.4760	H	0
3.0250	11.7120	-8.5400	C	0	-4.4310	16.7370	4.6370	C	0	-9.4580	21.0040	9.4930	O	0
3.2880	12.7390	-8.7950	H	0	-4.9370	17.6810	4.8360	H	0	-9.2460	20.9460	10.4270	H	0
3.9580	11.1500	-8.4950	H	0	-3.4230	16.9320	4.2710	H	0	-10.7290	19.1150	7.9530	C	0
2.2620	11.0410	-10.0100	S	0	-5.1420	15.9640	3.5160	C	0	-11.3130	19.5080	6.9480	O	0
2.6950	9.7770	-9.9770	H	0	-4.8650	14.9170	3.3910	H	0	-9.5820	18.3930	7.9160	N	0
2.9650	12.3430	-5.9980	C	0	-6.2170	16.1150	3.6080	H	0	-9.3270	17.9560	8.7910	H	0
4.1120	12.7630	-6.1490	O	0	-4.9620	16.5780	2.1780	N	0	-8.9860	17.7110	6.7540	C	0
2.2130	12.5570	-4.8910	N	0	-4.2890	16.2020	1.5250	H	0	-8.4160	16.8470	7.0960	H	0
1.2810	12.1770	-4.9770	H	0	-5.4380	17.7490	1.7900	C	0	-9.8050	17.4610	6.0790	H	0
2.5650	13.3800	-3.7720	C	0	-6.3010	18.4400	2.4670	N	0	-8.0500	18.6230	5.9980	C	0
3.6480	13.4980	-3.8190	H	0	-6.6340	18.0200	3.3220	H	0	-7.6710	18.3360	4.8330	O	0
1.7980	14.7240	-3.9760	C	0	-6.3780	19.4220	2.2430	H	0	-7.5730	19.6520	6.6740	N	0
0.7090	14.6810	-3.9950	H	0	-5.0930	18.2340	0.5850	N	0	-7.9140	19.8350	7.6060	H	0
1.9830	15.7570	-2.9340	C	0	-4.5330	17.7880	-0.1270	H	0	-6.7470	20.7240	5.9870	C	0
3.0390	15.8980	-2.7030	H	0	-5.6500	19.0410	0.3420	H	0	-6.9970	20.7910	4.9280	H	0
1.5890	16.7360	-3.2070	H	0	-3.8480	16.4880	8.4010	C	0	-7.1000	22.0580	6.6480	C	0
1.5720	15.3680	-2.0030	H	0	-3.9360	15.3770	8.9520	O	0	-7.0240	21.9110	7.7250	H	0
2.2040	15.3880	-5.1450	O	0	-4.3060	17.6120	8.9590	N	0	-6.2600	22.6100	6.2260	H	0
2.1010	14.8780	-5.9520	H	0	-4.1730	18.4920	8.4820	H	0	-8.4540	22.7070	6.1970	C	0
2.1580	12.7600	-2.4220	C	0	-5.0460	17.7240	10.2800	C	0	-8.4210	22.9040	5.1260	H	0
1.0710	12.2180	-2.2310	O	0	-4.4460	17.1420	10.9810	H	0	-9.2510	21.9920	6.4020	H	0
2.9470	13.0570	-1.4040	N	0	-5.0970	19.1640	10.7590	C	0	-8.6110	24.0870	6.8270	C	0
3.7960	13.5750	-1.5820	H	0	-5.3250	19.8190	9.9190	H	0	-7.7820	24.7170	6.5010	H	0
2.5970	12.9000	0.0500	C	0	-5.8690	19.2490	11.5240	H	0	-9.5490	24.4860	6.4410	H	0
1.9580	12.0200	0.1200	H	0	-3.7050	19.6650	11.3880	C	0	-8.5370	24.1140	8.4040	C	0
3.8920	12.6190	0.8670	C	0	-3.4710	19.0050	12.2230	H	0	-9.4440	23.6040	8.7280	H	0
4.5440	13.4820	1.0010	H	0	-2.8770	19.7720	10.6860	H	0	-7.6220	23.6950	8.8220	H	0
3.3430	12.1450	2.2200	C	0	-3.7660	21.0180	12.0310	C	0	-8.6240	25.5690	8.9350	N	0
2.4510	11.5210	2.2580	H	0	-4.1120	21.7490	11.3000	H	0	-9.5830	25.7140	9.2160	H	0
4.0370	11.4190	2.6430	H	0	-4.4770	20.9630	12.8550	H	0	-7.9210	25.7200	9.6440	H	0
3.2420	13.0260	2.8540	H	0	-2.4300	21.3990	12.5380	N	0	-8.3430	26.2010	8.1990	H	0
4.7200	11.4840	0.2030	C	0	-1.9430	20.7660	13.1560	H	0	-5.2350	20.3940	6.0600	C	0
3.9790	10.6860	0.2510	H	0	-1.8690	22.5320	12.3100	C	0	-4.7440	19.8360	7.0830	O	0
4.8390	11.7740	-0.8410	H	0	-2.5980	23.4930	11.8080	N	0	-4.5060	20.5730	5.0000	N	0
6.0430	10.9990	0.7410	C	0	-3.5630	23.3410	11.5500	H	0	-5.0090	20.9070	4.1900	H	0
5.9450	10.4910	1.7000	H	0	-2.1670	24.3970	11.6730	H	0	-3.1050	20.1810	4.8420	C	0
6.5070	10.3050	0.0400	H	0	-0.6350	22.8700	12.5390	N	0	-2.8800	19.2090	5.2820	H	0
6.7810	11.7890	0.8810	H	0	0.1010	22.2560	12.8610	H	0	-2.6420	20.2740	3.4350	C	0
1.9240	14.1570	0.4930	C	0	-0.3880	23.8310	12.3510	H	0	-3.3230	19.6800	2.8250	H	0
2.4800	15.2510	0.4350	O	0	-6.4870	17.0800	10.1980	C	0	-2.6380	21.2990	3.0650	H	0
0.7210	14.0820	1.0110	N	0	-7.2980	17.3380	9.3240	O	0	-1.6960	19.7410	3.3460	H	0
0.4550	13.1480	1.2880	H	0	-6.8690	16.2100	11.1820	N	0	-2.1920	21.0930	5.6900	C	0
0.0350	15.1970	1.7370	C	0	-6.0020	15.8060	12.2600	C	0	-2.2760	22.3390	5.7050	O	0
0.6230	16.1150	1.7460	H	0	-5.7150	16.6130	12.9350	H	0	-1.0850	20.5140	6.1890	N	0
-1.4760	15.3130	1.2770	C	0	-5.0860	15.2870	11.9800	H	0	-1.0080	19.5070	6.1620	H	0

0.0280	21.2010	6.8340	C	0	5.5650	16.5850	-3.2270	N	0	7.2540	16.4200	-20.4950	C	0
-0.2800	22.2470	6.8190	H	0	5.8970	17.5350	-3.1370	H	0	7.8470	16.2920	-21.3880	H	0
0.3590	20.6510	8.1900	C	0	5.4470	15.9260	-4.5720	C	0	7.9600	16.6960	-19.2850	C	0
-0.4560	20.8920	8.8720	H	0	4.5980	15.2480	-4.4910	H	0	9.0400	16.7180	-19.2810	H	0
0.4790	19.6200	7.8570	H	0	5.0650	17.0010	-5.6580	C	0	7.2460	16.9130	-18.1300	C	0
1.5880	21.0220	9.0250	C	0	4.1000	17.4660	-5.4570	H	0	7.8650	17.2030	-17.2940	H	0
1.4470	20.3680	9.8860	H	0	5.7810	17.8220	-5.6230	H	0	5.8670	16.6820	-18.0110	C	0
2.5150	20.8100	8.4930	H	0	4.9900	16.4430	-7.0510	C	0	4.8500	14.2010	-14.8710	C	0
1.5840	22.4580	9.5490	C	0	5.9890	16.3590	-7.4790	H	0	5.4850	14.0230	-15.8810	O	0
1.2370	23.1520	8.7840	H	0	4.5310	15.4550	-7.0860	H	0	4.4370	13.2630	-13.9890	N	0
0.8640	22.5190	10.3640	H	0	4.1150	17.3570	-7.9830	C	0	4.0780	13.5200	-13.0800	H	0
2.8620	22.8300	10.1410	N	0	4.5310	18.4880	-8.0940	O	0	4.5740	11.7740	-14.1560	C	0
2.8950	23.0400	11.1280	H	0	3.1380	16.9040	-8.7020	N	0	5.6170	11.5120	-13.9770	H	0
3.9330	23.1460	9.4850	C	0	2.8560	17.5110	-9.4580	H	0	3.7980	11.0330	-13.0510	C	0
3.9790	23.1480	8.1490	N	0	2.7570	15.9910	-8.4990	H	0	4.3900	11.2360	-12.1590	H	0
3.1160	22.9060	7.6820	H	0	6.7050	15.0960	-4.9010	C	0	2.8020	11.4770	-13.0590	H	0
4.7480	23.6250	7.7010	H	0	7.8130	15.6220	-5.1380	O	0	3.7070	9.5080	-13.3610	C	0
4.9220	23.4990	10.1820	N	0	6.5900	13.7810	-4.9310	N	0	2.6560	8.9000	-13.5910	O	0
4.8920	23.4890	11.1910	H	0	5.6460	13.4220	-4.9210	H	0	4.8390	9.0210	-13.5800	O	0
5.8040	23.7710	9.7720	H	0	7.6170	12.9020	-5.3390	C	0	4.1680	11.3270	-15.1510	C	0
1.2520	21.3130	6.0120	C	0	8.5370	13.1400	-4.8050	H	0	3.3070	11.8770	-16.2250	O	0
1.9170	22.3590	6.1130	O	0	7.2930	11.4770	-5.0800	C	0	4.8740	10.3670	-15.9790	N	0
1.6540	20.2890	5.3250	N	0	6.4080	11.1180	-5.6050	H	0	5.2480	9.7530	-15.2690	H	0
1.1090	19.4410	5.3780	H	0	8.0330	10.7980	-5.5030	H	0	4.7370	9.6950	-17.2710	C	0
2.7700	20.1430	4.4090	C	0	7.1210	11.1280	-3.5740	C	0	3.7290	9.8130	-17.6690	H	0
3.0100	21.1260	4.0050	H	0	7.9990	11.6150	-3.1480	H	0	5.7370	10.3360	-18.2490	C	0
4.0790	19.7780	5.1540	C	0	6.2100	11.6010	-3.2070	H	0	5.4020	10.3280	-19.2870	H	0
4.8340	19.9670	4.3910	H	0	6.9230	9.4480	-3.0600	S	0	5.8500	11.3980	-18.0320	H	0
4.3030	20.5270	5.9140	H	0	5.1650	9.1160	-3.3750	C	0	7.1240	9.9290	-18.0910	O	0
4.2360	18.4020	5.7410	C	0	4.5730	9.8460	-2.8220	H	0	7.3430	10.0870	-17.1690	H	0
4.2650	18.1790	7.0530	C	0	4.9100	9.1990	-4.4310	H	0	4.9530	8.1550	-17.2410	C	0
4.2180	19.0290	7.7190	H	0	5.0050	8.0570	-3.1730	H	0	5.3750	7.5470	-18.2940	O	0
4.4920	16.7780	7.2910	N	0	7.9100	13.1120	-6.8320	C	0	4.6180	7.5720	-16.1540	N	0
4.6020	16.3650	8.2060	H	0	9.0530	13.0310	-7.2370	O	0	4.2510	8.0540	-15.3460	H	0
4.8260	16.1500	6.0800	C	0	6.9610	13.1510	-7.7540	N	0	5.0320	6.1710	-15.9080	C	0
5.1420	14.8120	5.7760	C	0	5.9890	13.3030	-7.5250	H	0	5.1100	5.6070	-16.8370	H	0
5.5470	14.1390	6.5170	H	0	7.2690	12.9040	-9.1650	C	0	6.3820	6.0550	-15.2670	C	0
5.2530	14.3950	4.4290	C	0	8.2980	13.1550	-9.4260	H	0	6.2760	6.5850	-14.3200	H	0
5.4520	13.3600	4.1920	H	0	7.1400	11.4480	-9.6490	C	0	6.4930	5.0140	-14.9600	H	0
5.1300	15.3030	3.3930	C	0	6.0760	11.2200	-9.7070	H	0	7.5140	6.6050	-16.0240	C	0
5.2170	15.0700	2.3420	H	0	7.8110	11.1350	-11.0080	C	0	8.3240	5.9710	-16.9120	C	0
4.9500	16.6690	3.7260	C	0	8.8800	11.3440	-10.9660	H	0	8.2190	4.9120	-17.0960	H	0
4.8890	17.3500	2.8900	H	0	7.6420	10.1340	-11.4070	H	0	9.3440	6.7640	-17.3610	N	0
4.6450	17.1460	5.0770	C	0	7.2360	11.7300	-11.7190	H	0	10.1360	6.4510	-17.9040	H	0
2.5260	19.1630	3.2460	C	0	7.6230	10.5520	-8.6790	O	0	9.3370	7.9390	-16.5810	C	0
1.8130	18.1530	3.4010	O	0	8.5120	10.8390	-8.4610	H	0	10.1780	9.0960	-16.6610	C	0
3.1500	19.3500	2.1240	N	0	6.4100	13.8640	-10.0680	C	0	11.0390	9.1420	-17.3110	H	0
3.6770	20.1950	1.9530	H	0	5.3200	13.5060	-10.5640	O	0	9.9640	10.1510	-15.8000	C	0
3.0060	18.4690	0.9650	C	0	6.8370	15.1040	-10.1790	N	0	10.6490	10.9850	-15.8200	H	0
2.5340	17.5590	1.3340	H	0	8.0640	15.6760	-9.6900	C	0	8.8540	10.1280	-14.8770	C	0
2.0200	19.0190	-0.0720	C	0	8.9310	15.0500	-9.9030	H	0	8.6500	10.9690	-14.2320	H	0
2.4340	19.8480	-0.6450	H	0	8.0060	15.9420	-8.6350	H	0	7.9720	9.0120	-14.9220	C	0
1.7910	18.2810	-0.8410	H	0	8.1470	16.8490	-10.6530	C	0	7.1430	8.9910	-14.2300	H	0
1.0910	19.1820	0.4750	H	0	8.3730	16.4390	-11.6370	H	0	8.1820	7.8800	-15.7950	C	0
4.2890	18.3400	0.1950	C	0	8.8670	17.6350	-10.4210	H	0	4.0430	5.3460	-15.0750	C	0
5.0720	19.2530	-0.0500	O	0	6.7320	17.3520	-10.7050	C	0	4.1610	4.1670	-15.1660	O	0
4.6100	17.0710	-0.2090	N	0	6.5320	18.0960	-11.4760	H	0	3.0370	6.0550	-14.3840	N	0
4.0780	16.2480	0.0360	H	0	6.4310	17.8280	-9.7720	H	0	3.1620	7.0540	-14.2990	H	0
5.7800	16.7530	-0.9340	C	0	6.0160	16.0850	-10.9530	C	0	2.1580	5.3310	-13.3950	C	0
6.3000	17.6780	-1.1860	H	0	5.0350	16.2270	-10.5010	H	0	1.5900	6.1720	-12.9960	H	0
6.7550	16.0240	0.0060	C	0	5.8420	15.8270	-12.4820	C	0	1.1310	4.4530	-13.9620	C	0
6.9370	16.7200	0.8240	H	0	6.8090	15.4200	-13.0970	O	0	0.8240	4.6880	-14.9220	H	0
6.3200	15.0760	0.3220	H	0	4.6640	16.0020	-13.0490	N	0	1.5340	3.4690	-14.2000	H	0
8.0890	15.7120	-0.5880	C	0	3.8390	15.9430	-12.4690	H	0	-0.1070	4.2330	-13.0580	C	0
9.1100	16.6550	-0.7560	C	0	4.5600	15.6800	-14.5200	C	0	-0.7710	5.2400	-12.7670	O	0
9.0990	17.5950	-0.2250	H	0	3.5060	15.8080	-14.7690	H	0	-0.5260	3.2260	-12.5440	O	0
10.2760	16.3590	-1.5370	C	0	5.1830	16.7270	-15.4230	C	0	2.8990	4.8910	-12.1460	C	0
11.0910	17.0680	-1.5430	H	0	4.7470	17.6570	-15.0590	H	0	2.5000	3.9690	-11.4780	O	0
10.3440	15.0900	-2.1430	C	0	6.2660	16.6520	-15.3310	H	0	3.8710	5.7250	-11.6620	N	0
11.4540	14.7300	-2.7860	O	0	4.9410	16.6360	-16.9000	C	0	4.1940	6.4740	-12.2570	H	0
11.7890	15.3430	-3.4440	H	0	3.7300	16.3820	-17.4590	C	0	4.4070	5.6830	-10.2680	C	0
9.3580	14.1280	-2.0300	C	0	2.8290	16.2170	-16.8860	H	0	4.4760	4.6450	-9.9420	H	0
9.4100	13.1930	-2.5690	H	0	3.8710	16.3300	-18.8540	N	0	5.8250	6.4070	-10.1510	C	0
8.2490	14.4280	-1.2130	C	0	3.0620	16.2480	-19.4540	H	0	5.7140	7.4210	-10.5360	H	0
7.4360	13.7200	-1.1390	H	0	5.1840	16.4700	-19.1970	C	0	6.1300	6.4130	-9.1050	H	0
5.4880	15.9280	-2.1080	C	0	5.8040	16.4450	-20.4380	C	0	6.9320	5.7410	-11.0440	C	0
5.1400	14.7360	-2.1420	O	0	5.2550	16.1300	-21.3140	H	0	7.0770	4.3300	-11.1720	C	0

6.4210	3.6580	-10.6380	H	0	3.6700	5.2650	3.2420	H	0	8.4300	9.1740	16.0040	O	0
8.0480	3.7710	-12.0370	C	0	3.7830	6.1830	5.1900	C	0	12.4870	7.8930	15.1540	C	0
8.0940	2.6980	-12.1490	H	0	4.6240	6.7350	4.7720	H	0	12.8330	6.8690	15.6660	O	0
8.9360	4.6300	-12.7140	C	0	2.5530	7.1040	5.1740	C	0	13.3220	8.6710	14.4590	N	0
9.8750	4.1110	-13.5230	O	0	1.7960	6.4170	5.5530	H	0	12.9880	9.5190	14.0230	H	0
9.7000	3.1700	-13.6020	H	0	2.7920	7.9070	5.8720	H	0	14.6940	8.2910	13.9450	C	0
8.8250	6.0370	-12.6400	C	0	2.2350	7.7250	3.8630	C	0	15.0750	7.4360	14.5050	H	0
9.7010	6.6010	-12.9220	H	0	1.7230	6.9510	3.2920	H	0	14.6890	7.9050	12.4840	C	0
7.7930	6.5800	-11.8150	C	0	1.4520	8.4780	3.9520	H	0	14.5670	8.8510	11.9570	H	0
7.7940	7.6340	-11.5790	H	0	3.5150	8.5860	2.8450	S	0	15.7080	7.6680	12.1790	H	0
3.3340	6.4210	-9.3380	C	0	2.6090	8.5940	1.3150	C	0	13.7040	6.9030	11.8610	C	0
3.4930	7.5360	-8.8570	O	0	3.3760	8.2780	0.6090	H	0	12.6830	7.0850	12.1950	H	0
2.2600	5.6540	-9.0320	N	0	1.8190	7.8450	1.2710	H	0	13.8760	7.0660	10.3620	C	0
2.0470	4.7720	-9.4760	H	0	2.0880	9.4840	0.9630	H	0	13.6290	8.1040	10.1420	H	0
1.3220	6.0460	-7.9750	C	0	4.0850	5.7670	6.7390	C	0	14.8090	6.7520	9.8940	H	0
0.9210	7.0450	-8.1430	H	0	3.3540	6.1350	7.6310	O	0	13.0650	6.4920	9.9120	H	0
0.1740	5.1050	-7.9510	C	0	5.1040	4.9200	6.9840	N	0	13.9280	5.4600	12.2620	C	0
0.5490	4.1330	-7.6340	H	0	5.6510	4.7040	6.1630	H	0	14.0320	5.3490	13.3410	H	0
-0.5340	5.3570	-7.1610	H	0	5.4470	4.3700	8.2790	C	0	13.0130	4.9380	11.9840	H	0
-0.6600	4.8740	-9.1030	C	0	4.6410	3.7950	8.7350	H	0	14.7560	4.9920	11.7280	H	0
-1.2540	3.8070	-9.3290	O	0	6.7070	3.5030	8.0930	C	0	15.6710	9.3990	14.1650	C	0
-0.8050	5.6480	-9.9960	O	0	7.5480	4.1810	7.9480	H	0	15.3090	10.6210	14.2730	O	0
1.9900	6.0120	-6.5800	C	0	6.8210	2.6600	9.4240	C	0	16.9670	9.0450	14.0450	N	0
2.4340	4.9880	-6.0920	O	0	6.9120	3.3920	10.2270	H	0	17.2050	8.1200	13.7170	H	0
2.0070	7.2120	-5.9150	N	0	5.9330	2.0580	9.6170	H	0	18.1400	9.8980	14.4820	C	0
1.5710	7.9420	-6.4620	H	0	7.6350	1.9360	9.3990	H	0	17.7250	10.4460	15.3270	H	0
2.7830	7.6320	-4.7620	C	0	6.7780	2.4810	6.9160	C	0	19.3280	8.9840	14.9530	C	0
3.7620	7.1630	-4.8630	H	0	6.0350	1.6960	7.0540	H	0	20.1880	9.6180	15.1680	H	0
2.8700	8.7180	-4.7970	H	0	6.3910	2.8980	5.9870	H	0	18.9230	8.2010	16.1840	C	0
2.1540	7.3030	-3.4530	C	0	8.1900	1.9480	6.5170	C	0	18.0650	7.5820	15.9230	H	0
2.3180	8.0210	-2.4550	O	0	8.5400	1.3790	7.3780	H	0	19.7960	7.7160	16.6230	H	0
1.3610	6.2220	-3.4630	N	0	8.1990	1.3330	5.6180	H	0	18.6990	8.9520	16.9410	H	0
1.3400	5.7950	-4.3780	H	0	8.7980	2.8440	6.3890	H	0	19.6840	8.1030	13.9820	O	0
0.3870	5.7330	-2.3950	C	0	5.8440	5.6570	9.1880	C	0	19.1840	7.2850	14.0360	H	0
0.1460	6.5930	-1.7700	H	0	6.5250	6.5740	8.6680	O	0	18.6380	11.0540	13.5900	C	0
-0.9280	5.2260	-3.1530	C	0	5.4380	5.6780	10.4270	N	0	19.8270	11.2140	13.4560	O	0
-1.6420	4.9930	-2.3630	H	0	4.6310	5.1330	10.6950	H	0	17.6850	11.8000	12.9480	N	0
-1.5340	6.2540	-4.1070	C	0	5.7220	6.8340	11.3000	C	0	16.7130	11.5820	13.1110	H	0
-0.9830	6.3150	-5.0460	H	0	6.1980	7.5640	10.6460	H	0	17.9320	12.9350	12.0760	C	0
-2.5820	6.0650	-4.3410	H	0	4.3830	7.5060	11.7650	C	0	18.4860	12.6840	11.1720	H	0
-1.5340	7.2760	-3.7280	H	0	4.0880	6.9310	12.6430	H	0	16.5900	13.6380	11.6600	C	0
-0.6650	4.0120	-3.9710	C	0	4.6450	8.4990	12.1300	H	0	16.1540	14.0790	12.5560	H	0
-0.3100	3.1770	-3.3660	H	0	3.2600	7.7450	10.8780	C	0	16.7570	14.7790	10.6990	C	0
-1.6790	3.7740	-4.2940	H	0	3.0240	6.7470	10.5080	H	0	17.1650	14.4020	9.7620	H	0
-0.0570	4.2300	-4.8490	H	0	2.0630	8.4220	11.5390	C	0	15.8320	15.3050	10.4610	H	0
0.9830	4.6500	-1.4830	C	0	2.3600	9.4400	11.7920	H	0	17.4020	15.4790	11.2300	H	0
0.1780	3.9030	-0.9000	O	0	1.2620	8.4480	10.8000	H	0	15.6170	12.6900	11.0160	C	0
2.2730	4.7040	-1.1930	N	0	1.7810	7.8390	12.4150	H	0	15.9190	12.3310	10.0320	H	0
2.7530	5.5260	-1.5300	H	0	3.7560	8.6850	9.7670	C	0	15.3570	11.8260	11.6270	H	0
3.0030	3.7190	-0.3160	C	0	3.9110	9.6900	10.1600	H	0	14.7910	13.3220	10.6900	H	0
2.4060	2.8120	-0.4080	H	0	4.6870	8.3660	9.2990	H	0	18.8010	13.9800	12.7290	C	0
4.3690	3.4120	-0.9340	C	0	2.9700	8.6550	9.0120	H	0	18.5470	14.4140	13.8450	O	0
4.8790	4.3080	-1.2880	H	0	6.7090	6.5780	12.4480	C	0	19.8780	14.3850	12.0490	N	0
4.9380	2.8000	-0.2350	H	0	6.3420	6.7190	13.6300	O	0	19.9970	13.8840	11.1800	H	0
4.1110	2.3910	-2.0910	C	0	7.9680	6.1470	12.1900	N	0	21.0530	15.1340	12.6640	C	0
3.7520	1.2380	-1.7940	O	0	8.6640	5.8940	10.9070	C	0	21.9890	14.9540	12.1350	H	0
4.1890	2.8290	-3.2930	N	0	8.7620	6.8890	10.4710	H	0	20.7470	16.5770	12.6930	C	0
4.0680	2.1220	-4.0050	H	0	8.1910	5.1020	10.3260	H	0	19.7220	16.7440	13.0230	H	0
4.6280	3.6890	-3.5890	H	0	9.9940	5.1980	11.2280	C	0	21.3720	17.2270	13.3050	H	0
2.9280	4.0740	1.2010	C	0	10.7640	5.9550	11.0850	H	0	20.7040	17.2470	11.2840	C	0
2.3360	5.0820	1.5960	O	0	10.0730	4.2940	10.6240	H	0	19.9030	16.8320	10.6730	H	0
3.4070	3.0970	2.0000	N	0	9.8480	4.8400	12.7210	C	0	20.3090	18.2390	11.5040	H	0
3.8450	2.3280	1.5120	H	0	10.7230	4.9020	13.3680	H	0	21.9660	17.2520	10.4590	C	0
2.9260	2.7210	3.3590	C	0	9.3530	3.8880	12.9140	H	0	22.7380	17.8190	10.9780	H	0
1.8660	2.4760	3.2900	H	0	8.9350	5.9650	13.2360	C	0	22.1870	16.2010	10.2720	H	0
3.5530	1.3900	3.7430	C	0	8.3840	5.5230	14.0670	H	0	21.7090	17.9680	9.1040	C	0
3.1070	1.1100	4.6970	H	0	9.6210	7.2130	13.6760	C	0	20.9530	17.4930	8.4780	H	0
3.1590	0.6120	3.0890	H	0	9.7920	8.2100	12.8960	O	0	21.4380	19.0010	9.3240	H	0
5.0610	1.2430	3.7920	C	0	10.1500	7.3140	14.8360	N	0	22.9600	17.9150	8.2530	N	0
5.3370	2.2480	4.1130	H	0	10.0170	6.5880	15.5260	H	0	23.2500	16.9540	8.1410	H	0
5.4270	0.5530	4.5530	H	0	11.0280	8.3890	15.2450	C	0	22.7510	18.2880	7.3380	H	0
5.7920	1.1800	2.4080	C	0	10.9890	9.3010	14.6500	H	0	23.6980	18.4890	8.6350	H	0
6.9510	1.6390	2.2950	O	0	10.7250	8.8620	16.6720	C	0	21.3910	14.6290	14.0540	C	0
5.1710	0.6640	1.4170	O	0	11.0760	8.1540	17.4230	H	0	21.5840	15.4790	14.9440	O	0
3.0080	3.8490	4.5130	C	0	11.1580	9.8420	16.8700	H	0	21.5500	13.3210	14.3060	N	0
2.5940	3.5570	5.6380	O	0	9.2300	9.0630	16.9520	C	0	21.0130	12.6970	13.7210	H	0
3.5490	5.0670	4.2250	N	0	8.7730	9.1250	18.1050	O	0	21.9200	12.6860	15.5600	C	0



22.3290	11.7360	15.2150	H	0	9.6100	10.2670	12.8420	H	0	11.3050	1.2470	4.4880	H	0
22.7440	13.2280	16.0240	H	0	9.8720	10.7940	10.7330	C	0	10.6040	1.4460	2.4860	C	0
20.8120	12.6410	16.6730	C	0	9.9210	11.7530	10.2190	H	0	9.5650	1.2110	2.6630	H	0
21.0440	11.9440	17.6490	O	0	11.1770	10.0530	10.4010	C	0	8.5560	2.8940	-1.6190	C	0
19.6810	13.4060	16.5310	N	0	11.3690	9.1250	10.9420	H	0	8.0790	1.8550	-2.0490	O	0
19.4890	14.0290	15.7600	H	0	11.1820	9.8400	9.3320	H	0	8.4080	4.0590	-2.2790	N	0
18.5880	13.4970	17.5640	C	0	12.5560	11.1590	10.9080	S	0	8.7170	4.9210	-1.8520	H	0
18.9550	13.1390	18.5270	H	0	12.3320	11.1370	12.2240	H	0	7.4760	4.3050	-3.3650	C	0
18.0990	14.9830	17.7060	C	0	8.6460	10.1140	10.0940	C	0	6.5280	3.9730	-2.9430	H	0
17.8910	15.3920	16.7170	H	0	7.8240	9.5240	10.7700	O	0	7.2010	5.8210	-3.6230	C	0
17.1540	14.9510	18.2470	H	0	8.4860	10.2200	8.7570	N	0	7.0780	6.2990	-2.6520	H	0
19.0640	15.8600	18.5190	C	0	9.1920	10.8180	8.3510	H	0	8.0450	6.2910	-4.1280	H	0
18.4180	16.6190	18.9610	H	0	7.6590	9.5160	7.8160	C	0	5.9770	5.9600	-4.5060	C	0
19.5270	15.2790	19.3170	H	0	7.1150	8.8480	8.4840	H	0	6.0330	6.4390	-5.6530	O	0
20.1780	16.4990	17.6710	C	0	6.7300	10.4430	7.0860	C	0	4.9500	5.4280	-3.9740	O	0
20.8670	16.9860	18.3610	H	0	6.0200	10.8550	7.8040	H	0	7.7820	3.5750	-4.6800	C	0
20.8140	15.7710	17.1660	H	0	7.2320	11.3010	6.6370	H	0	8.8940	3.1770	-4.9530	O	0
19.7070	17.6340	16.7230	C	0	5.8830	9.8270	5.9600	C	0	6.7240	3.4160	-5.5590	N	0
19.0680	17.2060	15.9520	H	0	5.8370	8.7390	6.0080	H	0	5.9060	3.9570	-5.3180	H	0
19.1120	18.4010	17.2200	H	0	4.5380	10.4650	5.9810	C	0	6.7640	2.7930	-8.6270	C	0
20.9000	18.2630	16.0240	N	0	3.9310	10.2090	5.1130	H	0	7.0190	1.7350	-6.8050	H	0
21.4220	18.8930	16.6170	H	0	3.9990	10.4780	6.9290	H	0	5.4370	2.8390	-7.6030	C	0
21.6160	17.5810	15.8190	H	0	4.7470	11.5350	5.9580	H	0	4.9110	3.7800	-7.4470	H	0
20.5510	18.7890	15.2360	H	0	6.6040	10.0130	4.6380	C	0	5.6680	2.5450	-8.6270	H	0
17.3320	12.6380	17.1700	C	0	6.0640	9.4550	3.8720	H	0	4.5210	1.7270	-7.1310	C	0
16.9660	12.5150	16.0060	O	0	6.8160	11.0560	4.4050	H	0	4.8850	0.7870	-7.5450	H	0
16.6530	12.0730	18.1570	N	0	7.5690	9.5220	4.5120	H	0	4.4250	1.7700	-6.0460	H	0
16.8990	12.3150	19.1070	H	0	8.5850	8.7690	6.9290	C	0	3.0960	1.9280	-7.5080	C	0
15.3480	11.4450	17.9570	C	0	9.5710	9.3600	6.4120	O	0	2.6790	1.0800	-6.9650	H	0
15.3920	10.6730	17.1890	H	0	8.2990	7.5240	6.5850	N	0	2.8000	2.9150	-7.1530	H	0
14.8260	10.8260	19.2950	C	0	7.5090	7.0820	7.0340	H	0	2.8690	1.7750	-9.0320	N	0
15.4990	10.1180	19.7780	H	0	9.1310	6.6220	5.7360	C	0	3.4770	2.1810	-9.7280	H	0
14.6200	11.6520	19.9760	H	0	9.7200	7.2690	5.0860	H	0	1.7530	1.2380	-9.5500	C	0
13.5320	10.0780	19.0220	C	0	9.9680	5.6310	6.6140	C	0	1.1960	0.1620	-8.9550	N	0
12.8220	10.8340	18.6880	H	0	9.3600	5.0270	7.2880	H	0	1.4600	-0.1080	-8.0190	H	0
13.7500	9.3000	18.2890	H	0	10.8730	4.7690	5.6450	C	0	0.4610	-0.3310	-9.4430	H	0
12.8860	9.5480	20.3010	C	0	10.3160	4.1270	4.9620	H	0	1.2110	1.5980	-10.6920	N	0
13.5700	8.7640	20.6270	H	0	11.5490	5.4460	5.1240	H	0	1.7000	2.3280	-11.1890	H	0
12.8220	10.2830	21.1040	H	0	11.5320	4.0900	6.1870	H	0	0.3800	1.1300	-11.0250	H	0
11.4600	9.0590	20.0510	C	0	10.9380	6.4580	7.4390	C	0	7.8410	3.3620	-7.7800	C	0
11.3820	8.3440	19.2320	H	0	10.3790	7.0610	8.1550	H	0	8.4160	2.5610	-8.4730	O	0
11.1380	8.4110	20.8660	H	0	11.5670	5.6870	7.8830	H	0	8.0850	4.6620	-7.7080	N	0
10.4760	10.1100	20.0230	N	0	11.5000	7.0340	6.7040	H	0	7.4750	5.2630	-7.1730	H	0
9.6400	9.7400	19.5930	H	0	8.2360	5.7940	4.8710	C	0	9.2720	5.2580	-8.4080	C	0
10.2470	10.3710	20.9710	H	0	7.1380	5.4340	5.3100	O	0	9.1270	5.1150	-9.4790	H	0
10.8350	10.9330	19.5620	H	0	8.6210	5.5590	3.6680	N	0	9.0950	6.7890	-8.1790	C	0
14.4080	12.4740	17.3160	C	0	9.5100	5.9500	3.3900	H	0	9.7710	7.3540	-8.8210	H	0
14.0330	13.4880	17.9420	O	0	8.0170	4.7020	2.6680	C	0	8.0820	7.1310	-8.3930	H	0
13.8560	12.1900	16.1560	N	0	7.9310	3.7510	3.1950	H	0	9.3100	7.1350	-6.7750	C	0
14.0320	11.3100	15.6920	H	0	6.6370	5.1430	2.2640	C	0	10.3830	6.9610	-6.2100	O	0
13.0550	13.1440	15.3560	C	0	6.0790	4.2810	1.8990	H	0	8.2860	7.6400	-6.1120	N	0
12.8470	13.9440	16.0650	H	0	6.0010	5.4490	3.0950	H	0	8.4160	8.0450	-5.1960	H	0
13.8270	13.7580	14.1980	C	0	6.5400	6.2610	1.2570	C	0	7.3350	7.7280	-6.4420	H	0
14.4090	12.9440	13.7660	H	0	5.5500	6.3330	0.3340	N	0	10.6640	4.7290	-8.0770	C	0
13.0900	14.5140	13.0800	C	0	5.8420	7.3230	-0.4770	C	0	11.5340	5.0230	-8.8930	O	0
12.0780	14.7910	13.3730	H	0	5.2820	7.6140	-1.3540	H	0	10.8590	3.9670	-6.9690	N	0
13.6910	15.3960	12.8580	H	0	7.0080	7.8550	-0.0910	N	0	10.1130	3.9230	-6.2900	H	0
13.0310	13.8370	12.2270	H	0	7.5440	8.4560	-0.7010	H	0	12.0570	3.2270	-6.6970	C	0
14.8240	14.6730	14.6420	O	0	7.4010	7.2950	1.0900	C	0	11.6830	2.2740	-6.3200	H	0
15.6210	14.1800	14.8520	H	0	8.3560	7.3900	1.5840	H	0	12.4830	2.9060	-7.6470	H	0
11.8660	12.3920	14.9300	C	0	8.8710	4.4130	1.4210	C	0	13.0280	3.8610	-5.6900	C	0
12.0010	11.2820	14.3780	O	0	9.7970	5.2120	1.0710	O	0	13.9940	3.2130	-5.2610	O	0
10.6260	12.8070	15.0660	N	0	8.6620	3.2890	0.8290	N	0	12.7120	5.0210	-5.1980	N	0
10.2890	14.0430	15.7680	C	0	7.9370	2.6800	1.1800	H	0	11.8020	5.3540	-5.4850	H	0
10.4510	14.8860	15.0960	H	0	9.4450	2.8050	-0.2770	C	0	13.3400	5.7650	-4.0860	C	0
10.8280	14.3200	16.6740	H	0	10.3250	3.4230	-0.4590	H	0	14.3420	5.3380	-4.0400	H	0
8.7680	13.9270	15.9970	C	0	9.8760	1.4230	0.0260	C	0	13.5960	7.2350	-4.4410	C	0
8.2260	14.8720	16.0400	H	0	9.0420	0.8130	0.3710	H	0	12.5830	7.6350	-4.4950	H	0
8.7090	13.3670	16.9300	H	0	10.2930	0.8290	-0.7880	H	0	14.0730	7.7580	-3.6120	H	0
8.2470	13.0930	14.8470	C	0	10.9170	1.5540	1.0890	C	0	14.3880	7.5310	-5.6930	C	0
8.0240	13.5750	13.8950	H	0	12.2240	1.6610	0.7120	C	0	15.7720	7.7370	-5.5310	C	0
7.4020	12.5350	15.2520	H	0	12.3920	1.7690	-0.3500	H	0	16.1010	7.7870	-4.5040	H	0
9.4590	12.2390	14.4140	C	0	13.2450	1.5130	1.6970	C	0	16.6690	7.7890	-6.6210	C	0
9.2920	11.2440	14.8270	H	0	14.2890	1.5810	1.4300	H	0	17.7400	7.8380	-6.4880	H	0
9.6550	12.2610	12.8040	C	0	12.9190	1.5520	3.0630	C	0	16.1170	7.7050	-7.8810	C	0
9.8140	13.3670	12.2190	O	0	13.7070	1.4880	3.8000	H	0	16.7000	7.6780	-8.7900	H	0
9.6740	11.0120	12.1640	N	0	11.5580	1.4690	3.4620	C	0	14.7160	7.5650	-8.0560	C	0

14.2940	7.5700	-9.0500	H	0	9.7820	17.3100	11.0540	O	0	11.9020	19.7560	6.5300	H	0
13.8240	7.4270	-6.9910	C	0	9.0050	15.2750	9.0810	C	0	12.5890	18.1430	6.4740	H	0
12.7750	7.1950	-7.1090	H	0	8.4720	16.2600	8.4880	O	0	13.7120	19.5590	5.3020	C	0
12.7280	5.6320	-2.7340	C	0	8.2880	14.3670	9.7900	N	0	13.9940	18.8600	4.5140	H	0
11.5320	5.8070	-2.5850	O	0	8.7500	13.6330	10.3070	H	0	13.4050	20.5170	4.8820	H	0
13.5520	5.2600	-1.7030	N	0	6.8370	14.3040	9.7240	C	0	14.7670	19.8590	6.3180	C	0
14.5490	5.3670	-1.8300	H	0	6.7290	14.3060	8.6390	H	0	14.7520	19.3950	7.4320	O	0
13.0010	5.1930	-0.3370	C	0	6.2110	12.9430	10.1200	C	0	15.8310	20.5620	5.8030	N	0
12.0100	4.7410	-0.2990	H	0	5.1860	13.0080	9.7550	H	0	16.5670	20.7850	6.4570	H	0
13.6890	4.5730	0.2380	H	0	6.7150	12.1480	9.5700	H	0	15.9490	20.3780	4.8170	H	0
13.1040	6.5930	0.3620	C	0	6.1740	12.7400	11.6000	C	0	11.9220	17.1530	4.3370	C	0
14.2070	7.0430	0.7410	O	0	7.2450	12.6680	11.7860	H	0	11.7920	16.1780	5.0540	O	0
11.9830	7.2490	0.5300	N	0	5.7460	13.6390	12.0440	H	0	12.5910	17.0860	3.1680	N	0
11.1300	6.8240	0.1960	H	0	5.3550	11.4560	11.9280	C	0	12.6960	17.9600	2.6720	H	0
11.9870	8.5430	1.2060	C	0	4.3020	11.7300	11.8560	H	0	13.3310	15.9400	2.6520	C	0
12.8950	9.0950	0.9640	H	0	5.4950	10.6170	11.2470	H	0	12.6980	15.0750	2.8480	H	0
10.8550	9.3940	0.6180	C	0	5.4860	11.1710	13.4340	N	0	13.5070	16.1250	1.1530	C	0
9.8470	9.0920	0.9020	H	0	4.8350	11.5890	14.0830	H	0	12.5480	16.1900	0.6380	H	0
10.9560	10.3950	1.0380	H	0	6.2410	10.3170	14.0790	C	0	14.0080	17.0810	1.0020	H	0
10.8570	9.6050	-0.8850	C	0	7.2840	9.6900	13.6110	N	0	14.2870	15.0090	0.4740	C	0
10.3680	8.5820	-1.7200	C	0	7.3170	9.6280	12.6030	H	0	15.1570	14.8650	1.1140	H	0
10.0920	7.6410	-1.2690	H	0	7.9480	9.2980	14.2630	H	0	13.5750	13.7090	0.6560	C	0
10.3220	8.7170	-3.1480	C	0	6.0810	10.3050	15.3530	N	0	14.2520	12.9330	0.2970	H	0
10.0890	7.8820	-3.7930	H	0	5.1850	10.6260	15.6910	H	0	13.3340	13.4380	1.6840	H	0
10.9240	9.8420	-3.7120	C	0	6.7860	9.8230	15.8930	H	0	12.7140	13.6200	-0.0050	H	0
10.9420	9.8030	-5.0680	O	0	6.1000	15.6370	10.1790	C	0	14.9440	15.3490	-0.8460	C	0
11.1340	8.8930	-5.3050	H	0	4.9070	15.7080	9.9290	O	0	15.4010	14.4910	-1.3410	H	0
11.3900	10.8770	-2.9150	C	0	6.8000	16.5160	10.8960	N	0	14.2210	15.6490	-1.6050	H	0
11.7040	11.7660	-3.4400	H	0	7.8070	16.4450	10.9330	H	0	15.7550	16.0760	-0.8140	H	0
11.3650	10.7270	-1.5120	C	0	6.1620	17.7830	11.4590	C	0	14.6050	15.8340	3.4380	C	0
11.8170	11.5490	-0.9750	H	0	5.1770	17.5660	11.8730	H	0	15.4930	16.6790	3.4130	O	0
11.9810	8.5480	2.7400	C	0	7.1230	18.2100	12.6090	C	0	14.7700	14.6260	4.1260	N	0
11.0900	7.8790	3.2680	O	0	8.0170	18.6260	12.1440	H	0	13.9790	14.0060	4.2250	H	0
12.6820	9.5040	3.4030	N	0	6.7090	19.0580	13.1540	H	0	16.0020	14.2610	4.8920	C	0
13.2660	10.0540	2.7900	H	0	7.6070	17.2020	13.6830	C	0	16.5450	15.1660	5.1610	H	0
12.5660	9.9620	4.8130	C	0	6.7380	16.8760	14.2550	H	0	15.5310	13.6390	6.2210	C	0
11.6570	9.5150	5.2160	H	0	7.9950	16.3530	13.1220	H	0	15.1120	12.6570	6.0010	H	0
13.6910	9.3450	5.7990	C	0	8.7870	17.7230	14.6100	C	0	16.6940	13.3440	7.1720	C	0
14.6030	9.9060	5.5980	H	0	8.4580	18.6460	15.0880	H	0	17.5000	12.7460	6.7460	H	0
13.2570	9.5900	7.2730	C	0	8.8690	17.0350	15.4520	H	0	17.1530	14.3000	7.4220	H	0
13.8140	8.8750	7.8780	H	0	9.8880	18.0890	13.8210	N	0	16.3770	12.9450	8.1350	H	0
13.4060	10.6190	7.6000	H	0	9.7860	17.8720	12.8390	H	0	14.4790	14.4000	7.0550	C	0
12.1750	9.4710	7.3220	H	0	11.0410	18.6010	14.2440	C	0	13.5320	14.2630	6.5330	H	0
13.8400	7.9080	5.5290	C	0	11.1550	18.9290	15.5070	N	0	14.3920	13.8250	7.9770	H	0
14.5910	7.7660	4.7520	H	0	10.3200	19.1710	16.0200	H	0	14.7680	15.9510	7.2710	C	0
14.3090	7.4030	6.3730	H	0	12.1050	19.0960	15.8080	H	0	14.9000	16.4610	6.3170	H	0
12.9200	7.4160	5.2130	H	0	12.0790	18.7800	13.4700	N	0	13.9050	16.5260	7.6090	H	0
12.3860	11.4370	4.8750	C	0	11.9530	18.5950	12.4850	H	0	15.5190	16.2220	8.0130	H	0
13.2760	12.2420	4.4570	O	0	12.8610	19.3510	13.7570	H	0	16.9110	13.3470	4.1070	C	0
11.2240	11.7740	5.4110	N	0	6.1850	18.8600	10.4350	C	0	18.1480	13.4800	4.1820	O	0
10.5980	11.0120	5.6260	H	0	5.5210	19.8240	10.7280	O	0	16.4380	12.3490	3.3970	N	0
10.8760	13.1980	5.7400	C	0	6.9950	18.7930	9.3760	N	0	15.4510	12.1530	3.4930	H	0
11.7140	13.8700	5.5580	H	0	7.6170	18.0030	9.2720	H	0	17.2370	11.5060	2.5100	C	0
9.6110	13.5820	4.8910	C	0	7.1960	19.9400	8.4560	C	0	17.9710	12.1030	1.9680	H	0
8.7820	12.9700	5.2470	H	0	6.3860	20.6560	8.5980	H	0	18.0060	10.4350	3.3170	C	0
9.3760	14.6100	5.1650	H	0	8.5260	20.7240	8.7860	C	0	18.7310	11.0310	3.8710	H	0
9.8160	13.3870	3.3910	C	0	8.5780	21.6690	8.2440	H	0	17.3210	9.7980	3.8760	H	0
10.8790	13.3260	3.1600	H	0	8.5100	21.2170	10.2150	C	0	19.0160	9.5230	2.5980	C	0
9.2390	12.0530	2.9050	C	0	8.8090	20.3830	10.8510	H	0	19.5690	9.0030	3.3800	H	0
9.7700	11.8450	1.9760	H	0	9.4030	21.8230	10.3710	H	0	18.4430	8.7940	2.0250	H	0
9.4390	11.2310	3.5930	H	0	7.6360	21.7430	10.5990	H	0	19.9440	10.3470	1.6700	C	0
8.1700	11.9960	2.7020	H	0	9.6410	19.9250	8.5650	O	0	19.4790	10.9360	0.6250	O	0
9.0910	14.4960	2.5860	C	0	9.6850	19.2670	9.2640	H	0	21.1770	10.4450	1.9000	O	0
9.5450	15.4850	2.6470	H	0	7.2670	19.5130	6.9890	C	0	16.2520	10.8140	1.5360	C	0
9.0580	14.3420	1.5070	H	0	6.9940	20.3150	6.0910	O	0	15.1570	10.4830	1.8900	O	0
8.0640	14.6120	2.9300	H	0	7.5760	18.3160	6.5910	N	0	16.6600	10.5060	0.3220	N	0
10.6090	13.4160	7.2380	C	0	7.7900	17.5500	7.2140	H	0	17.5530	10.8700	0.0210	H	0
10.2870	12.5250	7.9940	O	0	7.7040	17.9050	5.2300	C	0	15.9740	9.5380	-0.5100	C	0
10.7620	14.6700	7.6400	N	0	7.5860	16.8220	5.2510	H	0	15.6180	8.7230	0.1210	H	0
11.0230	15.3520	6.9430	H	0	6.9480	18.3810	4.6070	H	0	14.8310	10.1790	-1.2840	C	0
10.5820	15.1370	9.0240	C	0	9.0380	18.2520	4.5380	C	0	14.5190	9.4430	-2.0240	H	0
10.8720	14.4190	9.7920	H	0	9.2200	18.3710	3.3380	O	0	14.0270	10.4680	-0.6060	H	0
11.3530	16.5170	9.3250	C	0	10.1080	18.3660	5.3680	N	0	15.0950	11.1280	-1.7520	H	0
12.3980	16.2290	9.4400	H	0	10.0660	18.2020	6.3640	H	0	17.0980	8.9650	-1.3930	C	0
11.2880	17.1110	8.4130	H	0	11.4980	18.5310	4.7840	C	0	17.6780	9.5980	-2.2600	O	0
10.8730	17.4210	10.5370	C	0	11.4550	19.1070	3.8590	H	0	17.3920	7.6710	-1.2500	N	0
11.6680	18.3960	10.7030	O	0	12.3730	19.0260	5.8720	C	0	16.8770	7.1020	-0.5950	H	0

18.1850	6.9180	-2.1850	C	0	19.8170	0.6160	-14.1640	C	0	20.4170	10.2450	-11.6270	C	0
18.3590	7.5880	-3.0270	H	0	20.2490	1.1400	-15.3400	O	0	20.6250	10.0820	-12.6840	H	0
19.6160	6.7020	-1.6240	C	0	20.8810	1.8550	-15.2310	H	0	20.0370	11.2510	-11.4460	H	0
19.5070	5.9710	-0.8230	H	0	18.6060	-0.0380	-14.1460	C	0	21.7120	10.1070	-10.9600	C	0
20.1910	6.2430	-2.4290	H	0	17.9650	0.1640	-14.9920	H	0	21.5860	10.1740	-9.8800	H	0
20.3740	7.9650	-1.1850	C	0	18.1710	-0.7260	-13.0270	C	0	22.1620	9.1270	-11.1200	H	0
19.8560	8.4210	-0.3410	H	0	17.1940	-1.1860	-13.0530	H	0	22.6930	11.2070	-11.2990	C	0
21.3950	7.7500	-0.8710	H	0	16.9350	0.5090	-10.4040	C	0	23.2970	10.8210	-12.1200	H	0
20.6080	8.9390	-2.2450	C	0	15.7000	0.2680	-10.5660	O	0	22.2250	12.1660	-11.5220	H	0
20.9590	8.6100	-3.3750	O	0	17.4600	1.7010	-10.8230	N	0	23.7370	11.4180	-10.2500	C	0
20.4850	10.2430	-1.9610	N	0	18.4640	1.8030	-10.7740	H	0	23.2020	12.0150	-9.5120	H	0
20.6500	10.8500	-2.7140	H	0	16.6510	2.7790	-11.3600	C	0	24.0620	10.4580	-9.5480	H	0
20.3410	10.4730	-0.9880	H	0	15.7850	2.2520	-11.7610	H	0	24.9310	12.1890	-10.6980	N	0
17.4670	5.7340	-2.7910	C	0	16.0120	3.7390	-10.3670	C	0	24.7400	13.0630	-11.1670	H	0
16.3590	5.4550	-2.3200	O	0	15.5810	3.0750	-9.6180	H	0	25.4920	12.5010	-9.9180	H	0
17.9650	5.0400	-3.8630	N	0	17.0870	4.5340	-9.6190	C	0	25.5360	11.6710	-11.3200	H	0
18.9910	5.5130	-4.7660	C	0	17.6050	5.1850	-10.3240	H	0	19.2210	9.3150	-9.7350	C	0
19.9810	5.2440	-4.3950	H	0	16.6690	5.1410	-8.8160	H	0	19.5240	8.4410	-8.9570	O	0
18.9890	6.5810	-4.9820	H	0	17.8040	3.8430	-9.1740	H	0	18.5440	10.3900	-9.2670	N	0
18.6750	4.9060	-6.1670	C	0	14.9290	4.6100	-10.9570	C	0	18.1330	10.9880	-9.9700	H	0
19.5130	4.7260	-6.8410	H	0	13.9940	4.0550	-10.8770	H	0	18.5180	10.7830	-7.8510	C	0
17.8700	5.5660	-6.4880	H	0	14.9640	5.5480	-10.4020	H	0	18.3800	9.8880	-7.2440	H	0
17.8790	3.6440	-5.7440	C	0	15.0720	4.7760	-12.0240	H	0	19.8410	11.4490	-7.3330	C	0
18.5860	2.8150	-5.7020	H	0	17.2900	3.5350	-12.5630	C	0	19.5710	11.7840	-6.3320	H	0
17.1710	3.3720	-6.5270	H	0	18.4210	3.9900	-12.4820	O	0	20.5880	10.6610	-7.2430	H	0
17.1660	3.9230	-4.3510	C	0	16.5560	3.7180	-13.6820	N	0	20.4460	12.6320	-8.0740	C	0
16.1450	4.2840	-4.4710	H	0	15.5780	3.5070	-13.5450	H	0	20.6980	12.3090	-9.0840	H	0
17.2650	2.6530	-3.4760	C	0	17.0400	4.5550	-14.7630	C	0	19.7350	13.4550	-8.1460	H	0
18.3170	2.3320	-2.9320	O	0	17.8620	5.1960	-14.4460	H	0	21.6050	13.2790	-7.3650	C	0
16.1290	1.9060	-3.3950	N	0	17.5810	3.6620	-15.8960	C	0	22.4580	14.0260	-7.8800	O	0
15.2690	2.2210	-3.8210	H	0	18.1300	4.3220	-16.5670	H	0	21.6450	13.1850	-6.1190	O	0
16.0380	0.5800	-2.7350	C	0	18.2060	2.9210	-15.3970	H	0	17.3470	11.7210	-7.6100	C	0
16.9170	0.4170	-2.1120	H	0	16.4610	2.9540	-16.7220	C	0	17.1050	12.5910	-8.4110	O	0
14.9060	0.6140	-1.6960	C	0	15.2910	3.2710	-16.7320	O	0	16.8080	11.5750	-6.4310	N	0
14.9010	-0.3100	-1.1190	H	0	16.8080	1.9640	-17.5260	N	0	17.2850	10.9380	-5.8090	H	0
15.1390	1.3960	-0.9730	H	0	16.0590	1.5790	-18.0840	H	0	16.1120	12.7690	-5.7720	C	0
13.5360	0.6860	-2.2930	C	0	17.7760	1.7170	-17.6790	H	0	15.5870	13.3500	-6.5300	H	0
12.9070	1.8980	-2.5890	C	0	16.0550	5.6170	-15.2310	C	0	15.0930	12.4030	-4.6710	C	0
13.4840	2.7660	-2.3080	H	0	16.4910	6.3630	-16.0580	O	0	15.6310	11.8200	-3.9230	H	0
11.6880	2.1110	-3.2870	C	0	14.7710	5.7550	-14.7780	N	0	14.3390	13.6660	-4.2250	C	0
11.3310	3.1150	-3.4610	H	0	14.3730	5.1570	-14.0680	H	0	15.0000	14.3490	-3.6910	H	0
11.0990	0.8770	-3.6820	C	0	13.9700	6.9730	-15.1320	C	0	13.7900	14.0910	-5.0660	H	0
10.1770	0.8700	-4.2450	H	0	14.0370	7.1560	-16.2050	H	0	13.5460	13.3050	-3.5700	H	0
11.6330	-0.3640	-3.3670	C	0	12.4780	6.8680	-14.7620	C	0	14.1350	11.3030	-5.2920	C	0
11.1280	-1.2430	-3.7390	H	0	11.8480	7.6230	-15.2320	H	0	14.7110	10.3930	-5.4570	H	0
12.8050	-0.4490	-2.6510	C	0	12.0840	5.8840	-15.0160	H	0	13.4500	11.0210	-4.4920	H	0
13.0870	-1.4540	-2.3760	H	0	12.3950	7.0820	-13.2550	C	0	13.3950	11.7180	-6.5780	C	0
15.9490	-0.5230	-3.7760	C	0	12.5250	6.1780	-12.3070	C	0	12.8140	10.8500	-6.8910	H	0
16.1270	-1.6820	-3.3500	O	0	12.6470	5.1480	-12.6090	H	0	12.7280	12.5630	-6.4070	H	0
15.9540	-0.1620	-5.0460	N	0	12.3800	6.6510	-11.0400	N	0	14.0350	12.0330	-7.4020	H	0
15.9790	0.8470	-5.0970	H	0	12.3550	6.1090	-10.1880	H	0	17.1160	13.7550	-5.2120	C	0
16.1240	-0.9700	-6.2140	C	0	11.9820	7.9240	-11.0920	C	0	17.7550	13.2860	-4.2600	O	0
16.6370	-1.8810	-5.9060	H	0	11.7240	8.8930	-10.1100	C	0	17.2920	14.8770	-5.8120	N	0
14.7780	-1.3310	-6.8870	C	0	11.7550	8.6690	-9.0540	H	0	16.5580	15.1680	-6.4410	H	0
15.0300	-2.0110	-7.7000	H	0	11.2780	10.1050	-10.6400	C	0	18.2710	15.8120	-5.4040	C	0
13.8360	-2.0730	-5.9300	C	0	10.8910	10.7990	-9.9080	H	0	19.2320	15.2980	-5.3860	H	0
13.0040	-2.4950	-6.4940	H	0	11.3220	10.4930	-11.9620	C	0	18.3140	16.8640	-6.4620	C	0
14.4070	-2.8370	-5.4020	H	0	10.9940	11.4780	-12.2590	H	0	18.5970	16.4120	-7.4130	H	0
13.3530	-1.3130	-5.3160	H	0	11.7430	9.5430	-12.9280	C	0	17.2680	17.1530	-6.5640	H	0
14.0350	-0.1260	-7.5720	C	0	11.7690	9.7950	-13.9780	H	0	19.2240	17.9420	-6.1690	O	0
13.8110	0.6430	-6.8330	H	0	12.0370	8.2340	-12.4980	C	0	19.9980	17.8030	-6.7200	H	0
14.6020	0.2870	-8.4070	H	0	14.5370	8.2860	-14.5540	C	0	17.9780	16.5220	-4.0500	C	0
13.1240	-0.5890	-7.9500	H	0	14.4100	9.3400	-15.1870	O	0	16.8020	16.7760	-3.7670	O	0
17.0760	-0.3410	-7.2720	C	0	15.1190	8.2170	-13.3590	N	0	18.9950	16.9400	-3.3070	N	0
17.5450	0.7630	-7.1480	O	0	15.1850	7.3290	-12.8810	H	0	19.9170	16.7290	-3.6630	H	0
17.3050	-1.0780	-8.4080	N	0	15.8950	9.2800	-12.7820	C	0	18.9160	17.6680	-2.0850	C	0
16.9960	-2.0390	-8.4320	H	0	16.2220	9.9490	-13.5790	H	0	18.0300	17.4360	-1.4930	H	0
17.8150	-0.4180	-9.6110	C	0	15.1210	10.1640	-11.7490	C	0	20.0550	17.3110	-1.1350	C	0
18.6500	0.1950	-9.2710	H	0	14.6280	9.4370	-11.1020	H	0	20.9700	17.8090	-1.4570	H	0
18.4860	-1.3630	-10.6390	C	0	15.8190	10.7800	-11.1820	H	0	19.8260	17.8010	-0.1890	H	0
19.3530	-1.8860	-10.2350	H	0	14.3090	10.7420	-12.1900	H	0	20.1220	15.8680	-0.7900	C	0
17.7350	-2.0780	-10.9750	H	0	17.2060	8.6090	-12.2790	C	0	19.1110	15.5220	-0.5730	H	0
18.9790	-0.6730	-11.8430	C	0	17.2620	7.3610	-12.0750	O	0	20.5250	15.3080	-1.6340	H	0
20.2000	-0.0240	-11.8430	C	0	18.1010	9.4960	-11.9230	N	0	20.9970	15.5600	0.4590	C	0
20.8060	-0.0480	-10.9500	H	0	18.0150	10.3960	-12.3710	H	0	22.0160	15.7040	0.1000	H	0
20.6190	0.6720	-12.9680	C	0	19.3820	9.1930	-11.1960	C	0	20.6750	16.2860	1.2060	H	0
21.5930	1.1390	-12.9980	H	0	19.7490	8.2160	-11.5080	H	0	20.8670	14.1800	0.9500	C	0

21.7540	13.9500	1.5410	H	0	11.5960	13.7210	-9.5170	C	0	15.1450	9.4760	-24.0460	H	0
19.9310	14.2670	1.5010	H	0	10.8730	13.5920	-10.3220	H	0	17.0300	8.4390	-23.6750	C	0
20.6950	13.2500	-0.1050	N	0	11.2590	13.0880	-8.6960	H	0	16.8190	7.9110	-24.6050	H	0
21.4640	13.1460	-0.7510	H	0	13.0160	13.2590	-9.9970	C	0	17.7840	9.1760	-23.9530	H	0
20.5000	12.3790	0.3670	H	0	12.9920	13.3600	-11.0820	H	0	17.7070	7.4880	-22.7290	C	0
19.8540	13.4040	-0.6420	H	0	13.2470	12.2630	-9.6210	H	0	17.6340	7.9540	-21.7460	H	0
18.8350	19.1620	-2.3320	C	0	13.9540	14.2500	-9.2760	C	0	17.1580	6.5500	-22.6420	H	0
18.0960	19.9220	-1.7010	O	0	14.5330	13.6970	-8.5360	H	0	19.1540	6.9660	-23.1270	C	0
19.5960	19.6090	-3.3330	N	0	14.8850	14.9220	-10.2590	C	0	19.8480	6.5920	-22.2060	O	0
20.1950	18.9610	-3.8250	H	0	14.6370	16.0010	-10.7670	O	0	19.5640	7.1600	-24.2620	O	0
19.6320	20.9730	-3.7110	C	0	15.9550	14.1180	-10.6870	N	0	14.8550	7.8810	-22.5210	C	0
19.7270	21.5780	-2.8100	H	0	16.1200	13.3140	-10.0980	H	0	14.6530	6.8660	-23.1590	O	0
20.8100	21.2400	-4.6310	C	0	16.9660	14.4440	-11.7130	C	0	14.3740	8.0370	-21.3230	N	0
20.9570	20.5570	-5.4670	H	0	16.9380	15.4760	-12.0630	H	0	14.6450	8.8440	-20.7790	H	0
20.6360	22.2490	-5.0040	H	0	18.2630	14.4240	-10.9490	C	0	13.5480	7.0620	-20.6320	C	0
22.1390	21.2110	-3.8760	C	0	18.3720	13.4980	-10.3840	H	0	13.3570	6.2420	-21.3240	H	0
22.8930	21.4570	-4.6240	H	0	19.4330	14.4240	-11.9610	C	0	14.2970	6.5430	-19.3950	C	0
22.2060	21.9490	-3.0770	H	0	19.1980	15.0670	-12.8090	H	0	14.3060	7.3230	-18.6340	H	0
22.6120	19.8820	-3.3820	C	0	20.3370	14.7890	-11.4730	H	0	13.7510	5.7950	-18.8200	H	0
23.2200	19.7700	-2.3270	O	0	19.6100	13.3860	-9.3240	H	0	15.7360	5.9170	-19.4770	C	0
22.4520	18.9600	-4.1870	O	0	18.4240	15.5780	-9.9530	C	0	16.4960	6.5500	-19.9350	H	0
18.3390	21.4880	-4.3720	C	0	19.3440	15.5830	-9.3690	H	0	16.0220	5.5100	-18.5070	H	0
17.9260	22.6160	-4.0810	O	0	18.4410	16.5160	-10.5070	H	0	15.7020	4.6760	-20.4110	C	0
17.8030	20.6810	-5.2360	N	0	17.5550	15.4770	-9.3020	H	0	14.8990	4.0150	-20.0850	H	0
18.3260	19.8300	-5.3820	H	0	16.8650	13.3390	-12.7330	C	0	15.4730	5.0470	-21.4100	H	0
16.5920	20.9120	-6.0120	C	0	17.5010	12.2310	-12.6930	O	0	17.0350	3.9990	-20.5150	C	0
16.3960	21.9810	-6.0950	H	0	15.8890	13.5390	-13.6570	N	0	17.8330	4.6460	-20.8800	H	0
16.7300	20.3820	-7.3680	C	0	15.4090	14.4190	-13.5330	H	0	17.2340	3.6340	-19.5080	H	0
16.6430	19.2960	-7.3550	H	0	15.3700	12.4550	-14.5990	C	0	17.0400	2.8400	-21.4810	N	0
15.7740	20.4850	-7.8800	H	0	15.1210	11.5180	-14.1010	H	0	17.8990	2.3200	-21.3710	H	0
17.8020	20.9610	-8.2540	C	0	14.0910	12.9330	-15.2990	C	0	16.2980	2.1880	-21.2710	H	0
18.2130	22.0730	-7.9940	O	0	14.4420	13.8080	-15.8470	H	0	16.9490	3.2130	-22.4150	H	0
18.1390	20.3000	-9.3430	N	0	13.7830	12.1370	-15.9780	H	0	12.2130	7.7290	-20.1950	C	0
18.8390	20.7020	-9.9510	H	0	12.9240	13.1590	-14.3920	C	0	11.3310	7.0270	-19.5840	O	0
17.6950	19.5050	-9.7810	H	0	12.7380	12.2010	-13.9060	H	0	12.1160	9.0590	-20.2680	N	0
15.3450	20.3700	-5.2160	C	0	13.1510	13.8660	-13.5940	H	0	13.0120	9.4410	-20.5330	H	0
14.1990	20.6500	-5.6590	O	0	11.7080	13.7220	-15.1540	C	0	10.8180	9.7600	-20.1940	C	0
15.3990	19.4240	-4.2750	N	0	10.7130	14.1500	-14.4630	O	0	10.1860	9.4320	-19.3680	H	0
16.3060	19.0230	-4.0850	H	0	11.6750	13.7220	-16.4310	O	0	11.1420	11.2460	-20.1380	C	0
14.2900	18.6400	-3.6830	C	0	16.4030	12.2290	-15.8100	C	0	11.8720	11.3110	-19.3320	H	0
14.7510	17.8290	-3.1200	H	0	17.4080	12.9800	-16.0400	O	0	11.5870	11.6360	-21.0530	H	0
13.5340	19.5130	-2.7010	C	0	16.1520	11.0960	-16.4940	N	0	9.8070	11.9880	-19.9990	C	0
12.9560	20.2430	-3.2670	H	0	15.3480	10.5250	-16.2770	H	0	9.3310	12.1250	-20.9700	H	0
12.8680	18.9060	-2.0870	H	0	16.9740	10.7250	-17.6530	C	0	9.0720	11.4820	-19.3730	H	0
14.3580	20.2750	-1.7030	C	0	17.9230	11.2560	-17.7160	H	0	9.7890	13.3450	-19.3080	C	0
14.5080	21.5490	-1.7270	O	0	17.4760	9.1950	-17.5690	C	0	10.7710	13.8170	-19.3060	H	0
14.8790	19.6850	-0.7750	O	0	16.5850	8.5690	-17.6110	H	0	9.0460	13.9550	-19.8220	H	0
13.2370	17.9580	-4.6610	C	0	18.4150	8.8950	-18.7690	C	0	9.4280	13.2100	-17.9120	N	0
12.1910	17.5670	-4.2630	O	0	18.7220	7.8790	-18.5210	H	0	10.1660	13.1580	-17.2250	H	0
13.5410	17.9610	-5.9770	N	0	17.7930	8.8150	-19.6610	H	0	8.2980	13.5490	-17.3720	C	0
14.2940	18.5980	-6.1970	H	0	19.2100	9.6320	-18.8830	H	0	7.1920	13.7340	-18.0870	N	0
12.8590	17.3550	-7.1530	C	0	18.0060	8.9240	-16.1440	C	0	7.2580	13.4040	-19.0390	H	0
11.9830	16.8420	-6.7550	H	0	17.1290	8.8690	-15.4990	H	0	6.2780	13.8650	-17.6780	H	0
12.4980	18.5550	-8.0760	C	0	18.4830	7.9440	-16.1680	H	0	8.3130	13.7480	-16.0390	N	0
13.3350	19.2530	-8.0400	H	0	19.1080	9.8830	-15.6870	C	0	9.1030	13.6140	-15.4250	H	0
12.3330	18.3180	-9.1270	H	0	19.6400	9.4750	-14.8280	H	0	7.4340	14.0570	-15.6480	H	0
11.2840	19.3210	-7.5430	C	0	19.8390	9.9290	-16.4950	H	0	10.0340	9.4340	-21.4600	C	0
10.5220	18.5720	-7.7580	H	0	18.7340	10.8950	-15.5320	H	0	10.5950	9.5600	-22.5570	O	0
11.3080	19.4020	-6.4560	H	0	16.1050	10.9690	-18.9110	C	0	8.7830	9.0240	-21.2220	N	0
10.9880	20.6520	-8.2010	C	0	15.1390	10.2330	-19.1320	O	0	8.4120	8.8690	-20.2960	H	0
10.2110	21.2260	-7.6950	H	0	16.4460	11.8220	-19.8830	N	0	7.9110	8.4500	-22.2430	C	0
11.8750	21.2680	-8.0520	H	0	17.3110	12.9370	-19.5580	C	0	8.5260	7.7920	-22.8570	H	0
10.6740	20.5080	-9.6320	N	0	18.3690	12.6770	-19.5420	H	0	6.7640	7.7440	-21.5780	C	0
11.4530	20.2740	-10.2310	H	0	17.0230	13.3580	-18.5940	H	0	6.0400	7.4030	-22.3180	H	0
9.5940	20.9120	-10.3070	C	0	17.0120	14.0450	-20.5750	C	0	7.0560	6.6030	-20.6070	C	0
8.6470	21.6170	-9.8160	N	0	17.8250	14.6040	-21.0380	H	0	7.6640	5.8800	-21.1520	H	0
8.7930	22.0180	-8.9010	H	0	16.2460	14.6930	-20.1500	H	0	7.4880	6.8290	-19.6330	H	0
7.8050	21.7540	-10.3570	H	0	16.3970	13.3040	-21.7190	C	0	6.0640	6.2040	-20.3930	H	0
9.3220	20.5010	-11.5370	N	0	17.0970	12.9170	-22.4590	H	0	6.0190	8.6390	-20.8580	O	0
9.9750	19.8910	-12.0090	H	0	15.6140	13.9030	-22.1840	H	0	5.8820	8.2500	-19.9920	H	0
8.4000	20.7600	-11.8560	H	0	15.6320	12.1930	-21.0240	C	0	7.3510	9.6120	-23.2150	C	0
13.7120	16.3090	-7.8680	C	0	14.6750	12.4070	-20.5490	H	0	7.3810	10.7820	-22.7900	O	0
14.9170	16.2680	-7.6030	O	0	15.1400	11.0680	-21.8970	C	0	7.0860	9.2460	-24.4710	N	0
13.1070	15.3150	-8.6260	N	0	13.9500	11.0740	-22.1870	O	0	7.1520	8.2500	-24.6190	H	0
11.7320	15.2380	-9.1410	C	0	15.9500	10.1370	-22.3340	N	0	6.6450	10.1190	-25.6350	C	0
11.6170	15.7840	-10.0770	H	0	16.8980	10.2380	-22.0000	H	0	6.1970	11.0370	-25.2560	H	0
10.9620	15.5730	-8.4450	H	0	15.6940	9.0130	-23.2260	C	0	7.8670	10.6600	-26.3620	C	0

7.4610	11.4270	-27.0210	H	0	11.1880	5.9210	-22.5470	H	0	10.1190	1.5500	-14.0360	O	0
8.4670	11.1460	-25.5920	H	0	11.9220	4.3500	-23.1460	H	0	9.6500	-0.6710	-14.2840	N	0
8.6740	9.6800	-27.1540	C	0	9.9390	6.3440	-24.6830	O	0	9.9320	-1.6000	-14.0050	H	0
9.0570	8.8480	-26.5640	H	0	9.1170	6.3610	-25.1790	H	0	8.3550	-0.6680	-14.9100	C	0
8.1180	9.1760	-27.9450	H	0	10.7500	2.7690	-25.0680	C	0	8.4410	0.0630	-15.7140	H	0
9.8820	10.3730	-27.8320	C	0	9.8320	1.9490	-24.9330	O	0	7.9960	-2.0600	-15.4180	C	0
10.4490	10.7790	-26.9940	H	0	12.0150	2.3830	-24.9110	N	0	7.1440	-1.9100	-16.0810	H	0
10.4340	9.6030	-28.3700	H	0	12.7270	3.0850	-25.0550	H	0	8.8220	-2.4190	-16.0310	H	0
9.5410	11.5030	-28.7050	C	0	12.4530	1.0550	-24.3840	C	0	7.6950	-3.1050	-14.3380	C	0
8.7240	11.3500	-29.4110	H	0	11.5460	0.4890	-24.1730	H	0	8.1400	-3.0240	-13.2590	O	0
9.3070	12.2500	-27.9470	H	0	13.3770	0.4020	-25.4210	C	0	6.7880	-4.0380	-14.6450	N	0
10.7850	11.9910	-29.3750	N	0	14.3770	0.8250	-25.3200	H	0	6.6150	-4.6940	-13.8960	H	0
11.5110	12.0580	-28.6760	H	0	13.4800	-0.6540	-25.1730	H	0	6.3760	-4.0200	-15.5670	H	0
11.1030	11.4030	-30.1320	H	0	12.8740	0.5250	-26.8730	C	0	7.1780	-0.0550	-14.0910	C	0
10.7890	12.9230	-29.7630	H	0	12.8590	-0.3620	-27.5070	H	0	7.3820	0.3100	-12.9620	O	0
5.5110	9.4600	-26.4950	C	0	11.7940	0.6770	-26.3910	H	0	5.9400	0.1290	-14.6590	N	0
5.4480	8.2390	-26.5480	O	0	13.5540	1.6350	-27.6480	C	0	5.9340	0.1900	-15.6670	H	0
4.5480	10.1870	-27.1060	N	0	13.5700	2.5870	-27.1180	H	0	4.9450	0.9900	-13.9520	C	0
4.6560	11.1910	-27.1340	H	0	14.5830	1.2730	-27.6590	H	0	5.3910	1.9780	-13.8370	H	0
3.4580	9.6810	-27.9170	C	0	13.0260	1.7460	-29.1350	C	0	3.6680	0.9630	-14.8000	C	0
3.0180	8.8340	-27.3910	H	0	13.7750	1.2730	-29.7710	H	0	3.4470	-0.0710	-15.0650	H	0
2.4670	10.8640	-28.0920	C	0	12.1110	1.1860	-29.3310	H	0	2.8260	1.4120	-14.2740	H	0
2.3730	11.1640	-27.0490	H	0	13.0290	3.0800	-29.6090	N	0	3.8740	1.7120	-16.0280	O	0
2.8460	11.7160	-28.6560	H	0	12.4350	3.7170	-29.0990	H	0	3.9280	2.6340	-15.7670	H	0
1.1070	10.3690	-28.6960	C	0	13.9410	3.4850	-29.4520	H	0	4.5270	0.5620	-12.5280	C	0
1.1260	9.9710	-29.7100	H	0	12.7580	3.2350	-30.5700	H	0	4.2730	1.3690	-11.6610	O	0
0.5950	9.5570	-28.1790	H	0	13.1500	1.1220	-23.0060	C	0	4.3090	-0.7060	-12.3110	N	0
0.0450	11.4360	-28.6020	C	0	13.7760	2.1260	-22.5600	O	0	4.4720	-1.3770	-13.0480	H	0
0.0990	12.3930	-27.8550	O	0	13.1990	-0.0190	-22.3910	N	0	4.0490	-1.4070	-11.0520	C	0
-0.9710	11.2190	-29.3960	N	0	12.7020	-0.7350	-22.9010	H	0	3.1600	-0.9390	-10.6300	H	0
-1.7180	11.8860	-29.2640	H	0	14.0840	-0.2680	-21.1880	C	0	3.6930	-2.9480	-11.2740	C	0
-1.0210	10.3960	-29.9790	H	0	13.8280	-1.2330	-20.7500	H	0	3.6940	-3.5420	-10.3610	H	0
3.9910	9.0960	-29.1940	C	0	15.1070	-0.5160	-21.4710	H	0	2.7540	-3.0980	-11.8070	H	0
5.0490	9.5370	-29.6720	O	0	13.9870	0.6700	-20.0020	C	0	4.7550	-3.6060	-12.1800	C	0
3.2340	8.1160	-29.7570	N	0	14.9290	1.0490	-19.3230	O	0	4.6180	-3.4110	-13.2440	H	0
2.6220	7.5830	-29.1550	H	0	12.7270	1.0660	-19.7270	N	0	5.7700	-3.3820	-11.8520	H	0
3.2990	7.4750	-31.0710	C	0	12.0320	0.6200	-20.3080	H	0	4.5800	-5.4320	-12.0440	S	0
2.6150	6.6270	-31.1010	H	0	12.3500	1.8190	-18.6040	C	0	3.0150	-5.7590	-12.6710	C	0
3.0960	8.1630	-31.8920	H	0	13.0450	2.6470	-18.4600	H	0	2.7460	-5.0210	-13.4270	H	0
4.6930	6.8950	-31.4580	C	0	10.8900	2.3910	-18.7090	C	0	2.8660	-6.7900	-12.9910	H	0
4.9080	6.5380	-32.6180	O	0	10.2310	1.5450	-18.8990	H	0	2.3090	-5.5650	-11.8630	H	0
5.6010	6.7240	-30.4670	N	0	10.3800	3.0070	-17.3960	C	0	5.2300	-1.1460	-10.0280	C	0
5.4270	7.0100	-29.5140	H	0	10.4530	2.2260	-16.6390	H	0	5.0550	-1.4880	-8.9140	O	0
6.8370	5.9940	-30.6630	C	0	10.8540	3.9080	-17.0070	H	0	6.3000	-0.4700	-10.4320	N	0
6.6890	5.1540	-31.3410	H	0	9.3010	3.1380	-17.4790	H	0	6.3350	-0.3330	-11.4320	H	0
7.9860	6.9130	-31.1660	C	0	10.8270	3.4170	-19.8780	C	0	7.3070	0.2170	-9.5810	C	0
8.8330	6.2850	-31.4450	H	0	11.0260	4.4330	-19.5380	H	0	7.8820	0.9000	-10.2070	H	0
7.6780	7.6870	-32.5020	C	0	11.5030	3.2640	-20.7190	H	0	6.8260	0.8170	-8.8080	H	0
8.5570	8.1140	-32.9860	H	0	9.3790	3.4430	-20.4120	C	0	8.2890	-0.7230	-8.8950	C	0
7.2520	7.0480	-33.2760	H	0	9.1150	2.4110	-20.6440	H	0	8.3970	-1.9150	-9.1630	O	0
6.8910	8.4260	-32.3490	H	0	8.7230	3.8150	-19.6250	H	0	9.1330	-0.1020	-8.0710	N	0
8.5490	7.8740	-30.1420	C	0	9.2360	4.0530	-21.3040	H	0	9.1310	0.9080	-8.0740	H	0
7.6840	8.2650	-29.6050	H	0	12.4770	1.0130	-17.3530	C	0	10.1650	-0.7890	-7.3960	C	0
9.2800	7.3410	-29.5350	H	0	11.6530	0.0560	-17.2040	O	0	10.7000	-1.2980	-8.1990	H	0
9.1100	8.6440	-30.6720	H	0	13.3170	1.2550	-16.4130	N	0	10.7630	-0.1560	-6.7410	H	0
7.2930	5.2430	-29.3900	C	0	13.9710	2.0200	-16.4960	H	0	9.7490	-1.9010	-6.3870	C	0
7.0390	5.7100	-28.2470	O	0	13.3190	0.5390	-15.0900	C	0	10.3700	-2.9780	-6.2630	O	0
7.8010	3.9790	-29.4860	N	0	12.5250	-0.2080	-15.0750	H	0	8.6700	-1.6320	-5.7200	N	0
8.1800	3.6510	-30.3630	H	0	14.6320	-0.0890	-14.9970	C	0	8.2780	-0.7080	-5.8340	H	0
8.3420	3.1660	-28.4070	C	0	15.3780	0.7040	-14.9590	H	0	7.6240	-2.6250	-5.3760	C	0
7.6040	3.0910	-27.6080	H	0	14.8800	-0.6630	-14.1050	H	0	7.7360	-3.4680	-6.0570	H	0
8.6390	1.6780	-28.8260	C	0	15.0710	-1.2250	-16.4260	S	0	7.7940	-3.0030	-3.9210	C	0
9.6670	1.7120	-29.1860	H	0	13.2350	1.4870	-13.8240	C	0	6.9720	-3.6730	-3.6690	H	0
8.7540	1.0240	-27.9630	H	0	13.8680	2.5150	-13.8400	O	0	8.7630	-3.4980	-3.8540	H	0
7.6330	1.0170	-29.7380	C	0	12.4520	1.1600	-12.7910	N	0	7.7180	-1.7960	-2.9430	C	0
6.7260	1.6460	-30.3050	O	0	12.4390	1.9470	-11.5910	C	0	8.5230	-1.0890	-3.1460	H	0
7.7670	-0.1950	-29.9740	O	0	12.2940	2.9940	-11.8560	H	0	6.7600	-1.3200	-3.1520	H	0
9.5960	3.7870	-27.6810	C	0	13.3780	1.8290	-11.0500	H	0	7.5330	-2.0790	-1.4000	C	0
10.6680	3.9540	-28.2980	O	0	11.1860	1.6150	-10.7610	C	0	7.0020	-3.0290	-1.4590	H	0
9.4580	4.1980	-26.4160	N	0	10.3970	2.3270	-11.0030	H	0	8.4940	-2.3040	-0.9390	H	0
8.5230	3.9670	-26.1120	H	0	11.3520	1.4840	-9.6910	H	0	6.8670	-0.9830	-0.6660	C	0
10.5050	4.2650	-25.5020	C	0	10.8010	0.2540	-11.3190	C	0	6.9470	-1.1770	0.4030	H	0
11.4170	4.6210	-25.9810	H	0	9.7280	0.0700	-11.2610	H	0	7.2920	0.0070	-0.8280	H	0
10.2260	5.0710	-24.2610	C	0	11.2900	-0.4870	-10.6860	H	0	5.4360	-0.7400	-0.9610	N	0
9.4690	4.6600	-23.5930	H	0	11.4010	0.1350	-12.6590	C	0	5.2750	-0.2910	-1.8510	H	0
11.4690	5.3080	-23.4030	C	0	11.8640	-0.8440	-12.7810	H	0	4.7740	-1.4960	-0.8550	H	0
12.2060	5.8920	-23.9540	H	0	10.3310	0.3670	-13.7270	C	0	5.0700	-0.0430	-0.3280	H	0

6.4060	-2.0320	-5.7950	C	0	8.8570	-4.9610	7.6660	H	0	16.4040	-2.8600	13.1870	O	0
6.3290	-0.9300	-6.3180	O	0	8.2510	-4.3870	9.2640	H	0	16.3700	-3.5450	12.5150	H	0
5.3000	-2.6570	-5.4770	N	0	7.1140	-4.7690	8.0710	H	0	17.8390	-0.7570	14.3470	C	0
5.4620	-3.4420	-4.8630	H	0	9.6520	-2.3850	8.4770	C	0	18.8430	-0.3190	13.8970	O	0
3.9290	-2.1080	-5.5040	C	0	10.5680	-2.0460	7.7030	O	0	16.7120	-0.0340	14.3620	N	0
3.8800	-1.0610	-5.8050	H	0	9.6730	-2.3860	9.8480	N	0	15.8090	-0.3340	14.6980	H	0
2.9670	-2.9360	-6.3890	C	0	8.8560	-2.7690	10.3020	H	0	16.6480	1.2450	13.6600	C	0
3.4530	-3.0390	-7.3590	H	0	10.6710	-1.6940	10.6390	C	0	15.8070	1.8050	14.0680	H	0
2.7870	-3.9220	-5.9610	H	0	11.6440	-1.8440	10.1710	H	0	17.5540	1.7940	13.9170	H	0
1.6600	-2.2320	-6.7850	C	0	10.2330	-0.2590	10.8610	C	0	16.4560	1.1750	12.0960	C	0
0.7960	-2.8380	-7.4050	O	0	10.0530	0.2930	9.9380	H	0	16.6340	2.2370	11.4980	O	0
1.5490	-1.0380	-6.4980	O	0	9.1980	-0.3300	11.1970	H	0	16.2880	-0.0770	11.6210	N	0
3.4150	-2.0910	-4.0270	C	0	11.0220	0.6950	11.7630	C	0	16.3250	-0.8180	12.3060	H	0
4.1670	-2.3310	-3.0550	O	0	12.2490	1.1860	11.3420	C	0	16.3660	-0.3880	10.2090	C	0
2.0820	-1.7840	-3.8600	N	0	12.5590	0.8820	10.3530	H	0	16.6430	0.4970	9.6360	H	0
1.6120	-1.5900	-4.7330	H	0	13.0380	1.9930	12.1820	C	0	17.5610	-1.3960	9.9700	C	0
1.4650	-1.4850	-2.5680	C	0	13.9860	2.3480	11.8080	H	0	17.2500	-2.3260	10.4440	H	0
2.0310	-0.6480	-2.1580	H	0	12.4830	2.3960	13.3960	C	0	17.4490	-1.6550	8.9170	H	0
0.0050	-0.9540	-2.7010	C	0	13.1080	3.0370	14.0000	H	0	18.9770	-1.0470	10.2940	C	0
-0.4780	-0.7680	-1.7410	H	0	11.2450	1.9110	13.9120	C	0	19.0450	-0.9750	11.3800	H	0
-0.2190	0.0040	-3.1700	H	0	10.9310	2.2870	14.8750	H	0	19.9270	-2.1100	9.9480	C	0
-0.8950	-1.9690	-3.4930	C	0	10.4870	1.0770	12.9910	C	0	20.9020	-1.6580	10.1290	H	0
-1.9320	-1.6350	-3.5420	H	0	9.5410	0.6110	13.2260	H	0	19.7670	-3.0370	10.4980	H	0
-0.5080	-2.2030	-4.4850	H	0	10.8730	-2.3360	12.0010	C	0	19.9010	-2.2800	8.8710	H	0
-1.0440	-3.4080	-2.9100	C	0	10.1350	-3.2710	12.3010	O	0	19.4030	0.2540	9.5510	C	0
-1.2820	-3.5360	-1.7250	O	0	11.8990	-2.0000	12.7680	N	0	19.3660	0.1750	8.4640	H	0
-1.1950	-4.5170	-3.6240	N	0	12.5480	-1.3300	12.3810	H	0	18.7770	1.0610	9.9330	H	0
-1.0650	-5.3310	-3.0410	H	0	12.1620	-2.4900	14.1510	C	0	20.4280	0.4820	9.8420	H	0
-1.0050	-4.4720	-4.6150	H	0	11.1720	-2.8440	14.4400	H	0	14.9730	-0.8070	9.6670	C	0
1.6530	-2.4720	-1.3760	C	0	13.0700	-3.7030	14.2620	C	0	13.9590	-1.0620	10.3050	O	0
1.0080	-2.1840	-0.3620	O	0	12.5770	-4.4550	13.6450	H	0	14.9190	-0.9250	8.3250	N	0
2.3800	-3.5570	-1.4800	N	0	14.0420	-3.4100	13.8660	H	0	15.7530	-0.8380	7.7610	H	0
2.8980	-3.6990	-2.3350	H	0	13.2280	-4.1370	15.6060	O	0	13.7080	-1.1600	7.5400	C	0
2.7470	-4.4240	-0.3420	C	0	13.2920	-5.0950	15.5750	H	0	12.9040	-1.1550	8.2760	H	0
1.8800	-4.5250	0.3110	H	0	12.7760	-1.3810	14.9850	C	0	13.4770	0.0760	6.6590	C	0
3.2330	-5.8100	-0.7060	C	0	13.8960	-0.9390	14.7080	O	0	14.3810	0.2460	6.0740	H	0
3.4070	-6.4030	0.1920	H	0	12.1570	-1.0890	16.1780	N	0	12.6590	-0.1050	5.9610	H	0
2.4320	-6.4740	-1.0290	H	0	10.7400	-1.1580	16.4320	C	0	13.2060	1.2740	7.4700	C	0
4.4800	-5.8000	-1.6740	C	0	10.4670	-2.0370	17.0160	H	0	14.2240	2.1860	7.8840	C	0
4.9030	-4.7990	-1.5810	H	0	10.1290	-1.0890	15.5320	H	0	15.2730	2.0280	7.6830	H	0
5.2830	-6.4970	-1.4360	H	0	10.5270	0.0070	17.3760	C	0	13.8480	3.2930	8.6950	C	0
4.1490	-5.9270	-3.1570	C	0	9.7150	-0.1890	18.0770	H	0	14.6460	3.9180	9.0690	H	0
4.9140	-5.9150	-4.1220	O	0	10.3870	0.8900	16.7530	H	0	12.4940	3.5740	8.9680	C	0
2.9110	-6.0550	-3.4650	N	0	11.7870	0.0390	18.1820	C	0	12.1340	4.3150	9.6660	H	0
2.6330	-6.0820	-4.4350	H	0	11.8120	-0.7940	18.8840	H	0	11.4960	2.6430	8.4480	C	0
2.2610	-6.0220	-2.6930	H	0	11.8820	1.0220	18.6430	H	0	10.4420	2.8480	8.5630	H	0
3.6800	-3.8030	0.6290	C	0	12.8690	-0.2430	17.1450	C	0	11.8490	1.6050	7.6150	C	0
4.6740	-3.2320	0.2030	O	0	13.1280	0.6460	16.5700	H	0	11.0940	0.9750	7.1680	H	0
3.3500	-3.6180	1.9570	N	0	14.1230	-0.8160	17.7530	C	0	13.8300	-2.5110	6.8460	C	0
2.1780	-4.1350	2.6420	C	0	14.8730	0.0190	18.1700	O	0	14.9070	-2.9460	6.4270	O	0
2.2670	-5.2210	2.6110	H	0	14.4200	-2.1090	17.6330	N	0	12.6490	-3.1030	6.5310	N	0
1.2860	-3.7260	2.1680	H	0	13.7300	-2.6230	17.1030	H	0	11.7720	-2.7420	6.8790	H	0
2.2850	-3.6910	4.0170	C	0	15.6030	-2.8080	18.1520	C	0	12.6210	-4.4780	5.9860	C	0
2.7200	-4.4440	4.6740	H	0	15.7120	-2.3940	19.1540	H	0	13.6140	-4.6830	5.5850	H	0
1.2840	-3.5090	4.4080	H	0	15.4220	-4.3490	18.1530	C	0	12.4390	-5.4420	7.1330	C	0
3.0760	-2.4050	4.0040	C	0	15.4060	-4.7090	17.1240	H	0	11.4440	-5.2950	7.5540	H	0
3.7560	-2.3200	4.8520	H	0	16.3160	-4.7670	18.6170	H	0	12.4890	-6.4510	6.7240	H	0
2.4380	-1.5340	3.8510	H	0	14.3590	-4.7570	19.1050	C	0	13.4430	-5.4100	8.2800	C	0
3.9500	-2.5290	2.8040	C	0	14.6390	-4.4770	20.1200	H	0	14.7070	-5.9650	8.0290	C	0
3.9580	-1.5720	2.2840	H	0	13.4000	-4.3500	18.7860	H	0	14.9450	-6.3720	7.0580	H	0
5.3640	-2.8880	3.1480	C	0	14.1570	-6.2180	19.1620	C	0	15.6660	-5.9670	9.1170	C	0
5.6630	-4.0870	3.1500	O	0	14.2470	-6.9320	18.1620	O	0	16.5370	-6.5950	8.9970	H	0
6.2120	-1.9050	3.4250	N	0	13.8350	-6.8450	20.3120	N	0	15.3620	-5.2970	10.3310	C	0
5.8630	-0.9590	3.4880	H	0	13.4090	-7.7430	20.1300	H	0	16.2740	-5.1650	11.2960	O	0
7.4940	-2.1860	4.1070	C	0	13.5440	-6.3390	21.1360	H	0	16.8180	-5.9410	11.4500	H	0
7.9240	-3.1170	3.7370	H	0	16.8610	-2.4560	17.2730	C	0	14.0800	-4.7500	10.5010	C	0
8.4800	-1.0990	3.6060	C	0	17.9490	-2.1010	17.8460	O	0	13.7840	-4.2530	11.4130	H	0
8.4660	-1.0770	2.5160	H	0	16.6580	-2.4090	15.9770	N	0	13.1330	-4.9230	9.5280	C	0
8.1280	-0.1690	4.0530	H	0	15.7520	-2.6630	15.6090	H	0	12.1650	-4.4970	9.7450	H	0
9.4980	-1.0900	3.9940	H	0	17.7880	-2.1480	14.9890	C	0	11.5790	-4.5420	4.8820	C	0
7.2340	-2.1710	5.6450	C	0	18.7270	-2.4110	15.4770	H	0	10.4550	-4.1800	5.2120	O	0
6.1540	-1.7000	6.0350	O	0	17.5930	-3.1120	13.8440	C	0	12.0300	-4.6980	3.6630	N	0
8.2410	-2.5890	6.4390	N	0	18.3310	-3.0690	13.0430	H	0	12.9680	-5.0350	3.5030	H	0
9.0690	-2.9080	5.9580	H	0	17.5870	-4.5940	14.3250	C	0	11.3420	-4.1450	2.4970	C	0
8.2970	-2.8210	7.8730	C	0	16.9420	-5.2560	13.7470	H	0	10.3530	-3.8230	2.8240	H	0
7.5110	-2.1970	8.2960	H	0	18.5550	-5.0950	14.3550	H	0	11.9740	-2.8790	1.9260	C	0
8.1150	-4.3520	8.1830	C	0	17.1590	-4.7130	15.3200	H	0	12.8980	-3.1710	1.4260	H	0

11.0920	-2.1950	0.9120	C	0	7.6040	-7.1070	-11.4460	C	0	4.4770	3.7650	-29.6340	H	0
10.1020	-1.9970	1.3220	H	0	7.9730	-6.1760	-11.0170	H	0	2.6460	2.6970	-29.9780	C	0
11.5070	-1.2160	0.6710	H	0	7.1260	-6.9760	-12.4180	H	0	2.0200	3.3150	-30.8750	O	0
11.0210	-2.7920	0.0030	H	0	6.8890	-7.5470	-10.7510	H	0	2.4970	1.4640	-29.9030	O	0
12.2850	-1.8140	2.9810	C	0	11.1930	-4.2390	-14.5390	C	0	3.1160	4.5490	-26.1160	C	0
11.4110	-1.4620	3.5280	H	0	11.2180	-3.2640	-13.8570	O	0	2.1450	4.0010	-25.5260	O	0
13.1190	-2.2250	3.5490	H	0	11.2280	-4.2300	-15.8400	N	0	3.1430	5.9120	-26.1750	N	0
12.7290	-0.9660	2.4590	H	0	11.2250	-5.1290	-16.3010	H	0	3.9670	6.4090	-26.4820	H	0
11.1360	-5.2710	1.4890	C	0	11.4720	-3.0920	-16.7930	C	0	1.9720	6.7350	-25.7120	C	0
12.1880	-5.8920	1.1410	O	0	11.2630	-2.1030	-16.3860	H	0	1.6380	6.3410	-24.7520	H	0
9.8960	-5.6280	0.9800	N	0	12.9150	-3.1690	-17.3260	C	0	2.1060	7.8130	-25.6330	H	0
8.6130	-5.0160	1.4260	C	0	12.9920	-4.1430	-17.8090	H	0	0.8250	6.6680	-26.6940	C	0
8.6290	-3.9330	1.3020	H	0	12.9560	-2.2830	-17.9590	H	0	1.1080	6.6870	-27.8840	O	0
8.4280	-5.2980	2.4620	H	0	14.2980	-3.0980	-16.1160	S	0	-0.3870	6.6400	-26.2620	N	0
7.5080	-5.6310	0.5520	C	0	10.6220	-3.2060	-18.0240	C	0	-0.5230	6.9490	-25.3110	H	0
7.0920	-4.8970	-0.1380	H	0	10.0330	-4.2960	-18.2550	O	0	-1.5910	6.5250	-27.0880	C	0
6.6100	-5.9840	1.0590	H	0	10.4540	-2.0880	-18.7730	N	0	-1.2920	6.6160	-28.1320	H	0
8.1740	-6.8430	-0.1700	C	0	10.9680	-1.2650	-18.4920	H	0	-2.1650	5.0780	-26.8770	C	0
7.8900	-6.8800	-1.2210	H	0	9.4070	-2.0400	-19.8950	C	0	-2.1710	4.9020	-25.8020	H	0
8.0840	-7.6970	0.5010	H	0	9.2010	-3.0630	-20.2090	H	0	-3.6370	4.9260	-27.3400	C	0
9.6560	-6.4910	-0.1560	C	0	8.1310	-1.5920	-19.2000	C	0	-4.1590	4.0880	-26.8790	H	0
10.2780	-7.3830	-0.0920	H	0	7.2510	-1.8180	-19.8030	H	0	-4.2820	5.7690	-27.0940	H	0
10.0760	-5.6860	-1.4320	C	0	8.1200	-2.0700	-18.2200	H	0	-3.7290	4.8870	-28.4250	H	0
9.6600	-4.5340	-1.4810	O	0	7.9680	-0.0630	-18.8290	C	0	-1.3130	3.9670	-27.5350	C	0
10.8420	-6.3230	-2.3060	N	0	8.7360	0.1770	-18.0940	H	0	-1.1920	4.0930	-28.6110	H	0
11.2710	-7.2130	-2.1000	H	0	8.0810	0.4950	-19.7590	H	0	-0.3150	3.8980	-27.1020	H	0
11.1140	-5.7180	-3.6930	C	0	6.4610	0.2950	-18.0340	S	0	-1.7010	2.9590	-27.3860	H	0
10.5120	-4.8330	-3.9020	H	0	6.2250	2.0380	-18.4880	C	0	-2.5850	7.6970	-26.7540	C	0
12.5920	-5.1680	-3.8590	C	0	5.1500	2.1670	-18.3640	H	0	-2.8220	7.9440	-25.5740	O	0
12.6040	-4.6440	-4.8150	H	0	6.7190	2.7470	-17.8230	H	0	-3.2500	8.2430	-27.7830	N	0
13.1320	-4.4120	-2.6760	C	0	6.2930	2.1650	-19.5690	H	0	-3.0190	7.9920	-28.7340	H	0
14.1770	-4.1970	-2.9020	H	0	9.6250	-1.1570	-21.1600	C	0	-4.1370	9.3480	-27.5090	C	0
12.5370	-3.5030	-2.5960	H	0	10.3500	-0.1760	-21.1660	O	0	-3.6980	10.1760	-26.9520	H	0
13.0350	-4.9670	-1.7430	H	0	8.9500	-1.5170	-22.2620	N	0	-4.4940	10.0400	-28.8230	C	0
13.4990	-6.1820	-4.1330	O	0	8.3170	-2.2980	-22.1610	H	0	-3.6580	10.0650	-29.5210	H	0
13.5520	-6.8000	-3.4000	H	0	8.7260	-0.6600	-23.4450	C	0	-5.2200	9.3780	-29.2960	H	0
10.8800	-6.5940	-4.8930	C	0	9.5560	0.0440	-23.5190	H	0	-5.1520	11.4030	-28.6750	C	0
10.9280	-7.8120	-4.7340	O	0	8.6440	-1.4540	-24.7250	C	0	-5.7740	11.6400	-29.5390	H	0
10.5810	-6.0090	-6.0250	N	0	7.7690	-2.0830	-24.5610	H	0	-5.7540	11.4540	-27.7690	H	0
10.5810	-4.9990	-5.9880	H	0	8.4730	-0.8750	-25.6330	H	0	-4.0630	12.4510	-28.5160	C	0
10.4020	-6.7490	-7.3190	C	0	9.8990	-2.3650	-24.8250	C	0	-3.5050	12.8260	-29.5760	O	0
10.5520	-7.8240	-7.2180	H	0	11.0030	-2.0930	-24.3930	O	0	-3.9330	13.0550	-27.4470	O	0
8.9230	-6.5070	-7.7330	C	0	9.7360	-3.5700	-25.3260	N	0	-5.4090	8.8900	-26.7620	C	0
8.7030	-5.4890	-8.0540	H	0	10.5830	-4.1190	-25.2870	H	0	-6.2780	8.1140	-27.2160	O	0
8.7340	-7.1350	-8.6040	H	0	8.9260	-3.8740	-25.8470	H	0	-5.5830	9.4220	-25.5520	N	0
7.9230	-6.9020	-6.6040	C	0	7.4480	0.1570	-23.2370	C	0	-4.9150	10.1600	-25.3840	H	0
8.1860	-7.9180	-5.9890	O	0	6.5490	-0.3360	-22.5980	O	0	-6.7180	9.2030	-24.6540	C	0
7.0530	-5.9950	-6.2800	N	0	7.2710	1.3710	-23.7820	N	0	-7.2710	8.2840	-24.8480	H	0
6.3730	-6.1370	-5.5470	H	0	8.0950	1.7930	-24.1850	H	0	-6.1170	8.9880	-23.2490	C	0
6.9450	-5.2640	-6.9690	H	0	5.9950	2.2040	-23.6830	C	0	-5.4930	8.0960	-23.2860	H	0
11.3850	-6.1380	-8.3450	C	0	5.1300	1.5500	-23.5770	H	0	-5.5020	9.8130	-22.8910	H	0
11.6680	-4.8760	-8.3240	O	0	6.1350	3.0760	-22.5410	C	0	-6.8880	8.8600	-22.4890	H	0
11.8410	-6.9640	-9.3240	N	0	6.3550	2.4950	-21.6450	H	0	-7.8190	10.4030	-24.7440	C	0
11.4630	-7.9000	-9.2890	H	0	7.0350	3.6860	-22.6200	H	0	-7.4430	11.5650	-24.6570	O	0
12.7970	-6.5890	-10.3600	C	0	4.9870	3.9540	-22.2040	C	0	-9.0700	10.1520	-24.9510	N	0
13.0350	-5.5260	-10.3520	H	0	4.6980	5.1000	-22.9720	C	0	-9.3570	9.1960	-25.1040	H	0
14.1100	-7.4040	-10.0830	C	0	5.3580	5.3380	-23.7940	H	0	-10.1530	11.1000	-24.6300	C	0
14.3820	-7.3070	-9.0320	H	0	3.6320	5.9610	-22.7150	C	0	-9.6890	12.0160	-24.2640	H	0
13.8070	-8.4390	-10.2370	H	0	3.4520	6.8520	-23.2990	H	0	-10.9370	11.5850	-25.8330	C	0
15.2710	-6.9140	-10.9110	C	0	2.6790	5.5490	-21.7870	C	0	-11.5170	10.7170	-26.1490	H	0
15.4720	-5.7110	-10.9620	O	0	1.5720	6.3520	-21.5820	O	0	-11.8610	12.7570	-25.6140	C	0
15.9650	-7.8460	-11.5300	N	0	1.1050	6.5710	-22.3920	H	0	-12.4820	12.8140	-26.5090	H	0
16.7380	-7.5760	-12.1200	H	0	3.0000	4.4230	-20.9320	C	0	-12.5680	12.5400	-24.8130	H	0
15.6080	-8.7900	-11.5120	H	0	2.4600	4.2490	-20.0130	H	0	-11.3280	13.7050	-25.5360	H	0
12.2640	-6.6960	-11.8360	C	0	4.1420	3.6220	-21.1060	C	0	-10.0230	11.8430	-26.8860	O	0
12.4790	-7.7690	-12.4330	O	0	4.3520	2.7600	-20.4910	H	0	-9.4990	11.0390	-26.9120	H	0
11.5220	-5.6770	-12.3000	N	0	5.9480	3.0160	-24.9470	C	0	-10.9560	10.7280	-23.3630	C	0
11.3770	-4.8110	-11.8000	H	0	6.9070	3.7380	-25.3230	O	0	-11.2740	9.5360	-23.1460	O	0
11.0700	-5.6520	-13.8120	C	0	4.8060	2.9560	-25.6460	N	0	-11.1170	11.6880	-22.4970	N	0
11.6720	-6.3510	-14.3920	H	0	4.2270	2.1910	-25.3300	H	0	-10.7140	12.6070	-22.6180	H	0
9.6420	-6.1850	-13.9660	C	0	4.3060	3.7530	-26.7100	C	0	-11.9230	11.5540	-21.2670	C	0
8.8770	-5.6180	-13.4350	H	0	5.1050	4.4460	-26.9710	H	0	-11.6270	10.6300	-20.7700	H	0
9.4110	-6.0010	-15.0150	H	0	3.9450	2.8380	-27.8390	C	0	-11.7750	12.7140	-20.2410	C	0
9.5580	-7.7120	-13.6270	C	0	4.7890	2.1550	-27.9330	H	0	-10.7310	12.9320	-20.0160	H	0
8.7260	-8.1190	-14.2020	H	0	3.1520	2.1900	-27.4670	H	0	-12.1420	13.6100	-20.7400	H	0
10.4440	-8.3030	-13.8610	H	0	3.5460	3.5650	-29.1030	C	0	-12.5480	12.4730	-18.9120	C	0
9.0680	-8.2130	-11.8910	S	0	2.9240	4.4310	-28.8750	H	0	-12.0240	11.5970	-17.9020	C	0

-11.1400	11.0230	-18.1390	H	0	-8.3690	11.1050	-20.8010	C	0	4.6650	-5.2750	-22.6170	H	0
-12.7440	11.3350	-16.7470	C	0	-8.4620	11.3400	-21.8510	H	0	6.1670	-4.9630	-24.2490	C	0
-12.2600	10.6020	-16.1180	H	0	-7.8720	11.9800	-19.7820	C	0	5.4250	-4.7790	-25.0260	H	0
-13.9210	12.0550	-16.4870	C	0	-7.5150	13.2660	-20.1080	O	0	6.9760	-4.2540	-24.4290	H	0
-14.5440	11.7860	-15.3430	O	0	-7.5580	13.4200	-21.0550	H	0	6.6150	-6.3880	-24.3610	C	0
-14.2210	10.9860	-14.9210	H	0	-7.7860	11.5300	-18.4640	C	0	7.1270	-6.6900	-23.4470	H	0
-14.4750	12.9170	-17.4810	C	0	-7.3100	12.2040	-17.7680	H	0	5.4520	-7.2580	-24.7180	C	0
-15.4240	13.3740	-17.2420	H	0	-8.2140	10.2580	-18.1420	C	0	4.8450	-6.9690	-25.5750	H	0
-13.7480	13.1800	-18.6470	C	0	-8.2840	9.9210	-17.1180	H	0	5.7630	-8.2780	-24.9430	H	0
-14.2900	13.7700	-19.3720	H	0	-6.9410	6.5070	-19.4160	C	0	4.6850	-7.3190	-23.9450	H	0
-13.3850	11.4210	-21.5470	C	0	-6.2640	7.3500	-18.7910	O	0	7.6240	-6.6180	-25.4670	C	0
-14.0570	12.1970	-22.1460	O	0	-6.4240	5.3790	-20.0250	N	0	7.2150	-6.1910	-26.3830	H	0
-13.9430	10.3750	-21.0240	N	0	-7.0450	4.8470	-20.6170	H	0	8.6060	-6.2020	-25.2440	H	0
-13.2770	9.6940	-20.6870	H	0	-5.0680	4.9860	-19.6950	C	0	7.7840	-7.6820	-25.6410	H	0
-15.3920	10.0550	-20.8910	C	0	-4.7770	5.1480	-18.6570	H	0	6.5140	-4.6420	-21.7750	C	0
-15.9100	11.0140	-20.8810	H	0	-4.8620	3.5250	-19.9970	C	0	7.4470	-3.8670	-21.7470	O	0
-15.8270	9.2370	-22.1620	C	0	-5.2090	3.2910	-21.0040	H	0	6.2950	-5.5810	-20.7960	N	0
-15.1680	8.3800	-22.2990	H	0	-3.4140	3.0050	-19.8030	C	0	5.4940	-6.1940	-20.8190	H	0
-17.3560	8.8530	-22.2220	C	0	-3.4970	1.9230	-19.7070	H	0	7.2480	-5.7120	-19.6600	C	0
-17.9250	9.7830	-22.1980	H	0	-2.6910	3.3040	-20.5620	H	0	7.9130	-4.8520	-19.5870	H	0
-17.4510	8.2290	-23.1110	H	0	-3.0480	3.3780	-18.8460	H	0	6.5460	-5.7700	-18.2770	C	0
-17.6390	8.1890	-21.4060	H	0	-5.9180	2.7450	-19.2370	C	0	6.0730	-6.7450	-18.1620	H	0
-15.6520	10.0910	-23.2250	O	0	-6.8880	2.8970	-19.7090	H	0	7.2670	-5.6800	-17.4640	H	0
-14.9430	10.7000	-23.0070	H	0	-5.7280	1.6800	-19.3660	H	0	5.6170	-4.5880	-18.0470	C	0
-15.6370	9.3000	-19.6260	C	0	-5.9980	3.0280	-18.1880	H	0	6.3050	-3.7450	-17.9770	H	0
-14.8370	8.4340	-19.2830	O	0	-4.0990	5.8600	-20.5030	C	0	4.9590	-4.4870	-18.9110	H	0
-16.5930	9.6840	-18.8000	N	0	-3.3340	6.6460	-20.0310	O	0	4.5850	-4.7220	-16.5710	S	0
-17.1420	10.4720	-19.1150	H	0	-4.1050	5.6230	-21.8130	N	0	3.4440	-3.3640	-17.0670	C	0
-16.9310	9.0160	-17.5510	C	0	-4.8110	4.9480	-22.0700	H	0	2.5070	-3.8760	-17.2880	H	0
-16.0940	8.9460	-16.8550	H	0	-3.1930	6.2180	-22.8260	C	0	3.3710	-2.7000	-16.2060	H	0
-18.0290	9.8900	-16.8320	C	0	-3.7240	6.2250	-23.7770	H	0	3.8550	-2.7610	-17.8770	H	0
-18.3030	9.5800	-15.8230	H	0	-2.8840	7.2150	-22.5090	H	0	8.1200	-6.9980	-19.7380	C	0
-17.5760	10.8750	-16.7110	H	0	-1.8700	5.4550	-23.0910	C	0	7.8240	-8.0440	-20.3270	O	0
-19.0140	9.9050	-17.2980	H	0	-0.8480	6.0770	-23.3810	O	0	9.2190	-6.9310	-19.0450	N	0
-17.4380	7.5260	-17.7280	C	0	-1.9570	4.1160	-23.1130	N	0	9.4930	-6.0500	-18.6350	H	0
-17.9640	7.0500	-18.7910	O	0	-2.8510	3.6950	-22.9040	H	0	10.1500	-8.0720	-18.8810	C	0
-17.1020	6.7560	-16.6970	N	0	-0.6970	3.4010	-23.2640	C	0	9.7090	-9.0670	-18.9380	H	0
-16.5280	7.1800	-15.9820	H	0	-0.0780	4.0510	-23.8820	H	0	11.1520	-8.0920	-20.1770	C	0
-17.3300	5.2910	-16.6290	C	0	0.0190	3.2980	-21.9420	C	0	12.0500	-8.6330	-19.8790	H	0
-17.0830	4.9810	-15.6140	H	0	-0.3900	2.4050	-21.4700	H	0	10.6080	-8.4900	-21.0330	H	0
-18.3890	5.1510	-16.8470	H	0	1.0960	3.1650	-22.0460	H	0	11.4960	-6.7130	-20.7350	C	0
-16.4900	4.4160	-17.6440	C	0	-0.0900	4.1490	-21.2690	H	0	12.5390	-5.8930	-20.2670	C	0
-16.8390	3.2200	-17.8780	O	0	-0.6590	2.0730	-23.8710	C	0	13.2430	-6.4580	-19.6740	H	0
-15.4680	4.9110	-18.2690	N	0	-1.4930	1.2080	-23.6650	O	0	12.7500	-4.6450	-20.6750	C	0
-15.1160	5.8050	-17.9590	H	0	0.4800	1.7770	-24.5360	N	0	13.6800	-4.1670	-20.4050	H	0
-14.6750	4.2730	-19.3810	C	0	1.1110	2.5380	-24.7410	H	0	11.8520	-3.9890	-21.6630	C	0
-14.7970	3.1920	-19.3170	H	0	0.8100	0.4380	-25.0750	C	0	12.1220	-2.7940	-22.2220	O	0
-15.3310	4.8370	-20.6840	C	0	0.1510	-0.3330	-24.6770	H	0	11.4210	-2.6010	-22.8490	H	0
-14.7160	4.4860	-21.5130	H	0	0.6570	0.4860	-26.6580	C	0	10.8590	-4.8270	-22.1250	C	0
-16.3990	4.6330	-20.7590	H	0	-0.3790	0.7020	-26.9170	H	0	10.1780	-4.4190	-22.8570	H	0
-15.3740	5.9260	-20.6600	H	0	1.3840	1.2070	-27.0330	H	0	10.6810	-6.1590	-21.7300	C	0
-13.1360	4.5190	-19.1580	C	0	1.1060	-0.8860	-27.2880	C	0	9.8470	-6.7000	-22.1530	H	0
-12.7880	5.7000	-18.8520	O	0	1.0930	-1.9040	-26.6430	O	0	10.9010	-7.9560	-17.4840	C	0
-12.2030	3.5490	-19.2940	N	0	1.5370	-0.9100	-28.5700	N	0	10.5850	-7.0900	-16.7070	O	0
-12.4290	2.1690	-19.8050	C	0	2.0750	-1.6730	-28.9570	H	0	11.8030	-8.9420	-17.2720	N	0
-13.2350	2.0780	-20.5330	H	0	1.6870	-0.0140	-29.0110	H	0	12.0040	-9.6460	-17.9670	H	0
-12.6620	1.5440	-18.9430	H	0	2.2210	0.1470	-24.5910	C	0	12.7140	-8.8980	-16.0650	C	0
-11.0350	1.6780	-20.2900	C	0	3.1950	0.8680	-24.8020	O	0	11.9820	-9.0150	-15.2660	H	0
-10.8520	2.0700	-21.2910	H	0	2.3160	-1.0290	-23.9120	N	0	13.5870	-10.1490	-15.9500	C	0
-11.0460	0.5880	-20.3020	H	0	1.4730	-1.5800	-23.8390	H	0	13.9620	-10.1570	-14.9270	H	0
-10.1700	2.2780	-19.2450	C	0	3.4180	-1.4710	-23.0720	C	0	13.0530	-11.0970	-16.0090	H	0
-9.1320	2.4790	-19.5110	H	0	4.3300	-0.9280	-23.3210	H	0	14.5670	-10.1530	-16.9750	O	0
-10.2780	1.6090	-18.3910	H	0	3.1350	-1.1580	-21.5250	C	0	15.3000	-10.6850	-16.6560	H	0
-10.7910	3.6460	-18.9550	C	0	2.1390	-1.4450	-21.1880	H	0	13.6380	-7.5990	-16.0710	C	0
-10.8450	3.8360	-17.8830	H	0	4.0360	-1.7080	-20.4810	C	0	13.6910	-6.8030	-17.0770	O	0
-10.1070	4.7720	-19.6890	C	0	4.0000	-1.1520	-19.5440	H	0	14.3180	-7.4000	-14.9360	N	0
-10.3290	4.9360	-20.8690	O	0	3.8560	-2.7780	-20.3740	H	0	14.1300	-7.9930	-14.1400	H	0
-9.1250	5.4810	-19.0940	N	0	5.0400	-1.6290	-20.8990	H	0	15.3190	-6.3460	-14.5790	C	0
-9.0160	5.3340	-18.1010	H	0	3.1360	0.3540	-21.3670	C	0	14.8620	-5.3580	-14.5180	H	0
-8.4800	6.6770	-19.5690	C	0	4.0840	0.8330	-21.6120	H	0	15.7340	-6.4500	-13.5760	H	0
-8.7530	6.8220	-20.6150	H	0	2.4750	0.8280	-22.0920	H	0	16.5450	-6.0900	-15.5130	C	0
-9.0540	7.9000	-18.7860	C	0	2.8290	0.5770	-20.3450	H	0	16.8290	-6.7850	-16.4960	O	0
-10.1440	7.8780	-18.8100	H	0	3.7780	-2.9390	-23.3180	C	0	17.0760	-4.9090	-15.2270	N	0
-8.7540	7.7130	-17.7550	H	0	2.9020	-3.6920	-23.8040	O	0	16.8070	-4.5680	-14.3160	H	0
-8.5810	9.3200	-19.1590	C	0	4.9610	-3.2700	-22.8880	N	0	18.2620	-4.4110	-15.9860	C	0
-8.7300	9.7770	-20.4860	C	0	5.6660	-2.5650	-22.7250	H	0	18.2770	-3.3360	-15.8020	H	0
-8.9400	9.1360	-21.3300	H	0	5.4940	-4.6340	-22.9160	C	0	19.5510	-5.1530	-15.3830	C	0



19.4580	-5.1450	-14.2970	H	0	19.6900	-14.7030	-16.1840	O	0	11.4020	-7.3310	4.6050	H	0
19.5670	-6.1640	-15.7890	H	0	16.7590	-13.7450	-12.8960	C	0	11.8980	-8.6360	2.9330	C	0
20.8030	-4.4230	-15.5600	C	0	16.3000	-14.9050	-12.8120	O	0	11.5050	-7.9730	2.1770	H	0
21.0020	-3.1370	-15.1380	N	0	16.5740	-12.7030	-12.1130	N	0	14.8270	-8.9210	0.8610	C	0
22.2430	-2.8280	-15.6220	C	0	16.9550	-11.7980	-12.3460	H	0	15.8380	-9.6420	0.7370	O	0
22.7270	-1.8660	-15.5400	H	0	15.5930	-12.7660	-11.0210	C	0	14.8470	-7.6820	1.3840	N	0
22.6950	-3.8800	-16.3480	N	0	15.1520	-13.7600	-10.9510	H	0	14.0040	-7.1260	1.4080	H	0
23.6290	-3.9500	-16.7250	H	0	16.3250	-12.5740	-9.6220	C	0	16.0000	-6.8760	1.7450	C	0
21.8600	-4.8990	-16.2690	C	0	15.6020	-12.7750	-8.8320	H	0	16.7860	-7.6190	1.8810	H	0
21.9110	-5.9000	-16.6700	H	0	17.0690	-13.3610	-9.4920	H	0	16.4480	-5.7880	0.7100	C	0
18.2190	-4.5010	-17.5600	C	0	16.8430	-11.2070	-9.3420	C	0	17.4780	-5.4650	0.8640	H	0
19.1030	-5.0440	-18.2920	O	0	18.1740	-10.9690	-9.7860	C	0	16.4770	-6.4320	-0.6570	C	0
17.0350	-4.0040	-18.0810	N	0	18.7100	-11.7300	-10.3330	H	0	15.4780	-6.6440	-1.0390	H	0
16.5200	-3.4670	-17.3980	H	0	18.7750	-9.7270	-9.5410	C	0	17.0890	-5.7200	-1.2100	H	0
16.5490	-4.2260	-19.4580	C	0	19.7930	-9.5230	-9.8380	H	0	16.9560	-7.4110	-0.6580	H	0
15.5420	-3.8100	-19.4350	H	0	18.1020	-8.8020	-8.6750	C	0	15.5550	-4.5510	0.7290	C	0
17.3060	-3.3460	-20.5060	C	0	18.7360	-7.6760	-8.4700	O	0	14.5180	-4.8800	0.6570	H	0
18.1510	-3.8930	-20.9240	H	0	19.2890	-7.4610	-9.2250	H	0	15.5240	-4.0840	1.7130	H	0
16.5900	-3.1490	-21.3050	H	0	16.8090	-9.0530	-8.1590	C	0	15.9530	-3.4110	-0.2870	C	0
17.6880	-1.8800	-19.9960	C	0	16.3340	-8.3800	-7.4610	H	0	16.9630	-3.0790	-0.0490	H	0
16.8580	-1.4210	-19.4600	H	0	16.1650	-10.2500	-8.4790	C	0	15.6070	-3.6950	-1.2810	H	0
18.5950	-1.9640	-19.3970	H	0	15.1830	-10.5370	-8.1340	H	0	15.3160	-2.5310	-0.1940	H	0
17.9070	-0.8480	-21.0780	C	0	14.5390	-11.6960	-11.0560	C	0	15.8540	-6.2400	3.1320	C	0
17.5810	-1.0580	-22.2760	O	0	14.6930	-10.6140	-11.5970	O	0	14.7730	-5.9860	3.6370	O	0
18.3530	0.3050	-20.8200	O	0	13.3700	-11.9240	-10.3170	N	0	17.0360	-5.9620	3.7850	N	0
16.3100	-5.6860	-19.9380	C	0	13.3290	-12.8140	-9.8410	H	0	17.9110	-6.2760	3.3900	H	0
16.7750	-6.0490	-20.9870	O	0	12.1080	-11.0600	-10.3190	C	0	17.0600	-4.8290	4.7930	C	0
15.5920	-6.5210	-19.1540	N	0	12.2850	-10.1360	-10.8700	H	0	16.0300	-4.6590	5.1080	H	0
15.2970	-6.2030	-18.2420	H	0	11.0240	-11.9200	-10.9170	C	0	17.7120	-5.3450	6.0260	C	0
15.4270	-8.0180	-19.4610	C	0	10.7890	-12.7890	-10.3030	H	0	17.1270	-6.1260	6.5110	H	0
14.7000	-8.3400	-18.7150	H	0	10.1310	-11.3090	-11.0460	H	0	18.6470	-5.8450	5.7750	H	0
14.9660	-8.3080	-20.4050	H	0	11.3020	-12.5200	-12.2700	C	0	18.0970	-4.0480	7.2380	S	0
16.6450	-8.8350	-19.2400	C	0	12.0090	-13.7790	-12.4030	C	0	16.9450	-3.3750	7.1790	H	0
16.5950	-9.9970	-19.6460	O	0	12.3480	-14.3200	-11.5310	H	0	17.7500	-3.5890	4.1590	C	0
17.7400	-8.2550	-18.7700	N	0	12.3590	-14.3720	-13.6610	C	0	18.5040	-3.6560	3.1600	O	0
17.7410	-7.2450	-18.7780	H	0	12.9480	-15.2760	-13.6780	H	0	17.3740	-2.4100	4.6780	N	0
19.0160	-9.0440	-18.6730	C	0	12.1180	-13.5780	-14.8350	C	0	16.6580	-2.3730	5.3900	H	0
19.0700	-9.8630	-19.3900	H	0	12.6910	-13.9180	-16.0110	O	0	17.7980	-1.0990	4.1030	C	0
20.2030	-8.0820	-19.0950	C	0	13.1850	-14.7350	-15.9160	H	0	18.7490	-1.1890	3.5770	H	0
20.2570	-7.2210	-18.4290	H	0	11.2320	-12.4360	-14.7260	C	0	16.7590	-0.4240	3.0850	C	0
21.1040	-8.6870	-19.0030	H	0	10.8140	-11.9390	-15.5890	H	0	16.3880	-1.2140	2.4310	H	0
20.1430	-7.6490	-20.6240	C	0	10.8640	-11.9260	-13.4620	C	0	15.8740	-0.0240	3.5790	H	0
19.3950	-6.8690	-20.7620	H	0	10.3850	-10.9590	-13.4860	H	0	17.2650	0.6590	2.1830	C	0
21.1270	-7.2650	-20.8950	H	0	11.7130	-10.4870	-8.9380	C	0	18.0270	0.3560	1.0200	C	0
19.6990	-8.7720	-21.5480	C	0	10.7630	-9.6670	-8.8370	O	0	18.1780	-0.6620	0.6910	H	0
20.3220	-9.6260	-21.2830	H	0	12.4240	-10.8900	-7.8620	N	0	18.6210	1.3260	0.1860	C	0
18.6410	-9.0260	-21.4830	H	0	13.1110	-11.6300	-7.8660	H	0	19.2960	1.1230	-0.6320	H	0
20.0270	-8.3130	-23.0120	C	0	12.1170	-10.3530	-6.5530	C	0	18.3300	2.6500	0.4480	C	0
19.4060	-7.4520	-23.2620	H	0	11.9010	-9.2870	-6.6220	H	0	18.6060	3.6230	-0.4040	O	0
21.0190	-7.8820	-23.1450	H	0	11.1620	-10.7420	-6.2000	H	0	18.4480	3.3670	-1.3160	H	0
19.8510	-9.5180	-23.8270	N	0	13.2720	-10.5270	-5.5630	C	0	17.4930	3.0190	1.5810	C	0
18.8680	-9.7360	-23.7500	H	0	14.2070	-11.2900	-5.8420	O	0	17.1220	4.0330	1.6090	H	0
20.1010	-9.3560	-24.7920	H	0	13.1870	-9.6870	-4.5890	N	0	16.9410	1.9880	2.3930	C	0
20.3190	-10.3460	-23.4860	H	0	12.4200	-9.0310	-4.5580	H	0	16.2620	2.2850	3.1790	H	0
19.2600	-9.7490	-17.3460	C	0	14.1020	-9.8510	-3.3870	C	0	17.8460	-0.0970	5.3210	C	0
19.9830	-10.7170	-17.2710	O	0	14.1400	-10.9320	-3.2570	H	0	16.9370	-0.0330	6.1980	O	0
18.5490	-9.2530	-16.3380	N	0	15.3960	-9.1840	-3.7240	C	0	18.8620	0.7660	5.3200	N	0
17.8050	-8.6070	-16.5600	H	0	16.2070	-9.6700	-3.1820	H	0	19.4660	0.7270	4.5110	H	0
18.5110	-10.0220	-15.0640	C	0	15.6770	-9.2700	-4.7740	H	0	19.0430	1.9090	6.2100	C	0
19.5730	-10.2200	-14.9220	H	0	15.4460	-8.1360	-3.4300	H	0	18.5670	1.8520	7.1890	H	0
17.9640	-9.1630	-13.8980	C	0	13.5300	-9.2190	-2.1450	C	0	20.5320	1.8740	6.5480	C	0
16.9280	-8.8330	-13.9760	H	0	13.1340	-8.0310	-2.1670	O	0	20.6800	0.8470	6.8830	H	0
18.1050	-9.7880	-13.0160	H	0	13.6800	-9.9830	-1.0630	N	0	21.0400	2.1380	5.6210	H	0
18.8110	-8.0170	-13.4890	C	0	14.0640	-10.9150	-1.1330	H	0	20.9630	2.7060	7.7330	C	0
20.0520	-8.1380	-13.5680	O	0	13.4430	-9.4120	0.2740	C	0	22.1300	2.7000	8.1270	O	0
18.1750	-7.0370	-13.0550	O	0	12.8610	-8.5210	0.0380	H	0	20.1270	3.4100	8.3270	O	0
17.8240	-11.4050	-15.1260	C	0	12.7460	-10.3460	1.1780	C	0	18.3970	3.1210	5.5660	C	0
16.9030	-11.6430	-15.9430	O	0	11.6820	-10.4350	0.9620	H	0	19.1300	3.8780	4.8480	O	0
18.2180	-12.2880	-14.1860	N	0	13.3220	-11.2720	1.2040	H	0	17.1270	3.3700	5.6280	N	0
19.1120	-12.0900	-13.7590	H	0	12.5910	-9.8140	2.6020	C	0	16.6530	2.8190	6.3300	H	0
17.7580	-13.6050	-14.0640	C	0	13.0810	-10.6570	3.6070	C	0	16.4590	4.4020	4.9100	C	0
17.2000	-13.9500	-14.9340	H	0	13.5610	-11.5180	3.1670	H	0	16.6240	4.3220	3.8270	H	0
18.8820	-14.5750	-13.9450	C	0	12.9080	-10.3430	4.8700	C	0	14.9600	4.2230	5.2570	C	0
19.3110	-14.5270	-12.9440	H	0	13.4490	-11.0420	5.4900	H	0	14.7000	3.1850	5.0500	H	0
18.5820	-15.6110	-14.1000	H	0	12.2420	-9.1490	5.2710	C	0	14.7870	4.4080	6.3180	H	0
19.9650	-14.3790	-15.0160	C	0	12.2360	-8.8230	6.3010	H	0	14.3770	4.9080	4.6430	H	0
20.9580	-13.7780	-14.7180	O	0	11.7990	-8.2830	4.2850	C	0	16.9760	5.8960	5.2390	C	0

17.1340	6.6980	4.3310	O	0	21.9200	-2.1180	-0.4230	H	0	16.6960	-12.9940	0.3460	C	0
17.2240	6.1090	6.5380	N	0	20.5850	-3.5530	0.2460	C	0	15.8340	-12.3560	0.5390	H	0
17.0520	5.4090	7.2460	H	0	21.3000	-4.1540	0.8070	H	0	16.1040	-14.3870	-0.0610	C	0
17.7440	7.3460	6.9720	C	0	19.6180	-3.4660	0.7420	H	0	15.8310	-15.0240	0.7810	H	0
17.0630	8.0960	6.5690	H	0	20.5560	-4.2110	-1.1750	C	0	15.1950	-14.2260	-0.6420	H	0
17.8360	7.3470	8.5390	C	0	21.5110	-4.0660	-1.6800	H	0	16.7720	-14.9540	-0.7090	H	0
16.8620	7.2370	9.0160	H	0	20.2370	-5.2260	-0.9380	H	0	17.4360	-13.2380	1.6860	C	0
18.4670	6.5090	8.8350	H	0	19.5720	-3.5870	-2.0520	N	0	17.9590	-14.1930	1.6300	H	0
18.4450	8.6910	9.0500	C	0	19.1130	-2.6940	-1.9420	H	0	18.1620	-12.4620	1.9280	H	0
19.3410	9.0350	8.5320	H	0	19.0520	-4.2190	-3.0970	C	0	16.5070	-13.2440	2.9490	C	0
17.3310	9.7310	8.7590	C	0	19.3710	-5.4620	-3.4010	N	0	15.5420	-13.7280	2.7990	H	0
16.3720	9.5040	9.2250	H	0	20.1470	-5.9220	-2.9470	H	0	17.0870	-13.7350	3.7300	H	0
17.6680	10.7410	8.9940	H	0	18.8500	-5.9640	-4.1060	H	0	16.3660	-12.2160	3.2830	H	0
17.2640	9.8360	7.6760	H	0	18.1070	-3.6670	-3.7540	N	0	17.0180	-12.5440	-2.1050	C	0
18.6270	8.6570	10.5800	C	0	17.7640	-2.7480	-3.5140	H	0	15.8180	-12.3610	-2.2080	O	0
17.7100	8.2390	10.9950	H	0	17.8840	-4.1650	-4.6040	H	0	17.7920	-12.8140	-3.1390	N	0
19.3700	7.9020	10.8380	H	0	21.9060	-2.1170	2.5230	C	0	18.7670	-12.8480	-2.8750	H	0
19.0800	9.5750	10.9540	H	0	23.0750	-1.8540	2.7040	O	0	17.3170	-12.8630	-4.5340	C	0
19.0910	7.5300	6.3070	C	0	21.2430	-3.0560	3.2420	N	0	16.7250	-11.9880	-4.8030	H	0
19.3240	8.6770	5.9240	O	0	20.2610	-3.2190	3.0720	H	0	18.5020	-13.0750	-5.4850	C	0
19.9790	6.5470	6.0790	N	0	21.9450	-3.8200	4.2400	C	0	18.9680	-13.9770	-5.0880	H	0
19.7950	5.6700	6.5440	H	0	22.9950	-3.5310	4.2990	H	0	18.2910	-13.2930	-6.5320	H	0
21.2780	6.7060	5.4720	C	0	21.3480	-3.5560	5.6250	C	0	19.4620	-11.9440	-5.7110	C	0
21.5090	7.7520	5.6720	H	0	20.3400	-3.9580	5.5140	H	0	20.5620	-11.9780	-6.5600	N	0
22.2580	5.7540	6.1050	C	0	22.0580	-4.2080	6.8860	C	0	21.1080	-10.7720	-6.5300	C	0
21.8040	4.7630	6.1200	H	0	23.0590	-3.8280	7.0910	H	0	22.0180	-10.4290	-7.0000	H	0
23.1460	5.6840	5.4780	H	0	21.4410	-3.9270	7.7400	H	0	20.3670	-9.9640	-5.7400	N	0
22.6320	6.2750	7.5500	C	0	22.0200	-5.2920	6.7820	H	0	20.4200	-8.9600	-5.6450	H	0
22.8310	7.3380	7.4180	H	0	21.2080	-2.0320	5.9020	C	0	19.3940	-10.6450	-5.1880	C	0
21.7610	6.0450	8.1630	H	0	22.1890	-1.5710	5.7840	H	0	18.5680	-10.1940	-4.6570	H	0
23.9790	5.5570	7.9670	C	0	20.6030	-1.4660	5.1940	H	0	16.3160	-14.0300	-4.6650	C	0
24.0790	4.5760	7.5020	H	0	20.7920	-1.7380	6.8650	H	0	16.6630	-15.1920	-4.2620	O	0
24.8320	6.1010	7.5600	H	0	22.1990	-5.3440	3.9440	C	0	15.0810	-13.7940	-5.0860	N	0
24.2300	5.3920	9.4520	C	0	23.3010	-5.8620	4.0620	O	0	14.8520	-12.8330	-5.2980	H	0
25.2480	5.0120	9.5460	H	0	21.2570	-6.0460	3.3640	N	0	14.0540	-14.7700	-5.3700	C	0
24.1830	6.3230	10.0160	H	0	20.3090	-5.6980	3.3760	H	0	14.3000	-15.7270	-4.9110	H	0
23.1420	4.5030	10.0140	N	0	21.3910	-7.3450	2.6940	C	0	12.7900	-14.1650	-4.8320	C	0
22.8470	3.8280	9.3240	H	0	22.2810	-7.2550	2.0710	H	0	12.6180	-13.2390	-5.3810	H	0
23.5370	3.8920	10.7150	H	0	21.6670	-8.4820	3.7390	C	0	12.0500	-14.9160	-5.1080	H	0
22.4530	5.1690	10.3320	H	0	21.5190	-9.4300	3.2220	H	0	12.4500	-13.7800	-3.3520	C	0
21.3660	6.5750	3.9240	C	0	22.7060	-8.4080	4.0600	H	0	13.0720	-12.9530	-3.0100	H	0
22.3730	6.9890	3.4060	O	0	20.6390	-8.5300	4.8890	C	0	11.4140	-13.4430	-3.3500	H	0
20.3320	6.0410	3.3840	N	0	20.9020	-8.1900	6.1860	C	0	12.4270	-15.0100	-2.4870	C	0
19.6200	5.6030	3.9520	H	0	21.8740	-7.8790	6.5380	H	0	13.1090	-16.0350	-2.7340	O	0
20.1930	5.7300	1.8920	C	0	19.7730	-8.2920	6.9560	N	0	11.5720	-15.1100	-1.5810	O	0
19.1980	5.3250	1.7090	H	0	19.8170	-8.0120	7.9250	H	0	13.8370	-14.9750	-6.8950	C	0
20.2610	6.6860	1.3720	H	0	18.7210	-8.6360	6.2330	C	0	13.8830	-14.0850	-7.7710	O	0
21.2020	4.7250	1.5050	C	0	17.3290	-8.7310	6.5330	C	0	13.2860	-16.1730	-7.2210	N	0
22.1250	4.9120	0.6850	O	0	17.0220	-8.5440	7.5520	H	0	13.2630	-16.8490	-6.4720	H	0
21.0660	3.5630	2.1440	N	0	16.5010	-9.2310	5.5520	C	0	12.7230	-16.6510	-5.8210	C	0
20.3650	3.5610	2.8710	H	0	15.4310	-9.2990	5.6840	H	0	13.4100	-16.4400	-9.3400	H	0
21.9650	2.4400	1.9250	C	0	17.0250	-9.6880	4.3100	C	0	12.6360	-18.1970	-8.4560	C	0
22.3330	2.3760	0.9010	H	0	16.2660	-10.0460	3.6300	H	0	12.0090	-18.4350	-7.5970	H	0
23.0880	2.5030	2.9660	C	0	18.3990	-9.5090	4.0010	C	0	12.2480	-18.6070	-9.3890	H	0
22.7200	2.8540	3.9300	H	0	18.6500	-9.8210	2.9990	H	0	13.9170	-18.8500	-8.1690	C	0
23.4910	1.5000	3.1090	H	0	19.2890	-8.9560	4.9550	C	0	15.0330	-18.6910	-9.0180	N	0
24.2860	3.2590	2.4380	C	0	20.2190	-7.5740	1.7850	C	0	16.0730	-18.9960	-8.1850	C	0
24.6510	2.6300	1.6260	H	0	19.2050	-6.8450	1.8960	O	0	17.1150	-18.8620	-8.4330	H	0
23.9130	4.1930	2.0180	H	0	20.2980	-8.5980	0.8990	N	0	15.6500	-19.3900	-6.9340	N	0
25.3410	3.5870	3.4710	C	0	21.0510	-9.2660	0.8250	H	0	16.2340	-19.7270	-6.1820	H	0
24.8680	3.9300	4.3910	H	0	19.1920	-9.0190	0.0470	C	0	14.2680	-19.1820	-6.9400	C	0
25.9830	2.7380	3.7060	H	0	18.2510	-8.6080	0.4150	H	0	13.7190	-19.2950	-6.0170	H	0
26.3910	4.6470	3.1340	C	0	19.4240	-8.3810	-1.3400	C	0	11.4020	-16.0300	-8.8440	C	0
26.9040	4.2830	2.2440	H	0	18.5380	-8.6430	-1.9190	H	0	10.8780	-16.1560	-9.9490	O	0
25.9790	5.6130	2.8420	H	0	19.4220	-7.2990	-1.2100	H	0	10.7660	-15.3790	-7.8750	N	0
27.5380	4.7610	4.1260	N	0	20.5360	-8.7530	-2.3910	C	0	11.1190	-15.3330	-6.9290	H	0
28.2990	5.2820	3.7150	H	0	20.5670	-9.8360	-2.2750	H	0	9.3560	-14.9100	-7.9820	C	0
27.2900	5.1970	5.0030	H	0	20.1540	-8.5810	-3.3970	H	0	9.2740	-14.6350	-9.0340	H	0
27.8670	3.8290	4.3370	H	0	21.7800	-7.9330	-2.0750	C	0	8.3780	-16.0850	-7.6760	C	0
21.3540	1.0510	2.1350	C	0	22.8090	-8.4260	-1.5840	O	0	8.5260	-16.3020	-6.6180	H	0
20.7570	0.7790	3.1300	O	0	21.8180	-6.7010	-2.4080	O	0	7.3430	-15.8370	-7.9110	H	0
21.5580	0.0820	1.1700	N	0	19.1200	-10.5400	0.0100	C	0	8.5760	-17.3110	-8.5340	C	0
22.2050	0.3110	0.4290	H	0	20.0820	-11.2120	0.3470	O	0	8.1460	-17.1410	-9.8850	C	0
21.1080	-1.3610	1.4060	C	0	17.9760	-11.0580	-0.4070	N	0	7.7010	-16.2220	-10.2380	H	0
20.0820	-1.2900	1.7650	H	0	17.1620	-10.4600	-0.4040	H	0	8.2050	-18.2290	-10.7620	C	0
20.9900	-2.0920	0.1450	C	0	17.6300	-12.4400	-0.7120	C	0	7.9950	-18.0730	-11.8100	H	0
20.3300	-1.5210	-0.5090	H	0	18.5310	-13.0520	-0.7580	H	0	8.6290	-19.5310	-10.3320	C	0

8.6610	-20.2710	-11.1180	H	0	4.9440	-7.9330	4.5460	C	0	13.8070	-12.2580	17.6380	C	0
8.8850	-19.6960	-8.9550	C	0	4.2510	-8.6690	5.2230	O	0	14.2990	-13.2830	17.1800	O	0
9.2510	-20.5950	-8.4820	H	0	6.2730	-7.8840	4.7750	N	0	14.1040	-11.0980	17.0790	N	0
8.9080	-18.5460	-8.0470	C	0	7.2350	-6.9430	4.1130	C	0	13.6450	-10.3090	17.5110	H	0
9.1010	-18.5990	-6.9860	H	0	6.9380	-5.8960	4.0430	H	0	15.1130	-10.8940	16.0230	C	0
9.0800	-13.5750	-7.2100	C	0	7.5710	-7.3000	3.1390	H	0	15.3190	-9.8350	15.8670	H	0
9.6940	-13.4050	-6.1500	O	0	8.3690	-6.9550	5.0950	C	0	16.0390	-11.3960	16.3030	H	0
8.1800	-12.7760	-7.6620	N	0	8.0710	-6.2840	5.9010	H	0	14.7420	-11.6160	14.6830	C	0
7.4020	-12.8670	-8.9830	C	0	9.3090	-6.6640	4.6270	H	0	15.6570	-11.8010	13.9060	O	0
6.6070	-13.6090	-8.9120	H	0	8.4670	-8.3950	5.6730	C	0	13.4710	-11.9450	14.5090	N	0
7.9290	-13.1810	-9.8840	H	0	9.0360	-8.4550	6.6010	H	0	12.8870	-11.7330	15.3060	H	0
6.8560	-11.4340	-9.1500	C	0	8.9250	-8.9820	4.8770	H	0	12.9610	-12.7280	13.3800	C	0
5.8500	-11.4070	-9.5690	H	0	6.9500	-8.6550	5.8580	C	0	13.8250	-12.9230	12.7440	H	0
7.5350	-10.7840	-9.7020	H	0	6.6660	-9.7070	5.8190	H	0	12.3350	-14.0510	13.9830	C	0
6.7620	-10.8230	-7.7960	C	0	6.4940	-8.0960	7.2520	C	0	13.0620	-14.4760	14.6750	H	0
5.7920	-10.8850	-7.3030	H	0	6.3190	-6.8860	7.4880	O	0	11.5540	-13.8360	14.7130	H	0
6.9030	-9.7440	-7.8700	H	0	6.4640	-9.0330	8.1850	N	0	11.7730	-15.0990	12.9960	C	0
7.8570	-11.4990	-6.9280	C	0	6.6830	-9.9670	7.8690	H	0	11.1620	-14.5740	12.2610	H	0
8.7310	-10.8500	-6.9830	H	0	6.1320	-8.8520	9.5820	C	0	12.8180	-15.9160	12.2510	C	0
7.4240	-11.4840	-5.4680	C	0	5.8740	-7.8030	9.7280	H	0	12.5280	-16.8360	11.7440	H	0
6.5970	-12.2730	-5.0490	O	0	4.8780	-9.6690	10.0540	C	0	13.2470	-15.2270	11.5230	H	0
7.8670	-10.6630	-4.6070	N	0	4.0580	-9.2030	9.5080	H	0	13.6410	-16.1870	12.9120	H	0
8.3410	-9.8640	-5.0050	H	0	4.8590	-11.1670	9.7630	C	0	10.7640	-16.1290	13.6610	C	0
7.5980	-10.5810	-3.1910	C	0	3.9030	-11.5980	10.0570	H	0	10.1100	-15.5190	14.2840	H	0
7.4310	-11.5900	-2.8130	H	0	5.0280	-11.4360	8.7200	H	0	10.1910	-16.6830	12.9170	H	0
8.8470	-10.0410	-2.4640	C	0	5.6030	-11.6310	10.4110	H	0	11.2300	-16.8620	14.3190	H	0
8.8170	-8.9660	-2.6400	H	0	4.7160	-9.5310	11.5180	C	0	11.9680	-11.8630	12.5330	C	0
8.9350	-10.4000	-0.9870	C	0	5.5350	-9.9890	12.0730	H	0	11.1910	-11.0530	13.1090	O	0
8.0550	-9.9500	-0.5270	H	0	4.8080	-8.4820	11.7970	H	0	11.9280	-12.0690	11.1780	N	0
8.7980	-11.4670	-0.8100	H	0	3.7890	-9.9610	11.8990	H	0	12.6400	-12.6490	10.7570	H	0
9.8030	-10.0050	-0.4600	H	0	7.3330	-9.1860	10.5070	C	0	10.8630	-11.6470	10.3600	C	0
10.1670	-10.5220	-2.9440	C	0	8.0240	-10.1610	10.2860	O	0	10.0790	-11.3980	11.0750	H	0
11.0320	-10.0410	-2.4860	H	0	7.7090	-8.3240	11.5060	N	0	11.3570	-10.3920	9.5460	C	0
10.3030	-11.5730	-2.6910	H	0	7.1360	-7.4910	11.5000	H	0	10.5410	-9.9990	8.9390	H	0
10.3830	-10.3030	-3.9900	H	0	9.0420	-8.2720	12.1390	C	0	11.6800	-9.5850	10.2030	H	0
6.3660	-9.7910	-2.7860	C	0	9.6990	-9.1150	11.9270	H	0	12.1250	-10.6540	8.8180	H	0
6.4060	-8.7380	-2.2060	O	0	9.8120	-6.9710	11.7670	C	0	10.2990	-12.8040	9.5300	C	0
5.2470	-10.2460	-3.2800	N	0	9.2880	-6.0940	12.1460	H	0	11.0530	-13.7120	9.0550	O	0
5.3350	-11.0550	-3.8780	H	0	11.1980	-6.8160	12.4500	C	0	8.9770	-12.8140	9.3340	N	0
3.9620	-9.4920	-3.3240	C	0	11.1050	-6.7440	13.5340	H	0	8.4350	-12.0490	9.7090	H	0
4.3120	-8.4800	-3.5270	H	0	11.7900	-7.6890	12.1750	H	0	8.2370	-13.6030	8.2830	C	0
3.0760	-9.8930	-4.4330	C	0	11.6190	-5.8320	12.2470	H	0	8.8920	-14.4160	7.9720	H	0
3.7090	-10.4610	-5.1150	H	0	9.9480	-6.8590	10.2010	C	0	6.9620	-14.3290	8.8070	C	0
2.3660	-10.6030	-4.0090	H	0	10.3890	-5.8810	10.0110	H	0	6.2600	-13.5390	9.0750	H	0
2.4110	-8.8230	-5.2710	C	0	10.5820	-7.6190	9.7460	H	0	6.5530	-14.8150	7.9210	H	0
1.2290	-8.3730	-5.0730	C	0	9.0240	-6.8190	9.6240	H	0	7.0690	-15.3030	9.9010	C	0
0.6060	-8.7800	-4.2900	H	0	8.8220	-8.3480	13.6310	C	0	7.2830	-14.8170	11.1950	C	0
0.8930	-7.3110	-5.9310	N	0	7.9960	-7.7270	14.1840	O	0	7.3540	-13.7560	11.3860	H	0
-0.0000	-6.8400	-5.9280	H	0	9.6380	-9.1040	14.3380	N	0	7.4260	-15.7130	12.2530	C	0
2.0250	-6.9030	-6.5480	C	0	10.2250	-9.6960	13.7680	H	0	7.5340	-15.1950	13.1950	H	0
2.2430	-5.9150	-7.4790	C	0	9.5070	-9.4020	15.8000	C	0	7.4770	-17.1060	12.0560	C	0
1.4730	-5.1770	-7.6480	H	0	8.5880	-9.0370	16.2590	H	0	7.7280	-17.8760	12.7700	H	0
3.4860	-5.9460	-8.1530	C	0	9.3790	-10.9710	15.9400	C	0	7.2060	-17.5890	10.7590	C	0
3.7090	-5.3610	-9.0330	H	0	9.1620	-11.1620	16.9910	H	0	7.0740	-18.6410	10.5520	H	0
4.4580	-6.8440	-7.7300	C	0	8.2110	-11.5540	15.1020	C	0	6.9880	-16.6970	9.6970	C	0
5.4110	-6.7680	-8.2320	H	0	8.6110	-11.8120	14.1220	H	0	6.8410	-17.0910	8.7030	H	0
4.2260	-7.8610	-6.7620	C	0	7.9430	-12.5060	15.5610	H	0	7.9330	-12.7740	7.0310	C	0
4.9480	-8.6310	-6.5300	H	0	7.3720	-10.8600	15.1540	H	0	7.7020	-11.5260	7.0870	O	0
2.9800	-7.8900	-6.2000	C	0	10.6370	-11.4770	15.6230	O	0	7.7920	-13.4160	5.9110	N	0
3.2800	-9.3240	-1.9310	C	0	10.7890	-11.1590	14.7300	H	0	7.7900	-14.4250	5.8700	H	0
2.1290	-9.0440	-1.8550	O	0	10.6150	-8.9180	16.8230	C	0	7.2720	-12.8000	4.6710	C	0
4.0300	-9.6100	-0.9020	N	0	11.7500	-8.7380	16.4640	O	0	6.4160	-12.1720	4.9180	H	0
5.0370	-9.5910	-0.9860	H	0	10.2780	-8.7410	18.0970	N	0	8.2900	-11.9440	3.9420	C	0
3.5670	-9.8960	0.4970	C	0	9.3180	-8.7410	18.4090	H	0	7.7900	-11.3080	3.2120	H	0
2.5020	-9.6620	0.5070	H	0	11.3110	-8.5730	19.1690	C	0	8.7250	-11.2990	4.7050	H	0
3.6710	-11.4120	0.8330	C	0	11.8770	-7.7110	18.8140	H	0	9.3950	-12.6250	3.2390	C	0
3.1110	-11.9760	0.0870	H	0	10.6990	-8.3210	20.5820	C	0	10.4270	-13.4220	3.8630	C	0
4.7390	-11.5270	0.6490	H	0	10.1180	-9.1740	20.9340	H	0	10.4480	-13.5630	4.9340	H	0
3.2850	-11.7180	2.1300	O	0	11.4990	-8.0910	21.2860	H	0	11.3330	-14.2140	3.0960	C	0
2.3340	-11.7430	2.2640	H	0	9.9760	-7.5210	20.4260	H	0	11.9760	-14.8570	3.6780	H	0
4.3290	-9.0440	1.5750	C	0	12.2700	-9.8250	19.2370	C	0	11.2910	-14.1190	1.7060	C	0
5.5370	-9.1780	1.6120	O	0	13.4760	-9.7700	19.5230	O	0	12.2550	-14.7530	0.9610	O	0
3.6020	-8.2340	2.4190	N	0	11.9370	-11.0660	18.8700	N	0	11.9240	-14.7600	0.0600	H	0
2.6280	-8.0970	2.1870	H	0	10.9440	-11.2140	18.7640	H	0	10.4130	-13.2610	1.0040	C	0
4.3280	-7.3010	3.2370	C	0	12.7740	-12.2670	18.7700	C	0	10.3040	-13.2410	-0.0710	H	0
5.1210	-6.9020	2.6050	H	0	13.4140	-12.3590	19.6470	H	0	9.4630	-12.5160	1.7800	C	0
3.6600	-6.5000	3.5550	H	0	12.1120	-13.1090	18.5680	H	0	8.7180	-11.9360	1.2570	H	0

6.7390	-13.9180	3.7140	C	0	9.2570	-24.7400	1.7940	H	0	16.3900	-13.8590	11.6150	H	0
6.8210	-15.1280	3.9850	O	0	8.3970	-23.1010	0.6440	C	0	18.2020	-14.7600	10.9130	C	0
6.4360	-13.5490	2.4950	N	0	8.0190	-22.5590	1.4980	H	0	17.8930	-15.5440	11.6040	H	0
6.4570	-12.5770	2.2210	H	0	7.9640	-22.6900	-0.6400	C	0	18.6810	-15.0520	9.9780	H	0
5.9890	-14.4960	1.4410	C	0	5.3780	-19.0520	1.0430	C	0	19.3120	-13.8490	11.5000	C	0
6.5440	-15.4160	1.6260	H	0	5.6150	-17.8450	0.7800	O	0	20.5030	-13.9430	11.1700	O	0
4.9120	-14.6590	1.4620	H	0	5.1820	-19.5180	2.2970	N	0	18.9630	-12.9680	12.3490	O	0
6.2090	-14.0990	0.0130	C	0	5.1710	-20.5180	2.4400	H	0	17.2200	-12.5270	10.1550	C	0
6.6590	-13.0010	-0.2810	O	0	5.4010	-18.7510	3.4450	C	0	17.9360	-12.3290	9.1620	O	0
5.8950	-14.9600	-0.8910	N	0	5.3100	-17.6810	3.2560	H	0	16.7080	-11.5090	10.8220	N	0
5.5400	-15.8130	-0.4810	H	0	4.3210	-19.1050	4.4090	C	0	16.3700	-11.6210	11.7670	H	0
6.0460	-14.8150	-2.3350	C	0	3.3550	-19.0860	3.9050	H	0	16.7590	-10.1470	10.3520	C	0
6.2790	-13.7620	-2.4920	H	0	4.3320	-20.1600	4.6800	H	0	16.4290	-10.1320	9.3140	H	0
7.3720	-15.4390	-2.9250	C	0	4.2560	-18.2820	5.6550	C	0	15.7370	-9.3130	11.1180	C	0
7.3390	-15.3110	-4.0070	H	0	4.5930	-16.9230	5.6440	C	0	15.5200	-8.4670	10.4660	H	0
8.7030	-14.7040	-2.4610	C	0	4.8220	-16.2990	4.7930	H	0	14.3530	-10.0190	11.1280	C	0
9.5780	-15.2530	-2.8090	H	0	4.4040	-16.2080	6.7950	C	0	13.5510	-9.3540	11.4490	H	0
8.7440	-13.6570	-2.7610	H	0	4.6970	-15.1720	6.7140	H	0	14.0270	-10.3850	10.1550	H	0
8.8250	-14.8280	-1.3850	H	0	4.1060	-16.8420	7.9710	C	0	14.4060	-10.7800	11.9060	H	0
7.4250	-16.8590	-2.6260	O	0	4.0940	-16.2960	8.9030	H	0	16.2040	-8.6250	12.4210	C	0
7.2200	-17.3020	-3.4520	H	0	3.9270	-18.2290	7.9910	C	0	16.8670	-9.3170	12.9400	H	0
4.8680	-15.2630	-3.2260	C	0	3.6570	-18.6300	8.9570	H	0	16.7650	-7.7190	12.1930	H	0
4.0930	-16.1150	-2.8990	O	0	3.8930	-18.9380	6.8420	C	0	15.0630	-8.2010	13.3680	C	0
4.7580	-14.5230	-4.3720	N	0	3.5590	-19.9620	6.7550	H	0	14.4330	-7.4580	12.8790	H	0
5.3780	-13.7310	-4.4620	H	0	6.8410	-19.1470	3.9240	C	0	14.3710	-8.9600	13.7300	H	0
3.8090	-14.7570	-5.4590	C	0	7.3270	-20.1810	3.5710	O	0	15.5240	-7.8100	14.2750	H	0
2.8620	-14.4190	-5.0380	H	0	7.4900	-18.2270	4.6350	N	0	18.1440	-9.4990	10.4330	C	0
4.0600	-13.7800	-6.6350	C	0	7.0000	-17.3520	4.7560	H	0	18.3980	-8.4160	9.9480	O	0
4.0710	-12.7940	-6.1700	H	0	8.9420	-18.2130	4.7700	C	0	19.0980	-10.1700	11.1170	N	0
4.9570	-14.0540	-7.1900	H	0	9.3870	-19.2010	4.8870	H	0	18.7400	-11.0170	11.5350	H	0
2.8490	-13.7490	-7.6110	C	0	9.5450	-17.5770	3.4380	C	0	20.4760	-9.8220	11.2940	C	0
2.7380	-14.7520	-8.0240	H	0	9.2140	-16.5390	3.4730	H	0	20.6310	-8.7430	11.2800	H	0
1.9950	-13.5580	-6.9620	H	0	10.6020	-17.4220	3.6560	H	0	20.8480	-10.2080	12.7070	C	0
2.8670	-12.6140	-8.9020	S	0	9.2660	-18.2420	2.0290	C	0	20.2740	-9.6910	13.4750	H	0
2.0470	-11.2120	-7.9430	C	0	9.2760	-19.3320	2.0220	H	0	20.9150	-11.2910	12.8010	H	0
0.9860	-11.4280	-7.8230	H	0	8.2670	-17.9500	1.7050	H	0	22.2820	-9.7360	12.9730	C	0
2.4080	-11.1500	-6.9160	H	0	10.2290	-17.6320	0.9110	C	0	23.0970	-9.9410	12.2790	H	0
2.2230	-10.3240	-8.5500	H	0	10.1210	-16.5490	0.8600	H	0	22.3010	-8.6460	12.9980	H	0
3.6510	-16.2070	-5.9210	C	0	11.2480	-17.9660	1.1020	H	0	22.7250	-10.2110	14.3890	C	0
2.5160	-16.5150	-6.3420	O	0	9.8040	-18.0910	-0.4880	C	0	22.9390	-11.2800	14.3800	H	0
4.6430	-17.1120	-5.8040	N	0	9.6890	-19.1750	-0.4620	H	0	23.7400	-9.8260	14.4920	H	0
5.5620	-16.7080	-5.6920	H	0	8.8660	-17.6230	-0.7890	H	0	21.8780	-9.8080	15.6740	C	0
4.5720	-18.5580	-6.1940	C	0	10.7860	-17.8390	-1.5720	N	0	20.8420	-10.1450	15.6660	H	0
3.9100	-18.4950	-7.0580	H	0	11.6720	-18.2480	-1.3120	H	0	22.1560	-10.3550	16.5760	H	0
5.9610	-19.0450	-6.5520	C	0	10.4640	-18.3060	-2.4080	H	0	21.8520	-8.3260	15.8050	N	0
5.9520	-20.0030	-7.0170	H	0	10.8490	-16.8510	-1.7740	H	0	21.6060	-7.8850	14.9300	H	0
6.4020	-18.3590	-7.2760	H	0	9.4600	-17.2760	5.9250	C	0	21.3420	-8.1830	16.6650	H	0
7.0250	-19.1830	-5.4620	C	0	8.7700	-16.3160	6.1870	O	0	22.7610	-7.9090	15.9440	H	0
6.9740	-18.4490	-4.4630	O	0	10.5840	-17.5230	6.5700	N	0	21.3900	-10.2710	10.1860	C	0
7.8560	-20.0990	-5.5160	O	0	10.9580	-18.4580	6.4810	H	0	22.1500	-9.4600	9.6480	O	0
3.8900	-19.4220	-5.0810	C	0	11.0670	-16.7640	7.7760	C	0	21.2320	-11.5560	9.6890	N	0
3.7890	-20.6480	-5.1740	O	0	10.7450	-15.7220	7.7690	H	0	20.7110	-12.2180	10.2460	H	0
3.6060	-18.8340	-3.8500	N	0	10.4360	-17.3840	8.9960	C	0	22.1190	-12.0580	8.6280	C	0
3.5850	-17.8240	-3.8470	H	0	10.5740	-18.4650	9.0020	H	0	22.8760	-11.3320	8.3330	H	0
2.8150	-19.5360	-2.8810	C	0	10.7420	-16.9950	9.9680	H	0	22.8720	-13.3590	8.9980	C	0
2.2240	-18.8150	-2.3180	H	0	9.3730	-17.1450	8.9480	H	0	23.5800	-13.6150	8.2100	H	0
2.1450	-20.1620	-3.4700	H	0	12.6150	-16.6970	7.7740	C	0	23.5450	-13.2500	10.3670	C	0
3.6800	-20.3410	-1.8640	C	0	13.3330	-17.6510	7.4260	O	0	22.8680	-12.8410	11.1170	H	0
3.4400	-21.5360	-1.7350	O	0	13.1180	-15.5930	8.3410	N	0	23.9120	-14.2170	10.7100	H	0
4.6240	-19.6540	-1.2470	N	0	12.4380	-14.8980	8.6130	H	0	24.4390	-12.6300	10.2900	H	0
4.6120	-18.6500	-1.3600	H	0	14.4790	-15.0410	8.0960	C	0	21.9260	-14.4060	8.9970	O	0
5.4380	-20.1450	-0.1100	C	0	15.1060	-15.8670	7.7610	H	0	21.2890	-14.2660	9.7010	H	0
5.1060	-21.0880	0.3240	H	0	14.3830	-13.9150	6.9540	C	0	21.4550	-12.2280	7.3190	C	0
6.8950	-20.2260	-0.5600	C	0	13.5640	-13.2510	7.2300	H	0	22.1780	-12.3030	6.2890	O	0
7.0810	-19.4320	-1.2830	H	0	15.7020	-13.1120	6.8300	C	0	20.1230	-12.0340	7.2800	N	0
7.5910	-20.0800	0.2660	H	0	15.8930	-12.4240	7.6540	H	0	19.6590	-11.9590	8.1740	H	0
7.2990	-21.5630	-1.1660	C	0	16.5440	-13.8000	6.7560	H	0	19.3830	-12.0320	6.0300	C	0
7.1620	-21.8380	-2.5200	C	0	15.6960	-12.5750	5.8820	H	0	18.3700	-11.6830	6.2280	H	0
6.7660	-21.1070	-3.2090	H	0	13.9920	-14.5080	5.6410	C	0	19.9670	-11.4580	5.3110	H	0
7.7430	-23.0230	-2.8860	N	0	14.7470	-15.2570	5.4020	H	0	19.3720	-13.4340	5.3590	C	0
7.7770	-23.3840	-3.8290	H	0	12.9780	-14.9030	5.5820	H	0	19.5770	-13.5310	4.1800	O	0
8.2710	-23.6750	-1.7420	C	0	14.1130	-13.7270	4.8900	H	0	19.1720	-14.4930	6.0950	N	0
8.9760	-24.7990	-1.5760	C	0	15.0310	-14.4030	9.3940	C	0	19.0560	-14.3360	7.0860	H	0
9.1690	-25.4880	-2.3850	H	0	14.3190	-13.6430	10.0390	O	0	19.0740	-15.9060	5.7240	C	0
9.4030	-25.1530	-0.2930	C	0	16.2330	-14.7770	9.6860	N	0	19.2010	-16.0060	4.6460	H	0
9.8950	-26.1090	-0.1880	H	0	16.7720	-15.4010	9.1020	H	0	20.2980	-16.5890	6.4230	C	0
9.0920	-24.3570	0.7980	C	0	16.9320	-13.9840	10.6770	C	0	20.4660	-16.3360	7.4690	H	0

20.1250	-17.6610	6.3270	H	0	9.8930	-22.0270	4.8970	C	0	-2.5490	-24.8550	-1.8080	H	0
21.5650	-16.3000	5.6270	C	0	9.2590	-21.2450	5.3150	H	0	-2.2430	-23.0880	-2.9910	C	0
21.4050	-16.7710	4.6570	H	0	10.5110	-21.3580	3.6180	C	0	-2.9670	-23.1690	-3.9780	O	0
21.6330	-15.2140	5.5700	H	0	9.6870	-21.0060	2.9980	H	0	-1.8660	-21.8430	-2.5890	N	0
22.7560	-16.8510	6.3710	C	0	11.0280	-20.4220	3.8330	H	0	-1.4580	-21.5590	-1.7090	H	0
22.8010	-16.3620	7.3440	H	0	11.3880	-22.2490	2.7600	C	0	-1.8350	-20.7150	-3.5870	C	0
22.6930	-17.9300	6.5130	H	0	12.3120	-22.3700	3.3240	H	0	-1.7160	-21.1360	-4.5850	H	0
23.9440	-16.6000	5.5010	C	0	10.8730	-23.2090	2.7370	H	0	-3.2430	-20.1010	-3.7850	C	0
23.8600	-17.2030	4.5970	H	0	11.6710	-21.8020	1.3610	C	0	-3.9210	-20.9410	-3.9390	H	0
23.9690	-15.5540	5.1950	H	0	11.0870	-20.9010	0.7380	O	0	-3.4560	-19.5640	-2.8610	H	0
25.1850	-17.0060	6.3080	N	0	12.6880	-22.4080	0.7880	N	0	-3.3200	-19.2120	-4.8220	O	0
25.1380	-17.9760	6.5850	H	0	12.9340	-22.1450	-0.1550	H	0	-3.2840	-19.6790	-5.6600	H	0
26.0440	-16.8310	5.8070	H	0	13.1910	-23.1510	1.2530	H	0	-0.8000	-19.6100	-3.2230	C	0
25.2680	-16.5100	7.1840	H	0	8.9950	-23.3070	4.7030	C	0	-0.3030	-19.4280	-2.1000	O	0
17.7840	-16.6490	6.1590	C	0	9.3180	-24.4430	5.0950	O	0	-0.4490	-18.7940	-4.3080	N	0
17.3730	-16.5330	7.2820	O	0	7.8410	-23.1020	4.1480	N	0	-0.8400	-19.1540	-5.1670	H	0
17.2600	-17.4380	5.2140	N	0	7.5740	-22.1420	3.9810	H	0	0.4300	-17.7110	-4.2930	C	0
17.6270	-17.5440	4.2780	H	0	6.7520	-24.1550	3.8750	C	0	1.4620	-18.0390	-4.1720	H	0
16.0430	-18.1900	5.4740	C	0	7.1290	-25.1440	3.6150	H	0	0.3330	-17.2630	-5.2820	H	0
15.3550	-17.5980	6.0770	H	0	5.8810	-24.3430	5.0740	C	0	0.1000	-16.6980	-3.1140	C	0
15.1050	-18.4230	4.1970	C	0	6.5050	-24.8530	5.8080	H	0	-1.0340	-16.3550	-2.8690	O	0
15.7920	-18.4290	3.3510	H	0	5.6380	-23.4030	5.5690	H	0	1.0860	-16.2940	-2.3560	N	0
14.3420	-19.8300	4.1390	C	0	4.4850	-24.9410	4.7370	C	0	2.0320	-16.6020	-2.5310	H	0
13.5210	-19.8340	4.8570	H	0	3.8610	-24.2050	4.2290	H	0	0.8460	-15.2380	-1.3840	C	0
13.9160	-19.9620	3.1450	H	0	4.6200	-25.7610	4.0320	H	0	-0.1900	-15.3090	-1.0530	H	0
15.0180	-20.6140	4.4820	H	0	3.6330	-25.4690	5.9470	C	0	1.7770	-15.3120	-0.1010	C	0
14.1180	-17.3330	3.8110	C	0	4.0220	-25.2780	7.0460	O	0	2.8070	-15.2720	-0.4560	H	0
13.3000	-17.6480	3.1640	H	0	2.4310	-25.8290	5.6850	N	0	1.5950	-14.2380	0.9980	C	0
13.7120	-16.8130	4.6790	H	0	1.7190	-25.9280	6.3940	H	0	2.4900	-14.1230	1.6110	H	0
14.7040	-16.6000	3.2570	H	0	2.3040	-25.9400	4.6890	H	0	1.4570	-13.2440	0.5730	H	0
16.2630	-19.4560	6.3610	C	0	5.9030	-23.6560	2.6440	C	0	0.7140	-14.4260	1.6120	H	0
17.0820	-20.3740	6.2000	O	0	5.6690	-22.4360	2.4460	O	0	1.5770	-16.6280	0.6180	C	0
15.6600	-19.4080	7.5500	N	0	5.4980	-24.6580	1.7870	N	0	0.5690	-16.6920	1.0270	H	0
15.1250	-18.6030	7.8430	H	0	5.8250	-25.5550	2.1160	H	0	1.5700	-17.4390	-0.1100	H	0
15.5970	-20.3570	8.6590	C	0	4.8200	-24.4200	0.4980	C	0	2.6470	-17.0550	1.6530	C	0
16.5480	-20.8750	8.7820	H	0	5.1190	-23.4680	0.0590	H	0	3.6560	-16.7300	1.3990	H	0
15.3500	-19.6450	10.0590	C	0	5.2110	-25.5500	-0.4900	C	0	2.3270	-16.6820	2.6270	H	0
14.4140	-19.1100	9.8960	H	0	6.2700	-25.4270	-0.7150	H	0	2.6390	-18.1410	1.5670	H	0
15.2590	-20.3560	10.8800	H	0	5.0590	-26.5220	-0.0210	H	0	1.0780	-13.8370	-1.9820	C	0
16.2860	-18.4860	10.4880	C	0	4.4010	-25.5000	-1.8150	C	0	2.1590	-13.4980	-2.4080	O	0
15.1260	-17.5110	10.0270	H	0	4.6330	-26.4650	-2.2670	H	0	-0.0130	-13.1240	-1.9270	N	0
16.0900	-18.1660	12.0450	C	0	3.3200	-25.5180	-1.6810	H	0	-0.9080	-13.4390	-1.5810	H	0
16.3600	-19.0920	12.5540	H	0	4.7810	-24.3400	-2.7690	C	0	-0.0070	-11.7450	-2.3390	C	0
16.7200	-17.3620	12.4250	H	0	5.0380	-23.4550	-2.1870	H	0	1.0120	-11.3590	-2.3760	H	0
15.0820	-17.8040	12.2450	H	0	5.6340	-24.7060	-3.3400	H	0	-0.7380	-11.6200	-3.6380	C	0
17.8410	-18.8300	10.3820	C	0	3.7280	-24.1210	-3.8400	C	0	-0.6350	-10.5730	-3.9250	H	0
18.0650	-19.2770	9.4140	H	0	3.1600	-25.0220	-4.0720	H	0	-0.3210	-12.5120	-4.8050	C	0
18.4410	-17.9250	10.4790	H	0	3.0430	-23.3310	-3.5330	H	0	-0.4410	-13.5390	-4.4600	H	0
18.1360	-19.5300	11.1640	H	0	4.2350	-23.4370	-5.0890	N	0	-0.8710	-12.4250	-5.7420	H	0
14.5740	-21.4840	8.3460	C	0	3.7840	-22.5330	-5.0770	H	0	0.7480	-12.3980	-4.9850	H	0
14.9600	-22.6940	8.4020	O	0	5.2340	-23.4270	-5.2330	H	0	-2.2440	-11.8600	-3.4780	C	0
13.3430	-21.0320	8.0230	N	0	3.7680	-23.7230	-5.9380	H	0	-2.3740	-12.9200	-3.6960	H	0
13.1480	-20.0420	7.9680	H	0	3.2900	-24.4100	0.7710	C	0	-2.5480	-11.8180	-2.4320	H	0
12.1490	-21.8550	7.8550	C	0	2.7740	-25.3130	1.4810	O	0	-3.1060	-10.9020	-4.2910	C	0
12.3280	-22.9310	7.8430	H	0	2.5730	-23.4510	0.2290	N	0	-3.1610	-9.9660	-3.7350	H	0
11.3150	-21.5840	9.1240	C	0	3.0600	-22.8660	-0.4350	H	0	-2.8790	-10.7840	-5.3500	H	0
11.9080	-21.9180	9.9760	H	0	1.1030	-23.4090	0.3130	C	0	-4.1010	-11.3340	-4.1860	H	0
11.1920	-20.5140	9.2890	H	0	0.7670	-24.1150	1.0730	H	0	-0.5950	-10.7650	-1.2550	C	0
10.0120	-22.1960	9.2400	C	0	0.6700	-22.0150	0.9300	C	0	-0.8290	-9.5760	-1.5190	O	0
9.7820	-23.2810	10.0050	C	0	0.9130	-21.2370	0.2060	H	0	-0.9180	-11.3220	-0.1050	N	0
10.5200	-23.7490	10.6400	H	0	-0.4000	-22.0450	1.1380	H	0	-0.7100	-12.3050	-0.0060	H	0
8.4770	-23.7770	9.8770	N	0	1.4440	-21.6500	2.1910	C	0	-1.3790	-10.5550	1.1010	C	0
8.0760	-24.5040	10.4510	H	0	2.5000	-21.4730	1.9890	H	0	-1.9260	-9.6340	0.9000	H	0
7.7530	-22.9570	9.0770	C	0	0.7450	-20.3900	2.6680	C	0	-2.1220	-11.2400	1.5110	H	0
6.4470	-22.9610	8.6010	C	0	1.0660	-20.1070	3.6710	H	0	-0.3360	-10.4270	2.1880	C	0
5.8590	-23.8260	8.8670	H	0	1.0490	-19.5710	2.0170	H	0	0.6520	-11.1730	2.0990	O	0
6.0150	-21.9650	7.7070	C	0	-0.3450	-20.3940	2.6640	H	0	-0.6190	-9.6690	3.3190	N	0
5.0410	-22.0600	7.2500	H	0	1.3510	-22.5740	3.3560	C	0	-1.5820	-9.3690	3.3820	H	0
6.9220	-20.9440	7.3360	C	0	1.6540	-22.1540	4.3150	H	0	0.3140	-9.4830	4.3840	C	0
6.6330	-20.0840	6.7500	H	0	0.2920	-22.8220	3.4210	H	0	1.2330	-9.7540	3.8640	H	0
8.2340	-20.9450	7.8420	C	0	1.9480	-23.4760	3.2200	H	0	0.4370	-8.0250	4.7930	C	0
8.9230	-20.1550	7.5840	H	0	0.4850	-23.6950	-1.1010	C	0	1.4230	-8.0090	5.2570	H	0
8.6950	-22.0180	8.5870	C	0	1.1780	-23.6820	-2.1710	O	0	0.3560	-7.3710	3.9250	H	0
11.3950	-21.4060	6.6310	C	0	-0.8260	-23.9600	-1.0530	N	0	-0.5140	-7.5870	5.8860	C	0
11.1280	-20.2000	6.5320	O	0	-1.2510	-23.9830	-0.1370	H	0	-0.2200	-7.8670	7.0700	O	0
10.9610	-22.3270	5.7720	N	0	-1.6830	-24.3030	-2.1730	C	0	-1.4620	-6.7930	5.5210	N	0
11.3820	-23.2420	5.8450	H	0	-1.1110	-24.9390	-2.8470	H	0	-2.1830	-6.7150	6.2230	H	0

-1.5400	-6.6300	4.5270	H	0	1.0870	-12.6290	22.5770	C	0	0.7640	-22.0900	21.9540	C	0
0.1360	-10.4200	5.5960	C	0	1.4310	-12.0300	21.7340	H	0	0.8420	-22.4860	22.9660	H	0
-0.9100	-10.6880	6.1150	O	0	1.3400	-11.8450	23.8990	C	0	-0.2650	-22.0690	21.5920	H	0
1.2390	-11.0920	6.0780	N	0	2.4090	-11.6380	23.9580	H	0	1.7080	-22.8770	21.0040	C	0
2.3770	-11.3870	5.2560	C	0	0.8070	-10.9020	23.7770	H	0	1.1540	-23.5930	20.3970	H	0
2.8800	-10.4820	4.9130	H	0	0.9050	-12.3800	24.7440	H	0	2.0400	-22.1120	20.3030	H	0
2.0170	-11.9750	4.4120	H	0	2.0710	-13.8140	22.4840	C	0	2.6900	-23.5550	21.8190	N	0
3.4120	-12.1400	6.0560	C	0	2.1890	-14.0640	21.4290	H	0	3.2410	-24.1800	21.2470	H	0
4.1620	-11.4170	6.3770	H	0	3.0330	-13.4930	22.8840	H	0	3.2450	-22.9580	22.4140	H	0
4.0440	-12.8940	5.5870	H	0	1.7450	-14.6310	23.1270	H	0	2.2240	-24.1500	22.4880	H	0
2.5480	-12.7580	7.0530	C	0	-2.4330	-13.9490	21.3130	C	0	0.8830	-17.4080	22.0820	C	0
3.0720	-12.9440	7.9910	H	0	-3.3590	-13.1010	21.2830	O	0	-0.1480	-16.7790	21.7220	O	0
2.3830	-13.7420	6.6140	H	0	-2.7690	-15.2400	21.6170	N	0	2.0710	-17.0900	21.5570	N	0
1.3190	-11.9090	7.3050	C	0	-1.9950	-15.8660	21.4460	H	0	2.8620	-17.6730	21.7900	H	0
0.4340	-12.5460	7.2700	H	0	-4.1270	-15.7360	21.7910	C	0	2.1440	-16.3920	20.2850	C	0
1.3460	-11.0700	8.5660	C	0	-4.8160	-15.3250	21.0530	H	0	1.4990	-15.5150	20.3390	H	0
1.9030	-9.9490	8.5500	O	0	-4.1920	-16.8130	21.6340	H	0	3.5910	-15.8960	20.1060	C	0
1.1060	-11.7070	9.6780	N	0	-4.6620	-15.4560	23.1570	C	0	3.9840	-15.5400	21.0580	H	0
1.0700	-12.7160	9.6770	H	0	-3.8850	-14.9400	24.0110	O	0	4.1580	-16.7880	19.8390	H	0
0.7860	-11.0130	10.9450	C	0	-5.9330	-15.8200	23.4520	N	0	3.7720	-14.8780	19.0060	C	0
1.3240	-10.0650	10.9390	H	0	-7.0150	-16.2520	22.5590	C	0	3.6050	-15.3350	18.0310	H	0
-0.7130	-10.5690	11.2410	C	0	-6.5780	-16.9810	21.8770	H	0	3.2020	-13.9510	19.0620	H	0
-0.6540	-9.9440	12.1320	H	0	-7.4640	-15.5270	21.8810	H	0	5.2480	-14.4200	18.9160	C	0
-1.2910	-9.6390	10.1500	C	0	-8.1150	-16.9800	23.3780	C	0	6.1300	-14.8940	19.5660	O	0
-0.5500	-8.8750	9.9160	H	0	-7.8650	-18.0400	23.3400	H	0	5.6250	-13.6220	17.9540	N	0
-1.4050	-10.2480	9.2530	H	0	-9.0610	-16.7530	22.8870	H	0	6.6150	-13.4220	17.9420	H	0
-2.2040	-9.1910	10.5420	H	0	-7.9690	-16.2390	24.7510	C	0	5.0390	-13.2260	17.2330	H	0
-1.5510	-11.7070	11.6520	C	0	-8.3920	-16.7710	25.6040	H	0	1.8050	-17.2560	19.0750	C	0
-1.8510	-12.1870	10.7210	H	0	-8.5200	-15.3080	24.6130	H	0	2.2380	-18.4110	18.9430	O	0
-1.0640	-12.4040	12.3340	H	0	-6.4280	-15.9850	24.8020	C	0	1.2300	-16.7120	18.0480	N	0
-2.8250	-11.2300	12.2550	C	0	-6.1980	-15.0230	25.2610	H	0	0.9650	-15.7590	18.2520	H	0
-2.6770	-11.3090	13.3320	H	0	-5.7270	-17.1010	25.5520	C	0	0.8790	-17.1590	16.7100	C	0
-3.0720	-10.1940	12.0240	H	0	-5.5250	-16.9660	26.7460	O	0	1.2630	-18.1650	16.5370	H	0
-3.6170	-11.8920	11.9050	H	0	-5.0840	-18.0860	24.9290	N	0	-0.6190	-17.3780	16.5900	C	0
1.3810	-11.7520	12.1400	C	0	-5.0030	-18.0210	23.9240	H	0	-1.1040	-16.4060	16.6850	H	0
1.6160	-12.9200	11.9940	O	0	-4.2800	-19.1260	25.5870	C	0	-0.8240	-17.6980	15.5680	H	0
1.5550	-11.1790	13.3260	N	0	-4.6740	-19.4010	26.5660	H	0	-1.3160	-18.4360	17.4990	C	0
1.4100	-10.1860	13.4430	H	0	-4.2910	-20.5180	24.8540	C	0	-1.8110	-18.0460	18.7670	C	0
1.6240	-12.0400	14.5660	C	0	-3.7580	-21.0930	25.6120	H	0	-1.7570	-17.0210	19.1020	H	0
1.3460	-13.0730	14.3570	H	0	-5.3280	-20.8370	24.7500	H	0	-2.1130	-19.0110	19.7310	C	0
3.1240	-12.0580	15.0740	C	0	-3.4600	-20.5370	23.5970	C	0	-2.3680	-18.7450	20.7460	H	0
3.7440	-12.3260	14.2190	H	0	-3.0620	-19.4870	23.0830	O	0	-2.1500	-20.3600	19.3120	C	0
3.6770	-10.5970	15.3990	C	0	-3.1510	-21.6230	23.0440	O	0	-2.5440	-21.3280	20.2270	O	0
4.6000	-10.8090	15.9400	H	0	-2.8270	-18.6440	26.0460	C	0	-2.5600	-20.9730	21.1190	H	0
3.7000	-10.0670	14.4470	H	0	-2.0620	-19.4520	26.4110	O	0	-2.0030	-20.6900	17.9160	C	0
2.9580	-10.1590	16.0910	H	0	-2.3600	-17.3890	25.7920	N	0	-2.2900	-21.6870	17.6170	H	0
3.2930	-12.8130	16.2830	O	0	-3.0530	-16.7810	25.3790	H	0	-1.5510	-19.7240	17.0330	C	0
2.8820	-13.6800	16.2490	H	0	-1.1560	-16.7130	26.1740	C	0	-1.3530	-20.0510	16.0230	H	0
0.6390	-11.5610	15.6130	C	0	-1.3200	-15.6490	25.9990	H	0	1.4740	-16.3070	15.6030	C	0
0.1560	-10.4010	15.6320	O	0	-0.8940	-16.8910	27.7110	C	0	1.8150	-15.1100	15.7470	O	0
0.3500	-12.4670	16.5530	N	0	-0.4180	-17.8680	27.8000	H	0	1.6020	-16.8440	14.3900	N	0
0.7840	-13.3780	16.6080	H	0	-0.1890	-16.1420	28.0720	H	0	1.2770	-17.8000	14.3700	H	0
-0.6260	-12.1480	17.5630	C	0	-2.1580	-16.7910	28.6750	C	0	1.7360	-16.1740	13.1140	C	0
-0.4950	-11.1350	17.9410	H	0	-2.9020	-17.5610	28.4710	H	0	1.4710	-15.1400	13.3340	H	0
-2.1190	-12.2950	17.0210	C	0	-1.8620	-17.1810	29.6490	H	0	3.1570	-16.2050	12.5670	C	0
-2.7610	-11.9460	17.8290	H	0	-3.0010	-15.5010	28.7820	C	0	3.2290	-15.7220	11.5930	H	0
-2.2070	-11.6900	16.1180	H	0	-2.3420	-14.6370	28.8710	H	0	4.1050	-15.3520	13.4790	C	0
-2.5600	-13.7210	16.5780	C	0	-3.4340	-15.3970	27.7870	H	0	3.7450	-14.3250	13.5210	H	0
-2.4260	-14.0710	15.1950	C	0	-4.1070	-15.3870	29.7780	C	0	4.3630	-15.9620	14.3450	H	0
-1.8150	-13.4760	14.5330	H	0	-3.6980	-15.6050	30.7650	H	0	5.0620	-15.4160	12.9600	H	0
-2.8490	-15.2830	14.7180	C	0	-4.5900	-14.4120	29.8360	H	0	3.7430	-17.5880	12.3650	C	0
-2.7130	-15.6030	13.6960	H	0	-5.1410	-16.3560	29.4510	N	0	4.8050	-17.7080	12.1470	H	0
-3.5430	-16.1830	15.5930	C	0	-5.9870	-16.1450	29.9600	H	0	3.5110	-18.1600	13.2630	H	0
-3.8720	-17.1130	15.1530	H	0	-5.4150	-16.4260	28.4820	H	0	3.1520	-17.9570	11.5270	H	0
-3.7600	-15.7860	16.9190	C	0	-4.8230	-17.2750	29.7240	H	0	0.6510	-16.6310	12.0970	C	0
-4.2590	-16.4650	17.5950	H	0	0.0460	-17.0610	25.2260	C	0	0.1040	-17.7150	12.3230	O	0
-3.1960	-14.5980	17.4370	C	0	1.1320	-16.4750	25.4440	O	0	0.2740	-15.8680	11.0250	N	0
-3.4800	-14.2940	18.4340	H	0	-0.1140	-17.9670	24.2760	N	0	0.7540	-14.9800	11.0640	H	0
-0.3950	-13.0270	18.8020	C	0	-1.0130	-18.4230	24.2220	H	0	-0.7000	-16.2090	10.1040	C	0
0.3220	-14.0510	18.7370	O	0	0.8130	-18.4130	23.2360	C	0	-0.7580	-17.2790	9.9040	H	0
-0.9370	-12.6630	19.9480	N	0	1.7740	-18.4360	23.7500	H	0	-2.0680	-15.9470	10.7060	C	0
-1.5200	-11.8390	19.9540	H	0	0.3850	-19.8790	22.8450	C	0	-2.3160	-16.6330	11.5160	H	0
-0.9510	-13.5230	21.0810	C	0	0.1400	-20.4080	23.7650	H	0	-2.2200	-14.9330	11.0770	H	0
-0.4990	-14.4680	20.7780	H	0	-0.5790	-19.7160	22.3630	H	0	-2.9050	-15.9930	10.0090	H	0
-0.4080	-12.9920	22.4000	C	0	1.3560	-20.6610	21.9240	C	0	-0.4980	-15.4410	8.7740	C	0
-0.9180	-12.0420	22.5610	H	0	1.2630	-20.2420	20.9220	H	0	0.2720	-14.5140	8.7910	O	0
-0.5530	-13.7570	23.1620	H	0	2.3960	-20.6580	22.2500	H	0	-0.9130	-15.9790	7.5770	N	0

-1.4390	-16.8320	7.7020	H	0	-2.5690	-10.1290	-8.7040	N	0	-1.4510	-14.3170	-15.8130	N	0
-0.7730	-15.3670	6.2120	C	0	-3.4070	-9.6110	-8.4820	H	0	-0.6000	-13.7740	-15.8370	H	0
-0.8220	-14.2970	6.4140	H	0	-1.5690	-9.1710	-9.1450	C	0	-1.3390	-15.6720	-16.4500	C	0
0.5380	-15.7430	5.5060	C	0	-1.9140	-8.2080	-8.7680	H	0	-1.8240	-15.6390	-17.4260	H	0
1.3390	-15.5530	6.2200	H	0	-0.6280	-9.5070	-8.7100	H	0	0.1570	-15.8620	-16.8530	C	0
0.5370	-17.2770	5.1920	C	0	-1.5820	-9.0530	-10.6720	C	0	0.2520	-16.8310	-17.3450	H	0
0.3970	-17.8870	6.0840	H	0	-1.6970	-10.0700	-11.3600	O	0	0.5200	-15.1450	-17.5900	H	0
-0.2770	-17.4660	4.4920	H	0	-1.3290	-7.8270	-11.1420	N	0	0.8010	-15.8070	-15.9760	H	0
1.4880	-17.4620	4.6910	H	0	-1.2450	-7.0220	-10.5390	H	0	-1.8170	-16.8380	-15.6040	C	0
0.7720	-14.7820	4.3160	C	0	-1.0940	-7.6320	-12.5150	C	0	-2.3020	-17.7900	-16.2180	O	0
0.6500	-13.7320	4.5830	H	0	-2.0460	-7.6670	-13.0440	H	0	-1.9370	-16.8130	-14.2960	N	0
1.8200	-14.8510	4.0240	H	0	-0.5950	-6.1820	-12.5760	C	0	-1.7520	-15.9400	-13.8240	H	0
0.1530	-15.0850	3.4710	H	0	-1.3130	-5.4790	-12.1550	H	0	-2.2690	-17.9480	-13.4200	C	0
-1.9920	-15.6880	5.2850	C	0	0.3310	-6.0700	-12.0110	H	0	-2.6170	-18.7380	-14.0850	H	0
-2.5400	-16.7750	5.4400	O	0	-0.4080	-5.5070	-13.8730	C	0	-0.9580	-18.4380	-12.8590	C	0
-2.4090	-14.7280	4.4340	N	0	-0.7890	-5.9960	-15.0660	C	0	-0.1930	-18.5370	-13.6290	H	0
-1.9040	-13.8560	4.3610	H	0	-1.3080	-6.9370	-15.1710	H	0	-0.3620	-17.4250	-11.8550	C	0
-3.3920	-15.0760	3.3480	C	0	-0.5290	-5.0510	-16.0350	N	0	0.0130	-16.5320	-12.3540	H	0
-4.1670	-15.7090	3.7800	H	0	-0.6010	-5.2560	-17.0210	H	0	-1.0770	-17.0110	-11.1440	H	0
-3.9190	-13.7420	2.8260	C	0	-0.0700	-3.8460	-15.5340	C	0	0.5140	-17.8460	-11.3620	H	0
-3.1060	-13.0330	2.6710	H	0	0.5140	-2.6210	-16.0850	C	0	-1.1620	-19.7840	-12.1460	C	0
-4.4340	-13.9260	1.8830	H	0	0.5410	-2.3570	-17.1320	H	0	-1.5850	-20.5210	-12.8300	H	0
-4.9040	-12.9450	3.8140	C	0	0.9050	-1.6100	-15.2580	C	0	-0.3050	-20.2460	-11.6560	H	0
-5.1930	-13.3580	5.1150	C	0	1.3080	-0.6820	-15.6340	H	0	-1.9420	-19.6590	-11.3960	H	0
-4.7050	-14.1850	5.6090	H	0	0.8220	-1.8030	-13.8850	C	0	-3.4530	-17.6600	-12.4690	C	0
-6.2290	-12.7720	5.8880	C	0	1.2630	-1.0510	-13.2470	H	0	-4.3620	-18.5060	-12.2620	O	0
-6.3800	-13.1460	6.8900	H	0	0.5040	-3.0490	-13.3770	C	0	-3.5630	-16.4450	-11.9770	N	0
-7.0430	-11.7650	5.3800	C	0	0.3460	-3.1650	-12.3140	H	0	-2.8130	-15.7970	-12.1740	H	0
-8.0300	-11.2360	6.2110	O	0	0.0250	-4.1380	-14.1250	C	0	-4.7530	-18.8920	-11.3370	C	0
-8.3450	-10.3960	5.8700	H	0	-0.0680	-8.6230	-13.1460	C	0	-4.9540	-16.4780	-10.4400	H	0
-6.8310	-11.3600	4.0600	C	0	-0.3070	-9.0010	-14.2950	O	0	-4.4390	-14.4250	-10.9690	C	0
-7.4290	-10.5360	3.7020	H	0	1.1050	-8.8910	-12.5560	N	0	-5.2480	-14.0200	-10.3620	H	0
-5.7360	-11.9150	3.3340	C	0	1.2440	-8.4510	-11.6570	H	0	-3.5080	-14.3390	-10.4070	H	0
-5.6130	-11.6380	2.2970	H	0	2.1890	-9.8080	-12.9180	C	0	-4.3960	-13.7230	-11.8020	H	0
-2.6630	-15.8310	2.2090	C	0	2.4560	-9.7300	-13.9720	H	0	-5.9620	-16.0020	-12.2820	C	0
-1.5710	-15.4580	1.7950	O	0	3.2950	-9.6280	-11.8960	C	0	-7.1220	-16.0550	-11.8810	O	0
-3.2120	-16.8790	1.6400	N	0	3.6190	-8.5890	-11.8400	H	0	-5.7190	-15.9340	-13.5260	N	0
-4.0840	-17.1420	2.0770	H	0	2.9040	-9.9910	-10.9460	H	0	-4.7740	-16.0060	-13.8760	H	0
-2.7360	-17.5940	0.4490	C	0	4.5750	-10.4390	-12.2020	C	0	-6.7460	-15.7720	-14.6040	C	0
-1.9760	-16.9820	-0.0370	H	0	4.6240	-11.7950	-11.8870	C	0	-7.6620	-16.1260	-14.1290	H	0
-2.2650	-18.9980	0.8660	C	0	3.7550	-12.2430	-11.4280	H	0	-6.9200	-14.2170	-14.9850	C	0
-1.3480	-18.9430	1.4530	H	0	5.7520	-12.5570	-12.2500	C	0	-6.1740	-13.9190	-15.7220	H	0
-2.9390	-19.4030	1.6210	H	0	5.8100	-13.6130	-12.0280	H	0	-7.8640	-14.1300	-15.5230	H	0
-2.0590	-19.9150	-0.1800	O	0	6.8330	-11.8540	-12.9280	C	0	-6.7550	-13.2470	-13.8520	C	0
-1.3820	-19.4900	-0.7120	H	0	7.7430	-12.3850	-13.1670	H	0	-7.3650	-13.6610	-13.0500	H	0
-3.8730	-17.6440	-0.5770	C	0	6.8100	-10.4350	-12.9880	C	0	-5.7040	-13.2170	-13.5670	H	0
-4.9190	-18.3030	-0.4000	O	0	7.6720	-9.9070	-13.3700	H	0	-7.3110	-11.8710	-14.2590	C	0
-3.6700	-16.9230	-1.6640	N	0	5.6540	-9.7350	-12.7070	C	0	-8.2690	-11.6630	-15.0530	O	0
-2.7660	-16.4820	-1.7580	H	0	5.5060	-8.6740	-12.8460	H	0	-6.7130	-10.8190	-13.7610	N	0
-4.5220	-16.8020	-2.7370	C	0	1.5980	-11.2330	-12.9270	C	0	-7.1400	-9.9690	-14.1010	H	0
-4.6360	-17.7760	-3.2140	H	0	1.8650	-11.9310	-13.8800	O	0	-5.9060	-10.8700	-13.1550	H	0
-5.5530	-16.5700	-2.4730	H	0	0.8650	-11.6760	-11.9480	N	0	-6.4460	-16.6090	-15.9100	C	0
-4.1460	-15.7170	-3.7360	C	0	0.7440	-11.0240	-11.1860	H	0	-7.3300	-16.6910	-16.7470	O	0
-4.5260	-14.5940	-3.6610	O	0	0.1870	-12.9480	-11.8590	C	0	-5.3770	-17.3110	-16.0140	N	0
-3.6370	-16.2220	-4.8560	N	0	0.8890	-13.7810	-11.8800	H	0	-4.6680	-17.3040	-15.2950	H	0
-3.4190	-17.2080	-4.8820	H	0	-0.1600	-13.0050	-10.8270	H	0	-5.1700	-18.3200	-17.1130	C	0
-2.8700	-15.4970	-5.9410	C	0	-0.9660	-13.2660	-12.7290	C	0	-4.1670	-18.7130	-16.9460	H	0
-1.9370	-15.0680	-5.5750	H	0	-1.5950	-14.3540	-12.6070	O	0	-6.2280	-19.5130	-16.9930	C	0
-2.2940	-16.5310	-7.0070	C	0	-1.3160	-12.3940	-13.6840	N	0	-7.1960	-19.0890	-17.2620	H	0
-1.7510	-17.3140	-6.4780	H	0	-0.9270	-11.4620	-13.6580	H	0	-5.9900	-20.3170	-17.6900	H	0
-3.3970	-17.2680	-7.8470	C	0	-2.5140	-12.4780	-14.6220	C	0	-6.1110	-20.3190	-15.7420	C	0
-4.0380	-17.8630	-7.1970	H	0	-3.3480	-12.5530	-13.9250	H	0	-4.9970	-20.6350	-15.3550	O	0
-3.9980	-16.5320	-8.3820	H	0	-2.5920	-11.1790	-15.4490	C	0	-7.1970	-20.6310	-15.0020	N	0
-2.9410	-17.9110	-8.6000	H	0	-2.4780	-10.3640	-14.7340	H	0	-6.9920	-21.1790	-14.1790	H	0
-1.3830	-15.9020	-8.1630	C	0	-1.3170	-11.0270	-16.3480	C	0	-8.1000	-20.3910	-15.3850	H	0
-1.9830	-15.1930	-8.7330	H	0	-1.5380	-11.6710	-17.1990	H	0	-5.1510	-17.6330	-18.5130	C	0
-0.5380	-15.3530	-7.7480	H	0	-1.1650	-10.0050	-16.6960	H	0	-5.5200	-18.2710	-19.5680	O	0
-0.9950	-16.6700	-8.8310	H	0	-0.3870	-11.3760	-15.8990	H	0	-4.5090	-16.4540	-18.5640	N	0
-3.6780	-14.3510	-6.5790	C	0	-3.9700	-11.0340	-15.9950	C	0	-4.1020	-16.0780	-17.7190	H	0
-4.9330	-14.4840	-6.6720	O	0	-4.1560	-11.9270	-16.5910	H	0	-3.9850	-16.0080	-19.8870	C	0
-3.0470	-13.2770	-6.8830	N	0	-4.7030	-11.0270	-15.1880	H	0	-4.8490	-15.9380	-20.5480	H	0
-2.0500	-13.2830	-6.7220	H	0	-4.1150	-9.9010	-16.9700	C	0	-3.6210	-14.5650	-19.7330	C	0
-3.5770	-12.1650	-7.7330	C	0	-3.9720	-8.9290	-16.4980	H	0	-2.9380	-14.5140	-18.8840	H	0
-4.2430	-12.5300	-8.5140	H	0	-3.4270	-9.9960	-17.8090	H	0	-3.0990	-14.2370	-20.6320	H	0
-4.0480	-11.5080	-7.0020	H	0	-5.1490	-10.0640	-17.2740	H	0	-4.8030	-13.5950	-19.5950	C	0
-2.4650	-11.4540	-8.5080	C	0	-2.5870	-13.7530	-15.4310	C	0	-5.3940	-13.6520	-18.6810	H	0
-1.4910	-12.0850	-8.8320	O	0	-3.6850	-14.3580	-15.4860	O	0	-4.1590	-12.1690	-19.5820	C	0

-4.9270	-11.4420	-19.3180	H	0	1.2230	-7.5010	-25.1680	C	0	1.0690	-11.0190	-21.6880	H	0
-3.4020	-12.1480	-18.7980	H	0	1.9950	-6.9340	-24.6490	H	0	1.0440	-13.1530	-21.7460	C	0
-3.6940	-11.9300	-20.5390	H	0	1.1270	-6.8290	-26.5450	C	0	0.1880	-13.2560	-22.4120	H	0
-5.8380	-13.5970	-20.7700	C	0	0.5100	-7.3050	-27.3070	H	0	2.0170	-13.2110	-22.2350	H	0
-6.4650	-12.7100	-20.6780	H	0	0.5750	-5.8930	-26.4660	H	0	1.0090	-14.0510	-21.1290	H	0
-5.2870	-13.4460	-21.6980	H	0	2.4320	-6.3800	-27.1860	C	0	-0.5230	-11.6620	-20.3250	C	0
-6.2760	-14.5950	-20.7570	H	0	3.2010	-7.2850	-28.0160	C	0	-0.7160	-12.5020	-19.6570	H	0
-2.7950	-16.8060	-20.4750	C	0	2.8310	-8.2910	-28.1520	H	0	-0.6500	-10.7120	-19.8060	H	0
-1.8500	-17.2170	-19.8320	O	0	4.4360	-6.8480	-28.5550	C	0	-1.1530	-11.7090	-21.2130	H	0
-2.7670	-16.9890	-21.7660	N	0	4.8860	-7.4940	-29.2930	H	0	3.3360	-12.0740	-20.1250	C	0
-3.7990	-16.7360	-22.7960	C	0	4.9510	-5.5380	-28.3080	C	0	3.8070	-13.2130	-19.7960	O	0
-4.0230	-15.6770	-22.9220	H	0	6.2710	-5.3360	-28.7170	O	0	4.0570	-11.2050	-20.7940	N	0
-4.7320	-17.2400	-22.5410	H	0	6.5320	-5.8680	-29.4720	H	0	3.6160	-10.3180	-20.9930	H	0
-3.4020	-17.3750	-24.1270	C	0	4.2460	-4.7010	-27.3790	C	0	5.4500	-11.4150	-21.2460	C	0
-2.7820	-16.7080	-24.7260	H	0	4.6290	-3.7550	-27.0280	H	0	5.4250	-12.1670	-22.0340	H	0
-4.2490	-17.7560	-24.6970	H	0	2.9370	-5.0850	-26.9110	C	0	5.9360	-10.5100	-21.6100	H	0
-2.4260	-18.4560	-23.6310	C	0	2.4220	-4.4060	-26.2490	H	0	6.3270	-11.8980	-20.1680	C	0
-1.7090	-18.6590	-24.4260	H	0	-0.0750	-7.4050	-24.3910	C	0	6.7820	-13.0130	-20.1480	O	0
-2.8680	-19.4150	-23.3620	H	0	-0.5000	-6.2970	-24.1800	O	0	6.4570	-11.0110	-19.2290	N	0
-1.6850	-17.7820	-22.4290	C	0	-0.6980	-8.5030	-23.9340	N	0	6.0160	-10.1110	-19.3540	H	0
-1.3170	-18.5650	-21.7660	H	0	-0.2830	-9.4080	-24.1020	H	0	7.1420	-11.2760	-17.9890	C	0
-0.5350	-17.0550	-23.0120	C	0	-1.8980	-8.5780	-23.1080	C	0	8.0930	-11.7320	-18.2630	H	0
-0.5680	-15.8510	-23.1370	O	0	-2.4940	-7.7510	-23.4950	H	0	7.5440	-9.9150	-17.2590	C	0
0.5550	-17.7190	-23.3290	N	0	-2.6580	-9.8440	-23.4900	C	0	8.0010	-9.2030	-17.9470	H	0
0.7640	-19.1510	-23.2550	C	0	-3.5540	-9.9320	-22.8750	H	0	6.4130	-9.2780	-16.3630	C	0
-0.0290	-19.7180	-23.7430	H	0	-2.9810	-9.8250	-24.5310	H	0	6.8220	-8.4270	-15.8170	H	0
0.9220	-19.4060	-22.2070	H	0	-2.0350	-10.7290	-23.3580	H	0	5.5080	-9.0250	-16.9140	H	0
1.9970	-19.4310	-24.0780	C	0	-1.6540	-8.3790	-21.6560	C	0	6.2180	-10.0670	-15.6370	H	0
1.7440	-19.6640	-25.1120	H	0	-0.4600	-8.5060	-21.1540	O	0	8.7230	-10.2170	-16.3860	C	0
2.5380	-20.2820	-23.6640	H	0	-2.7450	-7.9690	-20.9730	N	0	9.4820	-10.5990	-17.0690	H	0
2.7410	-18.0910	-23.9970	C	0	-3.6350	-7.9370	-21.4500	H	0	9.1050	-9.3940	-15.7820	H	0
3.5330	-17.9570	-24.7330	H	0	-2.8340	-7.5490	-19.5160	C	0	8.6140	-11.0450	-15.6850	H	0
3.2830	-18.0070	-23.0540	H	0	-3.8540	-7.2390	-19.2870	H	0	6.5020	-12.4090	-17.1150	C	0
1.6920	-17.0410	-23.9610	C	0	-2.6350	-8.3390	-18.7920	H	0	7.2850	-13.1600	-16.5230	O	0
1.8130	-16.1730	-23.3120	H	0	-1.9600	-6.3210	-19.2690	C	0	5.2160	-12.5990	-17.0820	N	0
1.3600	-16.5170	-25.3760	C	0	-1.1510	-6.3100	-18.3730	O	0	4.5480	-12.0060	-17.5540	H	0
2.2310	-16.0050	-26.0210	O	0	-1.9170	-5.4880	-20.3170	N	0	4.6830	-13.8160	-16.3880	C	0
0.1160	-16.7510	-25.8480	N	0	-2.4930	-5.6770	-21.1250	H	0	4.7950	-13.6380	-15.3180	H	0
-0.5310	-17.3860	-25.4010	H	0	-0.9610	-4.3050	-20.3560	C	0	3.1530	-13.8560	-16.5430	C	0
-0.2200	-16.5090	-27.2220	C	0	-1.1270	-3.7870	-21.3010	H	0	2.8820	-14.7230	-17.1470	H	0
0.5270	-17.0740	-27.7800	H	0	-1.3960	-3.1730	-19.3880	C	0	2.7370	-13.9360	-15.5390	H	0
-1.6300	-17.0240	-27.5840	C	0	-1.9640	-3.5820	-18.5520	H	0	2.8240	-12.9740	-17.0930	H	0
-2.3480	-16.3840	-27.0720	H	0	-0.4790	-2.7300	-18.9980	H	0	5.3060	-15.1960	-16.8240	C	0
-1.8650	-16.7750	-28.6190	H	0	-2.1040	-1.9820	-20.0710	C	0	5.6790	-16.0170	-15.9460	O	0
-2.0080	-18.5060	-27.3050	C	0	-2.8860	-2.3830	-20.7170	H	0	5.2490	-15.4820	-18.1280	N	0
-3.2230	-18.8180	-27.5970	O	0	-2.8350	-1.2820	-18.9300	C	0	4.7630	-14.8300	-18.7270	H	0
-1.1310	-19.3480	-26.8940	O	0	-3.5060	-0.5130	-19.3110	H	0	5.9600	-16.5700	-18.8200	C	0
-0.0830	-15.0260	-27.5980	C	0	-3.4790	-1.9340	-18.3400	H	0	5.6950	-17.4340	-18.2110	H	0
-0.0860	-14.7570	-28.8200	O	0	-2.2260	-0.6090	-18.3260	H	0	5.3140	-16.8240	-20.1440	C	0
-0.0130	-14.1320	-26.7230	N	0	-1.2860	-1.0090	-20.8590	C	0	5.3560	-15.8570	-20.6460	H	0
0.2910	-14.3870	-25.7940	H	0	-1.1200	-1.3800	-21.8700	H	0	5.8770	-17.5220	-20.7640	H	0
0.1070	-12.6630	-26.9170	C	0	-1.9240	-0.1420	-21.0300	H	0	3.8100	-17.3340	-20.1000	C	0
0.5990	-12.2730	-27.8080	H	0	-0.3510	-0.7230	-20.3770	H	0	2.7060	-16.4250	-20.0610	C	0
-1.3270	-12.1500	-27.1530	C	0	0.5500	-4.7240	-20.3330	C	0	2.8940	-15.3670	-20.1750	H	0
-1.7250	-12.6220	-28.0510	H	0	1.4290	-3.9520	-19.9380	O	0	1.4410	-16.9750	-19.9770	C	0
-1.9210	-12.4170	-26.2790	H	0	0.8710	-5.9320	-20.9340	N	0	0.5380	-16.3990	-20.1180	H	0
-1.4040	-10.6460	-27.3300	C	0	0.0900	-6.4370	-21.3280	H	0	1.2910	-18.3880	-19.7500	C	0
-0.3360	-10.0640	-27.3690	O	0	2.2840	-6.2660	-21.2310	C	0	0.0350	-18.8650	-19.5960	O	0
-2.5560	-10.1120	-27.3380	O	0	2.2740	-6.9900	-22.0460	H	0	-0.6430	-18.2240	-19.8230	H	0
0.7990	-12.0390	-25.6480	C	0	2.8050	-5.3520	-21.5160	H	0	2.3790	-19.3070	-19.9070	C	0
0.1540	-11.9120	-24.6560	O	0	2.9470	-7.0040	-20.1020	C	0	2.2870	-20.3720	-19.7510	H	0
2.1420	-11.7310	-25.7000	N	0	4.1390	-7.2430	-20.2500	O	0	3.6330	-18.7360	-20.0820	C	0
2.9830	-11.8330	-26.9420	C	0	2.2180	-7.4400	-19.0160	N	0	4.4710	-19.4070	-20.2050	H	0
2.5230	-11.4630	-27.8580	H	0	1.3100	-7.0360	-18.8400	H	0	7.4960	-16.4030	-18.9030	C	0
3.3500	-12.8320	-27.1760	H	0	2.7390	-8.2630	-17.9670	C	0	8.1120	-17.4610	-18.8420	O	0
4.1680	-10.9320	-26.7600	C	0	3.7570	-7.9380	-17.7510	H	0	8.1200	-15.1820	-18.7550	N	0
3.9430	-9.8990	-27.0270	H	0	2.0390	-8.0020	-16.6480	C	0	7.4780	-14.4020	-18.7710	H	0
5.0240	-11.3530	-27.2860	H	0	0.9520	-8.0790	-16.6880	H	0	9.6120	-15.0950	-18.6510	C	0
4.4210	-11.0710	-25.2500	C	0	2.4770	-8.6680	-15.9050	H	0	10.0440	-15.7800	-19.3800	H	0
4.9660	-10.2480	-24.7890	H	0	2.2830	-7.0280	-16.2240	H	0	10.0950	-13.6920	-18.8860	C	0
4.7840	-12.0760	-25.0330	H	0	2.6210	-9.7120	-18.3510	C	0	9.4870	-13.1910	-19.6390	H	0
2.9690	-11.0390	-24.7040	C	0	3.4290	-10.4990	-17.7520	O	0	9.9330	-13.0960	-17.9870	H	0
2.9910	-11.5970	-23.7680	H	0	1.8430	-10.1800	-19.2930	N	0	11.6270	-13.5930	-19.2010	C	0
2.5660	-9.5140	-24.5070	C	0	1.1170	-9.6010	-19.6890	H	0	12.1460	-14.2610	-18.5140	H	0
3.0420	-8.9780	-23.5120	O	0	1.8860	-11.6230	-19.7440	C	0	11.8220	-14.0290	-20.1810	H	0
1.6580	-8.8900	-25.2980	N	0	1.6180	-12.2340	-18.8820	H	0	12.3310	-12.2380	-19.1250	C	0
1.0700	-9.5070	-25.8400	H	0	0.8870	-11.7960	-20.9450	C	0	11.7340	-11.1620	-19.0570	O	0



13.6340	-12.1970	-19.2410	N	0	4.1140	-22.7060	-11.1970	N	0	-7.5190	-22.2280	3.1470	H	0
14.1060	-11.3250	-19.0460	H	0	4.3820	-21.8610	-11.6810	H	0	-7.7320	-22.1990	1.0330	C	0
14.0970	-13.0930	-19.1950	H	0	4.3750	-22.8640	-9.6870	C	0	-8.8560	-22.7360	1.0800	O	0
10.0540	-15.6950	-17.3400	C	0	4.8910	-23.8170	-9.5700	H	0	-7.2960	-21.7010	-0.0110	O	0
11.0380	-16.4670	-17.2520	O	0	5.4550	-21.8000	-9.2390	C	0	-6.5560	-18.4280	3.3850	C	0
9.3240	-15.4820	-16.2540	N	0	5.0370	-20.7950	-9.1790	H	0	-5.5370	-17.7630	3.1310	O	0
8.5830	-14.8010	-16.3430	H	0	5.8100	-22.1720	-8.2780	H	0	-7.1380	-18.3410	4.6340	N	0
9.6480	-15.9950	-14.9350	C	0	6.3130	-21.6990	-9.9040	H	0	-7.8470	-19.0220	4.8670	H	0
10.7210	-15.8680	-14.7920	H	0	3.1920	-22.8490	-8.7410	C	0	-6.3210	-18.0800	5.7870	C	0
8.8560	-15.1380	-13.9980	C	0	3.2520	-23.1980	-7.5370	O	0	-5.5720	-17.3440	5.4950	H	0
7.7760	-15.2830	-13.9740	H	0	2.0210	-22.5500	-9.2840	N	0	-7.2380	-17.6930	6.9440	C	0
9.2560	-15.2850	-12.9940	H	0	1.9880	-22.5720	-10.2930	H	0	-7.6500	-16.7200	6.6740	H	0
8.9950	-14.0810	-14.2260	H	0	0.8830	-22.2320	-8.4240	C	0	-7.9950	-18.4290	7.2140	H	0
9.2050	-17.4720	-14.7840	C	0	0.8220	-22.9150	-7.5770	H	0	-6.4450	-17.4920	8.2520	C	0
9.6620	-18.1940	-13.9100	O	0	1.0300	-20.8080	-7.8260	C	0	-5.8740	-18.3880	8.4970	H	0
8.4160	-18.0150	-15.7340	N	0	2.1070	-20.6500	-7.7750	H	0	-5.3740	-16.3780	8.2940	C	0
8.2060	-17.4090	-16.5140	H	0	0.4550	-19.7110	-8.6600	C	0	-5.6650	-15.5470	7.6520	H	0
7.7860	-19.4130	-15.6770	C	0	-0.6160	-19.5780	-8.5040	H	0	-5.0970	-16.1190	9.3160	H	0
7.4030	-19.6790	-16.6620	H	0	1.0100	-18.8100	-8.3980	H	0	-4.4930	-16.8750	7.8870	H	0
8.5490	-20.1550	-15.4400	H	0	0.5810	-20.0230	-9.6970	H	0	-7.4080	-17.1900	9.4100	C	0
6.6560	-19.5220	-14.6410	C	0	0.4270	-20.6020	-6.5690	O	0	-7.7860	-16.1770	9.2690	H	0
6.3060	-20.6700	-14.3010	O	0	0.8970	-21.1450	-5.9320	H	0	-8.2740	-17.8380	9.5430	H	0
6.0410	-18.4240	-14.1190	N	0	-0.5370	-22.4900	-9.0890	C	0	-6.8430	-17.2350	10.3400	H	0
6.2220	-17.5590	-14.6080	H	0	-0.6400	-22.9000	-10.2550	O	0	-5.5030	-19.3470	6.0820	C	0
5.1870	-18.3390	-12.9350	C	0	-1.6540	-22.3090	-8.2990	N	0	-5.9670	-20.5120	6.1070	O	0
5.7710	-18.7600	-12.1160	H	0	-1.4770	-21.9770	-7.3610	H	0	-4.2470	-19.1740	6.5440	N	0
4.7110	-16.9500	-12.4960	C	0	-3.0730	-22.5530	-8.6700	C	0	-3.7340	-18.3290	6.3370	H	0
5.5820	-16.3170	-12.3270	H	0	-3.3230	-22.4390	-9.7250	H	0	-3.4820	-20.1420	7.2590	C	0
4.1780	-16.5400	-13.3540	H	0	-3.5270	-23.9800	-8.4820	C	0	-4.1990	-20.8920	7.5920	H	0
3.7350	-16.8480	-11.2100	C	0	-2.8100	-24.6030	-9.0170	H	0	-2.3480	-20.6950	6.4150	C	0
2.7910	-17.2800	-11.5410	H	0	-3.5630	-24.4340	-7.0290	C	0	-1.7260	-19.8550	6.1070	H	0
4.2580	-17.4320	-9.8450	C	0	-2.5870	-24.2550	-6.5800	H	0	-1.7210	-21.2270	7.1300	H	0
3.5090	-17.9270	-9.0640	H	0	-4.3900	-23.9060	-6.5540	H	0	-2.6690	-21.6210	5.1950	C	0
4.3190	-18.5130	-9.9680	H	0	-3.6880	-25.5170	-6.9940	H	0	-2.6180	-21.2000	3.8270	C	0
5.2010	-17.0430	-9.4600	H	0	-4.7830	-24.1260	-9.0660	O	0	-2.3430	-20.1580	3.7680	H	0
3.4210	-15.4080	-10.9510	C	0	-5.0800	-25.0130	-8.8490	H	0	-2.8800	-22.1830	2.7960	C	0
4.2760	-14.7980	-10.6590	H	0	-3.9740	-21.5600	-7.9180	C	0	-2.9170	-21.8580	1.7670	H	0
3.0400	-15.1080	-11.9270	H	0	-3.5830	-20.8930	-6.9470	O	0	-3.2800	-23.4710	3.2100	C	0
2.5660	-15.2710	-10.2890	H	0	-5.2560	-21.2970	-8.3530	N	0	-3.6170	-24.2800	2.1900	O	0
3.9080	-19.3110	-13.0620	C	0	-5.5550	-21.5720	-9.2780	H	0	-3.5990	-23.7980	1.3600	H	0
3.5980	-19.9210	-12.0570	O	0	-6.1450	-20.3510	-7.5710	C	0	-3.2120	-23.9480	4.5160	C	0
3.2640	-19.5270	-14.2080	N	0	-5.5230	-19.4910	-7.3230	H	0	-3.4430	-24.9850	4.7110	H	0
3.3960	-18.7670	-15.4410	C	0	-7.3070	-19.9510	-8.5390	C	0	-2.9430	-22.9680	5.5090	C	0
4.3430	-18.9860	-15.9350	H	0	-7.6610	-20.8600	-9.0250	H	0	-3.0380	-23.3060	6.5300	H	0
3.4530	-17.7080	-15.1920	H	0	-8.4930	-19.2450	-7.8070	C	0	-2.8880	-19.4930	8.5360	C	0
2.1670	-19.1050	-16.2320	C	0	-9.2260	-18.7570	-8.4490	H	0	-2.5570	-18.2870	8.6040	O	0
2.2250	-18.8160	-17.2810	H	0	-9.0750	-20.0410	-7.3430	H	0	-2.7460	-20.3120	9.6190	N	0
1.4720	-18.3880	-15.7930	H	0	-8.1190	-18.5540	-7.0520	H	0	-3.1610	-21.2200	9.4680	H	0
1.8050	-20.5000	-15.8670	C	0	-6.8600	-18.8710	-9.4470	C	0	-2.2860	-19.9690	11.0130	C	0
2.3430	-21.2650	-16.4270	H	0	-6.7800	-17.9180	-8.9230	H	0	-1.8570	-18.9670	10.9930	H	0
0.7450	-20.7330	-15.9690	H	0	-5.8480	-19.0750	-9.7950	H	0	-3.4050	-19.8150	12.0150	C	0
2.2110	-20.5070	-14.3340	C	0	-7.5690	-18.7630	-10.2680	H	0	-3.8570	-20.8040	12.0940	H	0
1.3950	-20.2300	-13.6660	H	0	-6.6210	-21.0020	-6.1960	C	0	-3.0540	-19.3220	13.4250	C	0
2.5350	-21.9420	-14.0750	C	0	-6.9890	-22.1870	-6.1720	O	0	-3.9980	-19.0810	13.9140	H	0
1.6580	-22.7700	-13.8490	O	0	-6.5450	-20.1440	-5.1540	N	0	-2.5780	-20.1680	13.9210	H	0
3.8380	-22.2930	-13.9740	N	0	-6.2450	-19.2140	-5.4100	H	0	-2.4130	-18.4430	13.4890	H	0
4.5320	-21.5900	-14.1860	H	0	-7.0310	-20.5090	-3.8310	C	0	-4.4790	-18.8930	11.3550	C	0
4.2840	-23.6270	-13.4270	C	0	-7.8070	-21.2640	-3.9590	H	0	-4.0510	-17.9890	10.9230	H	0
3.6370	-24.3620	-13.9080	H	0	-6.3070	-21.0020	-3.1820	H	0	-5.0580	-19.5230	10.6800	H	0
5.7720	-23.9480	-13.8140	C	0	-7.4540	-19.2970	-3.0420	C	0	-5.2190	-18.6360	12.1120	H	0
6.4260	-23.2930	-13.2390	H	0	-7.5150	-18.1950	-3.6550	O	0	-1.2750	-20.9680	11.5480	C	0
6.0700	-24.8360	-13.2570	H	0	-7.7920	-19.3610	-1.7440	N	0	-1.4260	-22.1260	11.3460	O	0
6.1000	-23.9850	-15.3210	C	0	-8.0080	-20.2680	-1.3560	H	0	-0.2370	-20.5520	12.2470	N	0
5.4690	-24.7160	-15.8260	H	0	-8.2470	-18.2180	-0.9680	C	0	-0.1340	-19.5580	12.3980	H	0
5.8740	-23.0200	-15.7740	H	0	-7.6510	-17.3540	-1.2610	H	0	0.9970	-21.3340	12.6900	C	0
7.5830	-24.1930	-15.4310	C	0	-9.2290	-18.0610	-1.4160	H	0	0.7850	-22.3940	12.5530	H	0
8.1490	-23.3190	-15.1080	H	0	-8.3470	-18.4440	0.5360	C	0	2.0630	-20.8810	11.7290	C	0
7.9830	-25.0240	-14.8500	H	0	-9.3780	-18.3590	1.2200	O	0	2.2730	-19.8190	11.8500	H	0
7.8780	-24.4490	-16.9240	C	0	-7.2120	-18.8880	1.1090	N	0	2.9960	-21.3180	12.0870	H	0
7.1620	-25.1840	-17.2900	H	0	-6.3270	-18.9330	0.6240	H	0	1.8470	-21.2770	10.3040	C	0
7.8130	-23.5640	-17.5580	H	0	-7.0540	-19.5190	2.4420	C	0	1.2750	-20.3290	9.4150	C	0
9.2400	-24.9550	-16.9340	N	0	-8.0180	-19.9000	2.7800	H	0	0.9600	-19.3530	9.7540	H	0
9.7630	-24.7170	-16.1030	H	0	-6.0830	-20.8270	2.3390	C	0	0.9280	-20.5930	8.0800	C	0
9.2410	-25.9580	-16.8170	H	0	-5.4320	-20.6260	1.4890	H	0	0.3160	-19.9520	7.4630	H	0
9.7880	-24.6010	-17.7050	H	0	-5.4280	-20.7770	3.2090	H	0	1.2010	-21.8170	7.5600	C	0
3.9810	-23.7690	-11.9840	C	0	-6.9220	-22.1330	2.2400	C	0	1.0440	-21.9860	6.5050	H	0
3.5210	-24.8240	-11.5440	O	0	-6.1070	-22.8550	2.1850	H	0	1.8940	-22.7790	8.3660	C	0

2.1570	-23.7370	7.9410	H	0	<b>Yb-MDH (XoxF-type)</b>	40.7510	50.5630	61.9550	C	0
2.2770	-22.5270	9.7030	C	0		41.0140	51.0650	61.0240	H	0
2.8150	-23.3030	10.2270	H	0	39.2640	51.0710	68.8850	N	0	
1.4590	-20.9690	14.0700	C	0	40.0210	51.6500	69.2180	H	0	
1.2700	-19.8490	14.5210	O	0	39.4110	50.2020	69.3780	H	0	
1.9870	-21.9490	14.7530	N	0	38.3580	51.5080	68.9760	H	0	
2.1120	-22.7880	14.2050	H	0	39.4630	50.9430	67.4440	C	0	
2.4190	-21.9160	16.1780	C	0	38.7340	50.1670	67.2070	H	0	
2.9670	-20.9950	16.3790	H	0	39.1750	52.2840	66.6820	C	0	
1.1800	-22.0020	17.0590	C	0	38.4820	52.9470	67.2000	H	0	
1.3940	-21.9210	18.1250	H	0	40.0640	52.9090	66.5890	H	0	
0.5590	-21.2050	16.6500	H	0	38.5600	52.0650	65.2900	C	0	
0.8010	-23.0130	16.9080	H	0	37.7720	51.1730	65.1770	O	0	
3.4450	-23.0070	16.4790	C	0	39.0390	52.7400	64.2500	N	0	
3.7990	-23.8340	15.6010	O	0	38.7230	52.4320	63.3410	H	0	
4.0180	-23.0660	17.7000	N	0	39.8450	53.3300	64.4000	H	0	
3.7430	-22.4510	18.4530	H	0	40.8220	50.3730	67.0610	C	0	
4.9270	-24.1700	18.1410	C	0	40.9040	49.4680	66.2710	O	0	
5.4980	-24.5550	17.2960	H	0	41.8990	50.8550	67.6270	N	0	
5.9730	-23.5830	19.0560	C	0	41.8830	51.6550	68.2440	H	0	
5.3500	-23.3390	19.9160	H	0	43.2340	50.5810	67.1600	C	0	
6.6930	-24.2690	19.5020	H	0	43.2730	51.0690	66.1860	H	0	
6.8260	-22.3840	18.6130	C	0	44.3600	51.1490	68.0780	C	0	
6.2950	-21.5870	18.0920	H	0	44.2970	50.7320	69.0830	H	0	
7.5780	-21.7670	19.7650	C	0	45.3110	50.8850	67.6150	H	0	
8.1600	-20.9000	19.4530	H	0	44.3870	52.6710	68.2890	C	0	
6.8210	-21.5120	20.5070	H	0	45.2900	53.0880	69.0770	O	0	
8.2230	-22.5970	20.0550	H	0	43.5830	53.4440	67.7780	O	0	
7.8120	-22.8950	17.6120	C	0	43.5860	49.0440	67.0150	C	0	
8.3810	-22.0490	17.2280	H	0	44.2410	48.5790	66.1110	O	0	
8.5040	-23.5860	18.0940	H	0	43.0080	48.2820	67.9190	N	0	
7.2780	-23.3590	16.7820	H	0	42.5340	48.7770	68.6610	H	0	
4.2150	-25.4630	18.7190	C	0	43.0160	46.8340	68.0310	C	0	
3.3220	-25.4020	19.5690	O	0	44.0320	46.5790	68.3330	H	0	
4.5930	-26.5020	18.0600	O	0	42.0040	46.3250	69.1080	C	0	
-4.6830	-2.2510	-8.1290	N	0	42.2270	45.2770	69.3080	H	0	
-3.9580	-3.3730	-8.4190	C	0	42.3600	46.8280	70.0070	H	0	
-4.0710	-4.6220	-7.6550	C	0	40.5250	46.5840	69.0110	C	0	
-3.2240	-5.5220	-7.8330	O	0	40.1460	46.3590	68.0140	H	0	
-4.9180	-4.7520	-6.8070	O	0	40.0110	45.8610	69.6440	H	0	
-2.9510	-3.0820	-9.3110	C	0	39.9620	48.0130	69.2480	C	0	
-3.0510	-1.6650	-9.5590	C	0	40.6840	48.8400	69.8320	O	0	
-4.2110	-1.1860	-8.9260	C	0	38.8280	48.3760	68.8450	O	0	
-2.0360	-0.8080	-10.2170	C	0	42.5820	46.1220	66.6350	C	0	
-0.9570	-1.2180	-10.5530	O	0	43.0710	45.0190	66.3980	O	0	
-2.3840	0.7380	-10.3080	C	0	41.7530	46.7330	65.8380	N	0	
-1.8080	1.5680	-11.0250	O	0	41.3790	47.6190	66.1470	H	0	
-3.6230	1.2180	-9.5310	C	0	41.4920	46.1630	64.5330	C	0	
-3.9240	2.5280	-9.6880	N	0	41.7330	45.1030	64.4520	H	0	
-5.0700	3.0300	-9.1570	C	0	40.1010	46.6170	64.2210	C	0	
-5.2360	4.5230	-9.3650	C	0	39.4320	46.4280	65.0610	H	0	
-4.4550	4.9550	-10.2610	O	0	40.1240	47.7010	64.1080	H	0	
-6.2160	5.0930	-8.9290	O	0	39.3510	45.9610	62.9560	C	0	
-5.9080	2.1660	-8.4310	C	0	38.2790	45.9210	63.1500	H	0	
-5.6560	0.8160	-8.3380	C	0	39.7580	46.6590	61.6260	C	0	
-6.7330	0.0280	-7.5580	C	0	40.8200	46.5360	61.4130	H	0	
-6.6490	-1.0730	-7.0940	O	0	39.1870	46.3160	60.7630	H	0	
-7.8110	0.5320	-7.2960	O	0	39.5030	47.7160	61.7060	H	0	
-4.5190	0.2640	-8.9320	C	0	39.6380	44.5140	62.8250	C	0	
-5.5420	-2.2210	-7.5960	H	0	40.5600	44.3590	62.2650	H	0	
-6.7650	2.6520	-7.9710	H	0	39.7220	43.9730	63.7670	H	0	
-2.1730	-3.7400	-9.6850	H	0	38.9020	43.8890	62.3200	H	0	
-2.4020	4.1630	-11.3310	Eu	0	42.3610	46.7330	63.4480	C	0	
					42.8170	45.9920	62.6020	O	0	
					42.8340	47.9940	63.5320	N	0	
					42.7140	48.4620	64.4180	H	0	
					43.4370	48.8520	62.4300	C	0	
					42.7750	48.6810	61.5810	H	0	
					43.2950	50.3720	62.7490	C	0	
					43.7950	50.6930	63.6620	H	0	
					43.8630	51.2730	61.5960	C	0	
					43.3510	50.9120	60.7040	H	0	
					43.5190	52.3020	61.6990	H	0	
					44.9500	51.1940	61.5930	H	0	
					41.8660	50.8180	62.9760	C	0	
					41.5240	50.3380	63.8930	H	0	
					41.7540	51.9000	63.0520	H	0	
					40.7510	50.5630	61.9550	C	0	
					41.0140	51.0650	61.0240	H	0	
					40.7250	49.4830	61.8140	H	0	
					39.7650	50.8800	62.2930	H	0	
					44.8480	48.3910	62.1560	C	0	
					45.2570	48.1480	61.0240	O	0	
					45.5520	48.0060	63.1890	N	0	
					45.0410	48.1520	64.0470	H	0	
					46.9520	47.4820	63.1970	C	0	
					47.6100	48.1760	62.6760	H	0	
					47.3740	47.2860	64.6800	C	0	
					46.6230	46.6920	65.2010	H	0	
					48.3330	46.7670	64.6770	H	0	
					47.5300	48.6850	65.3740	C	0	
					46.6270	49.2300	65.1020	H	0	
					47.6200	48.4760	64.4400	H	0	
					48.7680	49.4410	64.8620	C	0	
					49.6780	48.8550	64.7350	H	0	
					48.4940	49.8770	63.9010	H	0	
					49.1270	50.4890	65.9320	C	0	
					48.3210	51.2050	66.0950	H	0	
					49.0980	49.9560	66.8830	H	0	
					50.3810	51.2360	65.5880	N	0	
					50.2160	52.0000	64.9480	H	0	
					50.7840	51.6470	66.4180	H	0	
					51.1240	50.7120	65.1490	H	0	
					47.0420	46.1700	62.5510	C	0	
					48.1960	45.8450	62.1510	O	0	
					45.9550	45.4510	62.4130	N	0	
					45.0580	45.7810	62.7410	H	0	
					45.8980	44.1790	61.7160	C	0	
					46.9080	43.7720	61.7540	H	0	
					45.0220	43.2460	62.5610	C	0	
					44.0740	43.7430	62.7620	H	0	
					44.7860	42.3010	62.0720	H	0	
					45.6870	42.8670	63.9230	C	0	
					45.4810	43.6490	64.6540	H	0	
					44.9710	41.6110	64.4020	C	0	
					45.3350	40.8000	63.7710	H	0	
					45.1980	41.3240	65.4290	H	0	
					43.8980	41.8020	64.4000	H	0	
					47.1580	42.5620	63.8820	C	0	
					47.3910	42.1050	62.9210	H	0	
					47.7010	43.5040	63.9650	H	0	
					47.4620	41.8690	64.6670	H	0	
					45.3780	44.2440	60.3190	C	0	
					45.8980	43.6390	59.4180	O	0	
					44.3680	45.0990	60.0980	N	0	
					43.9340	45.5750	60.8760	H	0	
					43.8580	45.5060	68.7480	C	0	
					43.3800	44.6270	58.3150	H	0	
					42.8860	46.6090	59.0050	C	0	
					42.1420	46.2210	59.7010	H	0	
					43.4880	47.4220	59.4110	H	0	
					42.2430	47.1270	57.7500	C	0	
					42.9690	47.8640	57.4060	H	0	
					42.0460	46.2770	57.0970	H	0	
					40.8730	47.8280	57.9510	C	0	
					40.0260	47.6370	57.0510	O	0	
					40.6030	48.4970	58.9810	O	0	
					44.9720	45.9360	57.7730	C	0	
					45.0050	45.5000	56.6590	O	0	
					45.9250	46.5990	58.3440	N	0	
					45.7860	46.9660	59.2740	H	0	

45.6400	52.1360	57.7850	H	0	45.2140	40.2600	50.7490	C	0	42.4230	43.9740	51.1170	H	0
45.2500	51.8980	55.7240	N	0	46.2060	40.5630	50.4480	H	0	44.0940	43.8550	52.2920	C	0
44.5930	52.6430	55.5420	H	0	45.1610	39.7290	52.0570	C	0	44.6670	44.5340	51.6610	H	0
46.1260	52.2150	55.3340	H	0	46.0770	39.7040	52.6290	H	0	43.6540	44.5110	53.0430	H	0
44.9970	51.1830	55.0570	H	0	43.9510	39.2140	52.4350	C	0	45.1970	42.9560	53.0010	C	0
48.2990	46.2170	57.7110	C	0	42.7430	39.2110	56.9410	C	0	44.6730	42.1890	53.5710	H	0
49.2320	46.3770	56.9030	O	0	42.1540	38.1500	57.0450	O	0	45.7680	42.3790	52.2740	H	0
48.3330	45.2240	58.6210	N	0	42.3090	40.3820	57.5240	N	0	46.0540	43.6620	54.0380	C	0
47.4400	44.9450	59.0000	H	0	42.9610	41.1440	57.4000	H	0	46.5610	44.5380	53.6320	H	0
49.4730	44.2740	58.6550	C	0	41.2270	40.5000	58.5180	C	0	45.3310	43.7950	54.8430	H	0
50.3000	44.9650	58.8200	H	0	41.1250	39.6700	59.2180	H	0	46.9950	42.7280	54.6260	N	0
49.2050	43.4160	59.8780	C	0	41.3310	41.7970	59.3050	C	0	47.6420	42.3950	53.9260	H	0
49.2530	43.9800	60.8090	H	0	40.5520	41.8780	60.0640	H	0	47.6480	43.2110	55.2270	H	0
48.2430	42.9150	59.7710	H	0	42.6610	41.7770	60.0640	C	0	46.5380	41.9420	55.0660	H	0
50.2810	42.4370	60.0030	C	0	42.6700	42.6460	60.7220	H	0	41.4530	43.1490	53.6520	C	0
50.0720	41.9020	60.9290	H	0	42.7460	40.9150	60.7250	H	0	41.6500	42.7720	54.7650	O	0
50.3200	41.6850	59.2150	H	0	43.5230	41.8560	59.4000	H	0	40.8010	44.2740	53.3410	N	0
51.6620	43.0430	60.3310	C	0	41.2240	43.0350	58.4170	C	0	40.7010	44.4460	52.3500	H	0
52.6620	42.2370	60.1840	O	0	41.4680	43.8010	59.1540	H	0	40.3190	45.3430	54.2710	C	0
51.8140	44.2120	60.8050	O	0	41.9660	42.9810	57.6200	H	0	40.4510	44.9000	55.2580	H	0
49.6400	43.5420	57.3320	C	0	40.2250	43.1900	58.0110	H	0	41.3090	46.5070	54.2640	C	0
48.6350	43.0040	56.8480	O	0	39.7730	40.5020	57.9740	C	0	41.0820	47.3840	54.8720	H	0
50.8270	43.5720	56.6770	N	0	38.6690	40.3240	58.6000	O	0	42.2160	46.0660	54.6770	H	0
52.0910	44.3080	56.9890	C	0	39.7820	40.7100	56.6810	N	0	41.5310	47.0750	52.9030	C	0
52.7700	43.5760	57.4260	H	0	40.6760	40.9430	56.2740	H	0	40.6610	47.4550	52.1810	O	0
51.9130	45.1530	57.6540	H	0	38.6020	40.8390	55.8230	C	0	42.7290	47.2590	52.4460	N	0
52.6620	44.8400	55.7160	C	0	37.7880	40.3480	56.3570	H	0	42.8300	47.5080	51.4730	H	0
53.7490	44.9180	55.6890	H	0	38.2100	42.2990	55.7150	C	0	43.5480	46.9950	52.9750	H	0
52.2530	45.8380	55.5530	H	0	37.8170	42.4930	56.7130	H	0	38.8900	45.7220	54.1880	C	0
52.1020	43.8190	54.7070	C	0	39.0580	42.9410	55.4760	H	0	38.2070	45.3050	53.2540	O	0
52.9010	43.1620	54.3620	H	0	37.1050	42.6470	54.7770	C	0	38.4080	46.4720	55.1300	N	0
51.7860	44.4470	53.8750	H	0	36.9000	43.7090	54.9150	H	0	38.8360	46.6880	56.0190	H	0
50.9000	43.1460	55.2380	C	0	37.5570	42.4540	53.8040	H	0	37.0600	47.0110	55.1190	C	0
49.9700	43.5320	54.8220	H	0	35.5130	41.7620	55.0100	S	0	36.4060	46.2410	54.7100	H	0
50.7790	41.6220	55.1620	C	0	34.4650	42.3930	53.6050	C	0	36.5840	47.2590	56.5340	C	0
50.1480	41.1050	54.1980	O	0	35.1220	42.5080	52.7430	H	0	37.2990	48.0140	56.8620	H	0
51.2050	40.8680	56.1530	N	0	33.5670	41.7800	53.5290	H	0	35.6060	47.7410	56.5110	H	0
51.6880	41.2480	56.9540	H	0	34.1530	43.4230	53.7770	H	0	36.3980	45.9910	57.2920	C	0
50.9390	39.4260	56.2180	C	0	38.7980	40.1880	54.5310	C	0	35.3820	45.0240	57.0130	C	0
51.2330	38.9600	55.2780	H	0	39.8260	40.2220	53.9110	O	0	34.6210	45.2640	56.2860	H	0
51.6690	39.0460	56.9330	H	0	37.7360	39.6740	53.9760	N	0	35.3610	43.7760	57.7350	C	0
49.5570	38.9170	56.5810	C	0	36.7990	39.6670	54.3540	H	0	34.5760	43.0470	57.5970	H	0
49.0920	37.9610	56.0210	O	0	37.7790	38.8420	52.7520	C	0	36.3900	43.4610	58.7240	C	0
48.8340	39.6500	57.4820	N	0	38.5630	38.1470	53.0540	H	0	36.3310	42.2930	59.4080	O	0
49.2310	40.5150	57.8210	H	0	36.4960	38.0490	52.5000	C	0	37.0170	42.3890	60.0720	H	0
47.4440	39.3450	55.9340	C	0	35.8190	38.8320	52.1600	H	0	37.3910	44.4560	58.9790	C	0
47.4020	38.2690	58.1030	H	0	36.6700	37.4450	51.6100	H	0	38.2430	44.3150	59.6270	H	0
47.0680	39.9810	59.3090	C	0	35.8530	37.1920	53.6270	C	0	37.3330	45.7260	58.3170	C	0
46.9230	41.0610	59.2760	H	0	36.5000	36.4480	54.0920	H	0	38.1030	46.4350	58.5850	H	0
46.1420	39.5390	59.6760	H	0	35.7340	37.7790	54.5380	H	0	36.9110	48.2220	54.1170	C	0
48.1410	39.8220	60.3940	C	0	34.4150	36.6800	53.3470	C	0	35.8130	48.6260	53.7510	O	0
49.1520	39.7330	59.9950	H	0	34.0800	36.3760	52.1730	O	0	38.0060	48.8420	53.6100	N	0
47.9780	40.6890	61.0340	H	0	33.6180	36.5510	54.3460	N	0	38.9270	48.5190	53.8710	H	0
48.0490	38.6410	61.2900	C	0	32.6980	36.2400	54.0670	H	0	38.0210	49.6590	52.4200	C	0
47.5410	38.7320	62.3800	O	0	33.9350	36.5890	55.3040	H	0	37.1620	50.3270	52.3660	H	0
48.4300	37.4610	60.8600	N	0	38.3180	39.5630	51.5140	C	0	39.3330	50.4580	52.4180	C	0
48.4970	36.6670	61.4800	H	0	38.8360	38.9040	50.5940	O	0	40.1170	49.9530	52.9820	H	0
48.9780	37.3870	60.0150	H	0	38.1690	40.9290	51.5650	N	0	39.6140	50.8170	51.4280	H	0
46.3860	39.6530	56.9390	C	0	37.7400	41.3080	52.3980	H	0	39.2180	51.3480	53.0370	H	0
46.6150	40.4210	56.0000	O	0	38.6120	41.9440	50.6290	C	0	37.8140	48.9400	51.0870	C	0
45.1600	39.0570	57.0570	N	0	38.7350	41.3010	49.7580	H	0	37.8090	49.6150	50.0120	O	0
44.9440	38.3640	57.7600	H	0	37.5250	42.9550	50.2710	C	0	37.6440	47.6160	51.0680	N	0
44.0640	39.2090	56.1220	C	0	37.2130	43.3930	51.2190	H	0	37.5740	47.1450	51.9580	H	0
44.0270	40.2140	55.7010	H	0	38.0590	43.6620	49.6360	H	0	37.6090	46.7130	49.9360	C	0
44.1640	38.1960	54.9850	C	0	36.3650	42.4310	49.4350	C	0	37.7600	45.7610	50.4450	H	0
45.1830	38.2720	54.6030	H	0	36.5930	41.4440	48.7260	O	0	36.1930	46.5710	49.3030	C	0
43.9100	37.2100	55.3740	H	0	35.1910	42.9810	49.5280	N	0	35.9240	47.5090	48.8180	H	0
43.4350	38.5710	53.7440	C	0	34.3800	42.6080	49.0570	H	0	36.3130	45.8120	48.5310	H	0
42.2560	37.9980	53.3580	C	0	35.0550	43.7740	50.1380	H	0	35.1360	46.2080	50.2740	C	0
41.5880	37.4440	54.0010	H	0	40.0120	42.5230	50.8400	C	0	35.2670	45.2430	51.0580	O	0
41.8690	38.5510	52.1320	N	0	40.1850	43.6270	50.4720	O	0	33.9950	46.9060	50.2600	N	0
40.9000	38.5310	51.8460	H	0	40.9140	41.8100	51.5870	N	0	33.4010	46.7360	51.0580	H	0
42.8410	39.1830	51.4380	C	0	40.5980	40.8840	51.8370	H	0	33.8330	47.7730	49.7690	H	0
42.9600	39.7380	50.1500	C	0	41.9730	42.4100	52.3870	C	0	38.8030	46.7300	48.9380	C	0
42.1860	39.6110	49.4080	H	0	42.3930	41.5440	52.8990	H	0	38.6040	46.2930	47.7890	O	0
44.1780	40.3180	49.8220	C	0	43.0280	43.1460	51.4880	C	0	39.9730	47.1740	49.3030	N	0
44.3750	40.7310	48.8440	H	0	43.4460	42.4220	50.7880	H	0	39.9970	47.5610	50.2350	H	0

41.0000	47.4840	48.2550	C	0	51.8330	47.5960	50.3220	H	0	56.4950	38.0930	41.8740	C	0
40.5940	48.2010	47.5410	H	0	50.3120	47.0940	51.8610	C	0	55.5830	38.6900	41.8780	H	0
42.2900	48.2490	48.7920	C	0	49.7930	46.0270	52.2800	O	0	57.5700	39.0000	42.3300	C	0
42.8910	48.5480	47.9370	H	0	49.6650	48.1120	51.8760	O	0	57.7550	39.8860	41.7220	H	0
41.9260	49.4610	49.6060	C	0	53.2280	44.1080	49.3120	C	0	57.4650	39.3800	43.3460	H	0
42.6650	49.7390	50.3570	H	0	54.4160	44.4080	49.0730	O	0	58.9010	38.2860	42.3450	C	0
41.9060	50.3010	48.9120	H	0	52.7260	42.8320	49.1730	N	0	59.4540	37.9610	41.2870	O	0
40.9210	49.3510	50.0120	H	0	51.7360	42.6330	49.1500	H	0	59.4340	38.0350	43.4730	N	0
43.0060	47.4270	49.6640	O	0	53.6470	41.6790	49.0020	C	0	60.3340	37.5760	43.4860	H	0
43.8060	47.9120	49.8770	H	0	54.4670	41.7870	49.7120	H	0	59.0360	38.5070	44.2720	H	0
41.4370	46.2730	47.3950	C	0	52.9170	40.4340	49.4050	C	0	56.7980	37.5850	40.4150	C	0
41.7050	46.3690	46.1660	O	0	52.0320	40.2990	48.7830	H	0	56.8900	36.3890	40.1040	O	0
41.5200	45.1280	48.0880	N	0	53.6570	39.6400	49.3080	H	0	56.7770	38.5020	39.4180	N	0
41.3440	45.1820	49.0810	H	0	52.3890	40.2540	50.8820	C	0	56.9200	39.4450	39.7500	H	0
42.0230	43.8780	47.5120	C	0	51.5040	40.8870	50.9450	H	0	56.9330	38.1870	37.9860	C	0
42.2220	43.1980	48.3400	H	0	51.9060	38.8180	51.0430	C	0	55.9980	37.7800	37.6010	H	0
40.9560	43.3780	46.5460	C	0	50.9440	38.7530	50.5340	H	0	57.1040	39.5060	37.1460	C	0
40.7130	44.0850	45.7530	H	0	52.5840	38.0940	50.5910	H	0	57.2640	39.2520	36.0980	H	0
41.2670	42.4580	46.0510	H	0	51.7520	38.6300	52.1060	H	0	55.8540	40.4340	37.2090	C	0
39.5690	42.9940	47.1170	C	0	53.4430	40.5430	51.9530	C	0	56.0710	41.2710	36.5460	H	0
39.6780	42.3660	48.0010	H	0	53.9760	41.4670	51.7320	H	0	55.0710	39.8530	36.7210	H	0
39.0140	43.9070	47.3330	H	0	52.8460	40.6900	52.8530	H	0	55.6310	40.7560	38.2270	H	0
38.7070	42.2630	46.1150	C	0	54.1280	39.7040	52.0750	H	0	58.3100	40.1430	37.5630	O	0
37.7320	42.1510	46.5890	H	0	54.3760	41.5630	47.6520	C	0	58.5880	40.6790	36.8160	H	0
38.6110	42.8600	45.2070	H	0	53.7770	41.8240	46.6180	O	0	58.0240	37.2150	37.6370	C	0
39.2140	40.9300	45.8870	N	0	55.5600	41.0000	47.5970	N	0	57.8330	36.4560	36.7240	O	0
39.7050	40.7690	45.0200	H	0	55.9750	40.6880	48.4630	H	0	59.1220	37.1180	38.4070	N	0
39.1680	39.7670	46.5330	C	0	56.3770	41.0420	46.4240	C	0	59.0400	37.7480	39.1920	H	0
38.6170	39.7160	47.7170	N	0	55.9140	41.1870	45.4480	H	0	60.3230	36.3460	38.1550	C	0
38.0540	40.4860	48.0490	H	0	57.1500	42.3510	46.6900	C	0	60.5970	36.3270	37.1000	H	0
38.7040	38.9540	48.3740	H	0	56.4050	43.0960	46.9690	H	0	61.4650	37.2250	38.6800	C	0
39.7110	38.7050	46.0530	N	0	57.7360	42.2890	47.6080	H	0	61.3130	37.6520	39.6700	H	0
39.9870	38.7060	45.0810	H	0	57.9030	42.9270	45.5500	C	0	62.4360	36.7310	38.7370	H	0
40.2390	38.0900	46.6550	H	0	58.6100	42.3070	44.7450	O	0	61.7090	38.3890	37.7370	C	0
43.4460	44.0630	46.8230	C	0	57.7320	44.2540	45.3930	N	0	62.1510	37.9620	36.8370	H	0
43.8290	43.2320	46.0080	O	0	58.2560	44.7320	44.6740	H	0	60.8450	38.9590	37.3980	H	0
44.1290	44.9900	47.4150	N	0	56.9890	44.7090	45.9030	H	0	62.7390	39.3790	38.2080	C	0
43.6020	45.4500	48.1430	H	0	57.2290	39.7420	46.5030	C	0	62.4800	39.8420	39.1600	H	0
45.5980	45.3090	47.1810	C	0	58.0690	39.5430	45.7060	O	0	63.5880	38.7770	38.5320	H	0
45.8930	45.0410	46.1670	H	0	56.9580	38.8100	47.3480	N	0	63.1270	40.3160	37.1000	C	0
45.9000	46.7860	47.4730	C	0	56.2020	39.0010	47.9910	H	0	63.5400	39.7820	36.2450	H	0
45.3010	47.5020	46.9110	H	0	57.7630	37.6460	47.7150	C	0	62.2680	40.8520	36.6970	H	0
45.5670	46.9930	48.4910	H	0	58.7790	38.0410	47.7010	H	0	64.2410	41.2490	37.4920	N	0
47.3330	47.1210	47.2120	C	0	57.4880	37.1040	49.1280	C	0	65.0500	40.6690	37.6630	H	0
47.9780	46.8390	45.9350	C	0	58.0960	37.5260	49.9280	H	0	64.4220	41.9280	36.7670	H	0
47.4360	46.3670	45.1290	H	0	56.4780	37.2390	49.5150	H	0	63.9240	41.6940	38.3420	H	0
49.2800	47.2180	45.6250	C	0	57.8710	35.6060	49.2170	C	0	60.3020	34.8710	38.6380	C	0
49.7550	47.1410	44.6590	H	0	57.3020	35.0710	48.4570	H	0	61.1990	34.0910	38.2870	O	0
50.0760	47.7850	46.6700	C	0	58.9500	35.5180	49.0930	H	0	59.3110	34.4970	39.4340	N	0
51.3990	48.0220	46.3180	O	0	57.6180	34.9800	50.6110	C	0	58.5920	35.1740	39.6460	H	0
51.7900	48.5690	47.0030	H	0	57.8750	33.8000	50.6820	O	0	59.2940	33.1700	40.1290	C	0
49.5230	47.9560	47.9640	C	0	57.0710	35.6680	51.6760	N	0	59.8390	32.4300	39.5430	H	0
50.1570	48.2700	48.7800	H	0	57.2150	35.3000	52.6060	H	0	59.8480	33.3200	41.5780	C	0
48.1720	47.6080	48.1880	C	0	56.9010	36.6620	51.6180	H	0	59.8940	32.3030	41.9700	H	0
47.8130	47.7410	49.1980	H	0	57.5490	36.5650	46.5870	C	0	60.8070	33.8350	41.5270	H	0
46.5060	44.4380	48.1200	C	0	58.5040	35.9330	46.1480	O	0	59.0850	34.1190	42.6070	C	0
46.0980	44.2400	49.2630	O	0	56.2520	36.3950	46.1790	N	0	57.9710	34.5380	42.4370	O	0
47.8110	44.1910	47.8200	N	0	55.5120	36.6980	46.7960	H	0	59.6860	34.4320	43.7210	N	0
48.1530	44.6060	46.9650	H	0	55.8420	35.8500	44.8940	C	0	59.2690	35.0910	44.3620	H	0
48.7430	43.6980	48.7750	C	0	56.6090	35.1900	44.4870	H	0	60.5170	33.9740	44.0680	H	0
48.4880	43.8410	49.8250	H	0	54.4720	35.1090	44.9900	C	0	57.9180	32.4720	40.0530	C	0
48.8360	42.1900	48.4970	C	0	53.6490	35.7480	45.3130	H	0	57.9490	31.3240	40.4700	O	0
47.8360	41.7560	48.5130	H	0	54.1570	34.5350	43.4990	C	0	56.8110	33.1080	39.7050	N	0
49.2560	41.9150	47.5300	H	0	55.0900	34.0820	43.1660	H	0	56.8500	34.0960	39.5000	H	0
49.6190	41.6690	49.5630	O	0	53.3270	33.8340	43.5880	H	0	55.5030	32.4210	39.7700	C	0
49.0700	41.4920	50.3300	H	0	53.9270	35.3990	42.8770	H	0	55.3590	31.9530	40.7440	H	0
50.0770	44.4260	48.5230	C	0	54.5060	33.8380	45.9130	C	0	54.4660	33.5020	39.5530	C	0
50.4670	44.6600	47.3810	O	0	55.1620	33.0590	45.5240	H	0	54.6360	34.2930	40.2840	H	0
50.7830	44.6940	49.6370	N	0	54.9970	34.1620	46.8300	H	0	54.3690	34.0650	38.0750	C	0
50.2920	44.4450	50.4830	H	0	53.1910	33.3140	46.4650	C	0	55.3550	34.4930	37.8950	H	0
52.1190	45.2000	49.6760	C	0	52.5270	34.1270	46.7590	H	0	54.1170	33.2590	37.3850	H	0
52.2060	45.9410	48.8810	H	0	52.7120	32.7030	45.7010	H	0	53.5800	34.8140	38.0110	H	0
52.4160	45.7800	51.1090	C	0	53.4190	32.7030	47.3380	H	0	53.0260	32.9970	39.6900	C	0
52.0380	45.0830	51.8560	H	0	55.6850	37.0800	43.9560	C	0	52.9090	32.7380	40.7420	H	0
53.4910	45.8940	51.2480	H	0	54.9910	38.0190	44.3450	O	0	52.2640	33.7510	39.4950	H	0
51.7390	47.1380	51.3060	C	0	56.3900	37.0660	42.7960	N	0	53.0360	32.0840	39.0940	H	0
52.3310	47.7810	51.9570	H	0	56.8600	36.1900	42.6150	H	0	55.3370	31.2720	38.7290	C	0

54.5500	30.3610	38.9940	O	0	51.2070	24.7010	44.1880	C	0	38.5360	20.3330	57.4550	H	0
56.1500	31.1170	37.6860	N	0	51.1070	25.5920	45.0590	O	0	37.5300	22.1110	56.6400	C	0
56.8840	31.7760	37.4720	H	0	50.4890	23.5620	44.2550	N	0	36.6750	22.2000	57.2930	H	0
56.0460	29.9880	36.7500	C	0	50.7070	22.8720	43.5500	H	0	37.6910	23.1820	55.7270	C	0
55.0430	30.0590	36.3290	H	0	49.3390	23.3750	45.1800	C	0	37.0080	24.0180	55.7670	H	0
57.0140	30.0940	35.6050	C	0	48.9090	24.3740	45.2600	H	0	38.6780	23.2020	54.7670	C	0
58.0630	29.9840	35.8800	H	0	48.3190	22.4770	44.4780	C	0	38.6810	24.0360	54.0800	H	0
56.8690	29.2530	34.9260	H	0	48.1360	22.8660	43.4770	H	0	38.7450	20.9200	52.0080	C	0
56.9480	31.3140	34.8050	O	0	48.6510	21.4490	44.3260	H	0	38.2190	21.8680	51.3220	O	0
56.2980	31.2840	34.0990	H	0	46.9720	22.4030	45.2950	C	0	38.1250	19.7450	52.3050	N	0
56.1060	28.6330	37.4510	C	0	47.3230	22.2650	46.3180	H	0	38.5580	18.9420	52.7380	H	0
55.5800	27.7040	36.8160	O	0	46.1920	23.6690	45.2050	C	0	36.6780	19.6280	51.9550	C	0
56.6600	28.4620	38.6820	N	0	46.9490	24.4170	45.4390	H	0	36.4600	20.1210	51.0080	H	0
56.9910	29.2830	39.1690	H	0	45.7720	23.7780	44.2050	H	0	36.2870	18.1940	51.5810	C	0
56.7520	27.1740	39.4480	C	0	45.4650	23.5720	46.0120	H	0	36.9320	17.9320	50.7420	H	0
56.4040	26.3570	38.8150	H	0	46.0210	21.2750	44.7840	C	0	36.5090	17.4780	52.3730	H	0
58.2190	26.8410	39.7540	C	0	46.4090	20.2870	45.0320	H	0	34.9540	18.1130	51.2690	O	0
58.1660	26.0130	40.4610	H	0	45.0870	21.3180	45.3440	H	0	34.8270	18.4540	50.3810	H	0
58.6900	26.5250	38.8230	H	0	45.8340	21.4260	43.7210	H	0	35.7350	20.0730	53.0920	C	0
59.0920	27.8870	40.4460	C	0	49.7740	22.9470	46.5360	C	0	35.7440	19.4750	54.1460	O	0
59.0160	28.8430	39.9280	H	0	50.3840	21.8690	46.6660	O	0	34.9940	21.1890	52.7990	N	0
58.7720	28.1230	41.4620	H	0	49.6530	23.7580	47.5670	N	0	35.0850	21.4340	51.8230	H	0
60.5430	27.5060	40.6290	C	0	49.2610	24.6780	47.4270	H	0	34.1450	21.8400	53.7750	C	0
60.9750	27.4120	39.6330	H	0	50.1840	23.4610	48.9060	C	0	34.7170	22.0950	54.6670	H	0
61.0290	28.3720	41.0780	H	0	51.1920	23.0640	48.7840	H	0	33.7450	23.2440	53.1700	C	0
60.6130	26.2490	41.3460	N	0	50.4560	24.7550	49.6530	C	0	33.2330	23.8260	53.9350	H	0
60.2570	26.2110	42.2900	H	0	51.0890	25.4200	49.0660	H	0	34.9410	24.1080	52.7620	C	0
60.9830	25.0640	40.8620	C	0	49.5310	25.3230	49.7650	H	0	35.1870	23.7640	51.7570	H	0
61.5120	24.9380	39.6680	N	0	50.8810	24.5780	50.6410	H	0	34.8380	25.1880	52.8630	H	0
61.8040	25.7870	39.2050	H	0	49.2600	22.4830	49.7090	C	0	35.8060	23.8320	53.3650	H	0
61.8710	24.0820	39.2690	H	0	49.7660	21.4520	50.1610	O	0	32.8480	23.1430	52.0590	O	0
60.9780	23.9830	41.6020	N	0	47.9100	22.7540	49.6950	N	0	33.3190	22.7560	51.3180	H	0
60.7510	24.0340	42.5850	H	0	47.5590	23.6120	49.2950	H	0	32.9800	20.9740	54.1670	C	0
61.3580	23.0920	41.3150	H	0	46.8730	21.8680	50.1780	C	0	32.3470	21.3850	55.1670	O	0
55.8740	27.1840	40.7000	C	0	46.9830	20.9000	49.6890	H	0	32.6570	19.8050	53.5760	N	0
56.1710	26.6290	41.7160	O	0	46.9240	21.6530	51.7010	C	0	33.1790	19.5420	52.7530	H	0
54.7240	27.8800	40.6380	N	0	46.1330	20.9800	52.0320	H	0	31.3760	19.1150	53.7630	C	0
54.5270	28.4050	39.7980	H	0	47.8610	21.1110	51.8260	H	0	31.3670	18.2090	53.1580	H	0
53.7360	27.8910	41.6480	C	0	47.1480	22.8510	52.5440	C	0	31.3660	18.8960	54.8310	H	0
54.1580	27.9210	42.6520	H	0	48.3870	23.3900	52.8580	C	0	30.0530	19.8930	53.4670	C	0
52.9440	29.1730	41.5400	C	0	49.3570	22.9720	52.6340	H	0	29.1250	19.7760	54.2470	O	0
53.6840	29.9710	41.6020	H	0	48.1850	24.6170	53.4160	N	0	29.9680	20.6680	52.3980	N	0
52.4180	29.2230	40.5860	H	0	48.9470	25.1450	53.8180	H	0	30.8210	20.7060	51.8590	H	0
51.7210	29.4460	42.5230	C	0	46.8430	24.7650	53.7850	C	0	28.8520	21.2070	51.6630	C	0
50.8770	28.7560	42.5400	H	0	46.2220	25.8170	54.4550	C	0	28.1630	20.3770	51.5050	H	0
52.1340	29.3670	43.9890	C	0	46.7070	26.6170	54.9960	H	0	28.1830	22.4110	52.3670	C	0
53.0940	29.8780	44.0620	H	0	44.7820	25.6490	54.5700	C	0	27.3740	22.8980	51.8230	H	0
51.3670	29.7890	44.6380	H	0	44.2280	26.4060	55.1050	H	0	27.7530	21.9570	53.2600	H	0
52.2690	28.3070	44.2040	H	0	44.1780	24.6270	53.8640	C	0	28.9550	23.1560	52.5560	H	0
51.0760	30.8010	42.2270	C	0	43.1040	24.5320	53.7980	H	0	29.3200	21.6660	50.2630	C	0
51.8290	31.5780	42.3570	H	0	44.8120	23.6810	53.0720	C	0	30.5830	21.7150	50.0310	O	0
50.6700	30.8680	41.2180	H	0	44.2920	22.9030	52.5320	H	0	28.4060	21.9740	49.3680	N	0
50.2520	30.8980	42.9340	H	0	46.1950	23.7510	52.9950	C	0	27.4570	21.8220	49.6800	H	0
52.8840	26.6120	41.6080	C	0	45.4890	22.3530	49.7500	C	0	28.5890	22.0960	47.8960	C	0
52.4870	26.1140	40.5760	O	0	45.2970	23.4760	49.3730	O	0	29.6480	22.1630	47.6470	H	0
52.6800	26.0250	42.8000	N	0	44.5080	21.5360	50.0130	N	0	27.8730	20.9280	47.1490	C	0
53.0900	26.5400	43.5660	H	0	44.7220	20.5790	50.2560	H	0	27.3720	20.2980	47.8830	H	0
52.1920	24.6970	43.0280	C	0	43.0750	21.7610	49.8980	C	0	27.1300	21.3640	46.4800	H	0
51.5910	24.3870	42.1730	H	0	43.0110	22.7770	50.2860	H	0	28.7480	19.9670	46.3520	C	0
53.3110	23.6740	43.2730	C	0	42.5820	21.5120	48.4580	C	0	29.1120	20.6020	45.5450	H	0
52.9380	22.6580	43.4120	H	0	41.5240	21.7700	48.4120	H	0	29.7940	19.3510	47.2100	C	0
53.8920	23.5360	42.3620	H	0	43.1790	22.0770	47.7430	H	0	29.3710	18.6310	47.9110	H	0
54.2860	23.9450	44.4110	C	0	42.4890	20.1280	48.2630	O	0	30.4510	18.7870	46.5470	H	0
55.1070	23.2740	44.1610	H	0	41.7500	19.9450	47.6790	H	0	30.4100	20.0230	47.8070	H	0
54.5880	24.9920	44.4100	H	0	42.3240	20.9870	51.0000	C	0	27.9480	18.7570	45.7520	C	0
53.9890	23.5760	45.8690	C	0	42.8310	20.0820	51.6890	O	0	28.5560	17.8840	45.5170	H	0
53.0660	24.0700	46.1700	H	0	41.0890	21.4280	51.2990	N	0	27.2610	18.4580	46.5440	H	0
54.0570	22.4940	45.9820	H	0	40.7870	22.2290	50.7630	H	0	27.3200	19.1370	44.9450	H	0
54.9050	24.1280	46.8330	N	0	40.2490	21.0520	52.4360	C	0	27.8690	23.4010	47.3810	C	0
55.4060	24.9600	46.5580	H	0	40.6370	20.0710	52.7110	H	0	26.8030	23.8190	47.8940	O	0
55.0630	23.8150	48.0980	C	0	40.5390	22.0320	53.5600	C	0	28.3170	23.7760	46.1990	N	0
54.5050	22.8320	48.7440	N	0	41.5190	21.7410	53.9370	H	0	29.1840	23.3770	45.8680	H	0
53.9730	22.1040	48.2890	H	0	40.6060	23.0280	53.1220	H	0	27.8330	24.8290	45.2270	C	0
54.5490	22.7420	49.7490	H	0	39.5860	22.1550	54.7240	C	0	28.7620	25.1620	44.7630	H	0
55.8660	24.5720	48.8460	N	0	39.5740	21.1890	55.7710	C	0	26.8890	24.1530	44.1890	C	0
56.3600	25.3390	48.4130	H	0	40.2600	20.3590	55.6870	H	0	26.5560	24.8910	43.4600	H	0
56.2620	24.2350	49.7130	H	0	38.5350	21.1100	56.7050	C	0	27.3970	23.3700	43.6250	H	0

25.5850	23.6650	44.7840	C	0	40.3810	32.2830	53.5800	C	0	47.1980	31.2710	62.7390	C	0
25.8380	23.0970	45.6780	H	0	41.2880	32.8870	53.5900	H	0	47.2650	30.0410	62.7020	O	0
24.9430	24.5090	45.0370	H	0	40.4350	31.5830	54.4130	H	0	46.0070	31.8930	62.5860	N	0
24.8180	22.7710	43.8260	C	0	39.1240	33.1600	53.6990	C	0	45.9530	32.8950	62.4750	H	0
24.5570	23.2750	42.8940	H	0	38.4130	32.6080	54.3140	H	0	44.7650	31.1940	62.3300	C	0
25.4720	21.9330	43.5840	H	0	39.6080	34.4720	54.3220	C	0	44.9670	30.1330	62.1820	H	0
23.6050	22.2720	44.4970	N	0	40.0060	35.4370	53.6650	O	0	43.8370	31.3770	63.5880	C	0
23.7090	21.4550	45.0820	H	0	39.7350	34.3840	55.6830	N	0	43.5230	32.4190	63.5200	H	0
22.3660	22.7570	44.3390	C	0	39.1610	33.6790	56.1220	H	0	42.6660	30.4160	63.6780	C	0
22.1360	23.7970	43.5850	N	0	40.4930	35.3140	56.5830	C	0	41.9600	30.6340	62.8770	H	0
22.8050	24.1550	42.9190	H	0	40.8380	36.2120	56.0700	H	0	42.9540	29.3810	63.4950	H	0
21.1670	24.0800	43.6200	H	0	39.6860	35.7400	57.7910	C	0	42.1010	30.4660	64.6090	H	0
21.3420	22.2200	44.9640	N	0	39.8450	34.9340	58.5070	H	0	44.6600	31.2310	64.7110	O	0
21.4750	21.5550	45.7120	H	0	40.2290	36.6060	58.1680	H	0	44.3760	31.9850	65.2330	H	0
20.5340	22.8120	45.0940	H	0	38.1820	36.0650	57.6680	C	0	44.0760	31.7070	61.1200	C	0
27.3210	26.2270	45.7510	C	0	37.6970	35.2170	57.1830	H	0	43.6010	32.8150	61.0880	O	0
26.3510	26.8360	45.2040	O	0	37.5700	36.4520	58.9480	C	0	44.0030	30.8780	60.1230	N	0
27.9390	26.8230	46.7860	N	0	37.9830	37.3720	59.3610	H	0	44.4870	30.0010	60.2550	H	0
28.6850	26.3090	47.2320	H	0	36.4970	36.4600	58.7550	H	0	42.9500	31.0070	59.1020	C	0
27.5830	28.2070	47.3000	C	0	37.7140	35.6550	59.6770	H	0	43.0740	32.0510	58.8140	H	0
27.1670	28.7200	46.4340	H	0	38.1170	37.1980	56.6910	C	0	43.2700	30.0370	57.8970	C	0
26.7630	28.0660	48.0050	H	0	38.7960	38.0160	56.9340	H	0	44.3350	30.0150	57.6650	H	0
28.7890	29.0250	47.8720	C	0	38.3840	36.8630	55.6880	H	0	42.9440	29.0350	58.1740	H	0
28.6070	29.9610	48.6180	O	0	37.1290	37.6570	56.6810	H	0	42.4210	30.4240	56.7290	C	0
30.0170	28.6050	47.5850	N	0	41.7460	34.5970	57.2250	C	0	41.3900	30.2470	57.0360	H	0
30.2290	27.7640	47.0660	H	0	41.7620	33.3520	57.2490	O	0	42.6350	31.4400	56.3970	H	0
31.2860	29.0840	48.2540	C	0	42.7070	35.3600	57.6130	N	0	42.4780	29.2350	55.3390	S	0
31.0620	29.3600	49.2840	H	0	42.5440	36.3470	57.4780	H	0	43.8130	29.9260	54.2980	C	0
32.2420	27.8520	48.3120	C	0	43.9810	34.9640	58.2430	C	0	44.4450	30.4990	54.9770	H	0
32.5490	27.5720	47.3040	H	0	43.7910	34.0560	58.8150	H	0	44.3410	29.1020	53.8180	H	0
33.1500	28.1170	48.8530	H	0	45.1100	34.9540	57.2160	C	0	43.3630	30.5200	53.5020	H	0
31.6630	26.6910	48.9890	C	0	45.3690	35.9430	56.8370	H	0	41.5230	30.7840	59.6600	C	0
30.6490	25.9390	48.5840	N	0	46.2550	34.2190	58.0020	C	0	41.2860	29.9380	60.5090	O	0
30.4970	24.9600	49.4800	C	0	47.0960	33.9690	57.3540	H	0	40.5500	31.3900	58.9820	N	0
29.7820	24.1580	49.3660	H	0	46.6860	34.8720	58.7600	H	0	40.9140	31.8570	58.1640	H	0
31.3840	25.0650	50.4830	N	0	45.9530	33.2640	58.4330	H	0	39.1270	31.1250	59.0880	C	0
31.6060	24.3480	51.1590	H	0	44.8610	34.0380	56.0070	C	0	38.9910	30.1410	59.5360	H	0
32.0640	26.2360	50.2020	C	0	43.8920	34.1610	55.5230	H	0	38.4800	32.2530	59.9610	C	0
32.8850	26.6520	50.7680	H	0	45.6940	34.2390	55.3320	H	0	38.4170	33.1950	59.4180	H	0
31.7520	30.3240	47.4770	C	0	44.9870	32.9990	56.3100	H	0	37.4400	32.0020	60.1740	H	0
32.9240	30.4380	47.1020	O	0	44.4190	35.9880	59.3320	C	0	39.0880	32.5040	61.3060	C	0
30.9390	31.3730	47.4720	N	0	44.9180	37.0490	59.0670	O	0	38.5970	31.9300	62.4910	C	0
30.0630	31.2690	47.9630	H	0	44.3540	35.6050	60.6130	N	0	37.7530	31.2710	62.3520	H	0
31.3690	32.7210	47.1530	C	0	43.9900	34.6670	60.6990	H	0	39.1690	32.2140	63.7410	C	0
32.1730	32.7100	46.4170	H	0	44.6320	36.3950	61.8070	C	0	38.7760	31.7420	64.6300	H	0
30.1980	33.4610	46.5530	C	0	45.2460	37.2590	61.5540	H	0	40.2670	33.0740	63.8600	C	0
29.2960	33.3760	47.1590	H	0	43.2790	37.0020	62.4180	C	0	40.9350	33.2890	65.0760	O	0
30.4050	34.5310	46.5300	H	0	42.6950	36.2480	62.9460	H	0	40.3650	32.9730	65.7810	H	0
29.9120	33.0640	45.0820	C	0	43.6180	38.1560	63.2900	C	0	40.8080	33.6180	62.6480	C	0
30.8010	33.0610	44.4510	H	0	44.3370	37.8940	64.0670	H	0	41.6680	34.2670	62.7330	H	0
29.6050	32.0240	45.1960	H	0	44.0450	39.0000	62.7470	H	0	40.2000	33.3750	61.3910	C	0
28.7900	34.0070	44.5570	C	0	42.7360	38.4730	63.8460	H	0	40.5980	33.9720	60.5840	H	0
29.0370	35.2200	44.5380	O	0	42.3310	37.5710	61.3490	C	0	38.4650	30.9280	57.6640	C	0
27.7820	33.5240	44.0700	O	0	42.8730	38.2960	60.7410	H	0	39.0000	31.3910	56.6190	O	0
32.0340	33.4100	48.4180	C	0	41.8930	36.7670	60.7570	H	0	37.3090	30.2210	57.5710	N	0
31.8160	32.9600	49.5470	O	0	41.4870	37.9750	61.9090	H	0	36.8640	29.8670	58.4060	H	0
32.7160	34.5650	48.2240	N	0	45.4320	35.5780	62.8000	C	0	36.7400	29.8310	56.2770	C	0
32.9070	34.8540	47.2750	H	0	45.0990	34.4720	63.1090	O	0	36.7410	30.7450	55.6840	H	0
33.5740	35.1180	49.3080	C	0	46.5360	36.2030	63.1600	N	0	37.5700	28.7670	55.5010	C	0
33.6880	36.1880	49.1320	H	0	46.7760	37.1180	62.8050	H	0	38.2000	29.3760	54.8520	H	0
33.1690	34.9020	50.2960	H	0	47.5030	35.5670	64.0700	C	0	38.4350	27.8290	56.3690	C	0
34.9150	34.4610	49.3520	C	0	48.2500	36.2640	64.4500	H	0	37.9010	27.4750	57.2520	H	0
35.3240	33.8290	48.3970	O	0	46.9420	35.1630	64.9130	H	0	38.7960	27.0090	55.7480	H	0
35.6620	34.5460	50.4800	N	0	48.2990	34.5070	63.2760	C	0	39.3240	28.3180	56.7660	H	0
35.3450	35.2070	51.1750	H	0	48.8550	34.8180	62.1690	O	0	36.7360	27.8370	54.4990	C	0
37.0310	34.0460	50.5240	C	0	48.2220	33.2850	63.8380	N	0	36.2090	27.1140	55.1210	H	0
37.1250	33.0780	50.0320	H	0	47.7560	33.1930	64.7290	H	0	36.0670	28.4340	53.8780	H	0
37.6210	34.8090	50.0170	H	0	48.4670	31.9990	63.1440	C	0	37.3910	27.2820	53.8270	H	0
37.4410	33.8980	52.0140	C	0	48.6940	32.3750	62.1460	H	0	35.2330	29.4200	56.5650	C	0
36.6040	34.2110	52.8560	O	0	49.6550	31.1230	63.6290	C	0	34.9260	28.8970	57.6610	O	0
38.6570	33.3300	52.2880	N	0	49.9070	30.3920	62.8610	H	0	34.3350	29.7870	55.6250	N	0
39.5470	32.4900	51.3880	C	0	50.9200	31.9000	63.6700	C	0	34.6660	30.3110	54.8280	H	0
40.2600	33.2190	51.0030	H	0	51.8000	31.2740	63.8160	H	0	32.8830	29.3430	55.6570	C	0
38.9080	31.9680	50.6750	H	0	51.0180	32.4710	62.7470	H	0	32.6400	29.1530	56.7020	H	0
40.2140	31.4470	52.2670	C	0	50.8040	32.6620	64.4410	H	0	31.9960	30.5590	55.2420	C	0
41.1110	30.9300	51.9230	H	0	49.4580	30.4930	64.8120	O	0	30.9270	30.3580	55.3180	H	0
39.4670	30.6710	52.4370	H	0	48.8510	29.7620	64.6720	H	0	32.1370	31.2600	56.0650	H	0

32.4510	31.2710	54.0050	C	0	27.0840	28.9900	54.4240	H	0	40.6510	24.9730	56.7240	H	0
33.3590	32.2910	53.9490	N	0	27.8350	26.9300	58.1020	C	0	41.3990	26.4250	56.7870	H	0
33.4770	32.6470	52.7060	C	0	28.2180	27.7480	58.9890	O	0	42.4300	24.9580	56.8980	H	0
33.8870	33.5900	52.3750	H	0	28.3280	25.6740	58.1120	N	0	41.4270	24.0330	59.3450	C	0
32.5860	31.9050	51.9300	N	0	28.0320	25.0870	57.3460	H	0	41.0840	24.1650	60.3710	H	0
32.1990	32.2570	51.0660	H	0	29.5690	25.3820	58.8160	C	0	40.7350	23.3580	58.8410	H	0
31.9490	31.0250	52.7730	C	0	29.3050	25.4790	59.8690	H	0	42.4420	23.6430	59.4210	H	0
31.0780	30.4390	52.5190	H	0	30.0670	23.9630	58.5920	C	0	44.0080	26.9820	61.3020	C	0
32.6380	28.0150	54.8700	C	0	30.9710	23.9790	57.9830	H	0	44.4130	28.0040	60.7870	O	0
33.5640	27.2180	54.4800	O	0	30.3000	23.5070	59.5540	H	0	44.4880	26.5200	62.4830	N	0
31.3560	27.8080	54.5910	N	0	29.1540	22.9980	57.9050	C	0	44.2550	25.5660	62.7170	H	0
30.7590	28.5720	54.8720	H	0	28.0400	22.4170	58.4880	N	0	45.7760	26.9860	63.0700	C	0
30.6760	26.9100	53.5930	C	0	27.5320	21.5390	57.6420	C	0	45.7750	28.0740	63.0000	H	0
31.4210	26.8550	52.7990	H	0	26.5850	21.0400	57.7870	H	0	45.9130	26.5460	64.5020	C	0
30.4960	25.5420	54.1830	C	0	28.2890	21.5600	56.4680	N	0	45.1350	27.0760	65.0520	H	0
30.1160	24.7890	53.4930	H	0	28.1490	20.9630	55.6660	H	0	45.5160	25.5330	64.5620	H	0
31.4780	25.2610	54.5630	H	0	29.2600	22.4570	56.6450	C	0	47.2310	26.7790	65.2250	C	0
29.6600	25.6480	55.3490	O	0	30.0730	22.5750	55.9440	H	0	47.8820	27.8280	64.8580	O	0
30.1580	26.0340	56.0740	H	0	30.7180	26.3850	58.5570	C	0	47.5930	26.0190	66.1250	O	0
29.3350	27.4330	53.0530	C	0	30.9310	26.8980	57.4760	O	0	46.9230	26.5180	62.1130	C	0
28.6610	28.2960	53.6770	O	0	31.4850	26.5410	59.6870	N	0	47.1260	25.3180	61.7640	O	0
28.7470	26.8650	51.9890	N	0	31.1700	26.1950	60.5820	H	0	47.8910	27.4190	61.9540	N	0
29.2170	26.2130	51.3770	H	0	32.6240	27.4940	59.7890	C	0	47.7890	28.2380	62.5350	H	0
27.3190	26.9800	51.7080	C	0	32.9500	27.5480	58.7500	H	0	49.0750	27.2750	61.0350	C	0
27.0400	28.0320	51.6490	H	0	32.3230	28.7960	60.5400	C	0	48.9420	26.3540	60.4680	H	0
27.1270	26.1650	50.4170	C	0	32.2950	28.5490	61.6010	H	0	49.0890	28.4440	60.0590	C	0
27.3120	25.1220	50.6760	H	0	33.4510	29.7540	60.4000	C	0	49.5900	29.2540	60.5890	H	0
26.1780	26.2500	49.8870	H	0	34.4280	29.3570	60.6750	H	0	49.7040	28.1440	59.2100	H	0
27.9030	26.5150	49.7360	H	0	33.5440	30.0260	59.3490	H	0	47.7750	28.9280	59.5550	C	0
26.4200	26.4680	52.8980	C	0	33.2870	30.7170	60.8820	H	0	47.1610	29.3550	60.3470	H	0
26.8630	25.7690	53.8110	O	0	30.9980	29.4610	60.2130	C	0	47.9680	30.1470	58.6190	C	0
25.0920	26.6240	52.8060	N	0	31.2120	29.9460	59.2610	H	0	48.1440	31.0150	59.2540	H	0
24.7800	27.1140	51.9800	H	0	30.1720	28.7610	60.0890	H	0	48.8460	29.9390	58.0080	H	0
24.0230	26.1580	53.7130	C	0	30.7730	30.2770	60.9000	H	0	47.0940	30.3290	57.9930	H	0
24.0810	26.6590	54.6790	H	0	33.7850	26.6920	60.4600	C	0	46.9740	27.8190	58.8370	C	0
22.6930	26.6500	53.1830	C	0	33.5500	25.7670	61.2300	O	0	46.6750	26.9710	59.4530	H	0
22.7470	27.7360	53.1070	H	0	34.9930	26.9690	59.9940	N	0	46.1030	28.3460	58.4480	H	0
22.5800	26.2020	52.1960	H	0	35.0790	27.6640	59.2660	H	0	47.6270	27.4440	58.0490	H	0
21.5210	26.1750	54.0670	C	0	36.2460	26.2420	60.3530	C	0	50.4890	27.1450	61.7070	C	0
20.8990	24.9390	53.8000	C	0	36.0780	25.7420	61.3070	H	0	51.5860	27.0810	61.0710	O	0
21.2680	24.3170	52.9980	H	0	36.6780	25.1450	59.3090	C	0	50.4880	27.0520	62.9970	N	0
19.8070	24.6190	54.6320	C	0	37.0160	25.6150	58.3860	H	0	49.5420	27.0840	63.3500	H	0
19.1550	23.8260	54.2980	H	0	37.5780	24.6180	59.6250	H	0	51.6240	26.8680	63.9300	C	0
19.3200	25.3550	55.6910	C	0	35.6420	24.0740	59.0390	C	0	52.1720	27.8100	63.9270	H	0
18.2700	24.9870	56.3930	O	0	35.3610	22.9150	59.8680	C	0	51.0800	26.6920	65.4400	C	0
17.5740	25.6370	56.5150	H	0	36.0740	22.7830	60.6670	H	0	50.4360	25.8350	65.6320	H	0
19.9690	26.5660	55.9360	C	0	34.3010	21.9970	59.5580	C	0	52.2120	26.7050	66.4720	C	0
19.4490	27.2120	56.6270	H	0	34.1860	21.1370	60.2020	H	0	52.5560	27.7230	66.6540	H	0
21.0260	27.0140	55.1010	C	0	33.6020	22.1370	58.3570	C	0	51.9100	26.1840	67.3810	H	0
21.4500	28.0040	55.1790	H	0	32.6300	21.2560	57.9740	O	0	53.0020	26.1300	65.9890	H	0
24.1580	24.6580	53.9530	C	0	32.4180	21.4310	57.0540	H	0	50.2600	27.8400	65.6700	O	0
24.2180	23.8510	52.9780	O	0	33.7700	23.3360	57.5590	C	0	49.5290	27.7240	65.0590	H	0
24.2770	24.2380	55.2250	N	0	33.0040	23.6070	56.8470	H	0	52.4410	25.6170	63.6010	C	0
24.5660	22.8050	55.5190	C	0	34.8200	24.2150	57.8780	C	0	53.6740	25.6680	63.7330	O	0
25.5790	22.5320	55.2240	H	0	34.8730	25.1610	57.3590	H	0	51.8150	24.4720	63.2640	N	0
23.8760	22.2540	54.8800	H	0	37.3750	27.2140	60.6800	C	0	50.8140	24.4440	63.1310	H	0
24.3620	22.6550	57.0390	C	0	37.5730	28.1900	59.9160	O	0	52.5110	23.2290	62.8680	C	0
25.3480	22.8020	57.4800	H	0	38.1980	26.9680	61.7210	N	0	53.5840	23.4220	62.8800	H	0
23.9810	21.6550	57.2490	H	0	38.0060	26.1020	62.2040	H	0	52.1680	22.0720	63.7900	C	0
23.4710	23.8530	57.5180	C	0	39.3540	27.7220	62.0960	C	0	52.5430	22.3090	64.7850	H	0
23.8030	24.1670	58.5080	H	0	39.4650	28.5820	61.4350	H	0	51.0820	22.0210	63.7200	H	0
22.4080	23.6180	57.4710	H	0	39.0890	28.1850	63.5500	C	0	52.8550	20.7190	63.4950	C	0
23.8370	24.9330	56.4670	C	0	38.7260	27.3840	64.1950	H	0	52.4660	19.9480	64.1590	H	0
22.9400	25.5340	56.3210	H	0	39.9530	28.7420	63.9090	H	0	52.5490	20.3890	62.5020	H	0
24.8280	25.9770	57.0970	C	0	38.3200	28.9470	63.4180	H	0	54.3770	20.6470	63.5300	C	0
24.5680	26.4470	58.2570	O	0	40.5710	26.7440	62.1260	C	0	54.9820	20.7560	62.4790	O	0
26.0010	26.2670	56.4690	N	0	40.4240	25.6500	62.6400	O	0	55.0180	20.4530	64.6820	N	0
26.1910	25.8100	55.5890	H	0	41.6200	27.1100	61.2950	N	0	56.0160	20.3210	64.6080	H	0
26.9710	27.2850	56.8980	C	0	41.5990	28.0520	60.9310	H	0	54.4680	20.3390	65.5220	H	0
27.6580	27.4060	56.0600	H	0	42.7120	26.3120	60.7760	C	0	52.1190	22.9300	61.4270	C	0
26.3500	28.7000	56.8960	C	0	42.7870	25.2980	61.1680	H	0	50.9310	22.9900	61.0280	O	0
25.8130	28.9090	57.8210	H	0	42.5900	26.1900	59.2510	C	0	53.0080	22.2830	60.6300	N	0
27.1410	29.4510	56.9010	H	0	42.5560	27.1280	58.6970	H	0	53.8590	21.9250	61.0390	H	0
25.5140	28.9530	55.6390	C	0	43.4540	25.6870	58.8170	H	0	52.7470	22.0520	59.1870	C	0
24.2860	29.1020	55.7530	O	0	41.3510	25.4150	58.7720	C	0	52.4670	23.0450	58.8360	H	0
26.0780	28.9690	54.5060	N	0	40.4300	25.9720	58.9470	H	0	53.9800	21.4840	58.4620	C	0
25.4510	29.1330	53.7310	H	0	41.5040	25.4320	57.2240	C	0	54.5500	20.8380	59.1290	H	0

53.7730	20.9520	57.5330	H	0	39.9350	19.1000	61.2370	H	0	27.1390	27.4400	67.0400	H	0
54.8890	22.6930	57.9500	C	0	41.7970	22.8520	64.3810	C	0	27.1400	28.6350	65.2570	C	0
55.4200	22.3750	57.0520	H	0	41.9560	21.9560	65.2590	O	0	25.8590	29.0780	65.6220	O	0
54.3190	23.5240	57.5350	H	0	41.6090	24.1680	64.7320	N	0	25.6450	28.9070	66.5430	H	0
55.8630	23.2350	58.9590	C	0	41.4670	24.8080	63.9630	H	0	27.8750	29.0910	64.1210	C	0
55.3850	23.6260	59.8570	H	0	41.5250	24.8470	66.1080	C	0	27.5010	29.9150	63.5320	H	0
56.6460	22.4870	59.0850	H	0	42.2320	24.3990	66.8070	H	0	29.1250	28.4310	63.9030	C	0
56.5510	24.4490	58.2930	C	0	41.9590	26.2710	65.9240	C	0	29.6390	28.8000	63.0280	H	0
57.2520	24.0140	57.5800	H	0	43.0220	26.3390	65.6910	H	0	30.0440	25.2360	63.0950	C	0
55.8810	25.0430	57.6710	H	0	41.3020	26.7600	65.2050	H	0	30.3220	25.4810	61.9090	O	0
57.2460	25.2890	59.3150	N	0	41.9210	27.0020	67.2530	C	0	28.8120	24.8900	63.4690	N	0
56.6690	25.6420	60.0640	H	0	40.9010	27.1910	67.8860	H	0	28.6350	24.6170	64.4250	H	0
58.0010	24.7220	59.6760	H	0	42.2320	26.3960	68.1040	H	0	27.6460	24.8140	62.5600	C	0
57.7190	26.0280	58.8140	H	0	42.6270	28.3930	67.3000	C	0	27.9190	25.3990	61.6820	H	0
51.6130	20.9870	59.0170	C	0	43.5880	28.1580	66.8410	H	0	27.2640	23.3540	62.0670	C	0
51.4920	20.0540	59.7950	O	0	42.0770	29.1870	66.7950	H	0	26.8940	22.7730	62.9120	H	0
50.8320	21.1170	57.9540	N	0	42.8460	28.6950	68.7790	C	0	26.0880	23.3590	61.0400	C	0
50.0740	19.9730	57.4620	C	0	41.8980	28.7370	69.3140	H	0	25.2140	23.8490	61.4700	H	0
49.3820	19.5010	58.1600	H	0	43.4620	27.8790	69.1580	H	0	26.3270	24.0340	60.2180	H	0
50.6910	21.1330	57.1420	H	0	43.4250	30.0850	68.8680	N	0	25.9470	22.3290	60.7130	H	0
49.2470	20.5130	56.2710	C	0	44.4250	30.0330	68.7370	H	0	28.3530	22.7370	61.4730	O	0
48.2690	20.8220	56.6410	H	0	42.9780	30.7350	68.2360	H	0	28.1030	22.8250	60.5500	H	0
49.2230	19.8360	55.4180	H	0	43.2470	30.6050	69.7160	H	0	26.4650	25.4740	63.2600	C	0
49.9520	21.7170	55.8100	C	0	40.0470	24.7260	66.6710	C	0	26.0270	24.9460	64.3080	O	0
49.3020	22.4020	55.2650	H	0	39.9700	24.4900	67.8970	O	0	25.8220	26.4930	62.7010	N	0
50.7720	21.5030	55.1240	H	0	39.0010	25.0180	65.9090	N	0	26.0640	27.1960	61.4140	C	0
50.5840	22.2790	57.0640	C	0	39.1240	25.2100	64.9250	H	0	26.0670	26.4410	60.6280	H	0
51.5090	22.7560	56.7380	H	0	37.6380	24.8500	66.2830	C	0	27.0110	27.7350	61.4470	H	0
49.5070	23.2110	57.7200	C	0	37.5160	23.8990	66.8020	H	0	24.8650	28.1300	61.2190	C	0
49.5040	24.4080	57.3960	O	0	37.1010	26.0010	67.1980	C	0	24.0130	27.6570	60.7310	H	0
48.6320	22.6500	58.5450	N	0	36.0350	25.8660	67.3760	H	0	25.2070	29.0730	60.7940	H	0
48.7610	21.6690	58.7500	H	0	37.6570	25.8380	68.1220	H	0	24.3370	28.2600	62.6860	C	0
47.6620	23.1740	59.4410	C	0	37.1710	27.4570	66.7340	C	0	23.3140	28.6340	62.7250	H	0
48.0210	24.0670	59.9520	H	0	38.0810	28.4040	67.1640	C	0	24.9780	28.9730	63.2030	H	0
46.3960	23.5820	58.6940	C	0	38.7840	28.2250	67.9640	H	0	24.5700	26.9650	63.3640	C	0
45.5990	23.9890	59.3160	H	0	37.7350	29.6460	66.6470	N	0	24.7570	27.0910	64.4300	H	0
46.7950	24.3320	58.0100	H	0	38.2740	30.4920	66.7630	H	0	23.3780	26.0030	63.0710	C	0
45.7460	22.5320	57.8250	C	0	36.5630	29.5640	65.9030	C	0	23.3100	25.3540	61.9910	O	0
44.8530	21.5830	58.3200	C	0	35.8620	30.5380	65.2070	C	0	22.3400	26.1380	63.8870	N	0
44.5650	21.5790	59.3610	H	0	36.2270	31.5500	65.2950	H	0	22.4960	26.6750	64.7280	H	0
44.2970	20.5940	57.4750	C	0	34.8330	30.1570	64.3460	C	0	21.0150	25.5700	63.6050	C	0
43.6650	19.8760	57.9770	H	0	34.3610	30.8910	63.7100	H	0	21.1500	24.6450	63.0450	H	0
44.7200	20.4850	56.1410	C	0	34.4070	28.7930	64.2460	C	0	20.2580	25.2430	64.9130	C	0
44.3870	19.4740	55.2960	O	0	33.6440	28.5040	63.5380	H	0	20.4230	26.1000	65.5660	H	0
45.0400	19.5860	54.6020	H	0	35.0510	27.8050	65.0650	C	0	18.7800	25.0320	64.8640	C	0
45.6440	21.3910	55.6520	C	0	34.8300	26.7510	64.9920	H	0	18.1980	25.8800	64.5050	H	0
45.9510	21.3890	54.6170	H	0	36.1930	28.2290	65.8680	C	0	18.5410	24.2720	64.1210	H	0
46.1740	22.4280	56.4410	C	0	36.6850	24.8230	65.0420	C	0	18.3760	24.7670	65.8410	H	0
46.9280	23.0720	56.0140	H	0	37.1140	25.2140	63.9760	O	0	20.9650	24.0960	65.7920	C	0
47.2180	22.1070	60.4550	C	0	35.5410	24.1120	65.2000	N	0	20.7710	23.1440	65.2990	H	0
47.7020	20.9540	60.4320	O	0	35.1940	23.9570	66.1360	H	0	22.0320	24.3150	65.7590	H	0
46.4640	22.5470	61.4290	N	0	34.6080	23.9410	64.1230	C	0	20.6710	24.0850	66.8420	H	0
46.3510	23.5450	61.5330	H	0	34.7830	24.7540	63.4190	H	0	20.0810	26.4670	62.8060	C	0
45.5780	21.6910	62.3130	C	0	34.8820	22.6350	63.3350	C	0	19.6850	27.6000	63.2180	O	0
45.3560	20.7660	61.7820	H	0	34.3570	22.7410	62.3850	H	0	19.8540	25.9590	61.6120	N	0
46.3310	21.3320	63.6710	C	0	35.9690	22.5920	63.2650	H	0	20.2410	25.0400	61.4550	H	0
45.7540	20.4710	64.0110	H	0	34.3670	21.4210	64.1160	C	0	19.0220	26.6480	60.6500	C	0
47.3850	21.1180	63.4960	H	0	34.5480	21.4610	65.1900	H	0	18.7110	27.6070	61.0650	H	0
46.2610	22.1320	64.4080	H	0	33.2880	21.4590	63.9600	H	0	19.7930	26.9380	59.3360	C	0
44.2730	22.4640	62.6940	C	0	34.9570	20.1280	63.4840	C	0	19.8320	26.0710	58.6770	H	0
44.2150	23.6960	62.8570	O	0	34.4360	19.5940	62.4910	O	0	19.1440	27.5680	58.7280	H	0
43.1220	21.7760	62.6780	N	0	36.1020	19.6840	64.0010	N	0	21.1700	27.7270	59.3890	C	0
43.0550	20.8110	62.3860	H	0	36.6700	18.9340	63.6340	H	0	21.2830	28.4510	60.1960	H	0
41.7590	22.3980	62.8980	C	0	36.6030	20.3340	64.5890	H	0	21.9940	27.0270	59.5270	H	0
41.7070	23.2050	62.1670	H	0	33.2250	24.3070	64.6040	C	0	21.6460	28.5240	58.1440	C	0
40.6880	21.3540	62.5690	C	0	32.8080	23.9100	65.6960	O	0	20.9500	29.2240	57.3980	O	0
40.9860	20.3810	62.9600	H	0	32.4420	25.0320	63.7770	N	0	22.9640	28.6590	58.0570	N	0
39.2950	21.6750	63.1860	C	0	32.8010	25.3310	62.8810	H	0	23.2470	29.0280	57.1600	H	0
38.6620	20.7870	63.2070	H	0	31.0700	25.5100	64.1450	C	0	23.5470	27.9150	58.4130	H	0
39.4890	21.8560	64.2430	H	0	30.7280	25.0680	65.0810	H	0	17.6090	25.9690	60.4070	C	0
38.7830	22.5170	62.7210	H	0	31.0940	27.0360	64.4970	C	0	17.4380	24.7530	60.6990	O	0
40.4910	21.1790	61.0590	C	0	31.6960	27.1680	65.3960	H	0	16.7070	26.7720	59.8610	N	0
40.0050	22.0910	60.7120	H	0	31.4200	27.6030	63.6250	H	0	16.8260	27.7750	59.8340	H	0
41.4080	21.0050	60.4970	H	0	29.7330	27.5700	64.8070	C	0	15.3390	26.3400	59.4720	C	0
39.6040	19.9700	60.6690	C	0	29.0140	27.1870	65.9700	C	0	14.9970	25.5570	60.1500	H	0
38.5510	20.1830	60.8520	H	0	29.5650	26.5660	66.6610	H	0	14.4930	27.6660	59.6680	C	0
39.6460	19.8100	59.5920	H	0	27.6910	27.6510	66.1360	C	0	14.5400	27.8090	60.7480	H	0



14.9300	28.5020	59.1230	H	0	14.0600	30.9180	51.5950	H	0	25.6680	33.1590	46.3900	H	0
13.0560	27.5880	59.1490	C	0	13.2110	32.7890	51.0900	C	0	25.8540	33.1520	48.1210	H	0
12.6900	26.7200	58.3970	O	0	12.3380	33.1520	50.5480	H	0	24.8670	30.7470	45.9990	C	0
12.2730	28.4510	59.7120	N	0	13.0700	33.0400	52.1410	H	0	24.5260	31.4140	45.2070	H	0
11.3670	28.5980	59.2930	H	0	14.1000	33.2130	50.6240	H	0	25.9150	30.6040	45.7380	H	0
12.4820	29.0210	60.5200	H	0	11.8090	30.8430	51.6240	C	0	24.2290	29.8730	45.8680	H	0
15.2630	25.7990	58.0630	C	0	11.7450	29.7550	51.5950	H	0	25.0080	31.3250	49.6980	C	0
15.9410	26.3710	57.1890	O	0	11.7310	31.1030	52.6800	H	0	23.9860	31.9250	50.0510	O	0
14.4860	24.7720	57.7670	N	0	10.9480	31.2030	51.0590	H	0	26.1620	31.5520	50.2910	N	0
14.0000	24.4150	58.5770	H	0	14.7380	31.2350	48.9130	C	0	26.9840	31.0320	50.0190	H	0
14.5180	24.1340	56.4470	C	0	14.6560	32.2700	48.1680	O	0	26.2690	32.3550	51.4590	C	0
15.5000	24.2930	56.0030	H	0	15.9100	30.6170	49.0330	N	0	25.5320	33.1580	51.4480	H	0
14.2100	22.6230	56.5840	C	0	15.8440	29.8640	49.7020	H	0	25.7740	31.5090	52.6010	C	0
13.3230	22.4720	57.2000	H	0	17.1280	31.0450	48.3750	C	0	24.8340	31.0140	52.3580	H	0
13.9480	22.2160	55.6070	H	0	17.1580	32.1180	48.5630	H	0	26.3960	30.6140	52.6100	H	0
15.1860	21.8000	57.0550	O	0	18.2870	30.2420	49.0970	C	0	25.8820	32.1660	53.9650	C	0
15.7770	21.6750	56.3090	H	0	18.2850	29.1580	48.9750	H	0	26.9780	32.4660	54.4820	O	0
13.6970	24.7480	55.3870	C	0	19.2490	30.6050	48.7350	H	0	24.7300	32.6110	54.4850	N	0
13.7720	24.3940	54.2130	O	0	18.2130	30.4920	50.1550	H	0	24.8500	33.1560	55.3270	H	0
12.8910	25.7280	55.7220	N	0	16.9590	30.9370	46.8430	C	0	23.9280	32.7150	53.8800	H	0
12.8850	26.0420	56.6820	H	0	16.7210	29.8560	46.3070	O	0	27.6720	32.8360	51.6310	C	0
12.1590	26.6190	54.7350	C	0	17.2680	31.9800	46.1220	N	0	28.5690	31.9750	51.3600	O	0
11.5400	25.9000	54.1970	H	0	17.4450	32.8840	46.5370	H	0	27.9970	34.0370	52.0880	N	0
11.2920	27.5980	55.5630	C	0	17.5100	32.0680	44.5980	C	0	27.1970	34.6170	52.2950	H	0
10.6240	27.0500	56.2260	H	0	16.5220	32.0480	44.1400	H	0	29.3360	34.6230	51.9830	C	0
11.9520	28.0270	56.3170	H	0	18.2030	33.4460	44.3780	C	0	29.9980	33.9270	51.4690	H	0
10.4540	28.6450	54.8110	C	0	18.2100	33.5360	43.2920	H	0	29.3920	35.8200	51.0060	C	0
10.1320	29.3650	55.5640	H	0	17.6810	34.2710	44.8640	H	0	28.7770	36.6370	51.3820	H	0
11.0680	29.2160	54.1150	H	0	19.8850	33.4500	44.9010	S	0	30.4010	36.2320	50.9890	H	0
9.2540	28.0660	54.1000	C	0	18.3770	30.9150	43.9930	C	0	28.8950	35.4090	49.5660	C	0
8.1800	28.6460	54.0220	O	0	18.1770	30.6670	42.8150	O	0	29.6260	34.6950	49.1850	H	0
9.4090	26.9900	53.4100	N	0	19.2950	30.3580	44.7950	N	0	27.9620	34.8480	49.6140	H	0
8.5170	26.7490	53.0040	H	0	19.3190	30.7470	45.7270	H	0	28.7480	36.6770	48.7630	C	0
10.2780	26.5260	53.1890	H	0	20.5070	29.7600	44.3630	C	0	28.2120	37.4370	49.3330	H	0
13.1420	27.4060	53.8030	C	0	20.3390	29.5140	43.3140	H	0	29.7100	37.1720	48.6270	H	0
12.8770	27.6990	52.6680	O	0	21.5610	30.8970	44.4340	C	0	28.1070	36.3240	47.4380	N	0
14.3640	27.7700	54.3270	N	0	21.6940	31.1490	45.4860	H	0	28.7570	36.2510	46.6690	H	0
14.5390	27.5090	55.2870	H	0	22.4530	30.4270	44.0200	H	0	26.8360	36.1310	47.0710	C	0
15.2010	28.7230	53.5650	C	0	21.1270	32.4400	43.5340	S	0	25.8640	36.0750	47.8860	N	0
14.5990	29.5900	53.2940	H	0	20.8100	28.5580	45.3020	C	0	26.0970	36.2390	48.8550	H	0
16.3530	29.0880	54.6010	C	0	21.9610	28.0500	45.4470	O	0	24.9080	35.8500	47.6530	H	0
16.8920	28.2630	55.0660	H	0	19.7890	28.1320	45.9940	N	0	26.5640	35.9220	45.8660	N	0
17.0990	29.6280	54.0180	H	0	18.8960	28.5630	45.7990	H	0	27.3410	35.8750	45.2220	H	0
15.9750	29.6900	55.4280	H	0	19.5100	27.1080	47.0750	C	0	25.6270	35.6600	45.5950	H	0
15.7730	28.1880	52.2180	C	0	18.4610	27.1270	47.3710	H	0	30.0520	34.7070	53.3300	C	0
16.0280	29.0290	51.4020	O	0	19.8410	25.7020	46.4440	C	0	31.1650	35.1760	53.3940	O	0
16.0100	26.9260	52.0610	N	0	20.8860	25.7300	46.1370	H	0	29.4080	34.1640	54.3640	N	0
15.7400	26.3950	52.8770	H	0	19.6480	24.9290	47.1880	H	0	28.5680	33.6620	54.1130	H	0
16.4830	26.2850	50.8190	C	0	18.9770	25.2970	45.2370	C	0	29.9730	33.9380	55.6640	C	0
17.4990	26.5890	50.5680	H	0	17.7940	25.7140	45.1350	O	0	29.2830	33.4270	56.3350	H	0
16.6100	24.7810	51.0130	C	0	19.4490	24.5580	44.3550	O	0	30.7690	33.1990	55.5720	H	0
15.6190	24.3640	51.1870	H	0	20.2490	27.2700	48.3590	C	0	30.4820	35.0310	56.5290	C	0
17.1660	24.1800	49.7630	C	0	19.6360	27.1370	49.4120	O	0	29.7320	35.7310	57.1930	O	0
16.5370	24.3330	48.8860	H	0	21.5510	27.6140	48.2580	N	0	31.8130	35.1570	56.6220	N	0
18.1060	24.6510	49.4770	H	0	21.8520	27.7990	47.3120	H	0	32.4120	34.7720	55.9060	H	0
17.3070	23.1240	49.9940	H	0	22.5340	27.4560	49.3610	C	0	32.4740	35.4590	57.8960	C	0
17.6730	24.4880	52.1330	C	0	22.0220	27.4430	50.3230	H	0	31.6840	35.7010	58.6060	H	0
17.5470	24.8290	53.1610	H	0	23.1800	26.0420	49.4140	C	0	33.1830	34.2350	58.3960	C	0
17.8760	23.4170	52.1290	H	0	23.9180	26.0260	50.2160	H	0	33.1910	34.4310	59.4680	H	0
18.6010	24.9330	51.7760	H	0	22.1810	24.8580	49.6210	C	0	32.4550	33.4240	58.3650	H	0
15.5330	26.6250	49.5980	C	0	21.6100	25.0190	50.5360	H	0	34.5910	34.0130	57.9720	C	0
16.0360	27.0340	48.5650	O	0	21.4820	24.8020	48.7870	H	0	35.1760	34.9250	58.0860	H	0
14.2470	26.5260	49.8800	N	0	22.7930	23.9610	49.5230	H	0	35.2470	32.9580	58.8140	C	0
13.9520	26.3420	50.8290	H	0	23.8640	25.7510	48.0980	C	0	36.2000	32.7010	58.3520	H	0
13.1870	26.8370	48.8850	C	0	24.2740	24.7420	48.1430	H	0	35.4570	33.3560	59.8060	H	0
13.3250	26.2500	47.9770	H	0	23.1510	25.7560	47.2740	H	0	34.6390	32.0620	58.9380	H	0
11.9040	26.3170	49.5480	C	0	24.5760	26.5240	47.8090	H	0	34.6040	33.4010	56.5350	C	0
12.0600	25.4070	50.1280	H	0	23.7540	28.4660	49.4600	C	0	34.0950	34.0660	55.8360	H	0
11.5040	27.0690	50.2290	H	0	24.5920	28.2660	50.3070	O	0	35.6320	33.3740	56.1750	H	0
11.1420	26.3210	48.7690	H	0	23.8920	29.3970	48.5330	N	0	34.1660	32.4030	56.5610	H	0
13.1270	28.4080	48.7050	C	0	23.0000	29.5110	48.0730	H	0	33.4300	36.6770	57.9000	C	0
12.7510	28.8980	47.6140	O	0	24.9940	30.4490	48.4880	C	0	34.1640	36.8730	56.9550	O	0
13.5390	29.2270	49.6910	N	0	25.9740	29.9810	48.3950	H	0	33.4730	37.4130	58.9980	N	0
13.9050	28.7970	50.5280	H	0	24.7550	31.4530	47.2730	C	0	32.7870	37.2140	59.7110	H	0
13.4360	30.6630	49.5710	C	0	23.7320	31.8230	47.3470	H	0	34.4650	38.5710	59.1900	C	0
12.6000	30.9490	48.9340	H	0	25.8470	32.5050	47.2440	C	0	35.4110	38.4120	58.6730	H	0
13.2150	31.2620	50.9980	C	0	26.8470	32.0740	47.2650	H	0	33.8930	39.8640	58.5720	C	0

32.9570	40.0040	59.1120	H	0	34.5280	38.0400	66.2770	C	0	21.5800	31.1040	58.7790	H	0
34.5870	40.6460	58.8820	H	0	34.5820	38.9610	65.4550	O	0	22.8870	31.3020	60.5040	C	0
33.7770	39.7590	57.4940	H	0	34.4210	36.7500	65.8900	N	0	23.1360	32.1050	61.1970	H	0
34.9230	38.6700	60.5770	C	0	34.1610	36.0260	66.5440	H	0	22.2310	30.6420	61.0710	H	0
34.0650	38.6780	61.5140	O	0	34.1660	36.3750	64.4300	C	0	23.8070	30.7970	60.2100	H	0
36.1480	39.0020	60.8190	N	0	34.6910	37.0400	63.7440	H	0	21.1140	32.7910	59.9090	O	0
36.8000	39.2060	60.0750	H	0	34.5300	34.9540	64.1210	C	0	20.3590	32.2690	60.1890	H	0
36.7870	39.1740	62.1560	C	0	34.1780	34.3120	64.9290	H	0	22.0420	32.9790	57.0420	C	0
36.2690	38.5540	62.8880	H	0	33.8570	34.4610	62.8090	C	0	21.4190	34.0410	57.0750	O	0
38.3100	38.8450	62.0210	C	0	32.7730	34.3460	62.8180	H	0	21.9210	32.0600	56.1030	N	0
38.5770	37.8280	61.7350	H	0	34.0230	35.0820	61.9280	H	0	22.5100	31.2390	56.1080	H	0
38.6540	39.5270	61.2440	H	0	34.1850	33.4380	62.6200	H	0	20.8930	32.0790	55.0960	C	0
39.1730	39.0890	63.2780	C	0	36.0050	34.6170	63.8680	C	0	20.9840	32.9640	54.4650	H	0
39.1990	38.1850	64.2940	C	0	36.5850	34.9550	64.7270	H	0	21.0130	30.7970	54.2150	C	0
38.4770	37.3820	64.2890	H	0	36.2640	33.5610	63.9430	H	0	22.0730	30.6060	54.0470	H	0
39.9440	38.3900	65.4910	C	0	36.6740	35.2800	62.6240	C	0	20.6530	29.9790	54.8380	H	0
39.8050	37.6880	66.3000	H	0	36.4680	36.3480	62.5570	H	0	20.1920	30.8140	52.9510	C	0
40.6890	39.5890	65.6480	C	0	37.7490	35.1250	62.5390	H	0	19.1940	31.2340	53.0800	H	0
41.2210	39.8670	66.8480	O	0	36.2030	34.8700	61.7300	H	0	20.8460	31.6400	51.8100	C	0
41.5280	40.7720	66.7490	H	0	32.6000	36.6920	64.2780	C	0	20.3780	31.4500	50.8450	H	0
40.6680	40.4940	64.5930	C	0	31.7850	36.0400	65.0520	O	0	20.7300	32.7120	51.9730	H	0
41.0730	41.4900	64.6940	H	0	32.1790	37.5310	63.3470	N	0	21.9250	31.4860	51.7860	H	0
39.9560	40.2480	63.4050	C	0	32.7680	38.0370	62.7010	H	0	20.0570	29.4040	52.4950	C	0
39.8330	41.0200	62.6600	H	0	30.7860	37.6000	62.9520	C	0	19.3050	29.2670	51.7180	H	0
36.6800	40.6250	62.7670	C	0	30.1550	37.3710	63.8100	H	0	20.9900	29.0540	52.0530	H	0
37.1290	41.5790	62.1180	O	0	30.4940	39.1200	62.6150	C	0	19.6630	28.7380	53.2620	H	0
36.4320	40.7010	64.1310	N	0	31.0120	39.3530	61.6840	H	0	19.4450	32.0790	55.6710	C	0
36.2870	39.8120	64.5880	H	0	29.4670	39.1430	62.2520	H	0	18.6520	32.8190	55.0870	O	0
36.7930	41.7970	65.0160	C	0	30.7140	40.0730	63.7970	C	0	19.0850	31.4360	56.7970	N	0
37.4990	42.5530	64.6720	H	0	29.8650	39.8850	64.9400	C	0	19.7480	30.8280	57.2560	H	0
35.4720	42.5050	65.2750	C	0	29.0650	39.1600	64.9710	H	0	17.7300	31.7300	57.3580	C	0
34.9340	41.6770	65.7370	H	0	30.0360	40.6930	66.0410	C	0	17.0120	31.7930	56.5410	H	0
35.5150	43.2130	66.1030	H	0	29.3500	40.5610	66.8650	H	0	17.2950	30.6660	58.3690	C	0
35.0420	42.7720	64.3100	H	0	31.0610	41.6700	66.0410	C	0	16.2350	30.8910	58.4860	H	0
37.4650	41.3330	66.3230	C	0	31.1440	42.3820	66.8490	H	0	17.4070	29.7490	57.7900	H	0
37.5540	40.1240	66.4590	O	0	31.8920	41.8300	64.9170	C	0	17.9860	30.4580	59.6400	C	0
37.8130	42.1520	67.3240	N	0	32.7410	42.4970	64.9310	H	0	19.0130	31.1060	59.9640	O	0
37.6480	43.1310	67.1370	H	0	31.7400	40.9980	63.8190	C	0	17.4920	29.5020	60.3410	O	0
38.5840	41.6720	68.5030	C	0	32.4680	41.0210	63.0220	H	0	17.4970	33.1490	57.9900	C	0
39.4430	41.1740	68.0550	H	0	30.4910	36.7300	61.7330	C	0	16.4070	33.5660	58.3440	O	0
39.1000	42.8650	69.2810	C	0	31.2540	36.6180	60.8300	O	0	18.6020	33.9280	58.2980	N	0
39.5430	43.5400	68.5490	H	0	29.2780	36.1880	61.6180	N	0	19.5070	33.4880	58.2120	H	0
38.1710	43.3290	69.6110	H	0	28.6080	36.5050	62.3040	H	0	18.5000	35.3530	58.6040	C	0
40.0290	42.4870	70.4290	C	0	28.7580	35.4820	60.4000	C	0	18.8800	35.9080	57.7470	H	0
40.6450	41.4530	70.3570	O	0	29.1580	36.0670	59.5710	H	0	17.4350	35.5360	58.7490	H	0
40.1110	43.2730	71.4930	N	0	29.3290	34.0270	60.2900	C	0	19.1160	35.9640	59.8910	C	0
40.7380	43.0500	72.2530	H	0	29.1200	33.5490	59.3330	H	0	18.8060	37.1330	60.2570	O	0
39.5780	44.1200	71.6220	H	0	30.4000	34.2130	60.3720	H	0	19.8500	35.1670	60.6730	N	0
37.8360	40.6070	69.3500	C	0	28.9220	33.0500	61.3540	C	0	20.1410	34.2920	60.2610	H	0
36.8530	40.9050	69.9440	O	0	29.6660	32.2820	61.5630	H	0	20.4880	35.5600	61.9750	C	0
38.2320	39.3530	69.2920	N	0	28.8940	33.6470	62.2660	H	0	19.8470	36.2810	62.4830	H	0
38.9750	39.1170	68.6500	H	0	27.2550	32.4240	61.0700	S	0	20.7390	34.2730	62.7950	C	0
37.6700	38.2540	70.0830	C	0	27.5030	31.4300	59.5470	C	0	21.6460	33.7710	62.4600	H	0
38.3430	37.4150	70.2620	H	0	27.6520	32.1020	58.7030	H	0	21.0290	34.4710	63.8270	H	0
37.4940	38.5340	71.1210	H	0	28.2320	30.6270	59.6600	H	0	19.6750	33.1810	62.7860	C	0
36.3890	37.6450	69.4060	C	0	26.5280	30.9670	59.3950	H	0	18.8580	33.3990	63.4740	H	0
35.8590	36.6650	69.9370	O	0	27.2570	35.5160	60.1760	C	0	19.1070	33.0950	61.8590	H	0
35.9240	38.1800	68.2850	N	0	26.5050	35.5570	61.1550	O	0	20.1560	31.8210	63.2580	C	0
36.5500	38.7970	67.7870	H	0	26.7470	35.6270	58.9430	N	0	20.5080	31.5940	64.4220	O	0
34.5850	38.1920	67.8090	C	0	27.4030	35.5580	58.1780	H	0	19.8720	30.7070	62.5460	N	0
34.1440	37.2910	68.2360	H	0	25.2640	35.6100	58.7020	C	0	20.1840	29.7880	62.8280	H	0
33.7620	39.4250	68.1880	C	0	24.7240	35.8950	59.6040	H	0	19.5980	30.7930	61.5780	H	0
34.2510	40.3410	67.8550	H	0	24.9610	36.7270	57.7540	C	0	21.8780	36.2160	61.6850	C	0
32.7810	39.3560	67.7200	H	0	23.8980	36.5670	57.5760	H	0	22.6070	35.7300	60.7870	O	0
33.4880	39.3920	69.7170	C	0	25.1310	38.1190	58.4210	C	0	22.3590	37.1180	62.5860	N	0
33.0200	38.4430	69.9790	H	0	26.1510	38.2030	58.7960	H	0	21.6710	37.4580	63.2430	H	0
34.4380	39.4370	70.2500	H	0	24.9460	39.0330	57.8570	H	0	23.7400	37.5650	62.6910	C	0
32.5120	40.4990	70.1300	C	0	24.3490	38.1390	59.1810	H	0	24.4480	37.2270	61.9350	H	0
32.9260	41.4510	69.7980	H	0	25.7400	36.7970	56.5840	O	0	23.7870	39.0950	62.4090	C	0
31.4730	40.3580	69.8350	H	0	25.6450	36.0500	55.9880	H	0	23.7100	39.2330	61.3300	H	0
32.4910	40.4350	71.6460	C	0	24.6930	34.2430	58.1770	C	0	22.5940	39.8860	63.0200	C	0
32.2190	39.4360	71.9840	H	0	25.2340	33.6940	57.2110	O	0	21.7330	39.7870	62.3580	H	0
33.5400	40.6670	71.8310	H	0	23.6830	33.7030	58.8350	N	0	22.3450	39.4340	63.9800	H	0
31.5800	41.4080	72.4340	N	0	23.3710	34.0420	59.7340	H	0	22.8250	40.9320	63.2200	H	0
31.5920	41.2120	73.4250	H	0	22.9490	32.5750	58.2770	C	0	25.2330	39.6210	62.8700	C	0
31.8920	42.3680	72.4020	H	0	23.7290	31.8850	57.9540	H	0	25.1610	40.6890	63.0740	H	0
30.6410	41.3620	72.0650	H	0	22.0790	31.9110	59.3150	C	0	25.4220	39.2080	63.8600	H	0

26.3510	39.1630	61.9870	C	0	38.3400	33.2790	69.9640	H	0	29.8230	36.4460	72.1370	H	0
26.5730	38.1040	62.1120	H	0	39.8140	31.8050	69.9550	C	0	31.3350	35.0150	71.9490	C	0
26.1730	39.5010	60.9660	H	0	40.7720	31.7380	69.4380	H	0	31.5440	34.1490	71.3210	H	0
27.2690	39.6640	62.2930	H	0	40.3020	32.2930	71.3040	C	0	32.2610	36.0670	71.4480	C	0
24.2000	37.0680	64.0740	C	0	40.7510	33.2850	71.2540	H	0	32.1570	36.9580	72.0680	H	0
23.7180	37.4380	65.1160	O	0	39.5030	32.3260	72.0440	H	0	33.3100	35.7750	71.3940	H	0
25.1900	36.1960	63.9440	N	0	41.3000	31.3840	71.9850	C	0	31.9340	36.2770	70.4300	H	0
25.6010	36.1000	63.0270	H	0	42.0750	30.6830	71.4110	O	0	31.6140	34.5870	73.4360	C	0
25.8480	35.4060	65.0230	C	0	41.1840	31.1140	73.2090	N	0	31.2210	33.5760	73.5430	H	0
25.2230	35.3510	65.9150	H	0	41.9090	30.6150	73.7050	H	0	32.6760	34.4850	73.6610	H	0
25.9790	33.8730	64.5990	C	0	40.3340	31.4760	73.6160	H	0	31.2530	35.3500	74.1250	H	0
26.6390	33.6900	63.7510	H	0	39.2610	30.3570	70.1950	C	0	27.3620	35.2590	72.1030	C	0
26.6820	33.1390	65.7700	C	0	39.9900	29.3640	69.9550	O	0	26.8450	35.5190	73.1730	O	0
27.7180	33.4770	65.7920	H	0	37.9320	30.1620	70.3790	N	0	26.8320	35.6010	70.9450	N	0
26.2640	33.2450	66.7710	H	0	37.3880	31.0090	70.4620	H	0	27.4510	35.4390	70.1650	H	0
26.8730	32.0900	65.5420	H	0	37.4260	28.7610	70.7050	C	0	25.3560	35.8680	70.8070	C	0
24.6480	33.3350	64.2240	C	0	38.1740	28.0180	70.4300	H	0	24.8490	35.1780	71.4810	H	0
23.8350	33.6850	64.8600	H	0	37.3510	28.6080	72.2750	C	0	25.0440	37.3520	71.1650	C	0
24.3970	33.8150	63.2780	H	0	37.2370	27.5360	72.4370	H	0	24.0230	37.5120	70.8170	H	0
24.3090	31.7950	64.1130	C	0	38.4740	29.1100	73.0420	C	0	25.0740	37.4710	72.2480	H	0
24.2830	31.3540	65.1090	H	0	39.3990	28.5680	72.8440	H	0	25.8060	38.4540	70.5450	C	0
23.3030	31.7590	63.6940	H	0	38.5780	30.1950	73.0320	H	0	26.9550	39.0470	71.0540	C	0
25.0590	31.3540	63.4560	H	0	38.2380	28.8540	74.0750	H	0	27.4950	38.7540	71.9430	H	0
27.2190	35.9790	65.3820	C	0	36.1340	29.1770	72.7730	O	0	27.4760	39.9140	70.1400	N	0
27.9290	36.5620	64.5570	O	0	36.3520	30.1080	72.8680	H	0	28.2640	40.5130	70.3440	H	0
27.5470	35.9590	66.7360	N	0	36.1320	28.2450	70.0410	C	0	26.6460	40.0880	69.0060	C	0
26.9680	35.3470	67.2930	H	0	35.6610	27.1350	70.3510	O	0	26.6190	41.0310	67.9420	C	0
28.8520	36.2610	67.2070	C	0	35.5310	28.9730	69.0670	N	0	27.3790	41.7760	67.7570	H	0
29.3980	36.4250	66.2780	H	0	35.9080	29.8580	68.7580	H	0	25.6060	40.9060	66.9760	C	0
28.9110	37.5240	68.0730	C	0	34.3450	28.5140	68.3830	C	0	25.6880	41.4810	66.0650	H	0
28.5900	38.3050	67.3840	H	0	34.1450	29.2920	67.6460	H	0	24.5970	39.9980	67.1720	C	0
28.1620	37.4870	68.8640	H	0	34.4950	27.5480	67.9020	H	0	23.9220	39.8450	66.3430	H	0
29.8640	37.6720	68.5820	H	0	33.0790	28.4130	69.2240	C	0	24.4890	39.1340	68.2800	C	0
29.4120	34.9390	67.7600	C	0	32.1200	27.8190	68.7600	O	0	23.6190	38.5060	68.3970	H	0
28.7060	34.2920	68.6030	O	0	32.9570	29.0910	70.3950	N	0	25.5600	39.1190	69.2430	C	0
30.5130	34.4690	67.2030	N	0	33.7370	29.6620	70.6870	H	0	24.8290	35.5630	69.3960	C	0
31.0320	35.0180	66.5320	H	0	31.6870	29.1940	71.1570	C	0	25.5170	35.2070	68.4880	O	0
31.3670	33.3810	67.6630	C	0	31.0550	28.3110	71.0690	H	0	23.5000	35.6370	69.2160	N	0
30.8740	32.8350	68.4680	H	0	31.9990	29.3590	72.6310	C	0	22.9610	35.8700	70.0380	H	0
31.7490	32.5230	66.4650	C	0	32.7340	30.1620	72.6920	H	0	22.6810	35.6470	67.9620	C	0
32.2900	33.1410	65.7480	H	0	31.0880	29.7060	73.1190	H	0	23.4300	35.8460	67.1960	H	0
32.4300	31.7200	66.7450	H	0	32.6020	28.0850	73.2610	C	0	22.1410	34.2480	67.6860	C	0
30.4920	31.8240	65.7450	C	0	33.5380	27.7920	72.7840	H	0	21.2930	34.1970	68.3690	H	0
29.6260	32.4460	65.5150	H	0	32.8100	28.3160	74.3060	H	0	21.7220	34.2380	66.6800	H	0
30.9550	31.2670	64.3960	C	0	31.6390	26.8500	73.2100	C	0	22.9810	32.9660	67.9880	C	0
31.5160	30.3340	64.3410	H	0	30.6840	27.1650	73.6290	H	0	23.9440	33.0890	67.4920	H	0
30.1230	31.1550	63.7000	H	0	31.5490	26.4140	72.2150	H	0	23.1360	32.9100	69.0660	H	0
31.5850	32.0640	64.0020	H	0	32.2320	25.7690	74.1820	C	0	22.2040	31.6890	67.6130	C	0
30.0480	30.7210	66.6380	C	0	33.2000	25.4080	73.8350	H	0	21.3480	31.5730	68.2780	H	0
30.7640	29.9110	66.5010	H	0	32.2010	26.2820	75.1430	H	0	21.9000	31.6940	66.5660	H	0
30.1070	31.0700	67.6690	H	0	31.2810	24.7100	74.3340	N	0	23.1830	30.5370	67.9400	C	0
28.9890	30.5660	66.4280	H	0	30.4240	24.9250	74.8240	H	0	24.0300	30.6890	67.2720	H	0
32.6900	33.9330	68.3160	C	0	31.1800	24.2410	73.4450	H	0	23.5160	30.6950	68.9660	H	0
33.2990	34.8930	67.8630	O	0	31.6350	23.9480	74.8950	H	0	22.5220	29.2000	67.7290	N	0
33.2040	33.1690	69.3100	N	0	30.7540	30.2380	70.6390	C	0	23.1700	28.4850	68.0260	H	0
32.5940	32.5000	69.7570	H	0	31.2150	31.2180	70.1920	O	0	21.6590	29.1560	68.2530	H	0
34.5400	33.4240	69.8840	C	0	29.4380	30.0910	70.8260	N	0	22.2960	29.0200	66.7610	H	0
34.6330	34.4990	70.0350	H	0	29.1440	29.1630	71.0960	H	0	21.5940	36.7120	67.9930	C	0
34.6310	32.7690	71.3220	C	0	28.3710	31.0550	70.5680	C	0	21.3070	37.2410	69.0620	O	0
34.0270	33.4020	71.9720	H	0	28.5510	31.5690	69.6230	H	0	21.0780	37.0720	66.8610	N	0
34.1010	31.8160	71.3350	H	0	27.0870	30.2490	70.5140	C	0	21.3890	36.6780	65.9850	H	0
35.9800	32.6690	71.8860	C	0	26.8930	29.7600	71.4690	H	0	20.0370	38.1260	66.6880	C	0
36.1320	31.9550	72.9390	O	0	26.2500	30.9190	70.3130	H	0	19.2060	38.0020	67.3820	H	0
36.8710	33.3730	71.4500	O	0	27.0110	29.2620	69.3360	C	0	20.6870	39.5290	66.9280	C	0
35.6700	32.9660	68.9260	C	0	27.0720	29.9890	68.5270	H	0	21.2050	39.5260	67.8870	H	0
35.8480	31.7990	68.5550	O	0	27.7920	28.5040	69.3920	H	0	21.4940	39.6550	66.2050	H	0
36.5050	33.9190	68.4630	N	0	25.6100	28.5700	69.3220	C	0	19.5840	40.6560	66.7970	C	0
36.2930	34.8140	68.8790	H	0	25.0410	28.3260	68.2270	O	0	20.1060	41.5430	67.1570	H	0
37.6190	33.6600	67.5320	C	0	25.0120	28.3350	70.3670	O	0	19.3060	40.7830	65.7510	H	0
37.1980	33.1310	66.6770	H	0	28.5260	32.1220	71.6650	C	0	18.1180	40.4490	67.7940	S	0
38.0960	35.0210	67.1470	C	0	28.3670	31.8630	72.8530	O	0	18.8450	40.3540	69.4630	C	0
38.4990	35.5800	67.9910	H	0	28.7310	33.3720	71.2430	N	0	19.3870	41.2700	69.6990	H	0
38.8310	35.0490	66.3420	H	0	28.8250	33.4830	70.2440	H	0	18.1460	40.0190	70.2300	H	0
37.2410	35.5970	66.7950	H	0	28.7620	34.5310	72.1160	C	0	19.6200	39.5870	69.4590	H	0
38.7010	32.7520	68.0450	C	0	28.8500	34.3280	73.1830	H	0	19.4830	38.0550	65.2980	C	0
39.5140	32.2090	67.2710	O	0	29.9000	35.4850	71.6280	C	0	20.1940	37.7990	64.2580	O	0
38.9040	32.7020	69.3570	N	0	29.7520	35.6070	70.5550	H	0	18.1910	38.2470	65.1510	N	0

17.6510	38.3070	66.0020	H	0	10.5760	33.5400	57.7680	H	0	22.9770	37.9060	55.1520	C	0
17.4830	38.3730	63.8520	C	0	8.6580	33.2290	56.8140	C	0	23.2420	38.4320	56.0690	H	0
17.6220	37.4090	63.3630	H	0	8.3840	32.3430	56.2430	H	0	23.8140	37.2300	54.9800	H	0
16.0090	38.4850	64.3270	C	0	7.8980	33.1140	58.1900	C	0	22.8650	38.5630	54.2910	H	0
15.8640	37.8440	65.1970	H	0	6.8320	32.9380	58.0420	H	0	20.8570	37.7610	56.3040	C	0
15.8880	39.5180	64.6540	H	0	8.4790	31.9870	58.9880	C	0	20.7630	38.7090	55.7760	H	0
15.2030	38.0030	63.1890	C	0	9.4580	32.2640	59.3790	H	0	19.9130	37.2250	56.3980	H	0
15.3980	38.6700	62.3490	H	0	7.8080	31.6950	59.7950	H	0	21.2130	37.9280	57.7650	C	0
15.5030	36.9810	62.9570	H	0	8.5770	31.1010	58.3600	H	0	22.1080	38.5490	57.8080	H	0
13.6820	38.1150	63.4330	C	0	8.1450	34.1850	59.0310	O	0	20.3920	38.2670	58.3970	H	0
13.4600	38.0040	64.4940	H	0	9.0740	34.4180	59.0890	H	0	21.5060	36.9600	58.1710	H	0
13.4630	39.1110	63.0510	H	0	7.9930	34.4490	56.1240	C	0	21.9160	35.5590	53.2510	C	0
12.8520	37.1640	62.6040	C	0	6.7640	34.4890	55.9810	O	0	22.5420	34.6050	53.7460	O	0
11.8300	37.5390	62.6550	H	0	8.8130	35.3850	55.6390	N	0	22.0620	35.9510	51.9730	N	0
13.1820	37.1940	61.5650	H	0	9.7900	35.2700	55.8680	H	0	21.5570	36.7420	51.6010	H	0
13.0140	35.7400	63.0450	N	0	8.4240	36.4560	54.7390	C	0	23.1070	35.3520	51.0650	C	0
13.9710	35.4630	62.8790	H	0	7.3420	36.4360	54.6120	H	0	23.2840	34.3130	51.3420	H	0
12.8360	35.7540	64.0390	H	0	8.7290	37.7940	55.4030	C	0	22.5630	35.3080	49.5850	C	0
12.3780	35.0950	62.5970	H	0	9.7680	37.8300	55.7310	H	0	23.3380	34.8370	48.9820	H	0
17.8800	39.5510	63.0560	C	0	8.6610	38.6740	56.7630	H	0	21.3240	34.3280	49.3930	C	0
17.7670	40.6610	63.6640	O	0	7.8250	38.0390	56.6090	C	0	20.4870	34.6050	50.0330	H	0
18.1370	39.4720	61.7390	N	0	6.7730	38.1820	56.3640	H	0	21.1310	34.1220	48.3400	H	0
18.2760	38.5860	61.2740	H	0	7.8720	37.2720	57.3830	H	0	21.5090	33.3250	49.7760	H	0
17.9680	40.6070	60.8480	C	0	8.2760	39.3670	57.3120	C	0	22.1680	36.4660	49.0660	O	0
17.6310	41.4570	61.4410	H	0	9.2660	39.3610	57.7680	H	0	22.4390	36.3850	48.0890	H	0
19.3450	40.8070	60.1750	C	0	8.1440	40.1980	56.6190	H	0	24.4160	36.0810	51.2420	C	0
19.9890	41.3770	60.8450	H	0	7.2600	39.6890	58.4960	C	0	25.4500	35.6970	50.6840	O	0
19.8900	39.9230	59.8420	H	0	7.5250	40.6600	58.9140	H	0	24.5000	37.0480	52.1360	N	0
19.2450	41.6780	59.0320	C	0	6.2600	39.8120	58.0790	H	0	23.6440	37.4440	52.4960	H	0
19.0640	43.0660	59.1480	N	0	7.2180	38.7150	59.6030	N	0	25.6930	37.9710	52.2100	C	0
19.2360	43.5950	57.9280	C	0	6.5850	39.0870	60.2960	H	0	26.0690	38.0070	51.1870	H	0
19.2260	44.6220	57.5960	H	0	6.8850	37.8410	59.2210	H	0	25.3350	38.9500	52.5310	H	0
19.4520	42.6140	57.1120	N	0	8.1140	38.5590	60.0420	H	0	26.7780	37.4600	53.1630	C	0
19.9270	42.7180	56.2270	H	0	9.1210	36.3930	53.3320	C	0	26.8020	36.3450	53.7280	O	0
19.5240	41.4250	57.7280	C	0	8.8130	37.2110	52.5270	O	0	27.7090	38.3480	53.4560	N	0
19.9030	40.5020	57.3150	H	0	9.9050	35.4200	52.9310	N	0	27.6300	39.2020	52.9240	H	0
16.8580	40.2800	59.8050	C	0	9.9760	34.6720	53.6070	H	0	28.5510	38.3990	54.6670	C	0
16.0260	41.1220	59.4980	O	0	10.7420	35.3760	51.7370	C	0	28.1210	37.6990	55.3830	H	0
16.9980	39.1020	59.2110	N	0	10.8560	34.3270	51.4620	H	0	29.9380	37.9690	54.2510	C	0
17.5820	38.3880	59.6220	H	0	10.2250	35.7010	50.8340	H	0	30.3440	38.7750	53.6390	H	0
15.9800	38.5800	58.3290	C	0	12.1600	35.9410	51.7750	C	0	30.6610	37.8820	55.0610	H	0
15.4270	39.4210	57.9130	H	0	12.8520	35.8370	50.8110	O	0	29.8920	37.1330	53.5530	H	0
16.6150	38.0640	57.0400	C	0	12.5740	36.4470	52.9260	N	0	28.5170	39.7790	55.2970	C	0
17.6830	38.2610	56.9540	H	0	12.0840	36.3270	53.8020	H	0	28.1190	40.7980	54.6690	O	0
16.4310	36.9970	56.9090	H	0	13.9000	36.9870	53.2390	C	0	28.9830	39.9350	56.6120	N	0
16.1810	38.5720	56.1780	H	0	14.1640	37.7000	52.4590	H	0	29.4020	38.9530	57.6260	C	0
14.9740	37.6250	58.9200	C	0	13.7950	37.8670	54.5210	C	0	30.3200	38.4490	57.3230	H	0
15.0790	37.1840	60.0200	O	0	13.8530	37.3600	55.4840	H	0	28.6590	38.1610	57.7180	H	0
13.9030	37.2710	58.2350	N	0	14.6500	38.5410	54.4640	H	0	29.6190	39.6860	58.8970	C	0
13.8530	37.6070	57.2840	H	0	12.5390	38.8860	54.5770	C	0	30.5840	40.1930	58.8840	H	0
12.8450	36.3320	58.6310	C	0	12.3870	39.2620	53.5650	H	0	29.5790	38.9630	59.7120	H	0
13.2080	35.6980	59.4400	H	0	11.6600	38.3340	54.9070	H	0	28.4930	40.6910	58.8690	C	0
11.7370	37.2860	59.1300	C	0	12.8410	40.0110	55.4960	C	0	28.6160	41.4980	59.5910	H	0
12.1130	37.7210	60.0560	H	0	12.3070	41.0750	55.2310	O	0	27.6040	40.1000	59.0920	H	0
11.5500	38.0190	58.3450	H	0	13.6120	39.8190	56.4460	O	0	28.6610	41.1390	57.4330	C	0
10.5050	36.6040	59.5270	C	0	14.9630	35.9240	53.4130	C	0	27.7110	41.5330	57.0720	H	0
10.4950	35.3270	59.6350	O	0	14.7930	34.8350	53.9630	O	0	29.8000	42.2300	57.2040	C	0
9.6110	37.3400	59.9640	O	0	16.2060	36.3770	53.1480	N	0	30.7410	41.9370	56.4840	O	0
12.4220	35.5930	57.3840	C	0	16.3600	37.3160	52.8090	H	0	29.8250	43.3790	57.9100	N	0
11.8070	36.1810	56.4760	O	0	17.4430	35.5770	53.4260	C	0	29.0630	43.7430	58.4660	H	0
12.7590	34.3110	57.3780	N	0	17.1290	34.9330	54.2470	H	0	30.8660	44.4370	57.8590	C	0
13.3100	33.9910	58.1610	H	0	17.7030	34.7120	52.1810	C	0	31.8600	44.0690	57.6050	H	0
12.5080	33.4000	56.2250	C	0	18.7790	34.5470	52.2350	H	0	30.2850	45.3720	56.7050	C	0
12.9610	33.8960	55.3660	H	0	16.8660	33.4020	52.0240	C	0	30.4570	44.7280	55.8420	H	0
13.3420	32.1220	56.5110	C	0	17.0120	32.7830	52.9100	H	0	29.2170	45.5860	56.7410	H	0
14.3870	32.3950	56.6590	H	0	15.7900	33.5700	52.0710	H	0	30.9870	46.7400	56.7360	C	0
12.8040	31.3770	57.7420	C	0	17.2750	32.9010	51.1470	H	0	30.8860	47.2000	57.7190	H	0
13.5020	30.6340	58.1290	H	0	17.6480	35.4190	50.9670	O	0	32.4960	46.8220	56.4400	C	0
12.8430	32.0820	58.5720	H	0	16.7790	35.3730	50.5610	H	0	32.7650	46.6030	55.4060	H	0
11.7840	31.0510	57.5420	H	0	18.6160	36.5020	53.8500	C	0	32.8610	47.8400	56.5790	H	0
13.3930	31.0300	55.4740	C	0	18.6280	37.6630	53.7340	O	0	32.9570	46.1700	57.1820	H	0
12.4370	30.8840	54.9720	H	0	19.7350	35.8400	54.2470	N	0	30.2850	47.6890	55.6900	C	0
14.2250	31.3060	54.8260	H	0	19.6280	34.8510	54.4220	H	0	29.2310	47.4290	55.7790	H	0
13.7820	30.1150	55.9210	H	0	21.0610	36.4430	54.1390	C	0	30.5430	48.7220	55.9220	H	0
11.0040	33.1410	55.9100	C	0	21.0140	37.3310	53.5090	H	0	30.6010	47.4280	54.6800	H	0
10.6520	32.8090	54.7520	O	0	21.7460	36.9680	55.4260	C	0	31.1390	45.0600	59.2550	C	0
10.1500	33.3110	56.8820	N	0	21.9770	36.0660	55.9940	H	0	30.2280	45.2890	60.0190	O	0

32.3680	45.2670	59.6680	N	0	27.6920	51.6490	65.1020	H	0	16.9830	43.2440	51.8240	H	0
33.0380	44.9600	58.9760	H	0	25.9820	51.0660	65.0940	H	0	16.2690	44.2540	52.9840	H	0
32.8310	45.6830	60.9790	C	0	26.4560	52.2400	66.6500	C	0	16.8870	41.9830	54.2280	C	0
31.9060	45.3970	61.4800	H	0	25.9240	52.9910	66.0660	H	0	17.1870	41.1960	54.9200	H	0
34.0960	44.9040	61.4350	C	0	25.7950	51.8280	67.4130	H	0	15.9810	42.3090	54.7390	H	0
34.8910	45.0890	60.7120	H	0	27.6290	53.0370	67.2270	N	0	16.7070	41.3040	53.3940	H	0
34.6740	45.4180	62.7300	C	0	28.5650	52.6820	67.3600	H	0	19.3260	41.7650	52.1770	C	0
33.9180	45.2720	63.5010	H	0	27.9500	53.7420	66.5790	H	0	19.7050	42.4340	51.2380	O	0
35.5210	44.7910	63.0100	H	0	27.3070	53.4680	68.0820	H	0	18.9340	40.5150	51.9910	N	0
34.9430	46.4520	62.5140	H	0	29.2460	46.9200	64.8360	C	0	18.8430	40.0940	52.9050	H	0
33.9030	43.3490	61.5820	C	0	30.0660	47.3520	64.1050	O	0	18.8130	39.7720	50.7900	C	0
34.8700	43.0170	61.9600	H	0	28.6130	45.7910	64.6460	N	0	19.2310	40.3040	49.9360	H	0
33.1990	43.2410	62.4070	H	0	27.9610	45.5870	65.3890	H	0	19.7210	38.5300	50.8150	C	0
33.5930	42.9630	60.6100	H	0	28.5810	44.9980	63.4020	C	0	19.5690	37.9180	51.7040	H	0
32.9970	47.2140	60.9880	C	0	29.3930	45.3650	62.7740	H	0	19.5820	37.9050	49.9330	H	0
33.6730	47.7540	60.1710	O	0	28.6880	43.4630	63.6160	C	0	21.0780	38.9850	50.9300	O	0
32.4770	47.8210	62.0020	N	0	29.5510	43.3980	64.2780	H	0	21.3270	39.0760	50.0070	H	0
31.9540	47.2210	62.6230	H	0	27.4420	42.8230	64.2560	C	0	17.3330	39.5220	50.5060	C	0
32.1870	49.2800	62.1010	C	0	26.5480	43.0940	63.6950	H	0	16.5370	39.1610	51.3850	O	0
32.9680	49.7480	61.5020	H	0	27.5700	41.7460	64.1480	H	0	16.9400	39.5020	49.2370	N	0
30.7680	49.5350	61.5400	C	0	27.3780	43.2240	65.2680	H	0	17.6050	39.6570	48.4930	H	0
30.1050	48.9110	62.1390	H	0	28.9790	42.7360	62.3110	C	0	15.5940	39.0780	48.7140	C	0
30.3830	51.0730	61.6730	C	0	29.7280	43.2800	61.7370	H	0	15.4380	38.0050	48.8250	H	0
31.2570	51.6860	61.4510	H	0	29.3070	41.7050	62.4400	H	0	14.8210	39.3690	49.4250	H	0
29.5440	51.4290	61.0760	H	0	28.0860	42.6600	61.6910	H	0	15.4020	39.4740	47.2240	C	0
30.1300	51.2830	62.7120	H	0	27.4140	45.4610	62.5520	C	0	16.3050	39.1410	46.4260	O	0
30.3450	49.1430	60.1640	C	0	26.4470	46.0150	63.1410	O	0	14.2870	40.0820	46.8470	N	0
30.7970	49.7720	59.3970	H	0	27.5940	45.4140	61.2220	N	0	13.5960	40.3450	47.5350	H	0
30.5430	48.0850	59.9890	H	0	28.5070	45.1790	60.8600	H	0	14.0040	40.2990	45.4200	C	0
29.2700	49.3190	60.1370	H	0	26.6230	45.9130	60.1530	C	0	14.7490	40.9600	44.9770	H	0
32.4170	49.6750	63.5400	C	0	25.7670	46.3260	60.6880	H	0	14.2990	39.4170	44.8530	H	0
31.4540	49.9530	64.2700	O	0	27.2310	47.2030	59.5180	C	0	12.5080	40.5770	45.1310	C	0
33.6440	49.7520	64.0330	N	0	27.5370	47.8460	60.3440	H	0	11.8220	40.9770	46.1130	O	0
34.4430	49.4710	63.4830	H	0	28.1300	46.8690	59.0010	H	0	12.0280	40.4260	43.9560	N	0
33.9870	50.0890	65.4470	C	0	26.3380	48.0510	58.5690	C	0	12.6980	40.1710	43.2440	H	0
35.0190	49.7730	65.6040	H	0	25.4010	47.5050	58.4590	H	0	10.8530	41.0830	43.3360	C	0
34.0480	51.6240	65.6550	C	0	25.9330	49.4300	59.2470	C	0	10.8830	42.1210	43.6680	H	0
33.0980	52.0770	65.9400	H	0	25.2810	49.2170	60.0940	H	0	10.9400	41.0590	41.7630	C	0
34.6590	51.6630	66.5560	H	0	26.8120	49.9740	59.5930	H	0	11.1270	40.0420	41.4190	H	0
34.7310	52.4160	64.5420	C	0	25.2210	49.9460	58.6030	H	0	9.9950	41.4070	41.3470	H	0
35.4370	51.8100	63.9750	H	0	27.0520	48.2950	57.2290	C	0	12.0050	42.0610	41.3010	C	0
33.9110	52.7610	63.9110	H	0	27.2020	47.3650	56.6810	H	0	11.8460	42.1990	40.2320	H	0
35.4250	53.7840	65.0060	C	0	26.5320	49.0100	56.5910	H	0	11.9210	43.0040	41.8410	H	0
36.1790	53.6450	65.7810	H	0	28.0860	48.6080	57.3690	H	0	13.4090	41.5990	41.4750	C	0
35.8940	54.1720	64.1020	H	0	26.2950	44.9340	59.1220	C	0	13.6990	40.4250	41.6370	O	0
34.3350	54.7300	65.5490	C	0	27.1230	44.1110	58.7410	O	0	14.2850	42.4890	41.4360	O	0
33.6130	54.7390	64.7320	H	0	25.0070	45.0390	58.6500	N	0	9.4990	40.5120	43.8080	C	0
33.8990	54.2130	66.4040	H	0	24.4430	45.7300	59.1240	H	0	8.4340	41.0830	43.6550	O	0
34.9290	55.9970	66.0390	N	0	24.3470	43.9100	57.9410	C	0	9.5600	39.4940	44.6270	N	0
35.5780	55.8460	66.7980	H	0	25.1850	43.4860	57.3880	H	0	10.4130	39.0130	44.8740	H	0
35.4610	56.4760	65.3270	H	0	23.7450	42.7940	58.9420	C	0	8.4490	38.9590	45.4690	C	0
34.2430	56.6870	66.3090	H	0	22.9170	43.1790	59.5370	H	0	7.4690	39.0830	45.0090	H	0
33.1760	49.1830	66.3860	C	0	22.9810	41.7070	58.1280	C	0	8.7830	37.5070	45.7020	C	0
33.1110	47.9570	66.3170	O	0	23.6180	41.2040	57.4010	H	0	8.0530	37.0860	46.3930	H	0
32.4230	49.7920	67.3460	N	0	22.5390	40.9180	58.7360	H	0	8.6840	37.0810	44.7040	H	0
32.2880	50.7920	67.3080	H	0	22.2300	42.1910	57.5030	H	0	10.1320	37.1840	46.1980	C	0
31.5500	49.1940	68.3300	C	0	24.7880	42.0960	59.7530	C	0	11.1880	36.8120	45.3270	C	0
32.1150	48.3700	68.7650	H	0	24.5060	41.2420	60.3690	H	0	10.9850	36.7610	44.2680	H	0
31.2760	50.3960	69.3420	C	0	25.5850	41.6510	59.1580	H	0	12.5130	36.5270	45.8020	C	0
30.8340	49.9660	70.2410	H	0	25.1590	42.8300	60.4690	H	0	13.3670	36.3800	45.1570	H	0
32.2260	50.7930	69.7010	H	0	23.3630	44.4660	56.9340	C	0	12.7510	36.7010	47.1350	C	0
30.4670	51.6660	68.9020	C	0	22.4230	45.2480	57.3190	O	0	13.7840	36.5640	47.4210	H	0
30.0080	52.3980	69.8080	O	0	23.4460	44.0990	55.6530	N	0	11.7040	36.9540	48.0420	C	0
30.4150	51.9030	67.6640	O	0	24.2300	43.5220	55.3850	H	0	11.8840	37.2130	49.0750	H	0
30.2090	48.6910	67.8230	C	0	22.4390	44.3420	54.6240	C	0	10.3640	37.1770	47.5560	C	0
29.3930	48.2990	68.6330	O	0	21.8420	45.2470	54.7330	H	0	9.6510	37.5520	48.2750	H	0
29.9760	48.5250	66.4980	N	0	22.8230	44.3480	53.6030	H	0	8.2070	39.7720	46.7330	C	0
30.7060	48.9150	65.9190	H	0	21.4240	43.2130	54.5390	C	0	7.4460	39.3700	47.5350	O	0
28.7610	47.8620	65.9390	C	0	21.5370	42.1600	55.2050	O	0	8.7020	41.0140	46.7850	N	0
28.3260	47.2460	66.7260	H	0	20.2560	43.4190	53.8700	N	0	9.3150	41.3520	46.0560	H	0
27.6890	48.8400	65.4390	C	0	20.0760	44.2490	53.3240	H	0	8.1000	42.0780	47.6560	C	0
28.1820	49.3230	64.5950	H	0	19.2980	42.3960	53.6000	C	0	7.9520	42.9880	47.0740	H	0
26.8870	48.3300	64.9050	H	0	19.5130	41.6030	54.3160	H	0	7.1510	41.6910	48.0270	H	0
27.2920	49.9000	66.4350	C	0	17.9150	43.0210	53.8500	C	0	8.9630	42.3620	48.9260	C	0
26.4910	49.5220	67.0700	H	0	18.0650	43.5250	54.8040	H	0	8.5180	42.9510	49.9390	O	0
28.1530	50.1480	67.0560	H	0	17.2400	43.8570	52.6880	C	0	10.2490	41.9800	48.9030	N	0
26.8880	51.1990	65.6850	C	0	17.9930	44.6140	52.4700	H	0	10.5680	41.4620	48.0960	H	0

11.2660	42.3960	49.9090	C	0	23.1530	47.9360	57.3010	H	0	28.6170	43.7850	71.6980	N	0
10.9440	42.2920	50.9450	H	0	23.6530	49.4250	56.3890	H	0	28.3380	44.7530	71.6270	H	0
12.4340	41.3650	49.8910	C	0	22.0020	48.3690	54.6150	C	0	28.5730	43.1160	73.0230	C	0
13.0380	41.3340	48.9840	H	0	22.7030	49.0680	54.1590	H	0	29.4560	42.5430	73.3060	H	0
13.2460	41.5650	51.1850	C	0	22.5260	47.4140	54.6510	H	0	28.5920	44.2400	74.0540	C	0
12.6990	41.1900	52.0490	H	0	21.1570	48.2080	53.9470	H	0	27.6630	44.7590	73.8180	H	0
14.1290	40.9430	51.0370	H	0	20.0340	48.3070	57.9790	C	0	28.5900	43.9340	75.1000	H	0
13.4410	42.6260	51.3420	H	0	19.2190	49.1280	58.2960	O	0	29.7980	45.1890	73.9630	C	0
11.8800	39.8810	50.0430	C	0	20.7420	47.6470	58.8480	N	0	30.9420	44.7980	74.2080	O	0
11.0960	39.8900	50.7990	H	0	21.4620	47.0020	58.5560	H	0	29.5970	46.3930	73.4670	N	0
11.4110	39.5270	49.1250	H	0	20.7590	47.8320	60.3370	C	0	30.3120	47.0940	73.5920	H	0
12.7260	39.2670	50.3530	H	0	20.2850	48.8040	60.4720	H	0	28.6860	46.6260	73.0980	H	0
11.7770	43.7960	49.7320	C	0	20.2150	47.0720	60.8980	H	0	27.3530	42.1830	73.2040	C	0
12.2050	44.1550	48.6360	O	0	22.1520	47.7160	60.8890	C	0	27.3870	41.1750	73.8830	O	0
11.6390	44.5740	50.7830	N	0	23.0780	47.0680	60.3310	O	0	26.2450	42.6640	72.6840	N	0
11.3730	44.1250	51.6480	H	0	22.3670	48.2550	62.0790	N	0	26.2750	43.5560	72.2110	H	0
12.0230	46.0010	50.8310	C	0	21.5410	48.6170	62.5340	H	0	24.8850	42.1090	73.0230	C	0
12.2070	46.3200	49.8050	H	0	23.5760	47.9910	62.8390	C	0	24.9440	41.1580	73.5530	H	0
10.9070	46.8180	51.4770	C	0	24.2620	47.3570	62.2780	H	0	24.1750	42.9580	74.0840	C	0
9.9270	46.5760	51.0630	H	0	24.2950	49.3690	62.9940	C	0	23.2110	42.5230	74.3470	H	0
10.8160	46.5230	52.5230	H	0	23.5500	50.0740	63.3620	H	0	24.7900	43.2000	75.3810	C	0
11.1940	48.3550	51.3820	C	0	25.1050	49.3480	63.7240	H	0	25.1480	42.2440	75.7610	H	0
12.2130	48.5780	51.6980	H	0	24.7160	49.6260	62.0220	H	0	25.5490	43.9100	75.0510	H	0
11.1060	48.7520	50.3700	H	0	23.2620	47.3120	64.1880	C	0	24.0290	43.5560	76.0750	H	0
10.3150	49.0140	52.4830	C	0	22.2760	47.5920	64.7850	O	0	23.8690	44.2260	73.5170	O	0
9.2560	48.8790	52.2620	H	0	24.2910	46.6220	64.7240	N	0	24.7140	44.5700	73.2190	H	0
10.4780	48.6190	53.4850	H	0	25.2090	46.5030	64.3210	H	0	23.9720	41.9050	71.7830	C	0
10.6110	50.4290	52.4780	N	0	24.0970	45.7530	65.8330	C	0	22.9330	41.3200	71.9200	O	0
11.2400	50.8100	51.7850	H	0	23.1490	46.0550	66.2790	H	0	24.3290	42.4440	70.6150	N	0
10.2100	51.3520	53.3520	C	0	23.8700	44.2990	65.3470	C	0	25.2800	42.7200	70.4180	H	0
9.4480	51.0830	54.3690	N	0	24.7400	43.8930	64.8310	H	0	23.4090	42.2310	69.4060	C	0
9.4160	50.1020	54.6060	H	0	23.7600	43.6720	66.2320	H	0	23.9890	42.5270	68.5320	H	0
9.1650	51.8080	55.0120	H	0	22.6840	44.0320	64.4590	C	0	23.1090	41.1830	69.4060	H	0
10.4140	52.5820	53.2150	N	0	22.8580	44.1100	63.1160	C	0	22.1630	43.1420	69.4170	C	0
11.0130	52.9310	52.4810	H	0	23.8030	44.2500	62.6120	H	0	21.3360	43.0840	68.4470	O	0
10.0690	53.1290	53.9910	H	0	21.6810	44.0870	62.2960	C	0	22.0430	44.0930	70.3740	N	0
13.4180	46.1870	51.4090	C	0	21.7680	44.1520	61.2220	H	0	22.7140	44.1000	71.1290	H	0
13.6600	45.8390	52.5270	O	0	20.4580	43.7570	62.9030	C	0	21.0100	45.0840	70.2920	C	0
14.3150	46.8250	50.6530	N	0	19.2980	43.7840	62.1490	O	0	20.1090	44.4980	70.4730	H	0
14.0670	47.2600	49.7760	H	0	19.4760	43.6290	61.2180	H	0	21.1940	46.2100	71.3340	C	0
15.7120	46.9160	50.9370	C	0	20.3330	43.5800	64.3030	C	0	21.0840	45.7570	72.3190	H	0
16.1050	45.9120	51.0970	H	0	19.3930	43.3570	64.7840	H	0	22.1960	46.6380	71.3670	H	0
16.1910	47.3790	50.0740	H	0	21.4200	43.8170	65.1220	C	0	20.1570	47.3300	71.3740	C	0
15.9090	47.8600	52.2180	C	0	21.3250	43.9400	66.1910	H	0	18.9690	47.0840	71.2590	O	0
15.2180	48.8720	52.3760	O	0	25.2570	45.8180	66.7820	C	0	20.6130	48.5330	71.7050	N	0
16.8440	47.3170	53.0830	N	0	26.3870	45.5390	66.4180	O	0	19.9260	49.2550	71.8700	H	0
17.1770	46.3740	52.9410	H	0	25.0120	46.2160	68.0400	N	0	21.5770	48.7710	71.8880	H	0
17.1770	47.9990	54.3640	C	0	24.0680	46.4200	68.3350	H	0	20.9850	45.7490	68.8720	C	0
17.1230	49.0730	54.1860	H	0	26.0610	46.2870	69.0460	C	0	22.0270	46.1730	68.3330	O	0
16.0510	47.7200	55.3560	C	0	26.7860	47.0710	68.8310	H	0	19.7620	45.8430	68.2800	N	0
16.1630	48.3410	56.2450	H	0	25.4360	46.5990	70.4560	C	0	18.9610	45.3590	68.6600	H	0
15.0930	48.0600	54.9640	H	0	25.1410	47.6490	70.4410	H	0	19.5880	46.6480	67.0550	C	0
15.8350	46.3120	55.8240	C	0	24.5480	45.9770	70.5690	H	0	20.3710	46.4080	66.3360	H	0
15.9850	45.6270	54.9890	H	0	26.3200	46.2040	71.6530	C	0	18.2630	46.3120	66.2920	C	0
16.6460	46.1970	56.5430	H	0	25.8560	45.5690	72.6720	O	0	18.1230	45.2420	66.1400	H	0
14.6270	45.9820	56.6710	C	0	27.4950	46.5470	71.6350	O	0	17.4560	46.5810	66.9740	H	0
14.5790	46.6650	57.5190	H	0	26.8250	45.0250	69.1830	C	0	18.2270	47.1360	65.0050	C	0
13.6950	46.1670	56.1370	H	0	26.2810	43.9350	69.3700	O	0	18.4590	48.1870	65.1730	H	0
14.7830	44.5660	57.0630	N	0	28.1710	45.1530	69.1130	N	0	18.9910	46.9060	64.2620	H	0
15.1710	44.2950	57.9560	H	0	28.4540	46.1150	68.9880	H	0	16.8000	47.0310	64.4400	C	0
14.2180	43.4890	56.5560	C	0	29.1770	44.0480	69.2780	C	0	16.7880	47.1060	63.3530	H	0
13.2880	43.5970	55.6440	N	0	28.9730	43.3600	68.4570	H	0	16.4920	46.0330	64.7500	H	0
13.1080	44.5290	55.3000	H	0	30.6720	44.5890	69.0940	C	0	16.0030	48.0260	65.1250	N	0
12.7850	42.7310	55.5100	H	0	31.2470	43.6670	69.1740	H	0	16.2070	48.3780	66.0500	H	0
14.4940	42.3420	57.0800	N	0	30.8230	45.1700	67.7290	C	0	14.8440	48.4050	64.6910	C	0
15.1280	42.2140	57.8550	H	0	30.2290	46.0810	67.6640	H	0	14.0950	47.7820	63.7580	N	0
14.1360	41.4480	56.7740	H	0	31.8590	45.4410	67.5240	H	0	14.4970	46.9440	63.3630	H	0
18.5220	47.5870	54.8590	C	0	30.4560	44.4290	67.0190	H	0	13.2650	48.2680	63.4510	H	0
18.9960	46.4670	54.6130	O	0	31.1270	45.5960	70.1540	C	0	14.3930	49.5420	65.0860	N	0
19.0790	48.3750	55.7590	N	0	30.6540	46.5590	69.9590	H	0	14.9980	50.0560	65.7110	H	0
18.6820	49.2850	55.9440	H	0	30.7640	45.3670	71.1560	H	0	13.5920	49.9360	64.6140	H	0
20.3350	48.0560	56.4770	C	0	32.6520	45.7460	70.3390	C	0	19.7160	48.1200	67.4540	C	0
20.5840	47.0000	56.3730	H	0	32.9850	44.7960	70.7570	H	0	18.9290	48.5070	68.2620	O	0
21.6200	48.8300	55.9810	C	0	33.1570	45.9380	69.3930	H	0	20.6320	48.9260	66.9090	N	0
21.3780	49.8870	55.8650	H	0	32.8980	46.4330	71.1480	H	0	21.3260	48.5470	66.2810	H	0
22.8530	48.9130	56.9230	C	0	29.1350	43.2710	70.5860	C	0	20.7930	50.2880	67.3850	C	0
22.5290	49.4260	57.8290	H	0	29.4910	42.0830	70.5990	O	0	20.5460	50.2940	68.4460	H	0

22.1920	50.9070	67.2410	C	0	11.8200	48.6480	56.7180	C	0	10.7300	61.4120	59.8470	C	0
22.3920	50.8840	66.1700	H	0	11.2110	47.6750	57.3910	O	0	11.2650	62.0860	59.1780	H	0
22.3860	52.3090	67.8360	C	0	11.1080	46.8840	56.8570	H	0	9.7180	61.7990	59.9630	H	0
21.6440	53.0780	67.6220	H	0	12.2980	48.4120	55.3900	C	0	11.4700	61.3910	61.1640	C	0
22.4600	52.2700	68.9230	H	0	12.2630	47.3900	55.0400	H	0	12.4450	62.2360	61.2560	O	0
23.3880	52.7010	67.6650	H	0	12.8760	49.4700	54.6810	C	0	11.1650	60.7130	62.1980	O	0
23.2570	50.0020	67.7840	C	0	13.3380	49.2180	53.7380	H	0	12.1880	58.0660	58.7560	C	0
23.0890	48.9540	67.5380	H	0	15.8840	52.2840	53.1710	C	0	12.0610	57.4790	59.8210	O	0
24.1960	50.3330	67.3410	H	0	16.6190	53.2730	53.2520	O	0	12.4420	57.3660	57.5870	N	0
23.2230	49.9470	68.8720	H	0	15.7020	51.6960	52.0030	N	0	12.3980	57.7810	56.6670	H	0
19.7570	51.1490	66.6010	C	0	15.2630	50.7880	52.0620	H	0	12.6680	55.9290	57.5610	C	0
19.1140	51.9310	67.2040	O	0	16.3940	52.0500	50.7410	C	0	13.0740	55.7590	58.5580	H	0
19.6240	50.9010	65.3350	N	0	17.3170	52.5940	50.9400	H	0	11.3560	55.2410	57.4010	C	0
20.1630	50.1630	64.9050	H	0	16.7790	50.8090	49.8770	C	0	11.4610	54.1960	57.6920	H	0
18.6920	51.5710	64.4680	C	0	15.9460	50.1250	49.7120	H	0	10.6010	55.7220	58.0230	H	0
17.7510	51.8150	64.9590	H	0	17.2090	51.0550	48.9060	H	0	10.7940	55.2920	55.9910	C	0
19.3080	52.9610	64.0870	C	0	17.8630	50.1330	50.4660	O	0	10.9330	56.2400	55.4720	H	0
18.7640	53.4100	63.2560	H	0	18.0530	49.4730	49.7950	H	0	11.3030	54.6330	55.2880	H	0
19.0550	53.5830	64.9460	H	0	15.6410	52.9770	49.8160	C	0	9.3900	54.7690	56.0130	C	0
20.7370	52.9040	63.8330	C	0	16.1610	53.3670	48.7900	O	0	8.5380	55.4200	56.5810	O	0
21.7150	53.3800	64.6200	C	0	14.4800	53.3650	50.2070	N	0	9.2040	53.6080	55.5850	O	0
21.5400	53.7930	65.6020	H	0	14.2950	53.0440	51.1470	H	0	13.7390	55.3530	56.6310	C	0
22.9110	53.4180	63.9650	N	0	13.5000	54.2710	49.4670	C	0	14.3870	54.3490	56.9830	O	0
23.7220	53.9510	64.2430	H	0	14.0150	55.1690	49.1280	H	0	14.0600	56.1140	55.5690	N	0
22.9200	52.7390	62.8140	C	0	12.9580	53.5640	48.2290	C	0	13.2960	56.6280	55.1560	H	0
23.9580	52.4870	61.9350	C	0	12.2760	54.2800	47.7730	H	0	15.3910	56.1260	54.9620	C	0
24.9590	52.8390	62.1390	H	0	13.7570	53.4100	47.5030	H	0	15.5910	55.0670	54.8000	H	0
23.5590	51.8560	60.7280	C	0	12.1200	52.2960	48.3530	C	0	15.2960	56.8430	53.6220	C	0
24.3190	51.7100	59.9760	H	0	11.2410	52.5540	48.9440	H	0	14.8680	57.8070	53.8970	H	0
22.2350	51.4940	60.5060	C	0	11.6730	52.0600	47.3870	H	0	16.6550	56.8360	52.9600	C	0
22.0220	50.8760	59.6460	H	0	12.8000	51.0910	49.0280	C	0	17.0160	55.8250	52.7710	H	0
21.2580	51.6740	61.4530	C	0	12.9020	50.9610	50.2440	O	0	16.6750	57.4070	52.0320	H	0
20.2140	51.4610	61.2800	H	0	13.3360	50.1690	48.2270	N	0	17.3280	57.3510	53.6450	H	0
21.5140	52.4080	62.6290	C	0	13.6530	49.3140	48.6600	H	0	14.3830	56.1060	52.7020	C	0
18.3860	50.7220	63.2430	C	0	13.1310	50.1800	47.2380	H	0	14.5810	56.5330	51.7190	H	0
19.0090	49.6360	63.1680	O	0	12.4010	54.7090	50.4940	C	0	14.5910	55.0360	52.6790	H	0
17.4980	51.1530	62.3320	N	0	12.2680	54.0620	51.5440	O	0	13.2980	56.1910	52.7570	H	0
16.9530	51.9120	62.7140	H	0	11.6560	55.7260	50.1480	N	0	16.4870	56.6610	55.9090	C	0
17.2180	50.5840	61.0110	C	0	11.9630	56.3360	49.4040	H	0	17.6200	56.3780	55.7150	O	0
18.0950	50.1020	60.5780	H	0	10.5270	56.2830	50.8680	C	0	16.1540	57.5210	56.9000	N	0
16.1020	49.5070	61.1580	C	0	9.7060	56.4150	50.1630	H	0	15.1720	57.7210	56.7810	H	0
16.3500	48.8010	61.9510	H	0	10.1620	55.6340	51.6630	H	0	16.8840	58.3120	57.8840	C	0
15.1720	50.0040	61.4340	H	0	10.7840	57.6140	51.6130	C	0	16.1690	59.0110	58.3190	H	0
15.7450	48.6700	59.8930	C	0	11.7130	58.3140	51.2130	O	0	17.4530	57.3780	58.9720	C	0
15.8410	49.2700	58.9880	H	0	10.1460	57.7710	52.8170	N	0	18.1700	56.6710	58.5540	H	0
16.5330	47.4320	59.7780	C	0	8.9100	57.1400	53.2500	C	0	18.1170	57.9930	59.5800	H	0
17.5530	47.8110	59.7060	H	0	9.3030	56.2670	53.7700	H	0	16.4820	56.6440	59.8400	C	0
16.3040	46.7890	60.6280	H	0	8.2900	56.8750	52.3930	H	0	15.7060	56.2390	59.1900	H	0
16.2660	46.8600	58.8900	H	0	8.1080	58.1310	54.0850	C	0	17.1500	55.6330	60.7480	C	0
14.2860	48.2370	60.0950	C	0	7.4650	57.6960	54.8500	H	0	18.0500	55.9830	61.2520	H	0
13.6700	49.1260	60.2350	H	0	7.4200	58.6450	53.4130	H	0	16.4530	55.1590	61.4390	H	0
13.9000	47.7420	59.2040	H	0	9.1330	59.1080	54.6590	C	0	17.4640	54.7650	60.1680	H	0
14.2040	47.5050	60.8990	H	0	9.4910	58.8030	55.6420	H	0	15.6770	57.5590	60.7960	C	0
16.9510	51.7460	59.9810	C	0	8.7490	60.1200	54.7900	H	0	15.0710	58.3510	60.3550	H	0
16.2760	52.7320	60.2890	O	0	10.2810	58.9550	53.6150	C	0	14.8860	56.9750	61.2660	H	0
17.4320	51.5250	58.7550	N	0	10.1610	59.8700	53.0340	H	0	16.3770	57.9300	61.5440	H	0
18.0410	50.7460	58.5480	H	0	11.6180	59.1490	54.2330	C	0	17.9550	59.2370	57.1820	C	0
17.2000	52.4400	57.6420	C	0	12.3680	58.2340	54.4360	O	0	19.0560	58.7740	56.7900	O	0
16.3830	53.1200	57.8860	H	0	11.9680	60.3960	54.5260	N	0	17.6860	60.5450	57.1560	N	0
18.4870	53.2820	57.5310	C	0	11.3090	61.1440	54.3650	H	0	16.7330	60.7340	57.4290	H	0
18.6660	53.9050	58.4070	H	0	13.2540	60.7250	55.2020	C	0	18.5470	61.5190	56.4190	C	0
19.3810	52.6690	57.4100	H	0	14.0990	60.2710	54.6840	H	0	19.3690	61.0520	55.8780	H	0
18.3310	53.9860	56.7130	H	0	13.5890	62.2380	55.0670	C	0	17.6070	62.3500	55.4390	C	0
16.8370	51.7640	56.2640	C	0	12.9490	62.8320	55.7190	H	0	16.5710	62.0510	55.6010	H	0
17.5310	50.8030	55.8680	O	0	14.5560	62.5040	55.4940	H	0	17.7010	63.4250	55.5950	H	0
15.8280	52.3090	55.5790	N	0	13.4640	62.8560	53.6710	C	0	17.8960	62.1000	53.8750	C	0
15.2480	52.8940	56.1630	H	0	13.3580	64.0820	53.6100	O	0	18.9400	62.3720	53.7160	H	0
15.2050	51.6460	54.4220	C	0	13.3900	62.1720	52.6390	O	0	17.6940	60.6330	53.5610	C	0
15.3700	50.5700	54.4640	H	0	13.2920	60.4300	56.7080	C	0	18.0840	60.2830	52.6060	H	0
13.6450	51.7840	54.4160	C	0	14.3500	60.4190	57.2470	O	0	18.2060	60.0840	54.3520	H	0
13.4540	52.7960	54.7720	H	0	12.1770	60.2070	57.3970	N	0	16.6190	60.4520	53.5770	H	0
13.3730	51.7380	53.3610	H	0	11.3090	60.4070	56.9200	H	0	16.9920	62.9280	52.9550	C	0
12.9700	50.7450	55.2290	C	0	12.0320	59.6000	58.7050	C	0	17.1280	62.7710	51.8850	H	0
12.3990	51.0050	56.5400	C	0	12.8270	59.9140	59.3810	H	0	15.9680	62.7190	53.2640	H	0
12.3620	52.0120	56.9290	H	0	10.6780	59.9850	59.2460	C	0	17.1560	63.9870	53.1540	H	0
11.7630	49.9540	57.2690	C	0	9.9960	59.8800	58.4020	H	0	19.1270	62.4610	57.5100	C	0
11.2930	50.2130	58.2070	H	0	10.3630	59.3160	60.0470	H	0	18.4200	62.8770	58.4350	O	0

20.3990	62.8130	57.3300	N	0	26.2340	69.1100	52.2830	H	0	26.3960	67.5920	40.0160	H	0
20.9460	62.4890	56.5460	H	0	26.6700	70.7600	51.7870	H	0	21.2290	66.6780	41.1670	C	0
20.9470	63.8710	58.0630	C	0	26.2820	70.6120	53.8930	C	0	20.3960	66.1170	40.5180	O	0
20.5300	63.8490	59.0700	H	0	26.1020	71.6870	53.8880	H	0	21.7450	66.0520	42.2350	N	0
22.4810	63.6040	58.2620	C	0	25.5660	70.1060	54.5400	H	0	22.4170	66.5130	42.8310	H	0
22.5580	62.5440	58.5040	H	0	27.6620	70.1910	54.4030	C	0	21.4150	64.6320	42.6110	C	0
23.0370	63.8740	57.3640	H	0	27.7250	69.1070	54.4990	H	0	21.5600	63.9310	41.7890	H	0
23.0310	64.3040	59.5450	C	0	28.3490	70.5100	53.6200	H	0	22.2790	64.2010	43.7830	C	0
24.1890	64.0380	59.8940	O	0	27.8710	70.8370	55.6870	N	0	22.0410	64.7930	44.6670	H	0
22.3210	65.1160	60.1270	O	0	28.2850	71.7580	55.6760	H	0	22.1560	63.1520	44.0540	H	0
20.6500	65.2330	57.4030	C	0	26.9590	71.0970	56.0350	H	0	23.7830	64.3520	43.5860	C	0
20.2160	65.3520	56.2850	O	0	28.3230	70.2010	56.3290	H	0	24.3570	65.2160	42.6560	N	0
20.8730	66.2780	58.2180	N	0	25.1810	70.6850	49.6280	C	0	25.6790	65.0370	42.6730	C	0
21.1340	66.1290	59.1820	H	0	24.9340	71.8250	49.2850	O	0	26.4570	65.4510	42.0480	H	0
20.7770	67.6710	57.7400	C	0	26.2160	69.9900	49.1450	N	0	25.9270	64.1590	43.6360	N	0
19.7590	67.9700	57.4920	H	0	26.3290	69.0240	49.4150	H	0	26.8740	63.8820	43.8510	H	0
21.3220	68.5320	58.8990	C	0	26.9550	70.6040	48.0400	C	0	24.7750	63.7260	44.2930	C	0
22.3960	68.3610	58.9620	H	0	27.0910	71.6670	48.2400	H	0	24.7120	63.0020	45.0920	H	0
21.3010	69.5980	58.6770	H	0	28.3290	69.8340	47.7910	C	0	20.0080	64.4690	43.1070	C	0
20.8620	68.2190	60.1850	O	0	28.0300	68.8100	47.5680	H	0	19.5730	63.3420	43.3900	O	0
20.2190	68.9100	60.3610	H	0	28.8730	70.1090	46.8870	H	0	19.3350	65.4930	43.5290	N	0
21.5950	68.0260	56.5590	C	0	29.2930	70.0020	48.9300	C	0	19.8410	66.3580	43.4050	H	0
21.1790	68.8230	55.7700	O	0	30.2390	69.5890	48.5800	H	0	18.1030	65.4810	44.3090	C	0
22.8380	67.4570	56.4930	N	0	29.4150	71.0730	49.0900	H	0	17.3430	66.1810	43.9600	H	0
23.0590	66.9100	57.3120	H	0	28.9370	69.3460	50.2620	C	0	17.7200	64.4700	44.1700	H	0
23.8850	67.7170	55.5820	C	0	28.2700	68.2740	50.3690	O	0	18.3940	65.7530	45.7500	C	0
23.9020	68.7860	55.3690	H	0	29.4190	69.8760	51.3560	O	0	19.5510	66.0010	46.1730	O	0
25.1850	67.2330	56.3040	C	0	26.2790	70.5040	46.6560	C	0	17.3490	65.5660	46.5720	N	0
25.2280	66.1630	56.5070	H	0	26.5690	71.3220	45.7260	O	0	16.5370	65.0680	46.2370	H	0
25.9510	67.4800	55.5680	H	0	25.3260	69.5700	46.4360	N	0	17.3630	65.9220	47.9980	C	0
25.5120	68.1470	57.5520	C	0	25.0660	68.9640	47.2000	H	0	18.3310	65.5640	48.3470	H	0
25.7550	67.5810	58.6410	O	0	24.7440	69.2150	45.1270	C	0	17.3490	67.0110	47.9780	H	0
25.5050	69.4210	57.3510	O	0	25.0400	70.0750	44.5280	H	0	16.1990	65.4310	48.8380	C	0
23.5880	66.9550	54.2100	C	0	25.3980	67.9000	44.5670	C	0	15.4850	64.4910	48.4230	O	0
24.4510	67.0590	53.3210	O	0	25.1150	67.0030	45.1170	H	0	15.9990	65.9980	50.0290	N	0
22.4220	66.3070	54.0300	N	0	25.1010	67.6360	43.5520	H	0	16.6440	67.2450	50.5660	C	0
21.6770	66.4790	54.6890	H	0	26.9180	67.9730	44.5990	C	0	16.6960	67.9860	49.7680	H	0
22.0630	65.4070	52.8610	C	0	27.5870	68.8850	43.7820	C	0	17.6830	67.1310	50.8770	H	0
22.7280	64.5420	52.8610	H	0	27.0290	69.4850	43.0780	H	0	15.7450	67.6300	51.7310	C	0
20.6030	64.8600	53.0410	C	0	28.9540	69.0930	43.8570	C	0	15.0150	68.4170	51.5440	H	0
20.6130	64.4080	54.0340	H	0	29.5220	69.8350	43.3150	H	0	16.3220	67.9800	42.5870	H	0
19.8090	65.6060	53.0320	H	0	29.6200	68.2460	44.7770	C	0	15.1480	66.2990	52.2890	C	0
20.3490	63.6880	52.0280	C	0	30.6810	68.3460	44.9480	H	0	14.2540	66.6290	52.8170	H	0
21.1290	62.5350	52.1610	C	0	28.9840	67.2590	45.4200	C	0	15.8320	65.6760	52.8650	H	0
21.8450	62.4500	52.9650	H	0	29.6380	66.8200	46.1580	H	0	14.9620	65.4960	50.9360	C	0
20.9230	61.5440	51.1550	C	0	27.6250	67.1400	45.4350	C	0	15.1940	64.4510	51.1390	H	0
21.4280	60.5890	51.1700	H	0	27.1610	66.4420	46.1150	H	0	13.5320	65.6180	50.3670	C	0
19.9210	61.6790	50.1760	C	0	23.2090	69.1610	44.9490	C	0	13.2020	66.6470	49.7730	O	0
19.7920	60.8460	49.5010	H	0	22.6020	68.1130	45.0120	O	0	12.6630	64.5280	50.5220	N	0
19.1310	62.8750	50.1350	C	0	22.5720	70.2840	44.5850	N	0	12.9480	63.8110	51.1740	H	0
18.3410	62.9940	49.4090	H	0	23.1100	71.6210	44.4140	C	0	11.2990	64.3710	49.9370	C	0
19.4240	63.8670	51.0210	C	0	23.6010	71.7050	43.4450	H	0	10.6610	63.7740	50.5890	H	0
18.8060	64.7520	51.0390	H	0	23.7300	72.0230	45.2160	H	0	10.8480	65.3510	49.7830	H	0
22.2070	66.1620	51.5300	C	0	21.9030	72.5660	44.2960	C	0	11.2510	63.5740	48.6240	C	0
21.4760	67.1120	51.4000	O	0	22.1880	73.3360	43.5800	H	0	10.1940	63.0930	48.1160	O	0
23.1400	65.8480	50.6490	N	0	21.5540	72.8320	45.2940	H	0	12.4260	63.5370	47.9380	N	0
23.8500	65.1940	50.9460	H	0	20.9120	71.6790	43.5890	C	0	13.2430	63.8870	48.4170	H	0
23.4030	66.5160	49.2990	C	0	21.1300	71.5170	42.5330	H	0	12.4830	62.9030	46.5520	C	0
24.3510	66.1500	48.9070	H	0	19.8920	72.0320	43.7400	H	0	11.7680	63.2650	45.8130	H	0
22.3280	65.9870	48.3120	C	0	21.1430	70.2820	44.1610	C	0	13.8580	63.2790	46.0010	C	0
21.3210	66.3430	48.5320	H	0	20.4680	70.0190	44.9750	H	0	14.6690	62.9460	46.6500	H	0
22.5530	66.5360	47.3970	H	0	20.8350	69.2420	43.0230	C	0	14.0170	62.7880	45.0410	H	0
22.3220	64.5020	48.1700	C	0	19.7620	68.6310	43.0140	O	0	13.9960	64.8250	45.6140	C	0
23.0810	63.7510	48.7550	O	0	21.7450	68.9950	42.1070	N	0	14.9230	65.0130	44.8410	O	0
21.3730	64.0160	47.3990	N	0	22.6510	69.4370	42.1690	H	0	13.2170	65.7370	45.9490	O	0
21.3140	63.0130	47.2920	H	0	21.4430	68.1960	40.9360	C	0	12.3720	61.3750	46.6630	C	0
20.8030	64.5920	46.7960	H	0	20.4980	68.6060	40.5790	H	0	11.8480	60.6770	45.8230	O	0
23.5500	68.0630	49.3900	C	0	22.4510	68.4350	39.8530	C	0	12.9910	60.8230	47.6650	N	0
23.2630	68.7110	48.3870	O	0	21.9610	68.0550	38.9560	H	0	13.4770	61.4380	48.3020	H	0
24.0600	68.5620	50.4730	N	0	22.4440	69.4740	39.5260	H	0	12.9400	59.3660	48.0180	C	0
24.1640	67.8810	51.2110	H	0	23.9010	67.8880	40.0400	C	0	13.2650	58.8270	47.1280	H	0
24.2000	69.9850	50.6730	C	0	23.8330	66.9270	40.5510	H	0	13.4850	59.1700	48.9410	H	0
23.2410	70.4260	50.3980	H	0	24.3110	67.6040	39.0710	H	0	11.4710	58.8280	48.2070	C	0
24.5080	70.3390	52.1320	C	0	24.9310	68.7550	40.7650	C	0	11.1200	57.6820	47.9640	O	0
24.1780	71.3520	52.3650	H	0	24.6370	69.6860	41.5000	O	0	10.6190	59.7500	48.6710	N	0
23.9620	69.7110	52.8360	H	0	26.2400	68.4210	40.5710	N	0	11.0050	60.6530	48.9060	H	0
26.0380	70.1690	52.4510	C	0	26.9690	68.9510	41.0260	H	0	9.1210	59.5210	48.5470	C	0



8.9700	58.4670	48.7820	H	0	3.9980	53.8550	39.6700	H	0	4.8420	49.6080	52.0670	H	0
8.3370	60.2310	49.6730	C	0	2.7300	55.0600	40.7880	C	0	4.8710	51.6690	52.0230	C	0
8.1980	61.2350	49.2710	H	0	1.8330	54.5050	41.0620	H	0	5.6380	51.8370	52.7800	H	0
6.8660	59.7900	49.9240	C	0	2.5070	55.4850	39.8090	H	0	4.8750	52.5010	51.3180	H	0
6.2540	59.9970	49.0460	H	0	3.1950	56.1120	41.7850	C	0	3.4060	51.7300	52.5830	C	0
6.9660	58.7190	50.1030	H	0	2.7760	57.0710	41.4800	H	0	2.8150	51.9620	51.6970	H	0
6.3890	60.1780	50.8240	H	0	2.8330	55.7950	43.2020	C	0	3.0630	50.7950	53.0260	H	0
8.9720	60.3090	50.9200	O	0	2.6260	54.6290	43.6820	O	0	3.3530	52.7990	53.6760	C	0
9.8030	60.7840	50.8400	H	0	2.4060	56.7940	43.9050	N	0	3.9720	52.4010	54.4800	H	0
8.4400	59.8550	47.2060	C	0	2.6070	57.7140	43.5410	H	0	3.7590	53.7530	53.3390	H	0
7.5400	59.1190	46.8130	O	0	1.8710	56.7770	45.3190	C	0	2.0260	52.9510	54.2270	N	0
8.6280	61.0810	46.7090	N	0	1.3660	57.6890	45.6370	H	0	1.5300	52.0790	54.3480	H	0
9.1960	61.7410	47.2200	H	0	1.0090	56.1200	45.1980	H	0	2.0480	53.3760	55.1430	H	0
7.7130	61.6860	45.7430	C	0	2.8100	56.2040	46.3910	C	0	1.5080	53.5800	53.6300	H	0
6.7380	61.2350	45.9260	H	0	4.0330	56.3820	46.2690	O	0	6.7010	48.7900	50.2810	C	0
7.5340	63.2300	45.9390	C	0	2.3230	55.4760	47.3960	N	0	6.8240	47.9230	51.1390	O	0
8.5340	63.6570	45.8680	H	0	1.3160	55.4520	47.4670	H	0	6.9000	48.5790	48.9630	N	0
7.0170	63.6560	45.0800	H	0	3.1480	54.8510	48.4750	C	0	6.7660	49.3320	48.3030	H	0
6.8850	63.6060	47.2460	C	0	4.0220	55.4740	48.6620	H	0	7.2270	47.3160	48.3250	C	0
5.9580	63.0580	47.0770	H	0	2.3900	54.6510	49.7960	C	0	7.5630	46.5170	48.9860	H	0
7.3180	63.2200	48.1690	H	0	2.9980	54.0970	50.5120	H	0	6.0090	46.6460	47.6970	C	0
6.7270	65.1020	47.4330	C	0	2.2360	55.6660	50.1610	H	0	6.3270	45.7150	47.2260	H	0
6.2800	65.6010	46.5730	H	0	1.0400	53.9670	49.6460	C	0	5.3140	46.2880	48.4560	H	0
6.2010	65.3160	48.3640	H	0	0.4530	54.6720	49.0580	H	0	5.2650	47.4960	46.6250	C	0
8.1530	65.6340	47.6780	C	0	1.0060	52.9850	49.1750	H	0	5.8990	48.1270	46.0020	H	0
8.5960	65.0810	48.5070	H	0	0.2050	53.9470	51.0070	C	0	4.7300	46.4530	45.6700	C	0
8.7710	65.5780	46.7820	H	0	-1.0220	53.7020	51.0420	O	0	4.1480	47.0380	44.9580	H	0
8.0340	67.0200	48.0360	N	0	0.7130	54.0620	52.1470	O	0	5.5420	46.0370	45.0740	H	0
7.6260	67.1540	48.9510	H	0	3.7310	53.4750	48.0270	C	0	4.1970	45.7180	46.2730	H	0
8.9860	67.3560	48.0480	H	0	3.9120	52.5410	48.7610	O	0	4.1420	48.3580	47.1960	C	0
7.5500	67.5990	47.3650	H	0	4.0510	53.3410	46.7180	N	0	3.2300	47.7720	47.3060	H	0
7.9470	61.3040	44.2720	C	0	4.0230	54.1440	46.1060	H	0	4.3640	48.8350	48.1500	H	0
7.0550	61.5080	43.4990	O	0	4.5610	52.1440	46.1420	C	0	3.9220	49.1100	46.4380	H	0
8.9880	60.5570	43.9780	N	0	4.0300	51.3200	46.6180	H	0	8.3790	47.4870	47.2670	C	0
9.7070	60.3260	44.6480	H	0	4.3800	52.0350	44.6350	C	0	8.6840	46.5810	46.5420	O	0
9.3070	60.0650	42.6100	C	0	3.3210	51.8200	44.4890	H	0	8.8960	48.6660	47.2710	N	0
8.8470	60.7710	41.9180	H	0	4.6120	53.0300	44.2550	H	0	8.6430	49.2440	48.0590	H	0
10.8070	60.1750	42.4670	C	0	5.0850	50.8600	43.9040	C	0	9.7020	49.3290	46.2090	C	0
11.0040	59.7850	41.4680	H	0	6.1030	51.1590	43.6540	H	0	9.1860	49.3270	45.2480	H	0
11.3760	61.5580	42.5160	C	0	4.9500	49.9690	44.5160	H	0	9.7370	50.3750	46.5150	H	0
11.2580	62.1460	43.4270	H	0	4.4230	50.4940	42.5570	C	0	11.1450	48.7900	45.9350	C	0
12.4430	61.4880	42.3060	H	0	3.4090	50.9050	42.1280	O	0	12.0450	49.5700	45.5930	O	0
10.7990	61.9650	41.6860	H	0	5.2640	49.7790	41.7380	N	0	11.4350	47.4790	46.1650	N	0
11.5130	59.3880	43.3650	O	0	4.8430	49.5890	40.8390	H	0	10.7320	46.8600	46.5420	H	0
11.5310	59.8750	44.1920	H	0	6.0790	49.3030	42.0980	H	0	12.7780	46.9370	45.9240	C	0
8.7140	58.6200	42.2220	C	0	5.9880	51.8070	46.6460	C	0	12.8610	45.8650	46.0990	H	0
9.4390	57.8970	41.5510	O	0	6.4530	50.6590	46.6730	O	0	13.1680	47.1480	44.9280	H	0
7.4830	58.3520	42.5740	N	0	6.6840	52.7860	47.1910	N	0	13.8650	47.4820	46.8340	C	0
6.9650	59.1550	42.9010	H	0	6.2980	53.7070	47.3400	H	0	13.7150	47.4640	48.0220	O	0
6.8040	57.0360	42.6180	C	0	7.9260	52.4720	47.9030	C	0	14.9820	47.8310	46.1520	N	0
7.2780	56.3750	41.8920	H	0	8.6560	52.1490	47.1600	H	0	14.9520	47.7180	45.1490	H	0
6.9180	56.4650	44.0430	C	0	8.4570	53.8650	48.4810	C	0	16.2310	48.4210	46.6380	C	0
6.5600	57.3010	44.6440	H	0	9.2510	53.5980	49.1790	H	0	16.8990	48.4260	45.7770	H	0
6.3870	55.5270	44.2060	H	0	8.8430	54.5790	47.7530	H	0	15.8720	49.3830	47.0040	H	0
8.3270	56.0490	44.5120	C	0	7.5270	54.7160	49.2760	C	0	17.1540	47.6510	47.6740	C	0
9.2220	56.7420	45.2440	C	0	7.0080	55.8990	48.8030	C	0	17.7630	48.2710	48.5350	O	0
9.0940	57.7090	45.7080	H	0	7.1020	56.2470	47.7850	H	0	17.2410	46.3500	47.5670	N	0
10.3040	55.9080	45.4920	N	0	6.1510	56.3730	49.7990	N	0	16.7700	45.9200	46.7830	H	0
11.0500	56.1710	46.1210	H	0	5.5220	57.1310	49.5800	H	0	17.9060	45.3670	48.4000	C	0
10.1490	54.6390	44.9710	C	0	6.1780	55.7050	50.9690	C	0	17.4060	45.3850	49.3680	H	0
10.9580	53.4700	44.8610	C	0	5.4660	55.8190	52.1410	C	0	17.7360	43.9420	47.7770	C	0
11.8900	53.3840	45.4010	H	0	4.7180	56.5800	52.3030	H	0	18.2770	43.9220	46.8310	H	0
10.5460	52.3420	44.1550	C	0	5.8380	55.0610	53.2210	C	0	18.2140	42.7600	48.5760	C	0
11.2930	51.5620	44.1340	H	0	5.3300	55.1220	54.1720	H	0	17.9280	42.8250	49.6260	H	0
9.3060	52.3670	43.4980	C	0	6.9750	54.2100	53.1270	C	0	17.8040	41.8800	48.0800	H	0
9.0400	51.5050	42.9030	H	0	7.2080	53.5650	53.9610	H	0	19.2840	42.5940	48.4540	H	0
8.5250	53.5130	43.4650	C	0	7.5480	54.0420	51.8550	C	0	16.3330	43.7080	47.4230	O	0
7.5770	53.5800	42.9520	H	0	8.5140	53.5710	51.7390	H	0	16.1760	43.4140	46.5230	H	0
8.8920	54.6770	44.2460	C	0	7.1280	54.7220	50.7410	C	0	19.4150	45.6530	48.4610	C	0
5.2920	57.1850	42.3260	C	0	7.8750	51.4160	48.9940	C	0	20.0090	46.3940	47.6760	O	0
4.8440	58.2890	42.6600	O	0	8.8920	50.7310	49.2200	O	0	20.0120	45.2200	49.5910	N	0
4.5910	56.1930	41.7970	N	0	6.7040	51.2490	49.5650	N	0	19.5260	44.5810	50.2040	H	0
5.1730	54.9520	41.2800	C	0	5.9030	51.8160	49.3270	H	0	21.2680	45.8780	50.1260	C	0
5.6020	54.3980	42.1150	H	0	6.4680	50.2630	50.6720	C	0	21.6370	46.5910	49.3890	H	0
5.8880	55.1140	40.4730	H	0	7.1350	50.4730	51.5090	H	0	20.9770	46.7620	51.3410	C	0
3.8970	54.1220	40.7220	C	0	5.0730	50.3680	51.3210	C	0	21.9020	47.1930	51.7250	H	0
3.7170	53.1880	41.2540	H	0	4.3760	50.2080	50.4980	H	0	19.9890	47.8660	50.9450	C	0

19.0220	47.4340	50.6880	H	0	28.0660	43.9240	54.0030	C	0	35.8990	60.7550	58.0810	H	0
19.7120	48.4750	51.8060	H	0	28.7390	43.2460	54.5070	H	0	35.1620	59.4200	56.5840	C	0
20.3880	48.4420	50.1100	H	0	28.5630	45.1470	53.5200	C	0	35.1620	58.3650	56.3120	H	0
20.3110	45.8770	52.2350	O	0	29.5980	45.3930	53.7090	H	0	34.2150	59.9390	56.4400	H	0
20.0000	46.3090	53.0340	H	0	30.8750	47.6050	52.1220	C	0	36.0380	60.1940	55.5870	C	0
22.4200	44.9180	50.4510	C	0	31.6450	46.6430	52.3160	O	0	37.0520	59.8310	55.7550	H	0
23.3080	45.2950	51.2440	O	0	31.1480	48.8380	52.5130	N	0	35.6580	59.9130	54.1320	C	0
22.4160	43.6710	49.9530	N	0	30.4780	49.5890	52.4240	H	0	36.3410	60.5150	53.5310	H	0
21.6990	43.3120	49.3390	H	0	32.4490	49.1870	53.1060	C	0	35.6950	58.8340	53.9860	H	0
23.6350	42.8810	49.8270	C	0	32.9020	48.2870	53.5220	H	0	34.6270	60.2390	53.9980	H	0
24.2320	43.0480	50.7230	H	0	33.3580	49.7410	52.0200	C	0	36.0720	61.7150	55.7680	C	0
23.3860	41.3520	49.8140	C	0	34.2250	50.1350	52.5480	H	0	36.5930	62.2350	54.9640	H	0
23.0630	41.0750	50.8180	H	0	33.9000	48.9690	51.4740	H	0	35.0430	62.0760	55.7850	H	0
22.5470	41.2000	49.1360	H	0	32.9350	50.7810	51.2030	O	0	36.3790	61.9630	56.7840	H	0
24.4080	40.4730	49.4510	C	0	33.1390	50.6580	50.2730	H	0	34.4730	59.3400	58.9950	C	0
24.3480	39.6660	48.3100	C	0	32.3220	50.2480	54.2080	C	0	33.5140	60.0880	59.1970	O	0
23.5110	39.5960	47.6310	H	0	31.2600	50.9570	54.3740	O	0	34.5600	58.1270	59.5960	N	0
25.6220	39.3440	47.9990	N	0	33.4600	50.4490	54.9210	N	0	35.2700	57.4760	59.2930	H	0
25.8650	38.8550	47.1490	H	0	34.2060	49.8520	54.5940	H	0	33.5330	57.4790	60.3430	C	0
26.5370	39.8880	48.8840	C	0	33.6330	51.4380	56.0000	C	0	33.9180	56.4660	60.4500	H	0
27.9410	39.8700	48.9340	C	0	32.9600	52.2830	55.8560	H	0	33.3600	57.9770	61.7390	C	0
28.4530	39.5540	48.0370	H	0	33.3760	50.7240	57.3190	C	0	34.3050	57.9600	62.2830	H	0
28.5910	40.3760	50.0350	C	0	32.3270	50.4270	57.3280	H	0	33.1630	59.0420	61.6220	H	0
29.6660	40.3540	50.1400	H	0	34.0220	49.8510	57.4070	H	0	32.3730	57.3210	62.7040	C	0
27.8160	40.9560	51.0500	C	0	33.4890	51.6530	58.5040	C	0	31.8530	58.0150	63.6160	O	0
28.3300	41.4130	51.8830	H	0	32.6060	52.7230	58.7370	C	0	32.1690	56.0840	62.5260	O	0
26.3920	40.8990	51.0660	C	0	31.7740	52.8800	58.0670	H	0	32.2310	57.4390	59.4950	C	0
25.8220	41.1470	51.9490	H	0	32.6780	53.5510	59.8960	C	0	31.2140	58.0070	59.8330	O	0
25.7680	40.3810	49.9550	C	0	31.9410	54.3350	59.9800	H	0	32.3100	56.8400	58.3070	N	0
24.5350	43.2960	48.7050	C	0	33.5530	53.2920	60.8740	C	0	33.2050	56.3990	58.1510	H	0
24.0710	43.3580	47.5760	O	0	33.5430	54.0960	61.9530	O	0	31.2440	56.7140	57.2850	C	0
25.7760	43.5200	49.0240	N	0	32.9970	54.8800	61.8610	H	0	30.3640	56.7830	57.9250	H	0
26.0740	43.4530	49.9870	H	0	34.4850	52.1610	60.7120	C	0	31.3200	57.8690	56.2650	C	0
26.9510	43.6500	48.1870	C	0	35.0060	51.8100	61.5910	H	0	32.3180	57.8130	55.8320	H	0
27.0440	42.7910	47.5210	H	0	34.3500	51.2740	59.5930	C	0	30.5880	57.6910	55.4770	H	0
26.7640	44.5940	47.6750	H	0	34.9920	50.4070	59.5370	H	0	31.0320	59.3250	56.6910	C	0
28.1640	43.8320	49.1030	C	0	35.0640	52.1010	56.1250	C	0	31.8210	59.5630	57.4050	H	0
28.0150	43.8340	50.3120	O	0	36.0350	51.3780	56.1910	O	0	31.2710	60.2160	55.3940	C	0
29.4260	44.0240	48.5960	N	0	35.1770	53.4440	56.2820	N	0	30.4420	59.9550	54.7370	H	0
29.5790	43.9590	47.6000	H	0	34.3460	54.0010	56.1380	H	0	31.1610	61.2760	55.6250	H	0
30.5800	44.3820	49.4510	C	0	36.4220	54.2230	56.6350	C	0	32.2080	60.0270	54.8700	H	0
30.5030	43.9740	50.4580	H	0	37.3020	53.5800	56.6480	H	0	29.6090	59.5670	57.2260	C	0
31.9270	44.0000	48.7260	C	0	36.8130	55.2380	55.4890	C	0	29.3830	59.3220	58.2630	H	0
31.9300	44.5640	47.7930	H	0	37.2260	54.6250	54.6880	H	0	29.4370	60.6340	57.0810	H	0
32.8290	44.3850	49.2020	H	0	35.9780	55.8590	55.1630	H	0	28.8190	59.1630	56.5930	H	0
31.9590	42.5110	48.4740	C	0	37.8370	56.2720	55.8270	C	0	31.2170	55.4180	56.6190	C	0
31.6800	41.8850	47.2690	C	0	38.0500	57.1310	54.9900	O	0	32.2490	54.8110	56.4120	O	0
31.5310	42.5250	46.4110	H	0	38.6320	56.0340	56.7270	O	0	30.0110	54.9170	56.2960	N	0
31.8200	40.5750	47.2940	N	0	36.1920	54.9680	58.0190	C	0	29.2120	55.5040	56.4880	H	0
31.8060	39.9900	46.4710	H	0	35.2710	55.7580	58.1820	O	0	29.7910	53.5820	55.7820	C	0
32.0540	40.1250	48.5900	C	0	36.9510	54.5880	59.1100	N	0	30.7200	53.1900	55.3680	H	0
32.1740	38.8520	49.1620	C	0	37.9090	53.5180	59.1080	C	0	29.1010	52.7170	56.8850	C	0
31.9770	37.8960	48.7010	H	0	38.6400	53.4910	58.2990	H	0	29.3040	51.6600	56.7170	H	0
32.3530	38.7780	50.5930	C	0	37.3330	52.5930	59.0840	H	0	29.5530	52.8600	57.8670	H	0
32.4080	37.8300	51.1060	H	0	38.7140	53.5310	60.4210	C	0	27.5850	52.8800	57.1100	C	0
32.4760	39.9400	51.3420	C	0	39.5170	54.2640	60.3430	H	0	27.2700	53.7210	58.1720	C	0
32.5880	39.8640	52.4140	H	0	39.1250	52.5680	60.7250	H	0	28.0070	54.2730	58.7360	H	0
32.4120	41.1880	50.7030	C	0	37.6810	54.1090	61.3490	C	0	25.9210	53.8850	58.4970	C	0
32.4830	42.0450	51.3560	H	0	38.2080	54.4400	62.2440	H	0	25.5410	54.5480	59.2610	H	0
32.2130	41.3440	49.3310	C	0	36.9160	53.3710	61.5860	H	0	24.9180	53.1490	57.8290	C	0
30.4380	45.8200	49.8710	C	0	36.9660	55.1480	60.4560	C	0	23.8630	53.2490	58.0370	H	0
31.1520	46.7090	49.3640	O	0	35.9170	55.2160	60.7460	H	0	25.2980	52.3470	56.7440	C	0
29.5620	46.1140	50.8390	N	0	37.4970	56.6030	60.5490	C	0	24.5600	51.7050	56.2870	H	0
29.0310	45.3510	51.2360	H	0	37.1210	57.3530	61.4470	O	0	26.6220	52.1240	56.4070	C	0
29.5000	47.4060	51.5060	C	0	38.4190	56.9140	59.6360	N	0	27.0220	51.3460	55.7740	H	0
29.4000	48.2040	50.7710	H	0	38.5440	56.2640	58.8730	H	0	28.8720	53.6460	54.4930	C	0
28.2540	47.4550	52.4280	C	0	38.9210	58.2120	59.5610	C	0	27.9360	54.4750	54.3670	O	0
28.4380	48.1110	53.2790	H	0	39.2710	58.5000	60.5530	H	0	29.0670	52.6810	53.5980	N	0
27.5360	47.9290	51.7590	H	0	40.0460	58.2750	58.5890	C	0	29.8080	52.0080	53.7340	H	0
27.7250	46.1200	52.9610	C	0	40.4380	59.2860	58.4790	H	0	28.6000	52.9030	52.2040	C	0
26.3390	45.9070	52.8130	C	0	40.8700	57.5720	58.7140	H	0	27.6910	53.5040	52.2340	H	0
25.6930	46.6370	52.3490	H	0	39.6070	58.1350	57.6020	H	0	29.6060	53.4800	51.2780	C	0
25.8820	44.6710	53.2070	C	0	37.8280	59.2470	59.1090	C	0	30.4020	52.8010	50.9740	H	0
24.8770	44.4210	52.9020	H	0	37.8080	60.3620	59.6280	O	0	29.0320	53.8750	50.4400	H	0
26.6880	43.6030	53.8130	C	0	36.8240	58.8680	58.3760	N	0	30.4660	54.6210	51.7910	C	0
26.2620	42.3800	54.2200	O	0	36.9090	57.9920	57.8810	H	0	31.6270	54.3580	52.5380	C	0
26.9660	41.7500	54.3900	H	0	35.6410	59.6980	58.0100	C	0	31.8610	53.3640	52.8890	H	0

32.3770	55.4390	53.0030	C	0	14.6010	47.5070	42.9790	O	0	8.9140	50.5000	35.2700	H	0
33.2930	55.2890	53.5560	H	0	13.8970	49.0690	41.5820	N	0	9.8090	50.7920	33.2310	C	0
32.0560	56.7810	52.5330	C	0	13.9980	49.7280	40.2160	C	0	9.4340	50.9650	32.2220	H	0
32.8440	57.8120	52.8590	O	0	14.0540	49.0360	39.3760	H	0	10.1360	51.7990	33.4910	H	0
32.4880	58.6810	52.6600	H	0	14.8290	50.4340	40.2340	H	0	10.5880	50.0600	33.4450	H	0
30.9110	57.0340	51.7970	C	0	12.6660	50.5410	40.1430	C	0	7.4320	51.3220	33.9460	C	0
30.5960	58.0260	51.5080	H	0	11.9460	49.8400	39.7190	H	0	7.2880	52.3850	34.5880	O	0
30.0830	55.9560	51.4510	C	0	12.7360	51.4780	39.5900	H	0	6.4960	50.8790	33.1640	N	0
29.1160	56.1130	50.9980	H	0	12.3050	50.8280	41.5860	C	0	6.5990	50.0160	32.6500	H	0
28.0200	51.5730	51.7360	C	0	11.2300	50.9480	41.7210	H	0	5.2250	51.5740	33.0060	C	0
28.5870	50.5190	51.9450	O	0	12.8770	51.6620	41.9940	H	0	5.4230	52.6340	32.8470	H	0
26.9710	51.6930	50.9390	N	0	12.7050	49.4550	42.2480	C	0	4.6310	50.9710	31.7200	C	0
26.4920	52.5730	50.8090	H	0	13.0310	49.7740	43.2380	H	0	5.1180	51.4550	30.8740	H	0
26.3120	50.6220	50.2460	C	0	11.6240	48.4100	42.3960	C	0	4.6430	49.8840	31.8030	H	0
27.0310	49.8400	50.0030	H	0	10.4390	48.7560	42.5300	O	0	3.0760	51.4060	31.6300	C	0
25.2890	49.9410	51.2650	C	0	11.9140	47.0860	42.3070	N	0	2.4970	50.8990	30.8580	H	0
24.8360	49.1040	50.7330	H	0	12.8810	46.8260	42.1750	H	0	2.5240	51.0570	32.5020	H	0
25.9020	49.6940	52.1320	H	0	10.8730	46.0700	42.4180	C	0	2.8090	52.9020	31.3560	C	0
24.1040	50.7740	51.6440	C	0	11.0110	45.2850	43.1610	H	0	1.6290	53.3000	31.5790	O	0
24.1280	51.3850	52.9060	C	0	9.9470	46.5940	42.6550	H	0	3.7290	53.6460	30.9590	O	0
25.0060	51.3650	53.5350	H	0	10.6790	45.4290	40.9780	C	0	4.3910	51.4760	34.3610	C	0
22.9200	52.0290	53.4040	C	0	11.5550	45.0040	40.3780	O	0	3.8400	52.4650	34.7480	O	0
23.0080	52.3240	54.4400	H	0	9.4930	45.3950	40.4640	N	0	4.4670	50.2900	35.0090	N	0
21.8040	52.0880	52.6330	C	0	8.8210	45.8630	41.0540	H	0	4.9880	49.5390	34.5800	H	0
20.6910	52.7000	53.0050	O	0	9.1550	44.7950	39.1410	C	0	3.7150	50.0190	36.1630	C	0
20.0010	52.0400	52.9070	H	0	9.3020	43.7190	39.2380	H	0	2.7190	50.3750	35.8990	H	0
21.7320	51.4810	51.3460	C	0	7.6620	44.9650	38.8590	C	0	3.7980	48.5110	36.5510	C	0
20.8760	51.5480	50.6900	H	0	7.0430	44.6690	39.7070	H	0	3.9030	47.8510	35.6900	H	0
22.9070	50.9080	50.8600	C	0	7.2540	46.4070	38.5540	C	0	4.6790	48.3270	37.1660	H	0
22.8800	50.5820	49.8310	H	0	7.2650	46.9830	39.4800	H	0	2.4630	48.1580	37.2100	C	0
25.6070	51.2050	48.9860	C	0	7.8940	46.7070	37.7240	H	0	1.7130	48.9050	36.9500	H	0
25.3250	52.4260	48.8600	O	0	6.2190	46.3870	38.2150	H	0	2.1520	47.1710	36.8670	H	0
25.2080	50.2770	48.1220	N	0	7.2660	44.2980	37.6630	O	0	2.4820	48.1420	38.7300	C	0
25.4350	49.3410	48.4240	H	0	6.3700	43.9580	37.7160	H	0	3.3320	48.7120	39.3910	O	0
24.2180	50.4980	47.0790	C	0	10.0400	45.3110	37.9290	C	0	1.4570	47.7890	39.4130	N	0
23.9320	51.5490	47.0200	H	0	10.3860	46.4600	37.7950	O	0	1.4920	47.8120	40.4220	H	0
24.5230	50.2000	46.0750	H	0	10.3720	44.4520	36.9380	N	0	0.6590	47.2830	39.0550	H	0
22.9210	49.7780	47.3190	C	0	9.9450	43.5370	36.9340	H	0	4.1700	51.0560	37.2750	C	0
22.8480	48.9190	48.1880	O	0	10.9310	44.7660	35.6360	C	0	3.4250	51.6320	38.0390	O	0
22.0110	49.9840	46.3820	N	0	11.8240	45.3570	35.8420	H	0	5.5520	51.2120	37.2650	N	0
22.3590	50.6450	45.7020	H	0	11.1800	43.5410	34.8090	C	0	6.0900	50.7200	36.5650	H	0
20.6330	49.4670	46.3430	C	0	10.2500	43.0870	34.4650	H	0	6.2970	52.2480	38.1750	C	0
20.4230	48.6890	47.0780	H	0	11.6650	43.8480	33.8830	H	0	5.7360	52.2560	39.1100	H	0
19.6760	50.6450	46.6200	C	0	11.9680	42.3420	35.5030	C	0	7.6060	51.6400	38.5380	C	0
18.6270	50.3490	46.6450	H	0	12.5550	42.3430	36.7100	C	0	8.2130	51.5540	37.6370	H	0
20.0420	51.2370	48.0180	C	0	12.6410	43.1790	37.3880	H	0	8.0930	52.3010	39.2550	H	0
19.2500	51.9640	48.1960	H	0	13.1530	41.1280	36.9770	N	0	7.6170	50.2810	39.1440	C	0
20.0930	50.4460	48.7670	H	0	13.7760	41.0150	37.7640	H	0	7.0730	50.4470	40.0740	H	0
20.9580	51.8230	47.9460	H	0	12.7110	40.2300	36.0330	C	0	7.1170	49.5720	38.4850	H	0
19.7190	51.6100	45.7210	O	0	12.8640	38.8750	35.8790	C	0	9.0650	49.7250	39.4940	C	0
19.1940	52.3100	46.1170	H	0	13.1210	38.3240	36.7720	H	0	9.6080	50.4610	40.0870	H	0
20.2430	48.8420	44.9850	C	0	12.5090	38.2510	34.6680	C	0	9.0040	48.7580	39.9940	H	0
20.6580	49.2600	43.8910	O	0	12.5660	37.1740	34.6030	H	0	9.7920	49.2940	38.2820	N	0
19.4660	47.7430	45.0200	N	0	12.0560	39.0300	33.5690	C	0	9.8200	48.2860	38.2140	H	0
19.3150	47.4040	45.9600	H	0	11.8690	38.5900	32.6010	H	0	10.5160	49.8640	37.4040	C	0
18.7410	47.0520	43.8930	C	0	11.8430	40.3690	33.7640	C	0	10.9530	51.0760	37.4920	N	0
19.5520	46.7600	43.2260	H	0	11.4110	40.9040	32.9320	H	0	10.7740	51.6550	38.3010	H	0
18.2250	45.6610	44.4060	C	0	12.1310	41.0250	35.0060	C	0	11.5980	51.3700	36.7730	H	0
18.3150	45.0470	43.5100	H	0	10.0200	45.7210	34.7980	C	0	11.0890	49.1180	36.5190	N	0
18.9200	45.2930	45.1610	H	0	10.6250	46.4360	33.9720	O	0	11.0670	48.1150	36.6330	H	0
16.8310	45.6360	44.8010	O	0	8.6810	45.6720	34.9240	N	0	11.6940	49.5530	35.8370	H	0
16.5820	44.7110	44.7320	H	0	8.2940	44.9160	35.4710	H	0	6.4160	53.7170	37.7240	C	0
17.7420	47.9360	43.0510	C	0	7.8020	46.6170	34.2320	C	0	7.2400	54.4850	38.2880	O	0
17.3570	49.0550	43.5030	O	0	8.0450	46.6040	33.1700	H	0	5.7000	54.0700	36.6370	N	0
17.1600	47.4320	41.9050	N	0	6.2590	46.1800	34.3870	C	0	5.1630	53.4150	36.0880	H	0
17.4130	46.4860	41.6570	H	0	6.0430	45.1250	34.2180	H	0	5.7290	55.4260	36.1250	C	0
16.1480	47.9940	41.1440	C	0	5.8890	46.3840	35.3920	H	0	6.7150	55.6670	35.7270	H	0
16.4180	49.0350	40.9660	H	0	5.3620	46.9540	33.4560	C	0	4.8290	55.5070	34.9370	C	0
16.1060	47.2740	39.8230	C	0	5.3190	48.1740	33.4440	O	0	5.1960	54.7770	34.2160	H	0
15.8770	47.9080	38.9660	H	0	4.6530	46.2370	32.6270	N	0	3.8120	55.2820	35.2590	H	0
17.0730	46.9220	39.4630	H	0	4.2720	46.6650	31.7950	H	0	4.8760	56.9700	34.3000	C	0
15.0420	46.1460	39.7820	C	0	4.8050	45.2410	32.5650	H	0	4.3590	57.6910	34.9320	H	0
15.0970	45.1760	40.5340	O	0	7.9750	48.0320	34.7130	C	0	5.9390	57.1810	34.1830	H	0
14.1910	46.1900	38.8510	N	0	7.6620	48.2550	35.8750	O	0	4.3530	57.0200	32.8620	C	0
13.5860	45.3860	38.9320	H	0	8.4650	48.9770	33.8870	N	0	4.5360	58.0220	32.4740	H	0
14.1180	46.9890	38.2370	H	0	8.9590	48.5850	33.0980	H	0	4.8820	56.2820	32.2580	H	0
14.8370	48.1700	41.9800	C	0	8.6670	50.3910	34.2140	C	0	2.9130	56.5780	32.7340	C	0

2.8090	55.6540	33.3030	H	0	17.0190	57.4340	47.6050	C	0	23.3350	54.2360	50.8020	H	0
2.2100	57.2930	33.1630	H	0	16.1360	57.9880	48.4720	C	0	23.4370	55.6540	51.9160	H	0
2.5810	56.1890	31.3390	N	0	15.5250	57.4150	49.1530	H	0	21.6760	55.5930	50.7320	C	0
2.8450	56.9450	30.7230	H	0	16.3250	59.3710	48.6000	N	0	21.1140	56.7400	51.3430	C	0
2.9250	55.3070	30.9860	H	0	15.7220	59.9850	49.1270	H	0	21.6760	57.2650	52.1010	H	0
1.5800	56.0890	31.2560	H	0	17.1800	59.7780	47.5950	C	0	19.7660	57.0540	51.0750	C	0
5.3210	56.4380	37.2130	C	0	17.4920	61.0320	47.1170	C	0	19.3500	57.8970	51.6060	H	0
4.2600	56.1930	37.7950	O	0	17.1330	61.8940	47.6600	H	0	18.9970	56.1940	50.1910	C	0
6.0950	57.4840	37.4550	N	0	18.3800	61.1690	46.0300	C	0	17.9460	56.4260	50.1070	H	0
6.9400	57.4900	36.9020	H	0	18.6530	62.1560	45.6880	H	0	19.6290	55.1430	49.5030	C	0
5.8490	58.6480	38.3710	C	0	18.8260	60.0450	45.4020	C	0	19.0110	54.6210	48.7880	H	0
5.2100	59.3670	37.8590	H	0	19.4100	60.0560	44.4930	H	0	20.8950	54.7880	49.8200	C	0
5.3100	58.2420	39.2270	H	0	18.5130	58.7630	45.8930	C	0	21.2850	54.0180	49.1710	H	0
7.0780	59.3370	38.9440	C	0	18.7660	57.8930	45.3050	H	0	25.5800	56.1920	50.9010	C	0
6.9410	60.0910	39.9150	O	0	17.6340	58.6080	46.9220	C	0	26.3610	55.2650	50.8840	O	0
8.2890	58.9590	38.4210	N	0	16.8680	54.1220	45.5570	C	0	25.8020	57.3320	51.6250	N	0
8.3280	58.0850	37.9160	H	0	17.7050	53.4770	46.1180	O	0	25.1250	58.0730	51.5100	H	0
9.5300	59.6270	38.6260	C	0	16.2650	53.6820	44.4440	N	0	26.8410	57.5590	52.6090	C	0
9.7370	60.3310	37.8200	H	0	15.5420	54.2650	44.0480	H	0	27.5680	56.7510	52.6770	H	0
9.5940	60.1620	39.5730	H	0	16.6990	52.4150	43.7320	C	0	27.7440	58.7190	52.0990	C	0
10.7350	58.6370	38.6000	C	0	16.9600	51.8150	44.6030	H	0	28.5050	58.9970	52.8270	H	0
10.6160	57.4380	38.1630	O	0	15.6060	51.8640	42.8420	C	0	28.1860	58.5290	51.1210	H	0
11.8070	59.2040	39.0860	N	0	15.9560	50.9660	42.3330	H	0	27.0700	59.5310	51.8250	H	0
11.7730	60.2090	39.1790	H	0	14.8030	51.5600	43.5130	H	0	26.2800	57.9130	53.9130	C	0
13.0980	58.4810	39.2050	C	0	15.1850	52.7620	41.8620	O	0	25.4490	58.8330	53.9910	O	0
13.3770	58.0950	38.2240	H	0	14.4980	53.3080	42.2510	H	0	26.6920	57.2240	55.0060	N	0
14.1830	59.4370	39.7280	C	0	18.0050	52.7280	42.9550	C	0	27.4640	56.5980	54.8260	H	0
13.7810	59.7560	40.6890	H	0	18.2780	53.8610	42.6060	O	0	25.8550	57.1990	56.3760	C	0
15.1580	58.9950	39.9330	H	0	18.7990	51.7180	42.7090	N	0	25.3290	58.1510	56.2990	H	0
14.3930	60.6500	38.8450	C	0	18.5410	50.7810	42.9830	H	0	24.9090	55.9510	56.4490	C	0
14.0950	60.5820	37.6290	O	0	20.0310	51.8910	41.8840	C	0	25.5610	55.1870	56.0250	H	0
14.9260	61.6720	39.3750	O	0	20.4900	50.9120	42.0220	H	0	24.5010	55.7650	57.4420	H	0
13.0620	57.1460	40.0570	C	0	19.5760	52.1330	40.4220	C	0	23.8430	56.0950	55.3730	C	0
14.0440	56.4510	40.1050	O	0	19.1290	53.1130	40.2520	H	0	23.2000	56.9370	55.6300	H	0
11.9290	56.8240	40.7140	N	0	20.4260	52.1550	39.7400	H	0	24.1730	56.2680	54.3480	H	0
11.1450	57.4530	40.6150	H	0	18.4230	50.8750	39.8520	S	0	23.0980	54.7170	55.2400	C	0
11.7890	55.6490	41.7050	C	0	19.2120	49.7970	39.8880	H	0	23.7900	54.0970	54.6700	H	0
10.7920	55.8260	42.0600	H	0	21.0080	53.0100	42.4330	C	0	22.8800	54.2710	56.2100	H	0
11.6940	54.2810	40.9340	C	0	21.4540	53.7640	41.5970	O	0	21.7980	54.8450	54.5640	N	0
12.6390	53.9990	40.4680	H	0	21.1310	53.1620	43.7930	N	0	21.7180	54.5560	53.6000	H	0
11.5380	53.5220	41.7010	H	0	20.6040	52.4930	44.3370	H	0	20.6520	55.3220	55.0060	C	0
10.6150	54.1000	39.8870	C	0	21.6470	54.3460	44.4250	C	0	20.3830	55.6830	56.2370	N	0
10.5640	53.0510	39.3050	O	0	22.2500	55.0180	43.8140	H	0	21.0050	55.5060	57.0120	H	0
9.6980	55.0110	39.5650	N	0	20.5730	55.1440	45.2120	C	0	19.4770	56.0830	56.4380	H	0
8.9850	54.6760	38.9330	H	0	19.9770	54.4750	45.8320	H	0	19.6600	55.3940	54.1870	N	0
9.7990	55.9630	39.8860	H	0	20.9730	56.3440	46.0700	C	0	19.9390	55.2360	53.2290	H	0
12.8700	55.6580	42.7660	C	0	21.7260	56.0520	46.8020	H	0	18.7220	55.6170	54.4870	H	0
13.6220	54.6590	42.9140	O	0	21.4590	57.1320	45.4950	H	0	26.8210	57.4550	57.5540	C	0
13.2250	56.7920	43.3610	N	0	20.1240	56.8620	46.5160	H	0	27.8350	56.7970	57.6740	O	0
12.7410	57.6530	43.1500	H	0	19.5720	55.6590	44.4400	O	0	26.3980	58.3210	56.5380	N	0
14.3740	56.9010	44.2400	C	0	19.3640	54.9270	43.8550	H	0	25.4870	58.7260	58.3760	H	0
15.3240	56.4900	43.8970	H	0	22.6900	54.0120	45.4970	C	0	27.0300	58.2630	59.8860	C	0
14.6860	58.3540	44.4300	C	0	22.4280	53.3400	46.4410	O	0	28.0910	58.1150	59.6840	H	0
13.7620	58.9170	44.5660	H	0	23.7960	54.7520	45.4980	N	0	26.7920	59.6480	60.5360	C	0
15.2130	58.3450	45.3840	H	0	23.8060	55.4960	44.8150	H	0	27.3070	59.7390	61.4920	H	0
15.4550	59.0480	43.2230	C	0	24.8610	54.7360	46.5650	C	0	27.3270	60.3620	59.9090	H	0
16.4490	58.6440	43.4130	H	0	24.8790	53.7600	47.0500	H	0	25.3090	60.0300	60.8210	C	0
14.9100	58.7390	42.3300	H	0	26.3040	55.0620	46.1670	C	0	24.7090	59.9380	59.9160	H	0
15.5500	60.5820	43.3490	C	0	26.3650	55.9920	45.6020	H	0	24.8860	59.4050	61.6080	H	0
14.5740	60.9580	43.0430	H	0	27.3110	55.0370	47.3200	C	0	25.2420	61.5050	61.1950	C	0
15.6300	60.6690	44.4330	H	0	27.0760	55.8610	47.9940	H	0	25.9820	61.9700	60.5440	H	0
16.8200	61.2380	42.6720	C	0	27.2590	54.1200	47.9070	H	0	24.2160	61.8520	61.0730	H	0
16.6490	62.3070	42.7910	H	0	28.3360	55.2250	47.0010	H	0	25.6760	61.6830	62.5860	N	0
17.7700	61.0980	43.1890	H	0	26.6850	54.0900	45.0190	C	0	25.8580	60.8750	63.1650	H	0
16.9910	60.8270	41.2190	N	0	25.7830	54.0160	44.4110	H	0	26.0570	62.8040	63.1510	C	0
16.1940	61.1460	40.6870	H	0	27.4210	54.5360	44.3500	H	0	25.9360	63.9810	62.5090	N	0
17.8570	61.2630	40.9320	H	0	27.0190	52.6570	45.4610	C	0	25.4960	63.8460	61.6100	H	0
17.0390	59.8280	41.0790	H	0	27.1210	52.1050	44.5260	H	0	25.8760	64.8330	63.0470	H	0
14.0770	56.2340	45.5730	C	0	28.0030	52.7120	45.9270	H	0	26.5730	62.8260	64.3360	N	0
12.9410	56.1910	46.0790	O	0	26.2620	52.2640	46.1400	H	0	26.6260	61.9750	64.8770	H	0
15.0640	55.5960	46.2480	N	0	24.4630	55.7060	47.6670	C	0	26.7120	63.7190	64.7880	H	0
14.8180	55.0880	47.0850	H	0	24.1370	56.8120	47.3420	O	0	26.5840	57.1210	60.7840	C	0
16.4800	55.5490	45.9640	C	0	24.5240	55.2920	48.9300	N	0	25.3300	56.9000	60.7880	O	0
16.8480	56.2450	45.2110	H	0	24.7190	54.3200	49.1270	H	0	27.4120	56.2650	61.4440	N	0
17.1720	56.0170	47.2620	C	0	24.2130	56.1070	50.0770	C	0	28.9090	56.1380	61.3080	C	0
16.7060	55.4840	48.0910	H	0	23.8850	57.1280	49.8810	H	0	29.3140	57.0330	61.7780	H	0
18.2470	55.8360	47.2400	H	0	23.1840	55.3100	50.9130	C	0	29.1330	55.8180	60.2900	H	0

29.2710	54.9840	62.1410	C	0	25.2330	62.4800	54.5520	C	0	22.2800	58.3830	42.5000	N	0
29.5280	55.3320	63.1410	H	0	24.9220	63.3320	55.1570	H	0	21.9970	59.3070	42.2080	H	0
30.1610	54.4420	61.8210	H	0	26.6960	62.2900	55.0440	C	0	21.6390	57.2470	41.7590	C	0
28.1020	54.0800	62.1670	C	0	26.6870	62.3330	56.1330	H	0	21.6310	56.3200	42.3320	H	0
28.2030	53.4120	63.0230	H	0	26.9780	61.2680	54.7890	H	0	20.1430	57.5460	41.6260	C	0
28.0630	53.4960	61.2470	H	0	27.7040	63.3010	54.5690	C	0	19.8690	57.6900	42.6710	H	0
26.9500	55.0550	62.1710	C	0	28.7020	63.0890	54.9510	H	0	19.9480	58.4660	41.0730	H	0
26.0390	54.7170	61.6790	H	0	27.8360	63.0740	53.5120	H	0	19.2560	56.4140	41.0170	C	0
26.4510	55.3070	63.5980	C	0	27.2550	64.7440	54.8270	C	0	19.5580	56.3250	39.9730	H	0
26.0580	54.2940	64.1620	O	0	26.2970	64.7670	54.3090	H	0	19.5500	55.4460	41.4220	H	0
26.4700	56.4910	64.1870	N	0	27.1690	64.8570	55.9080	H	0	17.7450	56.7600	41.0300	C	0
26.8240	57.3110	63.7160	H	0	28.1300	65.8420	54.4140	N	0	17.3620	57.9060	40.8800	O	0
25.8750	56.7740	65.5010	C	0	28.9180	65.9480	55.0370	H	0	16.8730	55.8130	41.0730	N	0
26.3100	55.9360	66.0450	H	0	28.0840	66.4440	53.2740	C	0	15.8910	55.9980	40.9240	H	0
26.3770	58.1160	66.0480	C	0	27.1480	66.2040	52.4000	N	0	17.1580	54.8530	41.2040	H	0
25.8920	58.3120	67.0040	H	0	26.3580	65.6110	52.6130	H	0	22.3280	57.0620	40.3890	C	0
27.4410	58.1960	66.2670	H	0	27.2270	66.6920	51.5190	H	0	22.4450	57.9650	39.5850	O	0
25.9190	59.3490	65.1820	C	0	28.9410	67.3930	52.9780	N	0	22.7170	55.7990	40.0910	N	0
25.6090	59.2490	63.9810	O	0	29.5050	67.5530	53.8010	H	0	22.5510	55.2260	40.9060	H	0
25.8250	60.4620	65.7050	O	0	28.9440	67.8410	52.0730	H	0	23.2510	55.2340	38.8160	C	0
24.2740	56.7430	65.5090	C	0	25.1000	62.8520	53.0420	C	0	24.0750	55.8520	38.4600	H	0
23.6660	56.2330	66.4600	O	0	24.8650	64.0090	52.7250	O	0	23.7570	53.7650	39.2470	C	0
23.7000	57.1450	64.4120	N	0	25.1960	61.8790	52.1680	N	0	22.9980	53.2510	39.8360	H	0
24.3280	57.2670	63.6310	H	0	25.4950	60.9700	52.4900	H	0	23.9050	53.1200	38.3800	H	0
22.2400	57.2150	64.1050	C	0	24.9310	61.9940	50.7030	C	0	25.0230	53.8820	40.1330	C	0
21.7300	56.6310	64.8710	H	0	24.2060	62.7700	50.4590	H	0	25.4850	52.8950	40.1180	H	0
21.8250	58.7510	64.2290	C	0	26.1360	62.5980	49.9490	C	0	25.7170	54.6670	39.8310	H	0
20.7930	58.8800	63.9040	H	0	25.8670	62.8730	48.9290	H	0	24.5620	54.1780	41.8790	S	0
22.0840	59.3660	65.6160	C	0	26.3580	63.5510	50.4290	H	0	24.4300	52.4480	42.5260	C	0
23.1630	59.4430	65.7520	H	0	27.4550	61.7160	49.8120	C	0	23.9740	52.4820	43.5160	H	0
21.7620	60.4070	65.6300	H	0	28.5480	61.7820	50.6430	C	0	23.8700	51.8110	41.8420	H	0
21.5360	58.7680	66.3450	H	0	28.6210	62.4440	51.4940	H	0	25.3930	52.0190	42.8040	H	0
22.7070	59.5770	63.4350	O	0	29.4990	60.9350	50.2790	N	0	22.1410	55.2320	37.6920	C	0
23.6140	59.4300	63.7160	H	0	30.3350	60.7450	50.8150	H	0	22.4190	55.7150	36.6090	O	0
21.9410	56.5970	62.7050	C	0	29.0560	60.0760	49.2360	C	0	20.9230	54.7120	37.9580	N	0
20.7640	56.6830	62.2580	O	0	29.6330	58.9510	48.6310	C	0	20.7960	54.2120	38.8260	H	0
22.9760	56.0970	61.9850	N	0	30.5710	58.4670	48.8580	H	0	19.9430	54.4740	36.8780	C	0
23.9210	56.0970	62.3410	H	0	28.9240	58.4380	47.4980	C	0	20.2050	54.9410	35.9290	H	0
22.7140	55.4270	60.6320	C	0	29.4080	57.6690	46.9140	H	0	19.9280	52.9690	36.5470	C	0
23.6340	54.9540	60.2870	H	0	27.6750	58.9150	47.1200	C	0	19.2970	52.4500	37.2690	H	0
21.9350	54.6700	60.7110	H	0	27.2170	58.5010	46.2340	H	0	19.3230	52.5970	35.1700	C	0
22.3200	56.5100	59.5940	C	0	27.0430	59.9840	47.8210	C	0	19.6540	53.1960	34.3220	H	0
21.9790	56.0560	58.4640	O	0	26.1380	60.3710	47.3760	H	0	19.4770	51.5230	35.0570	H	0
22.2820	57.8400	59.8480	N	0	27.6980	60.5750	48.9010	C	0	18.2660	52.7800	35.3620	H	0
22.7800	58.0730	60.6950	H	0	24.4440	60.7740	50.1020	C	0	21.1390	52.3170	36.5560	O	0
21.7000	58.8790	58.9830	C	0	24.6330	59.7060	50.6020	O	0	20.9670	51.4380	36.9000	H	0
20.7410	58.4820	58.6480	H	0	23.6160	60.8420	49.0530	N	0	18.6160	54.9810	37.3530	C	0
21.4920	60.1470	59.7440	C	0	23.3980	61.7610	48.6960	H	0	17.7550	54.1760	37.7070	O	0
22.3520	60.5410	60.2850	H	0	23.2550	59.7180	48.2370	C	0	18.2890	56.3000	37.3680	N	0
21.1490	60.9120	59.0470	H	0	23.9920	58.9310	48.3920	H	0	19.1560	57.4540	37.0960	C	0
20.3450	60.0170	60.7820	C	0	21.9550	58.9720	48.7140	C	0	19.8360	57.2500	36.2700	H	0
19.4500	59.7120	60.2400	H	0	22.0240	57.9790	48.2680	H	0	19.6910	57.7660	37.9930	H	0
20.6890	59.2970	61.5240	H	0	21.9880	58.9000	49.8010	H	0	18.1990	58.5310	36.6880	C	0
20.0000	61.2870	61.4770	C	0	21.0400	59.4280	48.3370	H	0	18.1620	58.4150	35.6050	H	0
20.0010	62.1070	60.7590	H	0	23.1560	60.2010	46.7180	C	0	18.6030	59.4870	37.0230	H	0
18.9650	61.2470	61.8150	H	0	22.8390	61.3760	46.4680	O	0	16.9340	58.3120	37.5120	C	0
20.8860	61.8030	62.6550	C	0	23.4950	59.3350	45.7660	N	0	16.1580	58.8130	36.9340	H	0
20.8380	60.9960	63.3870	H	0	23.6520	58.4140	46.1490	H	0	16.8700	58.7830	38.4930	H	0
21.9380	62.0200	62.4730	H	0	23.6120	59.5030	44.2660	C	0	16.8960	56.7570	37.6330	C	0
20.2800	63.0100	63.2510	N	0	22.9810	60.3330	43.9480	H	0	16.5950	56.5620	38.6620	H	0
20.1530	63.7840	62.6130	H	0	25.1100	59.8470	43.8360	C	0	15.9290	56.0280	36.6430	C	0
19.4160	62.7610	63.7110	H	0	25.3960	60.8550	44.1370	H	0	16.2540	55.9520	35.4360	O	0
20.9090	63.3120	63.9810	H	0	25.7650	59.1650	44.3770	H	0	14.7860	55.5920	37.1020	N	0
22.5080	59.0890	57.7250	C	0	25.4450	59.7850	42.3130	C	0	14.5430	55.6130	38.0830	H	0
23.7510	58.8990	57.7410	O	0	25.3980	60.9580	41.5440	C	0	13.7470	54.8480	36.3640	C	0
21.8980	59.3580	56.5910	N	0	25.3450	61.8850	42.0950	H	0	13.1020	54.4730	37.1580	H	0
20.8970	59.4700	56.6550	H	0	25.4820	60.8630	40.1650	C	0	12.8720	55.7880	35.5290	C	0
22.6430	59.6870	55.2910	C	0	25.4600	61.8140	39.6530	H	0	12.6410	56.6230	36.1910	H	0
23.5260	59.0490	55.2550	H	0	25.6740	59.6630	39.5380	C	0	13.4390	56.0640	34.6400	H	0
21.8430	59.4230	53.9760	C	0	25.8230	59.6150	38.1760	O	0	11.5860	55.1610	35.0140	C	0
22.4600	59.6480	53.1060	H	0	25.0780	60.0260	37.7320	H	0	10.7900	54.2300	35.6840	C	0
21.6340	58.3550	54.0220	H	0	25.7510	58.4590	40.2720	C	0	11.0180	53.6370	36.5570	H	0
20.9450	60.0340	54.0670	H	0	25.8840	57.4950	39.8030	H	0	9.7070	54.0100	34.8450	N	0
23.1330	61.1010	55.3190	C	0	25.6600	58.5690	41.6780	C	0	8.8380	53.5760	35.1180	H	0
22.3520	62.0360	55.5180	O	0	25.6800	57.6140	42.1810	H	0	9.7140	54.7370	33.6700	C	0
24.4120	61.2830	54.9380	N	0	23.1230	58.2310	43.5300	C	0	8.7700	54.8780	32.6310	C	0
24.7780	60.3710	54.7030	H	0	23.5630	57.1360	43.8660	O	0	7.8480	54.3190	32.5730	H	0

9.1710	55.6840	31.4650	C	0	21.4820	45.7800	34.7890	H	0	31.4120	47.8910	47.9170	H	0
8.5110	55.7540	30.6130	H	0	21.3270	46.3940	32.6540	C	0	31.8080	49.8890	47.3070	C	0
10.3090	56.4480	31.5200	C	0	21.6620	45.4310	32.3000	H	0	31.8800	50.3530	46.3230	H	0
10.5790	57.0670	30.6780	H	0	20.8320	47.4690	31.7960	C	0	30.7930	50.5160	48.1780	C	0
11.1030	56.3870	32.6860	C	0	21.0120	47.4560	30.4350	O	0	30.7650	50.0260	49.1510	H	0
12.0430	56.9180	32.6840	H	0	21.2460	46.5780	30.1260	H	0	31.1200	51.5360	48.3810	H	0
10.8710	55.5150	33.7940	C	0	20.2740	48.6470	32.3950	C	0	29.3340	50.5290	47.6280	C	0
14.2040	53.6270	35.6240	C	0	19.9410	49.3930	31.6890	H	0	28.7870	51.2640	48.2180	H	0
14.1920	53.6590	34.4030	O	0	20.0290	48.6700	33.7690	C	0	29.2410	50.9380	46.6220	H	0
14.7580	52.6200	36.2920	N	0	19.4100	49.4920	34.0980	H	0	28.4220	49.0030	47.7490	S	0
15.0570	52.6810	37.2550	H	0	19.7650	46.8860	38.4130	C	0	27.8740	48.8520	45.9910	C	0
15.1230	51.3490	35.6520	C	0	19.2700	47.8980	38.8630	O	0	27.5350	47.8820	45.6260	H	0
15.9810	51.3970	34.9810	H	0	20.2770	45.9230	39.2290	N	0	26.9980	49.4750	45.8170	H	0
15.5230	50.3900	36.7480	C	0	20.3040	44.9500	38.9600	H	0	28.7310	49.1690	45.3960	H	0
16.5640	50.6710	36.9130	H	0	20.5490	46.0020	40.6320	C	0	33.2420	49.9330	47.8860	C	0
15.0500	50.5750	37.7120	H	0	19.9650	46.8150	41.0640	H	0	33.5540	49.6620	49.0200	O	0
15.4240	48.9440	36.3850	C	0	20.2090	44.6430	41.2830	C	0	34.2640	50.1800	47.0100	N	0
16.1650	48.5140	35.4840	O	0	20.9310	43.9070	40.9320	H	0	34.0060	50.3270	46.0450	H	0
14.5710	48.2380	37.0100	O	0	20.3640	44.7000	42.3600	H	0	35.7340	50.1730	47.3070	C	0
13.9570	50.7850	34.8070	C	0	18.7820	44.1000	41.0380	C	0	35.9270	49.5860	48.2050	H	0
12.8040	50.7850	35.2930	O	0	17.7460	44.8410	41.1390	O	0	36.5730	49.7610	46.1360	C	0
14.2980	50.1370	33.6730	N	0	18.5450	42.9560	40.5650	O	0	36.7300	50.6680	45.5530	H	0
15.2130	50.2960	33.2770	H	0	21.9170	46.5330	40.9150	C	0	38.0440	49.3500	46.5750	C	0
13.3490	49.2840	32.9100	C	0	22.9360	45.7890	40.8730	O	0	38.6330	50.1450	47.0320	H	0
12.4400	49.2090	33.5070	H	0	22.0360	47.8510	41.0760	N	0	37.9970	48.5720	47.3370	H	0
13.0300	50.1640	31.6910	C	0	21.2240	48.4410	40.9670	H	0	38.6610	48.9950	45.7490	H	0
12.1940	49.7560	31.1240	H	0	23.2260	48.6230	41.3070	C	0	35.9550	48.6800	45.2430	C	0
12.7910	51.1810	32.0020	H	0	24.0200	48.3910	40.5980	H	0	36.1370	47.7280	45.7420	H	0
14.1080	50.2660	30.7390	O	0	22.9910	49.6790	41.1770	H	0	34.9160	48.9440	45.0470	H	0
14.7080	50.9670	31.0030	H	0	23.8510	48.4720	42.7080	C	0	36.3470	48.5880	43.7420	C	0
13.9210	47.9220	32.5270	C	0	24.0670	49.4770	43.4170	O	0	35.6580	47.9530	43.1840	H	0
13.3210	47.1720	31.7260	O	0	24.0810	47.2290	43.1160	N	0	36.3220	49.6360	43.4440	H	0
15.1020	47.6260	33.0410	N	0	23.8200	46.5090	42.4580	H	0	37.3980	48.3420	43.5910	H	0
15.5990	48.2690	33.6410	H	0	24.6880	46.8940	44.4280	C	0	36.0240	51.6030	47.7330	C	0
15.9160	46.4660	32.6610	C	0	25.1840	47.7860	44.8110	H	0	35.4990	52.5250	47.0420	O	0
15.4350	45.9830	31.8110	H	0	23.4500	46.6120	45.4130	C	0	36.8060	51.8140	48.7920	N	0
17.2780	46.8860	32.1280	C	0	22.8500	47.5060	45.5840	H	0	37.3020	51.0270	49.1860	H	0
17.8660	47.2140	32.9850	H	0	22.4840	45.5090	45.1850	C	0	37.2090	53.1160	49.2990	C	0
17.6900	45.9540	31.7410	H	0	23.0380	44.5830	45.0330	H	0	36.5870	53.8610	48.8030	H	0
17.2430	47.9680	31.0340	C	0	21.9150	45.5130	46.1150	H	0	36.8900	53.2540	50.8560	C	0
16.9820	47.7910	29.7360	C	0	21.7700	45.6500	44.3720	H	0	37.5710	52.5660	51.3570	H	0
16.8480	46.7810	29.3780	H	0	24.2070	46.2480	46.6910	C	0	37.1780	54.2590	51.1660	H	0
16.9630	49.0260	29.1550	N	0	23.5700	46.1730	47.5720	H	0	35.4170	53.0120	51.1640	C	0
16.8020	49.1460	28.1650	H	0	24.8090	45.3410	46.6360	H	0	35.2290	51.9650	50.9260	H	0
16.9350	50.0270	30.0480	C	0	24.9460	46.9990	46.9690	H	0	35.1810	53.3000	52.6490	C	0
16.9050	51.4800	29.8310	C	0	25.6580	45.6830	44.2250	C	0	35.9710	52.7820	53.1930	H	0
16.8900	51.9200	28.8450	H	0	25.3280	44.5130	44.1000	O	0	35.2170	54.3680	52.8600	H	0
17.0520	52.2990	30.9250	C	0	26.9140	45.9950	44.2090	N	0	34.2220	52.8850	52.9600	H	0
17.0950	53.3770	30.8620	H	0	27.1260	46.9810	44.2650	H	0	34.4110	53.7730	50.3500	C	0
17.1030	51.7430	32.1980	C	0	28.0420	45.0790	43.8820	C	0	34.4820	54.8490	50.5110	H	0
17.1380	52.4670	32.9980	H	0	27.6560	44.0610	43.9210	H	0	34.5990	53.6030	49.2900	H	0
17.1770	50.3480	32.4450	C	0	28.5710	45.3770	42.4700	C	0	33.4060	53.3940	50.5310	H	0
17.3200	49.9260	33.4290	H	0	28.8720	46.4050	42.2690	H	0	38.7200	53.3890	49.0420	C	0
17.1760	49.4130	31.3160	C	0	29.3690	44.6460	42.3390	H	0	39.5660	53.3430	49.9260	O	0
16.0350	45.4610	33.8520	C	0	27.6990	44.8080	41.3680	C	0	39.0760	53.4720	47.7290	N	0
16.4890	44.3670	33.6280	O	0	26.9910	43.8340	41.5030	O	0	38.3300	53.4140	46.4530	C	0
15.6940	45.8300	34.9920	N	0	27.8110	45.3370	40.1710	N	0	37.4650	54.0610	46.5970	H	0
15.3750	46.7670	35.1930	H	0	27.5000	44.8470	39.3440	H	0	38.1230	52.3590	46.2800	H	0
16.2920	45.2150	36.1700	C	0	28.5310	46.0360	40.0640	H	0	39.2400	54.0100	45.3440	C	0
16.0350	45.8530	37.0160	H	0	29.0920	45.1160	44.9900	C	0	38.9730	55.0660	45.3660	H	0
15.5350	43.9510	36.5270	C	0	29.2730	44.2120	45.8590	O	0	39.0340	53.4030	44.4620	H	0
14.4900	44.2590	36.4930	H	0	29.8810	46.1810	44.9260	N	0	40.5760	53.6380	45.8710	C	0
15.7400	43.1450	35.8220	H	0	29.9280	46.6900	44.0550	H	0	41.3270	54.2810	45.4130	H	0
15.8710	43.4580	37.9790	C	0	31.0000	46.5060	45.8830	C	0	40.8100	52.5940	45.6660	H	0
16.8780	43.8980	38.6090	O	0	30.6970	46.2570	46.9000	H	0	40.4070	53.9130	47.3640	C	0
15.1380	42.7600	38.7120	O	0	32.2340	45.7070	45.4180	C	0	41.0730	53.2300	47.8910	H	0
17.8750	45.1580	36.2230	C	0	32.8800	45.7900	46.2920	H	0	40.6410	55.3740	47.6980	C	0
18.5780	44.0980	36.2730	O	0	32.1000	44.6280	45.3350	H	0	39.7240	56.1590	47.5100	O	0
18.3880	46.3770	36.2420	N	0	33.1360	46.2730	44.2870	C	0	41.8580	55.7230	48.0670	N	0
17.7660	47.1160	35.9490	H	0	33.2630	47.3530	44.2250	H	0	42.6260	55.0690	48.1090	H	0
19.7330	46.6700	36.8720	C	0	34.1780	45.9900	44.4370	H	0	42.2880	57.1490	47.8700	C	0
20.3980	45.8060	36.8380	H	0	32.6790	45.8270	42.8960	C	0	41.4960	57.8860	48.0040	H	0
20.3950	47.8210	36.0700	C	0	31.4730	45.8380	42.5840	O	0	43.2430	57.4730	49.0030	C	0
19.8720	48.7630	36.2370	H	0	33.5630	45.4500	42.1090	O	0	44.0820	56.7780	48.9730	H	0
21.4280	47.8760	36.4130	H	0	31.2300	47.9750	45.8860	C	0	43.6570	58.4740	48.8770	H	0
20.4940	47.6580	34.6130	C	0	31.2040	48.5810	44.8270	O	0	42.6850	57.3220	50.4680	C	0
21.1460	46.5250	34.0830	C	0	31.4420	48.4760	47.0940	N	0	43.4630	57.7010	51.4380	O	0

41.7690	56.5520	50.8050	O	0	47.8220	66.2740	42.0500	H	0	39.0440	58.0300	48.0810	H	0
42.9050	57.3600	46.4140	C	0	47.6220	67.9880	42.4990	H	0	37.1840	58.4480	47.0400	C	0
43.4890	56.4130	45.8580	C	0	47.2650	66.6820	44.0930	C	0	36.4850	59.2640	47.2260	H	0
42.7860	58.5270	45.7960	N	0	48.1730	67.1310	44.8090	O	0	37.5690	58.5570	45.5270	C	0
42.1570	59.2200	46.1770	H	0	46.3230	65.9980	44.7200	N	0	38.2850	57.7920	45.2250	H	0
43.2890	58.8170	44.4360	C	0	45.5240	65.7130	44.1730	H	0	36.7230	58.5810	44.8410	H	0
43.9940	57.9990	44.2880	H	0	46.5360	65.4090	46.0810	C	0	38.3500	60.1340	45.0910	S	0
42.1820	58.7010	43.4270	C	0	47.6080	65.2570	46.2080	H	0	39.3430	59.9940	45.9730	H	0
41.4390	59.4870	43.5600	H	0	45.9250	66.4340	47.0850	C	0	36.4690	57.0850	47.3400	C	0
42.5210	58.9670	42.4250	H	0	46.0700	66.0290	48.0860	H	0	36.7450	56.3120	48.2090	O	0
41.3940	57.3330	43.2940	C	0	46.4170	67.4010	46.9830	H	0	35.3270	56.9520	46.6150	N	0
41.1130	57.0130	44.2970	H	0	44.3700	66.5860	46.9670	C	0	35.0090	57.6480	45.9560	H	0
40.0550	57.6810	42.6550	C	0	43.9960	66.5210	45.9450	H	0	34.6800	55.6370	46.4750	C	0
39.4280	58.4010	43.1810	H	0	43.9320	65.7700	47.5420	H	0	35.2650	54.8490	46.9510	H	0
40.2500	58.0430	41.6450	H	0	43.9140	67.8990	47.5780	C	0	33.3850	55.8010	47.3050	C	0
39.4320	56.7920	42.5640	H	0	44.1880	67.9350	48.6320	H	0	33.7330	56.0810	48.2990	H	0
42.0910	56.2740	42.5090	C	0	44.3780	68.7520	47.0820	H	0	32.8180	56.6140	46.8510	H	0
41.6020	55.3010	42.5640	H	0	42.3860	68.1470	47.5800	C	0	32.4220	54.6080	47.3850	C	0
42.2200	56.6680	41.5020	H	0	42.2360	69.0810	48.1220	H	0	33.0640	53.7300	47.4430	H	0
43.0660	56.1820	42.9880	H	0	42.0130	68.3840	46.5840	H	0	31.5680	54.8230	48.2680	C	0
43.9920	60.1650	44.3340	C	0	41.6560	66.9710	48.0490	N	0	30.8140	54.0360	48.6490	H	0
43.7200	61.0630	45.1010	O	0	41.8010	66.1350	47.5000	H	0	32.1570	55.0510	49.5360	H	0
44.9790	60.3590	43.4410	N	0	41.9170	66.6880	48.9830	H	0	30.8790	55.6640	48.5800	H	0
45.2160	59.5440	42.8920	H	0	40.6580	67.1200	48.0820	H	0	31.4800	54.3560	46.2680	C	0
45.7860	61.5440	43.2620	C	0	45.8970	64.0330	46.2420	C	0	32.0330	53.8750	45.4610	H	0
46.0810	62.0270	44.1930	H	0	44.9590	63.7490	45.4640	O	0	30.6800	53.6620	46.5250	H	0
47.1200	61.1460	42.6800	C	0	46.3590	63.3550	47.2930	N	0	31.0980	55.3110	45.9070	H	0
47.6920	62.0740	42.6560	H	0	47.1180	63.7810	47.8050	H	0	34.3780	55.2370	45.0000	C	0
47.8790	60.1550	43.6320	C	0	45.8120	62.0670	47.7320	C	0	34.1030	56.1960	44.2650	O	0
47.3220	59.2810	43.9680	H	0	45.7900	61.4210	46.8540	H	0	34.6810	53.9210	44.6320	N	0
48.7450	59.7480	43.1090	H	0	46.7520	61.4240	48.7440	C	0	34.9360	53.2240	45.3170	H	0
48.1950	60.7570	44.4840	H	0	47.8190	61.4700	48.5300	H	0	34.3720	53.4540	43.3280	C	0
46.9390	60.4830	41.4440	O	0	46.6300	61.9370	49.6980	H	0	33.6970	54.1800	42.8750	H	0
46.5180	61.0350	40.7810	H	0	46.4330	59.9100	49.0150	C	0	35.6710	53.0810	42.4750	C	0
45.0720	62.7090	42.4770	C	0	45.3550	59.7530	49.0560	H	0	36.3290	52.2690	42.7840	H	0
45.6470	63.5250	41.6390	O	0	46.7760	59.2620	48.2080	H	0	35.2310	52.6690	41.0920	C	0
43.7510	62.9420	42.7750	N	0	47.0390	59.2260	50.2500	C	0	36.1240	52.4400	40.5110	H	0
43.3600	62.2810	43.4310	H	0	46.4160	59.3600	51.1340	H	0	34.6070	51.7770	41.1500	H	0
42.8450	63.8330	42.0390	C	0	47.0160	58.1410	50.1440	H	0	34.5400	53.3930	40.6590	H	0
43.1680	63.7560	41.0000	H	0	48.4980	59.7560	50.3910	C	0	36.4400	54.4100	42.4310	C	0
41.3620	63.5440	42.1430	C	0	49.0020	59.8160	49.4260	H	0	36.7960	54.6530	43.4330	H	0
40.9590	64.2080	42.9070	H	0	48.3230	60.7630	50.7690	H	0	37.3350	54.3820	41.8090	H	0
40.5340	64.0070	40.9350	C	0	49.3210	58.9700	51.3110	N	0	35.7580	55.1930	42.1000	H	0
39.4610	63.9240	41.1090	H	0	49.2820	58.0250	50.9560	H	0	33.4120	52.2730	43.4630	C	0
40.9620	65.0090	40.9120	H	0	50.2440	59.3380	51.4910	H	0	33.4210	51.6110	44.4910	O	0
40.8180	63.4750	40.0270	H	0	48.9120	58.9180	52.2330	H	0	32.5050	52.2130	42.4890	N	0
40.9290	62.1150	42.4800	C	0	44.3720	62.3070	48.3310	C	0	32.6240	52.9370	41.7950	H	0
41.2850	61.3430	41.7980	H	0	44.0810	62.2210	49.5260	O	0	31.4620	51.2060	42.2230	C	0
41.1910	61.9310	43.5230	H	0	43.3650	62.5130	47.4580	N	0	31.9040	50.3530	42.7370	H	0
39.8410	62.0590	42.4580	H	0	43.6010	62.6860	46.4910	H	0	30.1580	51.6490	42.8510	C	0
43.2530	65.2860	42.4130	C	0	42.0090	62.8050	47.7320	C	0	30.3330	51.6420	43.9270	H	0
43.5390	65.6040	43.5660	O	0	41.9240	63.5380	48.5340	H	0	29.9910	52.6610	42.4820	H	0
43.2750	66.1430	41.3820	N	0	41.3890	63.3480	46.4300	C	0	29.0010	50.8070	42.3640	C	0
43.1510	65.6950	40.4860	H	0	41.5440	62.6770	45.5850	H	0	28.8810	49.4360	42.3720	N	0
43.6310	67.5580	41.4540	C	0	39.8750	63.6080	46.7020	C	0	27.6390	49.1840	41.8920	C	0
43.9150	67.8240	40.4360	H	0	39.6490	64.1030	47.6470	H	0	27.1500	48.2430	41.6910	H	0
42.4440	68.3660	42.0050	C	0	39.3640	64.1720	45.9210	H	0	26.9750	50.3410	41.5880	N	0
42.2590	68.1050	43.0470	H	0	39.3270	62.6660	46.7410	H	0	26.0310	50.3890	41.2330	H	0
42.8070	69.3930	41.9760	H	0	41.9430	64.5950	46.2030	O	0	27.8860	51.3780	41.8600	C	0
41.2290	68.1870	41.0670	C	0	42.7620	64.3900	45.7450	H	0	27.7250	52.4440	41.7990	H	0
41.6650	68.3930	40.0900	H	0	41.2210	61.5050	47.9870	C	0	31.3920	50.8640	40.7280	C	0
40.7350	67.2150	41.0920	H	0	41.2030	60.6170	47.1870	O	0	31.2930	51.6910	39.8480	O	0
40.1810	69.3130	41.3310	C	0	40.4910	61.3050	49.1310	N	0	31.4230	49.5330	40.3980	N	0
40.6980	70.2710	41.3860	H	0	40.4950	62.2390	50.2510	C	0	31.4190	48.8620	41.1530	H	0
39.4790	69.1930	40.5060	H	0	39.6740	62.9540	50.1960	H	0	31.2630	49.0250	39.0170	C	0
39.5620	69.0100	42.7420	C	0	41.4010	62.8080	50.4630	H	0	31.2070	49.8050	38.2580	H	0
39.3580	67.9390	42.7690	H	0	40.2010	61.3770	51.4820	C	0	32.4680	48.2000	38.6740	C	0
40.2300	69.4090	43.5050	H	0	39.6810	61.9430	52.2550	H	0	32.4660	47.3330	39.3340	H	0
38.3240	69.6770	42.9140	N	0	41.0750	60.9020	51.9280	H	0	32.3480	47.8560	37.6470	H	0
38.4370	70.6780	42.8440	H	0	39.2930	60.3410	50.9100	C	0	33.8680	48.7730	38.7780	C	0
37.6020	69.2840	42.3270	H	0	38.2890	60.7610	50.9790	H	0	34.3310	49.4960	37.6360	C	0
37.9400	69.4940	43.8310	H	0	39.3820	59.4860	51.5800	H	0	33.7520	49.4420	36.7260	H	0
44.9310	67.8940	42.2390	C	0	39.7630	60.1170	49.4450	C	0	35.6760	49.9390	37.6160	C	0
44.9870	68.8690	43.0280	O	0	40.4490	59.2770	49.3380	H	0	36.1480	50.3580	36.7400	H	0
45.9000	67.0120	42.0110	N	0	38.4850	59.9380	48.5250	C	0	36.4510	49.8810	38.7720	C	0
45.6860	66.2540	41.3790	H	0	37.6630	60.8020	48.4880	O	0	37.4770	50.2200	38.7870	H	0
47.2200	66.9820	42.6200	C	0	38.3140	58.7220	47.9810	N	0	35.9450	49.2540	39.9170	C	0

36.5930	49.0790	40.7630	H	0	28.3880	55.4490	29.8910	H	0	34.9950	63.5660	48.4900	O	0
34.6740	48.6500	39.9180	C	0	28.4560	54.5850	31.7850	C	0	33.4250	61.6780	47.7260	C	0
34.2990	48.0400	40.7260	H	0	29.4610	54.9270	31.9790	H	0	32.2080	62.0270	47.9170	O	0
29.8690	48.3950	38.8180	C	0	29.9910	52.1560	35.5940	C	0	34.1480	60.7700	48.4540	N	0
29.6680	47.2440	39.2190	O	0	29.5560	51.6400	36.6730	O	0	35.0290	60.6330	47.9790	H	0
28.8980	49.2190	38.4440	N	0	31.2510	52.5590	35.5860	N	0	33.6130	60.0500	49.5810	C	0
29.1950	50.1500	38.1880	H	0	31.6890	52.8620	34.7280	H	0	32.6140	59.8100	49.2190	H	0
27.5130	48.8530	38.5080	C	0	32.0880	52.5960	36.7380	C	0	34.3420	58.7770	49.8860	C	0
27.2510	48.4930	39.5030	H	0	31.8230	51.7920	37.4240	H	0	33.5700	58.1960	50.3900	H	0
26.7460	50.1400	38.2350	C	0	33.1050	52.3200	36.4620	H	0	34.5870	58.2760	48.9490	H	0
27.2700	50.9590	38.7260	H	0	32.1270	53.9800	37.4320	C	0	35.6390	58.7710	50.7960	C	0
26.7810	50.3730	37.1700	H	0	32.9890	54.7460	36.9930	O	0	36.4820	59.0890	50.1820	H	0
25.2680	50.0370	38.7750	C	0	31.2310	54.2470	38.4140	N	0	35.5070	59.5110	51.5840	H	0
24.4240	49.4670	38.0620	O	0	30.6600	53.4500	38.6580	H	0	35.8830	57.3110	51.2310	C	0
24.9640	50.4850	39.8690	O	0	30.9730	55.5110	39.0420	C	0	35.0510	56.9330	51.8250	H	0
27.0910	47.7700	37.4590	C	0	30.7910	56.3050	38.3180	H	0	35.9630	56.6980	50.3340	H	0
27.6560	47.6220	36.4380	O	0	29.6840	55.3590	39.8290	C	0	37.0890	56.9950	52.0910	N	0
26.1490	46.9380	37.8380	N	0	29.8000	54.5100	40.5020	H	0	37.0300	56.9860	53.0990	H	0
25.7750	47.0500	38.7690	H	0	29.7140	56.3530	40.2770	H	0	38.2950	56.7550	51.6210	C	0
25.4130	45.9460	36.9360	C	0	28.5100	55.2250	38.9040	C	0	38.6120	56.4980	50.3810	N	0
26.1660	45.3000	36.4850	H	0	28.1290	53.9890	38.4170	C	0	37.9570	56.5590	49.6150	H	0
24.3430	45.1890	37.6760	C	0	28.5920	53.0770	38.7640	H	0	39.6130	56.5030	50.2450	H	0
23.6340	45.8490	38.1770	H	0	26.9830	53.8500	37.5670	C	0	39.3280	56.7620	52.4040	N	0
23.7710	44.6870	36.8960	H	0	26.6780	52.8730	37.2250	H	0	39.1890	56.8030	53.4030	H	0
24.8470	44.0510	38.6810	C	0	26.3180	54.9710	37.0860	C	0	40.1980	56.4480	51.9980	H	0
25.6360	43.5160	38.1520	H	0	25.3110	54.8080	36.1400	O	0	33.2410	60.8890	50.7790	C	0
25.2900	44.5320	39.5540	H	0	24.9290	55.6110	35.7780	H	0	32.5480	60.3410	51.6430	O	0
23.7200	43.0790	39.0090	C	0	26.7180	56.2660	37.6050	C	0	33.5350	62.1490	50.8250	N	0
22.8400	43.6320	39.3370	H	0	26.0160	57.0630	37.4110	H	0	34.0660	62.5040	50.0440	H	0
23.3770	42.6440	38.0710	H	0	27.8160	56.3910	38.4800	C	0	33.1320	63.1750	51.8050	C	0
24.0930	42.0970	39.9610	N	0	28.0610	57.3830	38.8300	H	0	33.0540	62.7050	52.7850	H	0
24.6150	41.3270	39.5680	H	0	32.0770	55.8450	40.0830	C	0	34.1870	64.3350	51.9050	C	0
24.2490	42.2600	41.2710	C	0	32.4340	55.1020	40.9600	O	0	34.3390	64.7560	50.9110	H	0
23.8660	43.3740	41.9220	N	0	32.7210	56.9920	39.9150	N	0	33.7400	65.0280	52.6190	H	0
23.4100	44.1090	41.4000	H	0	32.5720	57.4770	39.0420	H	0	35.5130	64.0920	52.5160	C	0
24.2460	43.6510	42.8160	H	0	33.7090	57.5890	40.8180	C	0	36.0010	65.0100	52.8420	H	0
24.7870	41.3470	42.0140	N	0	34.0380	56.8170	41.5130	H	0	35.2210	63.5730	53.4300	H	0
24.7620	40.4190	41.6180	H	0	34.9450	58.0640	40.1210	C	0	36.5750	63.1800	51.7750	C	0
24.9220	41.3510	43.0150	H	0	34.7970	59.0040	39.5900	H	0	37.5050	63.1220	52.3410	H	0
24.8080	46.5530	35.6820	C	0	36.0530	58.2790	41.1750	C	0	36.2390	62.1630	51.5750	H	0
24.7340	45.8460	34.6970	O	0	36.3350	57.2670	41.4690	H	0	36.9480	63.8110	50.4680	N	0
24.4830	47.8600	35.6260	N	0	36.9570	58.6330	40.6800	H	0	36.3940	63.6530	49.6380	H	0
24.5880	48.3760	36.4880	H	0	35.8270	58.8530	42.0740	H	0	37.8430	64.7630	50.2490	C	0
24.0740	48.5580	34.4590	C	0	35.4660	57.0160	39.0910	C	0	38.7480	65.1730	51.0660	N	0
23.3070	48.0370	33.8860	H	0	35.5010	56.0290	39.5510	H	0	38.8240	64.7420	51.9760	H	0
23.4170	49.8670	34.9520	C	0	34.7430	57.0990	38.2800	H	0	39.1210	66.0990	50.9120	H	0
22.6900	50.1860	34.2050	H	0	36.4630	57.2550	38.7200	H	0	37.7560	65.1940	49.0470	N	0
22.8280	49.6580	35.8460	H	0	33.1070	58.6530	41.6460	C	0	37.0150	65.0510	48.3750	H	0
24.3480	51.0080	35.1820	C	0	32.7360	59.6440	41.0130	O	0	38.2670	66.0360	48.8240	H	0
25.5090	51.0910	34.8300	O	0	33.0670	58.6520	42.9470	N	0	31.7640	63.7610	51.4630	C	0
23.8990	52.1350	35.7810	N	0	33.4160	57.8040	43.3690	H	0	30.9750	63.8980	52.4480	O	0
24.5640	52.8290	36.0910	H	0	32.4880	59.7710	43.7870	C	0	31.4560	64.1110	50.2150	N	0
22.9850	52.1420	36.2100	H	0	32.5090	60.6460	43.1380	H	0	32.2200	64.0470	49.5570	H	0
25.2840	48.8330	33.4670	C	0	31.0180	59.5920	44.2380	C	0	30.4080	65.0800	49.9440	C	0
24.9750	49.3250	32.3520	O	0	30.9420	58.8860	45.0650	H	0	29.7680	65.3000	50.7990	H	0
26.5370	48.5440	33.8360	N	0	30.8080	60.5000	44.8020	H	0	31.0250	66.4840	49.4990	C	0
26.7770	48.1750	34.7450	H	0	29.9530	59.3520	43.1020	C	0	30.1900	67.1520	49.2880	H	0
27.6660	48.8260	32.9300	C	0	30.3700	59.8110	42.2060	H	0	31.8650	67.0930	50.6490	C	0
28.2730	47.9220	32.9820	H	0	29.8090	57.8360	42.8930	C	0	32.6400	66.3270	50.6450	H	0
27.3390	48.9150	31.8950	H	0	30.7480	57.4290	42.5140	H	0	32.1990	68.0790	50.3270	H	0
28.5940	49.9820	33.2430	C	0	29.6180	57.2850	43.8140	H	0	31.3130	67.1340	51.5880	H	0
29.6930	49.9990	32.6750	O	0	29.1400	57.7130	42.0410	H	0	31.8590	66.3000	48.2850	O	0
28.2740	51.0020	34.0490	N	0	28.6480	60.0150	43.4220	C	0	32.1580	67.1950	48.1090	H	0
27.3740	50.9770	34.5070	H	0	27.9740	59.2240	43.0940	H	0	29.4480	64.7010	48.7810	C	0
29.0930	52.2230	34.2510	C	0	28.4540	60.1750	44.4820	H	0	28.4080	65.3030	48.6890	O	0
29.7250	52.2960	33.3650	H	0	28.5220	60.9790	42.9290	H	0	29.7810	63.5390	48.1170	N	0
28.3710	53.6310	34.1020	C	0	33.3700	60.2640	44.9890	C	0	30.5320	62.9530	48.4560	H	0
27.5180	53.8410	34.7490	H	0	34.0010	59.4630	45.7390	O	0	28.9830	62.9170	47.0010	C	0
29.1440	54.3660	34.3260	H	0	33.4620	61.6080	45.1750	N	0	29.1080	61.8410	46.8790	H	0
27.7820	53.8150	32.7550	C	0	33.1750	62.2420	44.4430	H	0	27.9550	63.1150	47.3060	H	0
26.4570	53.3530	32.4740	C	0	34.0660	62.1930	46.4140	C	0	29.2260	63.4720	45.6080	C	0
25.9180	52.7480	33.1880	H	0	35.0730	61.7770	46.3890	H	0	28.3790	63.2680	44.7210	O	0
25.9130	53.4690	31.2050	C	0	34.1410	63.7030	46.2430	C	0	30.2610	64.1760	45.3120	N	0
24.9090	53.1400	30.9800	H	0	34.6340	63.8740	45.2860	H	0	30.9360	64.2740	46.0570	H	0
26.6070	54.2750	30.2900	C	0	33.1560	64.1650	46.3090	H	0	30.6540	64.6560	44.0250	C	0
26.1380	54.4520	29.3330	H	0	34.9680	64.2190	47.4390	C	0	29.8900	65.3130	43.6080	H	0
27.8660	54.8030	30.5810	C	0	35.6670	65.2850	47.4010	O	0	31.8950	65.5550	44.1330	C	0



31.7220	66.2090	44.9880	H	0	32.2610	55.7350	31.7490	C	0	26.8210	47.7550	21.8380	C	0
32.7780	65.0000	44.4500	H	0	31.5560	56.2130	31.0690	H	0	25.9050	48.1980	20.9480	O	0
32.2290	66.4410	42.8860	C	0	33.7020	55.9880	31.3330	C	0	25.3240	47.4490	20.7990	H	0
32.3530	65.7730	42.0340	H	0	34.3580	55.4110	31.9850	H	0	26.4610	46.6310	22.6090	C	0
31.5030	67.2040	42.6060	H	0	33.8000	55.6620	30.2980	H	0	25.4660	46.2380	22.4610	H	0
33.6390	67.0630	42.9910	C	0	34.1810	57.4800	31.1980	C	0	27.3410	46.1090	23.5690	C	0
34.4860	66.5790	43.7720	O	0	34.1450	57.8820	32.2110	H	0	26.9550	45.3540	24.2390	H	0
33.9440	68.1030	42.2280	N	0	35.2080	57.4790	30.8330	H	0	28.2640	47.4080	26.5530	C	0
34.9340	68.3000	42.2080	H	0	33.3600	58.3530	30.2800	C	0	27.5930	46.4670	27.0370	O	0
33.3020	68.4490	41.5300	H	0	32.8690	57.9980	29.2090	O	0	27.8200	48.6250	26.5180	N	0
30.9500	63.5310	43.0230	C	0	33.0670	59.5840	30.5970	N	0	28.4760	49.2710	26.1030	H	0
32.0080	62.9370	43.1430	O	0	32.3840	60.1440	30.1080	H	0	26.5160	49.1690	26.9090	C	0
30.1780	63.3240	41.9690	N	0	33.3260	59.9360	31.5080	H	0	25.9460	48.3490	27.3450	H	0
29.3260	63.8350	41.7860	H	0	31.9050	54.2240	31.5830	C	0	26.6370	50.2370	27.9680	C	0
30.5850	62.5240	40.8420	C	0	31.7800	53.5690	32.6190	O	0	27.3410	51.0040	27.6420	H	0
30.7760	61.4970	41.1550	H	0	31.6280	53.6480	30.3740	N	0	25.2680	50.8750	28.2580	C	0
29.2100	62.3000	40.0610	C	0	31.2990	54.3310	29.1110	C	0	25.0900	51.5340	27.4090	H	0
28.4510	62.1600	40.8310	H	0	32.1880	54.5790	28.5310	H	0	24.5120	50.1390	28.5360	H	0
28.9830	63.1860	39.4700	H	0	30.8210	55.2810	29.3510	H	0	25.1370	51.6410	29.0230	H	0
29.1350	61.1150	39.0100	C	0	30.4060	53.3650	28.2970	C	0	27.2660	49.7590	29.3680	C	0
28.1320	61.2310	38.6000	H	0	30.8930	53.2200	27.3330	H	0	27.6260	50.6120	29.9430	H	0
30.0410	61.3610	37.8390	C	0	29.3730	53.7110	28.2500	H	0	26.5310	49.2070	29.9550	H	0
31.0980	61.3120	38.1000	H	0	30.3350	52.0600	29.1050	C	0	28.2070	49.2140	29.2950	H	0
29.7550	60.6510	37.0630	H	0	30.7740	51.1930	28.6110	H	0	25.7920	49.6670	25.6810	C	0
29.7430	62.3580	37.5150	H	0	29.2930	51.9670	29.4110	H	0	26.4680	50.1190	24.7650	O	0
29.4300	59.6920	39.5890	C	0	31.2680	52.2230	30.3070	C	0	24.4560	49.5980	25.6110	N	0
28.6390	59.5300	40.3210	H	0	30.5990	51.9410	31.1200	H	0	24.0650	49.2280	26.4650	H	0
29.3290	58.9580	38.7900	H	0	32.4620	51.2440	30.4030	C	0	23.5630	50.2000	24.5990	C	0
30.4500	59.6280	39.9690	H	0	33.3010	51.3280	29.4740	O	0	24.2130	51.0400	24.3510	H	0
31.6890	62.9380	39.9270	C	0	32.4680	50.3430	31.3330	N	0	23.5480	49.3690	23.3370	C	0
31.5300	63.8870	39.1310	O	0	31.6280	50.2630	31.8880	H	0	23.4900	50.0200	22.4640	H	0
32.9220	62.4150	40.1920	N	0	33.5920	49.3280	31.5130	C	0	24.5020	48.8470	23.2600	H	0
32.9330	61.6450	40.8460	H	0	34.4950	49.8050	31.1330	H	0	22.5000	48.3220	23.2830	C	0
34.1150	62.7650	39.4990	C	0	33.9410	49.1070	33.0170	C	0	21.8300	48.0790	24.2240	O	0
34.1590	63.8440	39.3540	H	0	34.9170	48.6240	33.0670	H	0	22.4860	47.5210	22.2680	N	0
35.4190	62.4160	40.2600	C	0	34.1060	50.0140	33.5990	H	0	21.8390	46.7600	22.4170	H	0
35.1930	61.4340	40.6770	H	0	32.8640	48.3340	33.7520	C	0	23.0750	47.5720	21.4500	H	0
36.5700	62.4610	39.3170	C	0	31.8730	49.0600	34.5000	C	0	22.2200	50.8560	25.0310	C	0
36.3920	61.6360	38.6270	H	0	31.8550	50.1390	34.5430	H	0	21.5820	51.5290	24.2400	O	0
36.4230	63.3910	38.7690	H	0	30.8660	48.2740	35.1130	C	0	21.8280	50.7020	26.2530	N	0
37.4970	62.3220	39.8730	H	0	30.1420	48.7560	35.7520	H	0	22.2560	49.9670	26.7980	H	0
35.6410	63.3830	41.5080	C	0	30.7980	46.9080	35.1580	C	0	20.7360	51.4440	26.9010	C	0
36.0390	64.3490	41.1960	H	0	29.9970	46.4240	35.6960	H	0	19.8570	51.3600	26.2630	H	0
34.7110	63.5600	42.0470	H	0	31.8850	46.1980	34.6400	C	0	20.3430	50.7180	28.1970	C	0
36.6200	62.8270	42.6070	C	0	31.7910	45.1230	34.6850	H	0	19.3300	50.9430	28.5330	H	0
37.6860	62.9850	42.4420	H	0	32.8590	46.8940	33.8720	C	0	20.3070	49.6600	27.9370	H	0
36.4950	63.3560	43.5520	H	0	33.6170	46.3290	33.3500	H	0	21.2620	50.8730	29.3900	C	0
36.4230	61.7610	42.7250	H	0	33.4780	48.0090	30.6840	C	0	22.3060	50.0250	29.6810	C	0
34.0430	62.2690	38.0380	C	0	34.3350	47.1470	30.7790	O	0	22.5860	49.1400	29.1300	H	0
34.2440	62.9790	37.0680	O	0	32.4190	47.9380	29.8480	N	0	22.9820	50.5710	30.7030	N	0
33.6200	61.0130	37.8930	N	0	31.9000	48.8010	29.7610	H	0	23.7160	50.1000	31.2130	H	0
33.2810	60.4410	38.6540	H	0	31.9780	46.8730	29.0030	C	0	22.4520	51.7320	31.1990	C	0
33.5410	60.4050	36.6050	C	0	32.9030	46.4730	28.5880	H	0	22.7710	52.4570	32.3200	C	0
33.1200	61.1750	35.9580	H	0	31.0920	45.8930	29.7550	C	0	23.7020	52.2000	32.8030	H	0
35.0010	60.0640	36.2830	C	0	30.7200	45.1560	29.0430	H	0	21.9740	53.5100	32.6700	C	0
35.5640	60.9970	36.2970	H	0	31.8570	45.0840	30.7650	C	0	22.1410	54.1720	33.5070	H	0
35.3450	59.4810	37.1370	H	0	32.7230	44.5830	30.3320	H	0	20.9490	53.8590	31.8320	C	0
35.3030	59.3810	34.9640	C	0	32.2070	45.6040	31.6560	H	0	20.3680	54.7270	32.1060	H	0
36.3480	59.2780	34.6740	H	0	31.1750	44.3610	31.2120	H	0	20.6110	53.1100	30.6910	C	0
34.8170	58.4060	35.0030	H	0	29.8920	46.6200	30.4240	C	0	19.7610	53.4640	30.1260	H	0
34.7950	60.2120	33.8050	C	0	29.1820	46.9180	29.6520	H	0	21.3300	51.9560	30.3900	C	0
33.5990	60.1610	33.5370	O	0	29.3380	45.8230	30.9210	H	0	20.9530	52.9260	27.0330	C	0
35.5790	61.0730	33.2890	O	0	30.2090	47.4800	31.0140	H	0	19.9960	53.6300	26.8550	O	0
32.6270	59.1780	36.5990	C	0	31.0880	47.5080	27.8600	C	0	22.1690	53.3480	27.3910	N	0
32.2670	58.5640	37.6200	O	0	30.9780	48.6590	27.8240	O	0	22.8060	52.6420	27.7320	H	0
32.0650	58.8740	35.4240	N	0	30.6150	46.7170	26.8950	N	0	22.5280	54.8070	27.3030	C	0
32.3030	59.5010	34.6690	H	0	30.8770	45.7410	26.9140	H	0	21.8470	55.1990	26.5470	H	0
31.4230	57.6060	34.9770	C	0	29.6240	47.2290	25.9380	C	0	22.4310	55.4180	28.7220	C	0
32.0060	56.7590	35.3380	H	0	29.9480	48.1690	25.4910	H	0	22.7800	56.4490	28.6740	H	0
29.9780	57.4550	35.4950	C	0	29.5600	46.2560	24.8030	C	0	21.3850	55.4270	29.0310	H	0
29.4430	56.6630	34.9720	H	0	30.4910	46.3270	24.2410	H	0	23.1050	54.8460	29.3600	H	0
29.9470	57.2780	36.5700	H	0	29.1920	45.2880	25.1440	H	0	23.9210	54.9580	26.7310	C	0
29.4710	58.4060	35.3320	H	0	28.5950	46.7010	23.7240	C	0	24.8380	54.1240	26.7590	O	0
31.5040	57.3430	33.4690	C	0	28.9830	47.7800	22.8840	C	0	24.1300	56.0730	26.0690	N	0
31.0760	58.1080	32.6070	O	0	29.9950	48.1480	22.9640	H	0	23.3820	56.7510	26.0520	H	0
32.0840	56.1920	33.0980	N	0	28.1020	48.3130	21.9500	C	0	25.4500	56.4930	25.5440	C	0
32.4570	55.5690	33.8000	H	0	28.4890	49.1750	21.4270	H	0	25.8370	55.6290	25.0040	H	0

25.4730	57.7660	24.5720	C	0	32.3240	64.5850	33.7960	H	0	21.3990	57.1360	33.4660	C	0
24.8070	57.5350	23.7410	H	0	33.0330	66.1750	33.6090	H	0	20.7540	56.3280	33.8100	H	0
25.1050	58.6880	25.0220	H	0	33.0100	65.5740	35.6070	N	0	22.3890	56.7820	33.7540	H	0
26.8170	58.1020	23.9310	C	0	32.6170	66.2790	36.2150	H	0	21.5130	57.3430	31.9100	C	0
26.6090	58.9030	23.2220	H	0	33.0220	64.6860	36.0880	H	0	20.5180	57.4400	31.4760	H	0
27.4250	58.5550	24.7140	H	0	33.9640	65.8940	35.5260	H	0	22.1690	56.6030	31.4520	H	0
27.3690	56.8790	23.1580	C	0	26.9460	67.4270	33.3370	C	0	22.1630	58.7130	31.9210	C	0
27.9830	56.3140	23.8590	H	0	27.1640	68.1300	34.3450	O	0	23.2190	58.5380	31.7140	H	0
26.5090	56.3490	22.7500	H	0	25.8460	67.7360	32.6120	N	0	21.5730	59.4480	30.7510	C	0
28.3240	57.3360	21.9790	C	0	25.8200	67.1980	31.7580	H	0	20.4270	59.7860	30.7440	O	0
28.2140	56.5420	21.2400	H	0	24.8740	68.8280	32.9730	C	0	22.3580	59.5950	29.7220	N	0
27.9120	58.2390	21.5300	H	0	25.4010	69.7770	33.0730	H	0	23.3340	59.4800	29.9540	H	0
29.7840	57.4620	22.3440	N	0	23.9960	69.1130	31.6910	C	0	21.9390	60.0230	28.3740	C	0
29.9740	56.7090	22.9910	H	0	24.6830	69.3140	30.8690	H	0	21.0480	60.6370	28.5100	H	0
30.4310	57.5740	21.5770	H	0	23.4270	68.2240	31.4200	H	0	22.9660	60.7750	27.5430	C	0
29.8560	58.3510	22.8180	H	0	22.9800	70.2070	31.8620	C	0	23.8680	60.1760	27.4220	H	0
26.3780	56.7250	26.6930	C	0	22.4610	70.3890	30.9210	H	0	22.3540	61.1100	26.1960	C	0
27.4990	56.2170	26.6090	O	0	22.2300	69.9130	32.5960	H	0	21.5030	61.7660	26.3780	H	0
26.0310	57.6100	27.6500	N	0	23.5000	71.5990	32.3100	C	0	23.0370	61.6820	25.5680	H	0
25.0600	57.8850	27.6150	H	0	22.9370	72.3150	33.1850	O	0	22.0490	60.2170	25.6500	H	0
26.8950	58.2160	28.5800	C	0	24.6590	71.8710	31.9160	O	0	23.4170	62.0290	28.2760	C	0
27.5560	57.4570	28.9990	H	0	24.0800	68.4800	34.2700	C	0	22.5850	62.6680	28.5710	H	0
27.7720	59.3190	27.9500	C	0	23.8910	69.3800	35.1070	O	0	23.9380	61.6520	29.1560	H	0
28.5870	59.5800	28.6260	H	0	23.6420	67.1780	34.4230	N	0	23.9400	62.7190	27.6130	H	0
28.2590	59.0530	27.0120	H	0	23.8110	66.7280	33.5350	H	0	21.4630	58.7190	27.6540	C	0
26.9290	60.5990	27.6950	C	0	22.6480	66.6080	35.3340	C	0	22.2030	57.9790	27.0000	O	0
25.9880	60.5750	27.1460	H	0	22.5630	67.3870	36.0920	H	0	20.2260	58.2920	27.8870	N	0
26.5680	60.9990	28.6430	H	0	21.2810	66.4950	34.6300	C	0	19.6900	58.9980	28.3720	H	0
27.7560	61.7350	27.0410	C	0	21.3880	65.7450	33.8460	H	0	19.5810	57.1420	27.3580	C	0
28.7810	62.0920	27.6080	O	0	20.4940	66.2180	35.3310	H	0	20.2230	56.3030	27.6260	H	0
27.3690	62.2240	25.9880	O	0	20.8910	67.7220	33.8510	C	0	18.3310	56.8930	28.1160	C	0
26.2150	58.7870	29.8790	C	0	20.4450	68.7100	34.4280	O	0	17.5250	57.5830	27.8660	H	0
25.0440	59.0670	29.9140	O	0	20.7270	67.7780	32.5660	N	0	17.9310	55.9440	27.7590	H	0
27.0630	59.1930	30.8690	N	0	20.1480	68.5350	32.2320	H	0	18.4740	56.8240	29.6550	C	0
28.0600	59.1680	30.7110	H	0	20.9830	67.0280	31.9390	H	0	19.0830	55.9420	29.8520	H	0
26.5330	59.8810	32.0530	C	0	23.1610	65.4190	36.1990	C	0	18.9810	57.7360	29.9700	H	0
25.4750	59.6590	32.1900	H	0	22.3730	65.0350	37.1040	O	0	17.1540	56.7290	30.4320	C	0
27.1400	59.3290	33.3070	C	0	24.2960	64.8000	35.9070	N	0	17.0930	56.7450	31.6910	O	0
28.1890	59.6200	33.2500	H	0	24.8640	65.3170	35.2510	H	0	16.1210	56.4660	29.7570	O	0
26.5040	59.9160	34.6060	C	0	24.8640	63.7050	36.7370	C	0	19.3370	57.1360	25.8370	C	0
25.4630	59.6550	34.7990	H	0	25.7560	63.4430	36.1680	H	0	18.8670	58.1400	25.2770	O	0
27.0090	59.5790	35.5110	H	0	25.3460	64.1920	38.1270	C	0	19.1590	55.9250	25.2350	N	0
26.4610	61.0010	34.5120	H	0	24.5940	64.5550	38.8280	H	0	19.4690	55.0850	25.7020	H	0
27.0100	57.7270	33.4910	C	0	25.7830	63.2790	38.5300	H	0	18.5930	55.7180	23.8690	C	0
27.8090	57.1860	32.9850	H	0	26.5110	65.1910	38.0960	C	0	18.5520	56.6510	23.3070	H	0
27.1830	57.4990	34.5430	H	0	26.7300	65.9650	39.0620	O	0	19.3680	54.6880	23.0340	C	0
25.5250	57.2330	33.1700	C	0	27.3320	65.1650	37.1710	O	0	19.5580	53.7280	23.5130	H	0
25.3450	57.4570	32.1180	H	0	23.9380	62.4940	36.6570	C	0	18.6050	54.1860	21.7960	C	0
25.4400	56.1790	33.4340	H	0	23.7630	61.7070	37.5930	O	0	19.2060	53.5790	21.1190	H	0
24.7850	57.6350	33.8620	H	0	23.2890	62.2370	35.4850	N	0	17.6890	53.6260	21.9850	H	0
26.7080	61.4280	32.0130	C	0	23.5650	62.8520	34.7330	H	0	18.2410	55.0500	21.2400	H	0
27.7350	62.0660	32.0390	O	0	22.4570	60.9610	35.2590	C	0	20.7370	55.2480	22.5790	C	0
25.5540	62.0240	31.7230	N	0	22.9130	60.1000	35.7490	H	0	21.1230	54.5110	21.8740	H	0
24.7010	61.4870	31.6620	H	0	20.9450	61.3060	35.6380	C	0	20.6140	56.2080	22.0770	H	0
25.4430	63.5080	31.4420	C	0	20.3160	60.4340	35.4620	H	0	21.7870	55.5160	23.6650	C	0
25.7400	63.7700	30.4260	H	0	20.8780	61.7650	36.6240	H	0	22.7500	55.5770	23.1590	H	0
24.0070	63.8920	31.5650	C	0	20.4300	62.4370	34.7610	C	0	21.5970	56.3720	24.3120	H	0
23.4730	63.3140	30.8110	H	0	20.7300	63.3830	35.2120	H	0	21.7860	54.6080	24.2680	H	0
23.7380	63.7250	32.6080	H	0	20.8240	62.3670	33.7470	H	0	17.1020	55.2010	24.1070	C	0
23.7920	65.2470	31.2300	O	0	18.8810	62.4820	34.9000	C	0	16.8680	54.1540	24.7370	O	0
23.9130	65.2570	30.2770	H	0	18.3800	63.2190	34.2730	H	0	16.1070	55.9460	23.6430	N	0
26.1680	64.3790	32.4730	C	0	18.5230	61.5220	34.5270	H	0	16.1930	57.4000	23.3330	C	0
25.8700	64.3240	33.6580	O	0	18.5050	62.6720	36.3060	N	0	16.7390	57.5220	22.3980	H	0
27.1560	65.2030	32.1120	N	0	19.0070	63.3810	36.8210	H	0	16.7980	57.9270	24.0710	H	0
27.4150	65.1610	31.1370	H	0	17.3890	62.2830	36.8530	C	0	14.8270	58.0280	23.3240	C	0
27.8540	66.2230	32.9770	C	0	16.6460	61.4090	36.2970	H	0	14.5930	58.7690	22.5600	H	0
28.0010	65.7210	33.9340	H	0	16.8760	61.0060	35.4000	H	0	14.6730	58.5380	24.2750	H	0
29.1790	66.6980	32.3630	C	0	15.8450	61.0210	36.7750	H	0	13.9100	56.7980	23.1840	C	0
29.0470	66.7670	31.2830	H	0	17.0980	62.7320	38.0200	N	0	13.8540	56.5960	22.1140	H	0
29.3700	67.7440	32.6000	H	0	17.7780	63.3550	38.4300	H	0	12.9610	56.9940	23.6830	H	0
30.3860	65.7870	32.6600	C	0	16.1740	62.5820	38.4000	H	0	14.6800	55.6110	23.7770	C	0
30.2110	64.7120	32.6620	H	0	22.6020	60.4090	33.7980	C	0	14.5880	55.5620	24.8620	H	0
31.1160	66.0070	31.8810	H	0	23.4310	60.9640	33.1120	O	0	14.1020	54.3050	23.2160	C	0
30.9750	66.1740	34.0730	C	0	21.8990	59.3260	33.3230	N	0	13.1340	53.7660	23.7400	O	0
31.0300	67.2400	34.2960	H	0	21.1540	58.4590	34.1360	C	0	14.8180	53.8480	22.2320	N	0
30.3230	65.7990	34.8610	H	0	20.1230	58.8070	34.0680	H	0	15.5530	54.4100	21.8280	H	0
32.4090	65.5660	34.2630	C	0	21.5380	58.3950	35.1540	H	0	14.6610	52.5370	21.5720	C	0

13.6530	52.6220	21.1650	H	0	7.8450	49.8160	25.0910	H	0	14.7440	46.7210	23.5460	H	0
15.6070	52.3530	20.4160	C	0	6.5390	50.8300	25.9080	H	0	13.7600	48.0410	23.1520	H	0
15.6490	53.2260	19.7640	C	0	8.5460	51.5760	25.7890	C	0	11.5440	47.0860	24.4160	O	0
16.6130	52.0810	20.7360	H	0	8.3290	52.3420	26.5340	H	0	11.0090	46.4120	24.8430	H	0
15.0380	51.3070	19.4370	C	0	9.6090	51.3400	25.7480	H	0	13.4480	44.7090	22.2140	C	0
14.2680	50.7230	19.9410	H	0	8.3690	52.2220	24.4110	C	0	13.5070	43.5340	22.7230	O	0
14.5520	51.8110	18.6020	H	0	8.4430	51.4370	23.6590	H	0	14.3310	45.1020	21.2820	N	0
16.2010	50.3180	19.0230	C	0	7.4250	52.7640	24.3540	H	0	14.4050	46.0530	20.9500	H	0
17.2800	50.6030	18.4560	O	0	9.5650	53.1070	24.0530	C	0	15.4950	44.1800	20.9040	C	0
15.9990	49.1320	19.2970	O	0	9.2460	53.8480	23.3210	H	0	15.5480	43.4620	21.7230	H	0
14.8070	51.2900	22.4810	C	0	9.7970	53.7450	24.9060	H	0	15.3230	43.5090	19.4910	C	0
14.0330	50.3340	22.3930	O	0	10.8340	52.3780	23.7520	N	0	15.3000	44.2030	18.6510	H	0
15.7530	51.4050	23.4290	N	0	11.1200	51.7150	24.4580	H	0	16.0050	42.6760	19.3170	H	0
16.1290	52.3410	23.4840	H	0	10.7040	51.8640	22.8930	H	0	13.9610	42.8930	19.4870	C	0
16.3060	50.3630	24.2580	C	0	11.6040	53.0320	23.7600	H	0	13.7250	42.3440	20.3980	H	0
15.9740	49.3900	23.8960	H	0	6.7630	48.4290	27.2590	C	0	13.2820	43.7440	19.4440	H	0
17.8820	50.4400	24.3920	C	0	6.9570	47.2960	26.7980	O	0	13.7060	42.0660	18.2720	C	0
18.1220	51.4430	24.7440	H	0	5.6560	48.8160	27.8610	N	0	14.3380	42.3960	17.4470	H	0
18.2940	49.6370	25.0040	H	0	5.6380	49.7270	28.2960	H	0	13.7870	40.9900	18.4210	H	0
18.6640	50.2830	23.0080	C	0	4.3730	48.0620	28.0290	C	0	12.2590	42.2600	17.8460	C	0
18.5500	51.1710	22.3860	H	0	4.5640	47.2170	28.6890	H	0	11.5520	41.7890	18.5290	H	0
19.7320	50.1920	23.2060	H	0	3.4740	48.9980	28.7230	C	0	11.9520	43.3050	17.7960	H	0
18.3800	48.9610	22.2180	C	0	4.0060	49.2490	29.6400	H	0	12.0440	41.6970	16.4600	N	0
18.2560	48.0870	22.8580	H	0	3.4280	49.8490	28.0440	H	0	11.0840	41.3960	16.3730	H	0
17.4110	49.0940	21.7370	H	0	2.0730	48.4280	29.0950	C	0	12.1030	42.4640	15.8060	H	0
19.3030	48.7850	20.9680	C	0	1.4020	49.2810	29.1900	H	0	12.6510	40.9010	16.3260	H	0
19.5570	49.7980	20.6550	H	0	1.6390	47.8080	28.3100	H	0	16.9320	44.6900	21.0390	C	0
20.2350	48.3160	21.2840	H	0	2.0100	47.5980	30.3690	C	0	17.1980	45.9020	20.9890	O	0
18.6390	48.0250	19.9230	N	0	2.8560	46.7600	30.6210	O	0	17.9190	43.8150	20.9880	N	0
18.0670	47.2690	20.2730	H	0	1.0130	47.8710	31.2250	N	0	17.6560	42.8440	21.0770	H	0
18.0340	48.7030	19.4820	H	0	0.8790	47.2560	32.0160	H	0	19.3400	44.1710	21.1550	C	0
19.2750	47.7730	19.1800	H	0	0.2800	48.4720	30.8760	H	0	20.0490	43.3440	21.1220	H	0
15.7540	50.4230	25.7170	C	0	3.7910	47.4360	26.7090	C	0	19.5360	44.7440	20.2480	H	0
15.9120	49.4410	26.4760	O	0	3.6950	48.2070	25.7210	O	0	19.6890	45.0270	22.3810	C	0
15.0720	51.5040	26.0750	N	0	3.3720	46.1670	26.5410	N	0	20.2580	46.0720	22.0790	O	0
15.1110	52.2460	25.3920	H	0	3.5660	45.3900	27.1560	H	0	19.1970	44.7500	23.5830	N	0
14.1900	51.6750	27.2530	C	0	2.7110	45.5740	25.3390	C	0	18.7190	43.8610	23.6000	H	0
14.7350	51.0930	27.9960	H	0	2.3000	44.6090	25.6380	H	0	19.5850	45.4740	24.7930	C	0
13.9200	53.1520	27.5820	C	0	1.8030	46.1700	25.2450	H	0	19.9260	46.4620	24.4840	H	0
14.8370	53.6400	27.9140	H	0	3.3860	45.3580	23.9780	C	0	18.5830	45.5090	25.9560	C	0
13.6430	53.6570	26.6560	H	0	2.6610	45.0320	23.0070	O	0	18.6260	44.4770	26.3040	H	0
12.9350	53.2820	28.6740	C	0	4.6770	45.5530	23.9070	N	0	18.9980	46.4090	27.1300	C	0
12.0280	52.8630	28.2370	H	0	5.0810	45.9060	24.7620	H	0	18.6640	47.4380	27.0030	H	0
13.0400	52.6710	29.5710	H	0	5.5620	45.6430	22.7000	C	0	18.5550	46.0490	28.0580	H	0
12.6930	54.6570	29.2390	C	0	5.0780	45.1430	21.8610	H	0	20.0560	46.2920	27.3690	H	0
12.6320	55.4150	28.4580	H	0	5.7060	47.1230	22.2550	C	0	17.1000	45.9020	25.4970	C	0
11.7760	54.8200	29.8050	H	0	6.3160	47.0670	21.3530	H	0	17.0840	46.9720	25.2890	H	0
13.8150	55.0490	30.0970	N	0	4.3840	47.7110	21.8640	C	0	16.8420	45.3480	24.5950	H	0
14.5940	55.5130	29.6520	H	0	3.5910	46.9630	21.8540	H	0	15.9860	45.5330	26.4730	C	0
13.9260	54.6810	31.3990	C	0	4.0840	48.4640	22.5930	H	0	16.2350	44.6160	27.0070	H	0
13.0680	53.8600	31.9780	N	0	4.5710	48.2200	20.9180	H	0	15.8110	46.3100	27.2170	H	0
12.1890	53.6540	31.5240	H	0	6.4140	48.1340	23.1860	C	0	15.0490	45.3360	25.9530	H	0
13.2220	53.6780	32.9590	H	0	7.4170	47.8040	23.4560	H	0	20.8160	44.8520	25.4380	C	0
15.0090	54.9920	32.1670	N	0	6.5480	49.1400	22.7880	H	0	21.0450	43.6070	25.4300	O	0
15.7220	55.5490	31.7190	H	0	5.8260	48.1780	24.1030	H	0	21.7840	45.6950	25.8210	N	0
15.0740	54.7350	33.1410	H	0	6.9260	45.0190	22.9320	C	0	21.6740	46.6470	25.5010	H	0
12.9810	50.8710	26.9240	C	0	7.3770	44.8900	24.0480	O	0	23.0910	45.3590	26.3940	C	0
12.2150	51.2350	26.0060	O	0	7.6190	44.5870	21.8950	N	0	22.9320	44.3740	26.8340	H	0
12.7160	49.8490	27.7060	N	0	7.3490	44.8440	20.9570	H	0	24.2300	45.2720	25.3250	C	0
13.2360	49.7960	28.5700	H	0	8.9190	43.8960	22.0020	C	0	24.5420	46.2770	25.0390	H	0
11.6110	48.9250	27.5460	C	0	9.0430	43.5120	23.0150	H	0	25.1060	44.8010	25.7700	H	0
11.5820	48.6510	26.4920	H	0	9.0100	42.7040	21.0360	C	0	23.9540	44.2700	23.8450	S	0
11.8270	47.5950	28.2250	C	0	9.9960	42.2570	20.9040	H	0	23.4640	46.3820	27.5370	C	0
11.0760	46.8890	27.8730	H	0	8.2770	41.9790	21.3900	H	0	23.4930	47.5390	27.2730	O	0
13.1930	46.9050	27.9370	C	0	8.6880	42.9680	19.5500	C	0	23.8700	46.0090	28.7510	N	0
13.2690	46.1470	28.7160	H	0	9.6190	42.8460	18.6990	O	0	24.3630	46.9040	29.7300	C	0
13.1030	46.4480	26.9510	H	0	7.4620	43.0650	19.2510	O	0	23.4860	47.2070	30.3010	H	0
13.9860	47.6530	27.9060	H	0	10.0770	44.9570	21.8300	C	0	24.9330	47.7350	29.3150	H	0
11.6730	47.7620	29.6070	O	0	10.0770	45.7090	20.8820	O	0	25.3910	46.2290	30.6790	C	0
12.3810	47.3720	30.1250	H	0	11.0540	44.8970	22.7690	N	0	25.2540	46.5210	31.7200	H	0
10.1840	49.4930	27.8480	C	0	11.0510	44.1630	23.4620	H	0	26.3820	46.4550	30.2840	H	0
10.1230	50.4340	28.6320	O	0	12.3200	45.6670	22.6380	C	0	24.9550	44.7300	30.5390	C	0
9.2040	48.9910	27.0710	N	0	12.2180	46.3870	21.8260	H	0	24.3740	44.3440	31.3770	H	0
9.4410	48.3840	26.3000	H	0	12.6550	46.3680	23.9640	C	0	25.8580	44.1430	30.3710	H	0
7.8230	49.5200	27.1870	C	0	12.8930	45.5950	24.6950	H	0	23.9970	44.6650	29.2640	C	0
7.8270	50.1820	28.0530	H	0	13.8680	47.2610	23.9050	C	0	24.3410	43.9960	28.4750	H	0
7.5600	50.4500	25.9310	C	0	14.2090	47.7050	24.8400	H	0	22.6380	44.1140	29.6420	C	0

21.6250	44.8000	29.7930	O	0	28.7320	42.4470	37.4670	C	0	42.6620	44.8610	42.6630	H	0
22.6400	42.7760	29.7360	N	0	28.0210	43.3700	37.8100	O	0	41.7050	43.8680	43.8630	H	0
23.4940	42.2660	29.5610	H	0	28.7140	41.3190	38.2010	N	0	41.4270	43.6430	42.1540	H	0
21.4700	41.9740	30.2120	C	0	29.2560	40.4870	38.0140	H	0	41.1150	46.9430	42.5620	C	0
20.6100	42.4160	29.7090	H	0	27.9530	41.0190	39.3530	C	0	40.6400	47.5100	41.5670	O	0
21.7540	40.5500	29.7850	C	0	27.0460	41.6220	39.3240	H	0	41.9000	47.5590	43.3880	N	0
20.7560	40.1220	29.6940	H	0	27.5340	39.5510	39.3900	C	0	42.0670	47.1020	44.2730	H	0
22.2800	40.4410	28.8360	H	0	27.3980	39.1730	38.3770	H	0	42.7680	48.7600	43.1590	C	0
22.5100	39.7650	30.7820	C	0	28.2580	38.8680	39.8340	H	0	42.7150	49.0220	42.1020	H	0
23.6090	40.1730	31.1600	O	0	26.2940	39.2920	40.2050	C	0	42.3060	49.8470	44.0390	C	0
21.8230	38.6680	31.2150	N	0	25.1690	39.7180	39.7830	O	0	41.2540	49.9710	43.7820	H	0
22.4090	37.9200	31.5570	H	0	26.4740	38.7540	41.3190	O	0	42.4040	49.5980	45.0950	H	0
20.8640	38.4930	30.9510	H	0	28.7760	41.3520	40.5770	C	0	42.9750	51.1600	43.9380	C	0
21.1880	42.1540	31.7710	C	0	29.8300	41.9890	40.6460	O	0	42.9770	51.8230	42.7060	C	0
22.0770	42.5100	32.5370	O	0	28.3260	41.0440	41.8370	N	0	42.3750	51.4730	41.8810	H	0
19.9260	41.8100	32.1360	N	0	27.5270	40.4300	41.8990	H	0	43.6090	53.0660	42.5260	C	0
19.2680	41.4160	31.4780	H	0	28.9210	41.4660	43.1750	C	0	43.4730	53.5040	41.5480	H	0
19.5400	41.7900	33.5840	C	0	29.0930	42.5390	43.0800	H	0	44.1190	53.7660	43.6440	C	0
19.6680	42.7770	34.0280	H	0	27.9820	41.3060	44.3870	C	0	44.5940	54.7340	43.5990	H	0
18.0740	41.3890	33.6580	C	0	28.6000	41.5050	45.2630	H	0	44.2220	53.0300	44.8530	C	0
17.6380	41.4760	34.6530	H	0	27.1770	42.0400	44.3510	H	0	44.5560	53.5550	45.7350	H	0
17.5290	42.1360	33.0810	H	0	27.3900	39.9090	44.7450	C	0	43.6750	51.7740	45.0370	C	0
17.7150	40.0910	33.1170	O	0	27.1280	39.9310	45.8030	H	0	43.6970	51.3020	46.0090	H	0
16.7810	39.9500	33.2920	H	0	26.4290	39.8110	44.2380	H	0	44.1630	48.4170	43.5830	C	0
20.4390	40.9320	34.5510	C	0	28.3060	38.7190	44.4650	C	0	44.4080	47.7710	44.5950	O	0
20.3670	41.0440	35.7420	O	0	29.1490	38.4960	45.3240	O	0	45.1030	48.9710	42.8220	N	0
21.4290	40.0960	34.1050	N	0	28.0450	37.8750	43.5290	N	0	44.8960	49.4240	41.9440	H	0
21.5920	39.8760	33.1330	H	0	28.3990	36.9520	43.7340	H	0	46.4740	49.0810	43.3290	C	0
22.4220	39.4750	34.9700	C	0	27.3770	38.1190	42.8120	H	0	46.5740	48.6160	44.3100	H	0
22.0040	39.1190	35.9120	H	0	30.3070	40.8590	43.3630	C	0	47.4990	48.3510	42.5110	C	0
22.9540	38.3000	34.1790	C	0	30.9200	41.1070	44.3320	O	0	47.4720	47.2690	42.6360	H	0
22.1210	37.6820	33.8440	H	0	30.9530	40.1310	42.3790	N	0	47.4780	48.5080	41.4330	H	0
23.5610	38.6650	33.3510	H	0	30.4570	40.0580	41.5020	H	0	48.7650	48.8180	42.9340	O	0
23.6700	37.4300	35.1770	C	0	32.3940	39.7060	42.3980	C	0	49.3810	48.0980	42.7800	H	0
24.4000	38.0320	35.7180	H	0	32.5430	39.0590	43.2620	H	0	46.8680	50.5440	43.5550	C	0
22.9830	37.0660	35.9410	H	0	32.7540	38.8590	41.2200	C	0	47.1110	51.2450	42.5540	O	0
24.4910	36.0830	34.3560	S	0	33.8440	38.8400	41.2310	H	0	47.0930	50.9600	44.7910	N	0
23.3100	34.7030	34.5050	C	0	32.5440	37.8050	41.3970	H	0	46.9170	50.3080	46.0710	C	0
23.1670	34.4560	35.5570	H	0	32.3270	39.2070	39.8180	C	0	47.7260	49.5970	46.2350	H	0
22.4090	35.0620	34.0070	H	0	32.2390	40.2880	39.7100	H	0	45.9230	49.9020	46.2590	H	0
23.6800	33.8100	34.0010	H	0	33.1110	38.9060	39.1230	H	0	46.9770	51.4080	47.1270	C	0
23.4610	40.4350	35.3390	C	0	30.9720	38.5310	39.3600	C	0	47.3560	51.0650	48.0900	H	0
24.0770	40.2210	36.3680	O	0	30.4340	38.9560	38.3610	O	0	46.0570	51.9880	47.1940	H	0
23.7150	41.4600	34.5430	N	0	30.4180	37.5610	40.0970	N	0	48.0940	52.2480	46.5470	C	0
23.1310	41.5480	33.7240	H	0	29.5830	37.1710	39.6850	H	0	49.0100	51.6880	46.7360	H	0
24.6020	42.6700	34.7310	C	0	30.7480	37.0840	40.9240	H	0	48.0380	53.2280	47.0220	H	0
23.9260	43.5020	34.5330	H	0	33.2470	41.0400	42.4860	C	0	47.7520	52.2330	45.0320	C	0
24.9440	42.8520	35.7500	H	0	33.1570	41.8140	41.5500	O	0	47.0170	53.0150	44.8430	H	0
25.8370	42.6640	33.8520	C	0	33.9650	41.2810	43.6040	N	0	49.0750	52.5060	44.2550	C	0
26.2900	41.6270	33.3200	O	0	34.2350	40.3800	44.6310	C	0	49.4620	53.7000	44.0100	O	0
26.5000	43.8460	33.7380	N	0	34.6720	39.4170	44.3680	H	0	49.8700	51.4750	43.9000	N	0
26.0090	44.6810	34.0240	H	0	33.3410	40.0550	45.1630	H	0	49.4810	50.5450	43.8310	H	0
27.8820	43.7300	33.0620	C	0	35.1540	41.1250	45.7040	C	0	51.2010	51.5440	43.2860	C	0
27.8560	43.1340	32.1500	H	0	36.1830	41.0310	45.3570	H	0	51.8400	52.1350	43.9410	H	0
28.2220	44.6540	32.5960	H	0	34.9890	40.7260	46.7050	H	0	51.7720	50.1570	43.2040	C	0
29.1030	43.2490	33.8750	C	0	34.7870	42.6020	45.3840	C	0	51.4550	49.5500	44.0520	H	0
30.1900	42.8430	33.4200	O	0	35.6750	43.1920	45.6100	H	0	51.3350	49.6890	42.3220	H	0
28.8250	43.2850	35.2040	N	0	33.8870	42.8240	45.9580	H	0	53.2800	50.2060	42.9020	C	0
27.9910	43.6890	35.6050	H	0	34.4840	42.5990	43.8840	C	0	53.4650	50.7310	41.9650	H	0
29.5990	42.5360	36.1980	C	0	33.6960	43.3360	43.7340	H	0	53.6800	50.7350	43.7670	H	0
29.8370	41.5320	35.8450	H	0	35.7580	42.9550	43.0920	C	0	53.7170	48.7370	42.7670	C	0
30.8130	43.3550	36.5630	C	0	36.7020	42.1170	43.0100	O	0	52.9460	47.8630	42.3030	O	0
31.4410	43.5090	35.6860	H	0	35.8980	44.2040	42.6430	N	0	54.8300	48.2930	43.2840	N	0
30.4820	44.2980	36.9980	H	0	35.1100	44.8210	42.7710	H	0	54.9360	47.2950	43.3970	H	0
31.8090	42.8160	37.7010	C	0	37.1280	44.7230	41.9560	C	0	55.4350	48.8500	43.8710	H	0
31.2660	42.3200	38.5060	H	0	37.3980	43.9390	41.2490	H	0	51.0970	52.1010	41.8480	C	0
32.5050	42.0790	37.2990	H	0	36.6790	45.7950	40.9630	C	0	51.9390	52.8600	41.3830	O	0
32.8000	43.8230	38.2970	C	0	35.9140	45.3800	40.3070	H	0	50.0560	51.6370	41.1760	N	0
33.5970	43.3460	38.8690	H	0	36.2830	46.6150	41.5630	H	0	49.3440	51.1980	41.7410	H	0
33.2880	44.3580	37.4820	H	0	37.5430	46.1420	40.3950	H	0	49.7870	51.9610	39.7850	C	0
32.0740	44.7960	39.3350	C	0	38.2630	45.0760	42.9480	C	0	50.7160	52.2290	39.2820	H	0
32.7190	45.6370	39.5910	H	0	38.1110	45.3340	44.1300	O	0	49.1980	50.7500	39.0640	C	0
31.1670	45.1820	38.8700	H	0	39.4770	45.1020	42.3730	N	0	48.9530	51.0720	38.0520	H	0
31.7570	44.0160	40.5560	N	0	39.5200	44.9530	41.3750	H	0	50.1460	49.5030	39.0380	C	0
31.0390	43.3060	40.5340	H	0	40.6620	45.4980	43.0030	C	0	49.9370	48.7770	39.8240	H	0
32.6360	43.7050	40.9450	H	0	40.5330	45.5590	44.0830	H	0	50.3460	49.0330	38.0750	H	0
31.4270	44.5190	41.3670	H	0	41.7130	44.3820	42.9020	C	0	51.1580	49.8030	39.3130	H	0

48.0100	50.4460	39.7060	O	0	36.1400	45.8680	36.9700	C	0	26.9480	36.1300	31.0040	C	0
47.7190	49.6520	39.2510	H	0	35.9110	45.8770	38.0360	H	0	27.8550	36.0290	30.4080	H	0
48.7470	53.2050	39.6670	C	0	35.7970	46.8020	36.5250	H	0	26.9310	37.1430	31.4060	H	0
48.8670	54.1140	38.8320	O	0	35.5660	45.0740	36.4920	H	0	26.8850	35.4160	31.8250	H	0
47.8570	53.2550	40.6760	N	0	38.2420	46.9650	37.3100	C	0	24.6030	40.3490	27.4170	C	0
47.9390	52.5330	41.3780	H	0	39.2520	47.1100	36.9270	H	0	24.6310	41.3620	28.1140	O	0
46.7420	54.1980	40.6540	C	0	37.8330	47.8660	36.8520	H	0	23.6950	40.1790	26.5130	N	0
46.3740	54.3860	41.6630	H	0	38.1270	47.1430	38.3790	H	0	23.5370	39.2350	26.1920	H	0
47.0200	55.1810	40.2760	H	0	37.6050	43.0670	36.6240	C	0	22.6360	41.0540	26.0430	C	0
45.4860	53.6090	39.8940	C	0	38.0470	42.7890	35.5440	O	0	22.6370	41.9290	26.6920	H	0
44.6120	54.3720	39.6310	O	0	36.9290	42.1320	37.3250	N	0	23.0420	41.4600	24.6110	C	0
45.4720	52.3350	39.4410	N	0	36.3570	42.3440	38.6440	C	0	23.2220	40.5660	24.0130	H	0
46.2850	51.7870	39.6840	H	0	35.8400	43.2620	38.9220	H	0	22.2580	42.0390	24.1230	H	0
44.5550	51.7060	38.5090	C	0	37.1960	42.1950	39.3240	H	0	24.5650	42.3980	24.4840	S	0
43.8880	52.4760	38.1200	H	0	35.4190	41.1080	38.8700	C	0	21.2830	40.3070	26.0560	C	0
45.3240	51.2320	37.3090	C	0	34.3790	41.4140	38.7560	H	0	21.2180	39.1470	26.4350	O	0
45.8780	50.3670	37.6740	H	0	35.5960	40.6580	39.8460	H	0	20.2130	40.9850	25.6610	N	0
44.6300	50.8660	36.5530	H	0	35.6060	40.0940	37.7300	C	0	20.3090	41.9690	25.4570	H	0
46.4030	52.2300	36.6900	C	0	34.6440	39.6330	37.5070	H	0	18.8940	40.4010	25.8210	C	0
47.1630	52.4450	37.4420	H	0	36.4100	39.3930	37.9560	H	0	19.0460	39.3880	25.4470	H	0
47.0640	51.7200	35.4090	C	0	36.1480	41.0150	36.6510	C	0	18.4310	40.4170	27.3110	C	0
46.9960	50.6340	35.3470	H	0	36.8510	40.4030	36.0860	H	0	17.5300	39.8140	27.4240	H	0
46.5480	52.1710	34.5610	H	0	34.9850	41.5980	35.8160	C	0	19.1450	39.8120	27.8710	H	0
48.1190	51.9910	35.4360	H	0	34.4310	42.6810	36.1510	O	0	18.2720	41.7590	27.9820	C	0
45.8120	53.5730	36.2950	C	0	34.6150	40.9490	34.6560	N	0	19.1530	42.3930	27.8680	H	0
46.5900	54.1570	35.8030	H	0	35.0320	40.0620	34.4110	H	0	17.5940	42.3640	27.3800	H	0
45.0000	53.4540	35.5780	H	0	33.3560	41.3230	33.8780	C	0	17.5030	41.8720	29.5600	S	0
45.6220	54.2160	37.1550	H	0	32.6640	41.7570	34.5990	H	0	17.4900	43.5980	30.0220	C	0
43.7200	50.5700	39.0810	C	0	33.6970	42.2920	32.7640	C	0	16.8850	43.8270	30.8990	H	0
44.1450	49.9700	40.0810	O	0	32.7800	42.7250	32.3650	H	0	18.5100	43.8890	30.2710	H	0
42.6510	50.2090	38.4110	N	0	34.5220	43.5510	33.1700	C	0	17.1860	44.2650	29.2160	H	0
42.4500	50.7510	37.5830	H	0	33.9650	44.1200	33.9150	H	0	17.8170	41.0730	24.9860	C	0
41.7250	49.1600	38.8670	C	0	35.5130	43.2070	33.4660	H	0	17.8760	42.3130	24.6680	O	0
42.0790	48.9360	39.8740	H	0	34.6740	44.2260	32.3280	H	0	16.8240	40.2370	24.6340	N	0
40.2330	49.6380	38.8390	C	0	34.3650	41.6900	31.6830	O	0	16.9260	39.2770	24.9280	H	0
39.9300	49.7240	37.7950	H	0	35.1800	41.3310	32.0430	H	0	15.3880	40.6720	24.2560	C	0
39.5520	48.8910	39.2470	H	0	32.6400	40.1160	33.2570	C	0	15.6070	41.6670	23.8690	H	0
39.9270	50.9520	39.6810	C	0	33.1540	39.0530	32.9280	O	0	14.7080	39.8050	23.1770	C	0
40.4840	52.1570	39.3090	C	0	31.3380	40.3050	32.9550	N	0	14.7050	38.7600	23.4860	H	0
41.1230	52.3730	38.4650	H	0	30.9660	41.2450	32.9570	H	0	13.7080	40.1150	22.8730	H	0
40.3430	53.2570	40.2830	C	0	30.4620	39.4320	32.2280	C	0	15.4640	39.9520	21.7750	C	0
40.6960	54.2500	40.0510	H	0	30.9340	38.4950	31.9350	H	0	16.5390	40.4750	21.6840	O	0
39.6910	53.0680	41.4700	C	0	29.2430	39.0680	33.1200	C	0	14.9030	39.4920	20.6810	N	0
39.5160	53.9050	42.1290	H	0	28.6230	39.9280	33.3720	H	0	15.3720	39.7040	19.8120	H	0
39.1630	51.8090	41.7500	C	0	28.6790	38.3340	32.5440	H	0	13.9710	39.1040	20.6410	H	0
38.5540	51.7110	42.6360	H	0	29.7780	38.4990	34.4110	C	0	14.4850	40.8320	25.5080	C	0
39.3070	50.7890	40.8650	C	0	30.6800	37.6360	34.5600	O	0	14.7160	40.0770	26.4510	O	0
39.0490	49.7780	41.1430	H	0	29.1410	38.7030	35.4950	N	0	13.4890	41.7310	25.4330	N	0
41.9520	47.7930	38.1630	C	0	29.4610	38.3240	36.3750	H	0	13.3100	42.2350	24.5760	H	0
42.4040	47.7740	37.0410	O	0	28.2500	39.1630	35.3660	H	0	12.4520	41.9010	26.4180	C	0
41.5680	46.7180	38.8300	N	0	30.1310	40.0830	30.8850	C	0	12.3900	40.9740	26.9890	H	0
41.0890	46.8370	39.7110	H	0	30.3460	41.3020	30.7280	O	0	12.9800	43.1450	27.1640	C	0
41.7380	45.3370	38.3640	C	0	29.6330	39.3920	29.8570	N	0	13.8840	42.7110	27.5920	H	0
41.9280	45.3070	37.2910	H	0	29.7880	38.3950	29.8960	H	0	13.2110	43.9630	26.4820	H	0
42.8630	44.6750	39.1410	C	0	29.3770	39.8970	28.4850	C	0	12.1100	43.6030	28.3030	C	0
42.5140	44.5640	40.1680	H	0	29.3610	40.9840	28.5600	H	0	10.9560	44.3050	28.0400	C	0
43.0470	43.6730	38.7530	H	0	30.6300	39.6620	27.6880	C	0	10.5690	44.3240	27.0320	H	0
44.1960	45.3860	38.9060	C	0	31.4430	40.0660	28.2910	H	0	10.1680	44.7430	29.1410	C	0
44.9410	45.1440	37.7590	C	0	30.8880	38.6030	27.6960	H	0	9.1790	45.1650	29.0350	H	0
44.6100	44.3760	37.0750	H	0	30.5860	40.3440	26.3140	C	0	10.6030	44.6940	30.4500	C	0
46.0880	45.8850	37.4380	C	0	29.8780	41.3320	26.1350	O	0	9.8970	45.1630	31.5260	O	0
46.5480	45.7140	36.4760	H	0	31.2600	39.7820	25.3010	N	0	10.4690	45.5040	32.2180	H	0
46.4400	47.0040	38.2540	C	0	31.1260	40.2140	24.3980	H	0	11.7790	43.9860	30.7020	C	0
47.4760	47.9250	37.9210	O	0	31.7630	38.9140	25.4140	H	0	12.0130	43.8150	31.7420	H	0
47.7570	47.7600	37.0180	H	0	28.0880	39.2780	27.7310	C	0	12.5210	43.4200	29.6350	C	0
45.6780	47.2560	39.3430	C	0	28.2210	38.3260	26.9890	O	0	13.4270	42.8970	29.9050	H	0
45.9130	48.0890	39.9890	H	0	26.9180	39.9290	28.0370	N	0	11.0930	42.0380	25.8120	C	0
44.5920	46.4580	39.7310	C	0	26.9880	40.9000	28.3040	H	0	10.9340	42.5940	24.6750	O	0
44.0010	46.7570	40.5830	H	0	25.6230	39.3440	27.6990	C	0	10.0580	41.6520	26.5310	N	0
40.3100	44.6460	38.5420	C	0	25.6330	38.7480	26.7860	H	0	10.1500	41.0390	27.3280	H	0
39.8300	44.4910	39.6720	O	0	25.2180	38.4140	28.7300	C	0	8.6840	41.9700	26.1540	C	0
39.6170	44.4200	37.4130	N	0	25.6140	38.8310	29.6560	H	0	8.6920	42.7330	25.3750	H	0
40.0730	44.5050	36.5150	H	0	24.1330	38.4170	28.8410	H	0	8.1510	40.7100	25.5750	C	0
38.1400	44.3780	37.3470	C	0	25.7890	36.9760	28.5140	C	0	8.2740	39.8770	26.2680	H	0
37.7380	44.3830	38.3600	H	0	25.2190	36.5190	27.7050	H	0	7.0830	40.8630	25.4180	H	0
37.5980	45.6890	36.7450	C	0	26.8280	36.8920	28.1950	H	0	8.7570	40.2530	24.2860	C	0
37.8290	45.7360	35.6810	H	0	25.4150	35.9150	29.9010	S	0	8.5930	41.0880	23.6040	H	0

9.8370	40.1100	24.2810	H	0	2.4900	43.8340	41.1990	H	0	2.4400	42.0810	37.2230	C	0
7.9640	39.0600	23.6420	C	0	2.8370	44.0120	43.3290	C	0	1.7160	41.6710	36.5340	H	0
6.7460	39.1860	23.3700	O	0	3.8720	43.7470	43.1720	H	0	2.8010	43.4480	37.1210	C	0
8.6100	38.0840	23.2170	O	0	2.1740	44.0990	44.5860	C	0	2.3460	44.2040	36.0950	O	0
7.8930	42.4510	27.3560	C	0	2.8320	43.8610	45.7190	O	0	1.5150	43.8310	35.7940	H	0
7.7810	41.7190	28.3200	O	0	3.7250	43.6010	45.4800	H	0	3.5740	44.0220	38.1570	C	0
7.4790	43.6930	27.3680	N	0	0.7810	44.1970	44.5620	C	0	3.7600	45.0850	38.1060	H	0
7.7300	44.2850	26.5890	H	0	0.2850	44.1580	45.5200	H	0	4.0390	43.1980	39.1390	C	0
6.6460	44.2970	28.4820	C	0	0.0230	44.4690	43.4040	C	0	4.6310	43.6650	39.9120	H	0
7.0390	44.0250	29.4610	H	0	-1.0550	44.5160	43.4560	H	0	6.5620	40.8510	39.0040	C	0
6.5410	45.3770	28.3780	H	0	-0.5510	41.9460	40.9300	C	0	7.1330	41.8390	39.5200	O	0
5.2170	43.7800	28.3050	C	0	-1.7490	41.6030	40.9490	O	0	6.8780	40.4720	37.7270	N	0
4.6550	43.8920	27.2230	O	0	0.3420	41.3600	41.7230	N	0	6.3190	39.7360	37.3200	H	0
4.5980	43.3800	29.4130	N	0	1.2330	41.8020	41.8980	H	0	7.7750	41.2010	36.7500	C	0
5.1730	43.3410	30.2430	H	0	0.1210	40.2350	42.6420	C	0	8.2010	41.9930	37.3660	H	0
3.3710	42.6070	29.4080	C	0	-0.7920	40.3770	43.2200	H	0	8.9700	40.3170	36.3610	C	0
2.8660	42.7060	28.4470	H	0	0.0490	38.8940	41.9420	C	0	9.6650	40.8550	35.7150	H	0
3.6630	41.0620	29.7770	C	0	-0.5480	38.9940	41.0350	H	0	9.7870	40.0680	37.6330	C	0
4.3060	41.0960	30.6570	H	0	1.3490	38.2980	41.4420	C	0	9.9880	41.0610	38.0350	H	0
2.2960	40.3400	30.0200	C	0	1.8710	38.9140	40.7100	H	0	9.2900	39.4800	38.4050	H	0
2.5310	39.2770	30.0620	H	0	1.9820	38.1310	42.3140	H	0	10.7370	39.5520	37.4960	H	0
1.7780	40.5980	30.9440	H	0	1.0800	37.3630	40.9500	H	0	8.5750	39.0520	35.6180	C	0
1.6150	40.4120	29.1720	H	0	-0.4570	37.8950	42.8520	O	0	8.4010	38.2730	36.3610	H	0
4.3730	40.4320	28.5310	C	0	-1.2670	38.2030	43.2650	H	0	7.6640	39.1080	35.0220	H	0
4.5780	39.3680	28.6550	H	0	1.2530	40.1390	43.6640	C	0	9.4010	38.7150	34.9920	H	0
3.6830	40.4940	27.6890	H	0	2.3760	40.6050	43.3590	O	0	7.0500	41.8760	35.5230	C	0
5.3040	40.9150	28.2320	H	0	0.9800	39.5960	44.8240	N	0	7.6330	42.8280	34.9150	O	0
2.2950	43.2890	30.3540	C	0	0.0400	39.2660	44.9900	H	0	5.8120	41.5230	35.2080	N	0
2.6170	43.7260	31.4810	O	0	1.9160	39.6080	46.0000	C	0	5.4410	40.8060	35.8140	H	0
1.0620	43.3740	29.8460	N	0	2.7750	40.2620	45.8510	H	0	5.0340	42.1670	34.1250	C	0
0.8490	42.9510	28.9540	H	0	1.0920	40.2920	47.1790	C	0	4.1920	41.5090	33.9110	H	0
-0.0640	44.0340	30.3990	C	0	0.8840	41.3340	46.9390	H	0	4.7560	43.1010	34.6120	H	0
0.3080	44.9310	30.8930	H	0	0.1310	39.7790	47.2040	H	0	5.7860	42.2620	32.7580	C	0
-1.0580	44.4930	29.3590	C	0	1.6470	40.4240	48.1080	H	0	5.6740	43.2240	31.9890	O	0
-1.5120	43.7220	28.7360	H	0	2.5590	38.2520	46.1770	C	0	6.7230	41.3220	32.4270	N	0
-1.8390	45.1260	29.7820	H	0	2.1200	37.2590	45.6130	O	0	6.8690	40.6530	33.1700	H	0
-0.2560	45.3850	28.3360	C	0	3.6330	38.1320	46.9920	N	0	7.5330	41.1940	31.2130	C	0
0.5990	45.8190	28.8550	H	0	3.9910	38.9680	47.4300	H	0	6.9120	41.6590	30.4470	H	0
0.0970	44.8970	27.4280	H	0	4.3380	36.9860	47.4700	C	0	8.7610	42.0160	31.3660	C	0
-1.1520	46.5400	27.8850	C	0	5.0720	37.4340	48.1390	H	0	9.3280	41.9090	30.4410	H	0
-2.1580	46.2770	27.1480	O	0	3.6020	36.3920	48.0120	H	0	8.3780	43.0190	31.5560	H	0
-0.9270	47.7130	28.2160	O	0	5.0900	36.0090	46.4810	C	0	9.2140	41.6460	32.2860	H	0
-0.6560	43.2470	31.6920	C	0	5.8400	35.0310	46.8350	O	0	7.8150	39.7280	30.8560	C	0
-1.8440	43.4360	32.0580	O	0	4.8930	36.2950	45.1920	N	0	7.5680	38.8990	31.7250	O	0
0.1880	42.4180	32.3610	N	0	4.1410	36.9540	45.0480	H	0	8.4390	39.4030	29.7180	N	0
1.1460	42.5770	32.0850	H	0	5.5920	35.7530	43.9860	C	0	8.3790	40.0550	28.9490	H	0
-0.2330	41.6730	33.5150	C	0	6.4320	35.1390	44.3130	H	0	9.2930	38.2040	29.5440	C	0
-1.1600	41.1840	33.2170	H	0	4.5680	34.9280	43.3390	C	0	9.3250	37.5340	30.4030	H	0
0.7270	40.4750	33.8000	C	0	5.0130	34.3760	42.5110	H	0	8.6620	37.3520	28.4190	C	0
1.0180	39.9450	32.8930	H	0	4.2850	34.0910	43.9770	H	0	7.6070	37.1580	28.6100	H	0
1.6900	40.8660	34.1280	H	0	3.7070	35.5600	43.1220	H	0	8.8400	37.8390	27.4600	H	0
0.2190	39.8320	34.5190	H	0	6.1400	36.8990	43.1710	C	0	9.3880	35.9640	28.2830	C	0
-0.5870	42.4950	34.7470	C	0	5.5260	37.9870	43.1380	O	0	9.3530	35.0350	29.0630	O	0
0.1570	43.3970	35.0940	O	0	7.2770	36.7330	42.4130	N	0	10.0230	35.7160	27.1320	N	0
-1.7210	42.2720	35.4510	N	0	8.0430	35.5010	42.1060	C	0	10.2700	34.7390	27.0590	H	0
-2.3800	41.5810	35.1210	H	0	7.3590	34.7510	41.7090	H	0	10.2130	36.4550	26.4690	H	0
-2.1010	42.8510	36.7740	C	0	8.6070	35.2260	42.9970	H	0	10.7260	38.5910	29.0400	C	0
-2.0310	43.9270	36.6150	H	0	9.0360	35.8810	41.0240	C	0	10.9090	39.7080	28.5270	O	0
-3.4910	42.4040	37.2520	C	0	8.7000	35.6580	40.0110	H	0	11.8230	37.8870	29.2730	N	0
-3.6640	42.7440	38.2730	H	0	9.9950	35.3880	41.1880	H	0	11.7850	37.1170	29.9260	H	0
-4.6280	43.0410	36.4060	C	0	9.2370	37.3810	41.1910	C	0	13.1610	38.2350	28.8190	C	0
-4.3920	42.9980	35.3430	H	0	9.4800	37.8300	40.2280	H	0	13.1020	39.0120	28.0560	H	0
-5.5370	42.4580	36.5530	H	0	9.9940	37.5150	41.9640	H	0	13.9790	38.6930	30.0480	C	0
-4.6610	44.0850	36.7170	H	0	7.8630	37.8270	41.6970	C	0	13.8790	38.0110	30.8920	H	0
-3.5920	40.9770	37.2950	O	0	8.0310	38.6580	42.3810	H	0	15.4710	38.9530	29.7220	C	0
-3.1510	40.7610	38.1190	H	0	6.9630	38.3110	40.5400	C	0	15.9370	37.9830	29.5470	H	0
-1.1240	42.4010	37.8430	C	0	6.9710	37.7090	39.4420	O	0	15.5750	39.5380	28.8080	H	0
-0.5960	41.3320	37.6650	O	0	6.1730	39.3170	40.7440	N	0	15.9800	39.2810	30.6280	H	0
-0.8900	43.3570	38.7740	N	0	6.2060	39.6940	41.6810	H	0	13.6250	39.9710	30.7130	C	0
-1.5370	44.1290	38.6950	H	0	5.4540	40.0120	39.6770	C	0	14.1690	40.7720	30.2140	H	0
-0.1110	43.1680	40.0430	C	0	5.0530	39.2260	39.0370	H	0	12.5670	40.2340	30.6800	H	0
0.8970	43.0290	39.6510	H	0	4.3470	40.9590	40.2490	C	0	14.0390	39.9790	31.7210	H	0
-0.0730	44.4790	40.8310	C	0	3.5240	40.2730	40.4490	H	0	13.8660	36.9410	28.2050	C	0
0.2790	45.2800	40.1810	H	0	4.6950	41.5800	41.0750	H	0	13.6400	35.8040	28.5270	O	0
-1.0730	44.7870	41.1340	H	0	3.7690	41.8480	39.1780	C	0	14.7590	37.2230	27.2480	N	0
0.6710	44.4100	42.1430	C	0	2.8730	41.2700	38.3050	C	0	14.8650	38.2090	27.0600	H	0
2.0810	44.1000	42.1630	C	0	2.4920	40.2620	38.3800	H	0	15.6290	36.1550	26.7550	C	0

15.6510	35.3390	27.4770	H	0	29.2040	43.2360	21.2190	H	0	32.5300	31.1220	20.9360	O	0
15.1310	35.6660	25.4050	C	0	28.6600	42.2240	19.9610	H	0	31.7020	34.2480	23.0610	C	0
14.2100	35.1810	25.7290	H	0	28.6000	44.3400	19.5000	C	0	31.1730	33.4630	23.9220	O	0
14.8170	36.5580	24.8630	H	0	29.6110	44.3880	18.5590	N	0	32.7110	35.0190	23.4180	N	0
16.0870	34.6700	24.6510	C	0	29.3980	45.4600	17.7620	C	0	33.0430	35.6520	22.7040	H	0
16.9790	35.2130	24.3380	H	0	30.0220	45.8070	16.9520	H	0	33.3210	35.1560	24.7760	C	0
16.5790	33.4450	25.4860	C	0	28.2970	46.1270	18.1740	N	0	33.6850	34.1580	25.0230	H	0
17.2930	32.9100	24.8590	H	0	27.8770	46.9460	17.7580	H	0	34.6540	35.9780	24.6980	C	0
17.1870	33.8010	26.3180	H	0	27.6960	45.3470	19.2360	C	0	34.3610	36.9560	24.3150	H	0
15.7500	32.8090	25.7960	H	0	26.7480	45.5700	19.7020	H	0	35.0370	36.0460	25.7160	H	0
15.3580	34.1380	23.4570	C	0	25.8940	42.8290	20.3530	C	0	35.7980	35.4910	23.8660	C	0
15.9430	33.3150	23.0470	H	0	25.9960	42.7050	19.0850	O	0	36.4580	36.4520	22.9890	C	0
14.4190	33.7060	23.8030	H	0	24.7230	42.7780	20.9170	N	0	36.1840	37.4910	22.8760	H	0
15.2400	34.8810	22.6680	H	0	24.7980	43.0040	21.8990	H	0	37.6240	36.0620	22.3380	C	0
17.0720	36.6480	26.6390	C	0	23.4630	42.2310	20.3020	C	0	38.2410	36.7240	21.7470	H	0
17.2300	37.5570	25.7840	O	0	22.7480	42.0240	21.0990	H	0	38.0600	34.6830	22.4200	C	0
18.0780	36.2210	27.4080	N	0	22.7660	43.2110	19.2840	C	0	39.3160	34.2280	22.0240	O	0
17.7680	35.5880	28.1310	H	0	23.3280	43.1710	18.3510	H	0	39.5030	34.5280	21.1320	H	0
19.5600	36.4910	27.3390	C	0	21.7890	42.8330	18.9820	H	0	37.3520	33.7470	23.1770	C	0
19.5940	37.5630	27.1460	H	0	22.5520	44.7050	19.7230	C	0	37.7990	32.8190	23.5010	H	0
20.2660	36.2610	28.6260	C	0	21.7240	45.0510	19.1030	H	0	36.2250	34.1720	23.9020	C	0
21.2700	36.6600	28.4830	H	0	22.2610	44.6900	20.7740	H	0	35.7300	33.4380	24.5210	H	0
19.7210	36.8430	29.3690	H	0	23.8560	45.5880	19.4490	C	0	32.4290	35.7410	25.9340	C	0
20.4330	34.8140	29.0870	C	0	24.1630	45.8300	18.2580	O	0	32.0800	36.9210	25.8380	O	0
19.4900	34.2880	29.2330	H	0	24.3940	46.1130	20.4510	O	0	31.9850	34.9110	26.9020	N	0
20.8690	34.2880	28.2380	H	0	23.4840	40.7480	19.8420	C	0	32.1650	33.9200	26.8210	H	0
21.5690	34.5680	30.5020	S	0	22.5350	40.2800	19.1880	O	0	30.9030	35.3210	27.7780	C	0
20.3120	34.9240	31.7340	C	0	24.5010	40.0110	20.2420	N	0	30.1540	35.9070	27.2450	H	0
19.4040	34.3450	31.5660	H	0	25.1080	40.5170	20.8720	H	0	29.9740	34.1620	28.2170	C	0
20.7030	34.8040	32.7440	H	0	24.7090	38.5730	20.0140	C	0	30.6460	33.3970	28.6050	H	0
20.0580	35.9820	31.7970	H	0	24.7780	38.1580	21.0200	H	0	29.3850	34.5000	29.0700	H	0
20.2990	35.6810	26.2490	C	0	23.7740	38.2300	19.5690	H	0	29.0550	33.5600	27.1580	C	0
19.7970	34.5370	25.9740	O	0	25.8570	38.2290	19.0680	C	0	27.8840	34.2840	26.7460	C	0
21.3460	36.1950	25.7100	N	0	26.0240	37.0470	18.8420	O	0	27.6370	35.2210	27.2240	H	0
21.5480	37.1530	25.9590	H	0	26.6600	39.1990	18.5660	N	0	26.9740	33.6920	25.8210	C	0
22.2580	35.7590	24.7420	C	0	26.4770	40.1790	18.7230	H	0	26.0210	34.1460	25.5950	H	0
22.3190	34.6780	24.8640	H	0	27.7720	39.0110	17.5610	C	0	27.3330	32.5750	25.1130	C	0
21.7030	35.9030	23.3120	C	0	27.3080	38.3400	16.8390	H	0	26.5080	32.1560	24.1700	O	0
22.5800	35.7860	22.6750	H	0	28.0390	40.3740	16.9330	C	0	27.0790	31.6350	23.6000	H	0
21.2220	34.9670	23.0290	H	0	28.0210	41.1540	17.6940	H	0	28.5600	31.8810	25.4420	C	0
20.9760	37.1380	22.8450	C	0	28.9880	40.3540	16.3980	H	0	28.8110	30.9970	24.8750	H	0
19.5770	37.3170	22.9510	C	0	26.9040	40.7280	15.9820	C	0	29.3640	32.3970	26.4790	C	0
18.8820	36.5290	23.2020	H	0	27.0070	39.9660	15.2090	H	0	30.3300	31.9380	26.6290	H	0
19.0310	38.5120	22.6290	C	0	25.8750	40.6530	16.3310	H	0	31.3180	36.1870	28.9590	C	0
17.9540	38.4800	22.5560	H	0	27.1300	42.0740	15.2810	C	0	30.5560	36.6470	29.7760	O	0
19.8070	39.6290	22.3460	C	0	28.1490	42.2000	14.9140	H	0	32.6520	36.4760	29.0240	N	0
19.2070	40.8420	22.1110	O	0	26.3890	42.2080	14.4930	H	0	33.2490	35.9090	28.4410	H	0
18.2860	40.6700	21.9010	H	0	27.1160	43.2770	16.2590	C	0	33.1840	37.4670	29.9440	C	0
21.1770	39.5300	22.3390	C	0	27.5090	43.0320	17.2450	H	0	32.5930	38.3730	30.0730	H	0
21.8110	40.4040	22.3110	H	0	27.7560	44.0510	15.8360	H	0	33.2000	36.9890	30.9240	H	0
21.7810	38.2500	22.5810	C	0	25.7270	43.8390	16.4180	N	0	34.6170	37.9680	29.6240	C	0
22.8560	38.1540	22.5480	H	0	25.1150	43.2390	16.9510	H	0	35.1480	37.6090	28.5530	O	0
23.5510	36.5320	24.9560	C	0	25.8800	44.5610	17.1070	H	0	35.1930	38.7410	30.5640	N	0
23.7040	37.4550	25.8010	O	0	25.3760	44.2570	15.5680	H	0	34.5780	39.0350	31.3100	H	0
24.6030	36.1790	24.1940	N	0	28.9770	38.4380	18.1820	C	0	36.6190	39.1700	30.5760	C	0
24.5230	35.4050	23.5500	H	0	29.7390	37.8610	17.4520	O	0	37.1470	38.2810	30.2310	H	0
25.9720	36.7610	24.2450	C	0	29.1540	38.5030	19.4840	N	0	36.8420	40.3940	29.6190	C	0
26.3960	36.6610	25.2440	H	0	28.5020	39.0540	20.0240	H	0	36.6560	39.9260	28.6520	H	0
26.7810	35.9980	23.2330	C	0	30.1940	37.8620	20.2780	C	0	36.0920	41.1840	29.6630	H	0
27.8110	36.1690	23.5470	H	0	31.0790	38.0220	19.6620	H	0	37.8710	40.7300	29.7430	H	0
26.4540	34.9830	23.4570	H	0	30.4030	38.6070	21.5800	C	0	37.0770	39.6020	31.9830	C	0
26.5770	36.2960	21.8700	O	0	29.4020	38.6440	22.0100	H	0	36.2090	40.0640	32.7360	O	0
27.4120	36.6720	21.5820	H	0	31.0370	38.1620	22.3470	H	0	38.3340	39.5230	32.2000	N	0
26.0340	38.2660	23.8230	C	0	30.8090	40.1040	21.4500	C	0	38.7710	39.4020	31.2970	H	0
25.1000	39.0210	23.5400	O	0	30.8960	40.7300	20.3640	O	0	39.0050	40.2430	33.3170	C	0
27.2170	38.8860	23.9160	N	0	31.0990	40.6620	22.5170	O	0	38.3380	40.7770	33.9940	H	0
27.9590	38.3410	24.3310	H	0	29.9950	36.3900	20.5980	C	0	39.7930	39.2270	34.2390	C	0
27.4790	40.3380	23.7760	C	0	28.8910	35.8330	20.4640	O	0	38.9890	38.6490	34.6940	H	0
26.7460	40.9200	24.3350	H	0	31.0110	35.7620	21.1080	N	0	40.1260	38.3810	33.6370	H	0
28.4630	40.6310	24.1430	H	0	31.8980	36.2420	21.0690	H	0	40.9340	39.7860	35.1770	C	0
27.2470	40.9370	22.3530	C	0	31.0350	34.3490	21.6510	C	0	42.2770	39.4110	34.9710	C	0
27.2180	40.2320	21.3530	O	0	30.0390	33.9600	21.8620	H	0	42.5340	38.8150	34.1070	H	0
27.2150	42.3010	22.3430	N	0	31.7610	33.4030	20.6520	C	0	43.3260	39.7750	35.8550	C	0
27.3140	42.7170	23.2580	H	0	31.4120	33.5590	19.6320	H	0	44.3370	39.4160	35.7270	H	0
27.0810	43.1560	21.1790	C	0	32.8260	33.6340	20.6570	H	0	43.0100	40.7000	36.8640	C	0
27.0030	44.1930	21.5040	H	0	31.5440	31.9080	20.9990	C	0	43.8320	41.0380	37.4770	H	0
28.4620	43.1920	20.4220	C	0	30.4540	31.4830	21.4830	O	0	41.6560	41.0780	37.1230	C	0

41.4050	41.7820	37.9030	H	0	37.4060	56.5680	36.5830	O	0	41.1910	48.6890	28.5450	H	0
40.6720	40.6770	36.2380	C	0	39.6550	56.5750	37.0660	N	0	39.1670	48.6410	29.2070	C	0
39.6320	40.9330	36.3760	H	0	40.5000	56.0420	37.2110	H	0	39.3700	48.1370	30.1510	H	0
39.8380	41.3740	32.6830	C	0	39.8030	58.0100	37.2970	C	0	38.4150	49.4110	29.3790	H	0
40.5500	41.1720	31.7330	O	0	38.9680	58.3370	37.9180	H	0	38.6760	47.5620	28.1860	C	0
39.7930	42.6330	33.2350	N	0	41.1710	58.2510	38.0000	C	0	38.7400	47.9730	27.1780	H	0
39.0590	42.7890	33.9110	H	0	41.2100	57.5900	38.8660	H	0	39.3200	46.7000	28.3550	H	0
40.4890	43.7920	32.6470	C	0	42.0220	57.9100	37.4110	H	0	37.3760	47.1190	28.5820	N	0
41.2270	43.5420	31.8850	H	0	41.4450	59.6610	38.4200	C	0	36.8980	47.7510	29.2080	H	0
39.5130	44.7600	31.8990	C	0	41.6250	60.2560	37.5250	H	0	36.7730	46.0640	28.1770	C	0
40.1440	45.3930	31.2760	H	0	40.3020	60.3320	39.1960	C	0	37.3010	45.4150	27.1930	N	0
38.6150	44.0580	30.8760	C	0	39.4200	60.3630	38.5570	H	0	38.1500	45.6850	26.7180	H	0
38.1370	44.6560	30.1000	H	0	40.1260	59.6440	40.0230	H	0	37.0110	44.5390	26.7830	H	0
39.2060	43.3130	30.3420	H	0	40.6570	61.3140	39.5100	H	0	35.6630	45.7120	28.6800	N	0
37.8700	43.4030	31.3280	H	0	42.6400	59.7040	39.2990	C	0	35.3770	46.1360	29.5520	H	0
38.6930	45.6020	32.8590	C	0	43.5090	59.2430	38.8300	H	0	35.1660	45.0040	28.1590	H	0
38.2660	45.0100	33.6680	H	0	42.9280	60.6950	39.6480	H	0	42.3490	50.5540	29.7050	C	0
39.4050	46.2130	33.4130	H	0	42.4500	59.2300	40.2620	H	0	42.8430	51.4270	29.0020	O	0
37.4410	46.2890	32.3530	C	0	39.5400	58.8820	36.0420	C	0	43.1260	49.6270	30.2750	N	0
37.1430	47.0920	30.0260	H	0	38.8240	59.9060	36.0600	O	0	42.6340	48.9690	30.8630	H	0
37.7420	46.8790	31.4870	H	0	39.9160	58.3530	34.8030	N	0	44.5590	49.3980	30.2220	C	0
36.6020	45.6110	32.1950	H	0	40.4650	57.5100	34.7080	H	0	45.0070	50.2570	29.7230	H	0
41.3860	44.4950	33.7090	C	0	39.3810	58.9810	33.5330	C	0	45.2230	49.4500	31.6440	C	0
41.0700	44.3480	34.9760	O	0	38.8850	59.9260	33.7550	H	0	44.6490	48.7360	32.2340	H	0
42.2270	45.4250	33.2460	N	0	40.4720	59.3320	32.5800	C	0	46.7170	48.9490	31.6820	C	0
42.3730	45.4180	32.2470	H	0	40.7540	58.4140	32.0640	H	0	47.1410	49.2840	32.6290	H	0
42.7140	46.5530	33.9920	C	0	39.9550	59.9260	31.8270	H	0	46.7760	47.8640	31.7710	H	0
42.3670	46.4680	35.0220	H	0	41.6540	60.0550	33.1600	C	0	47.3780	49.2900	30.8860	H	0
44.2310	46.5140	34.0260	C	0	41.4330	60.5310	34.1150	H	0	45.2100	50.8280	32.2630	C	0
44.4330	45.5570	34.5070	H	0	42.3530	59.2280	33.2880	H	0	45.6400	50.6670	33.2510	H	0
44.5760	46.6270	32.9980	H	0	42.4480	61.1010	32.3570	C	0	45.6880	51.5860	31.6410	H	0
44.8650	47.8600	35.0700	S	0	41.8930	62.0340	32.2600	H	0	44.1710	51.1070	32.4420	H	0
44.6720	47.5240	36.3490	H	0	43.3500	61.1980	32.9620	H	0	44.9070	48.1220	29.3890	C	0
42.0830	47.8880	33.4530	C	0	42.8200	60.5370	30.9290	C	0	45.7760	48.1180	28.4980	O	0
41.8070	48.0030	32.2220	O	0	43.4660	59.6590	30.9290	H	0	44.3470	46.8960	29.7450	N	0
41.7960	48.9070	34.3430	N	0	41.8450	60.4270	30.4540	H	0	43.8140	46.7740	30.5940	H	0
42.0540	48.8680	35.3190	H	0	43.6490	61.5320	30.3110	N	0	44.4620	45.6960	28.9500	C	0
41.0480	50.0410	33.9390	C	0	44.5120	61.7690	30.7790	H	0	44.2790	45.8650	27.8890	H	0
41.2460	50.3850	32.9240	H	0	43.9640	61.2150	29.4060	H	0	45.8210	45.0160	29.1540	C	0
39.5420	49.5570	34.0240	C	0	43.2310	62.4490	30.2410	H	0	45.8720	44.0550	28.6400	H	0
39.5520	48.6620	33.4020	H	0	38.3490	58.0780	32.9510	C	0	46.6050	45.6800	28.7900	H	0
39.3650	49.1830	35.0320	H	0	37.6760	58.5100	32.0310	O	0	46.2200	44.7060	30.6080	C	0
38.5030	50.6430	33.6730	C	0	38.2000	56.7950	33.3800	N	0	47.2300	45.3800	31.1700	C	0
37.9480	50.6620	32.4360	C	0	38.6670	56.5080	34.2280	H	0	47.8960	46.1270	30.7650	H	0
38.2600	49.9370	31.7000	H	0	37.2660	55.7620	32.8610	C	0	47.2880	45.0260	32.4760	N	0
36.7630	51.4100	32.1550	C	0	37.2180	54.9970	33.6370	H	0	47.9430	45.4300	33.1300	H	0
36.2520	51.4710	31.2060	H	0	36.2350	56.1050	32.7740	H	0	46.4370	44.0170	32.8170	C	0
36.2590	52.2070	33.2280	C	0	37.6080	55.0950	31.5380	C	0	46.1660	43.3480	34.0350	C	0
35.2790	53.0210	32.8630	O	0	36.7030	54.8230	30.7640	O	0	46.6750	43.6100	34.9510	H	0
35.0730	53.7330	33.4730	H	0	38.8560	54.6150	31.3710	N	0	45.0700	42.4840	34.1160	C	0
36.7660	52.0790	34.5950	C	0	39.4920	54.8930	32.1040	H	0	44.8330	42.0910	35.0940	H	0
36.3720	52.6660	35.4110	H	0	39.5040	54.0000	30.2540	C	0	44.2800	42.2480	33.0110	C	0
37.9490	51.3250	34.7370	C	0	38.7360	53.7360	29.5270	H	0	43.4160	41.6220	33.1760	H	0
38.4160	51.3690	35.7100	H	0	40.6020	55.0170	29.6820	C	0	44.6110	42.8380	31.7930	C	0
41.2400	51.2000	34.8370	C	0	41.3120	55.1710	30.4950	H	0	44.0400	42.7570	30.8800	H	0
41.0240	51.1880	36.0400	O	0	41.0340	54.4500	28.8570	H	0	45.7220	43.7970	31.6400	C	0
41.8530	52.2150	34.2940	N	0	39.9190	56.3150	29.1890	C	0	43.3230	44.7900	29.2820	C	0
41.7410	52.3110	33.2950	H	0	39.1010	56.0670	28.5120	H	0	42.5810	45.1040	30.2040	O	0
41.9210	53.5520	34.8860	C	0	39.4800	56.9160	29.9850	H	0	43.0470	43.7420	28.5800	N	0
42.4690	53.5610	35.8280	H	0	40.8620	57.1340	28.3740	C	0	43.7280	43.4570	27.8910	H	0
42.7750	54.5630	34.0250	C	0	40.3570	58.0770	28.1650	H	0	41.9080	42.7950	28.8060	C	0
43.7650	54.1250	33.8950	H	0	41.7270	57.3270	29.0090	H	0	41.6240	42.8940	29.8540	H	0
42.3760	54.6700	33.0160	H	0	41.1960	56.5450	26.9270	C	0	40.7190	43.4080	28.0500	C	0
42.8980	55.8920	34.7280	C	0	41.3570	55.4740	27.0420	H	0	39.7980	42.8590	28.2470	H	0
42.9430	55.9320	35.9840	O	0	40.3020	56.6640	26.3150	H	0	40.5380	44.4020	28.4600	H	0
43.0440	56.9080	34.0250	O	0	42.3160	57.1960	26.2820	N	0	40.9480	43.4600	26.5030	C	0
40.5580	54.2800	35.1190	C	0	42.3930	56.8270	25.3450	H	0	41.9870	43.7080	26.2860	H	0
40.0610	55.0300	34.2730	O	0	42.2170	58.1740	26.0510	H	0	40.7140	42.5090	26.0240	H	0
39.7810	53.9480	36.1870	N	0	43.1360	57.1560	26.8710	H	0	40.2000	44.6180	25.8690	C	0
40.0750	53.0680	36.5880	H	0	40.1730	52.7000	30.6060	C	0	39.2440	44.3230	25.1570	O	0
38.4850	54.4750	36.5370	C	0	40.9180	52.6130	31.5810	O	0	40.5420	45.8150	26.1110	O	0
37.7110	54.2970	35.7900	H	0	40.1040	51.6420	29.7480	N	0	42.1630	41.3370	28.3910	C	0
37.8280	53.8980	37.8370	C	0	39.5630	51.7880	28.9070	H	0	42.7310	41.0900	27.3250	O	0
37.9380	52.8170	37.7630	H	0	40.8860	50.4110	29.8110	C	0	41.8470	40.3330	29.2230	N	0
38.4630	54.2500	38.6500	H	0	40.6330	49.9490	30.7650	H	0	41.5100	40.5720	30.1450	H	0
36.7760	54.1590	37.9590	H	0	40.4060	49.4170	28.7530	C	0	41.9910	38.9510	28.8990	C	0
38.5080	56.0240	36.6920	C	0	40.2380	49.9580	27.8210	H	0	42.4970	38.7970	27.9460	H	0



42.7040	38.1620	29.9600	C	0	33.0350	26.3000	29.0710	H	0	38.4030	38.8260	42.5860	C	0
42.1560	38.3880	30.8750	H	0	34.1380	27.7830	30.0590	C	0	38.9750	38.1680	43.4940	O	0
42.7540	36.6060	29.8290	C	0	35.0550	27.2370	29.8950	H	0	39.1110	39.5440	41.6310	N	0
41.7900	36.1700	29.5670	H	0	34.0160	28.9520	30.7760	C	0	38.5420	40.1620	40.4430	C	0
43.5880	36.4480	29.1450	H	0	34.8660	29.4000	31.2680	H	0	38.2080	41.1730	40.6790	H	0
42.8910	36.1460	30.8080	H	0	32.6480	33.5260	31.3590	C	0	37.7070	39.5900	40.0420	H	0
44.1540	38.7640	30.0650	C	0	33.6540	34.2180	31.4130	O	0	39.6020	40.1660	39.3590	C	0
44.7210	38.3960	29.2100	H	0	31.5140	33.9100	31.9730	N	0	39.4850	41.0430	38.7220	H	0
44.1500	39.8470	29.9380	H	0	30.2360	33.2290	31.8790	C	0	39.6530	39.2280	38.8070	H	0
44.8280	38.3860	31.3120	C	0	30.2720	32.1400	31.8390	H	0	40.9170	40.2060	40.2120	C	0
44.9720	37.3110	31.4280	H	0	29.6470	33.5590	31.0240	H	0	41.1630	41.2590	40.3510	H	0
45.8080	38.8620	31.2740	H	0	29.5190	33.4930	33.1920	C	0	41.6730	39.7150	39.6000	H	0
44.3360	38.8240	32.1800	H	0	29.8400	32.7530	33.9260	H	0	40.5800	39.4660	41.4930	C	0
40.5060	38.6120	28.7730	C	0	28.4400	33.4830	33.0350	H	0	41.0170	38.4680	41.4760	H	0
39.7290	38.7400	29.7590	O	0	29.9950	34.9100	33.5130	C	0	41.3750	40.0720	42.6590	C	0
40.0740	38.1900	27.5940	N	0	29.9960	35.1160	34.5840	H	0	40.7770	40.8190	43.4390	O	0
40.7210	38.1590	26.8190	H	0	29.3660	35.6280	32.9870	H	0	42.5800	39.6640	42.9480	N	0
38.7200	37.5830	27.4290	C	0	31.4620	35.0430	32.9560	C	0	42.9150	38.9860	42.2790	H	0
37.9590	38.1950	27.9120	H	0	31.5390	36.0410	32.5230	H	0	43.4940	40.4080	43.8510	C	0
38.3040	37.6700	25.9630	C	0	32.5230	34.8590	34.0400	C	0	42.9290	41.2560	44.2380	H	0
39.0470	37.0950	25.4100	H	0	32.7510	33.7520	34.4530	O	0	43.7660	39.4350	44.9730	C	0
37.3550	37.1420	25.8630	H	0	33.1220	35.9490	34.5070	N	0	42.8400	39.1090	45.4470	H	0
38.1940	39.0400	25.3380	C	0	32.6290	36.8120	34.3280	H	0	44.4290	38.1170	44.5730	C	0
39.2650	39.6760	24.7570	N	0	34.0630	35.9440	35.6410	C	0	43.7430	37.5870	43.9120	H	0
38.8880	40.9350	24.5190	C	0	34.5220	34.9580	35.7110	H	0	45.3690	38.3460	44.0720	H	0
39.4380	41.6530	23.9300	H	0	35.1730	36.9830	35.2860	C	0	44.6650	37.5080	45.4460	H	0
37.6110	41.0690	24.8460	N	0	34.8080	38.0100	35.3080	H	0	44.5650	40.0180	46.1240	C	0
37.0610	41.9070	24.7240	H	0	36.3590	36.8010	36.1630	C	0	44.0120	40.8300	46.5960	H	0
37.1660	39.9130	25.3780	C	0	36.1270	36.9940	37.2100	H	0	44.5770	39.1950	46.8380	H	0
36.2060	39.8040	25.8600	H	0	36.7730	35.8080	35.9860	H	0	45.5360	40.3120	45.7250	H	0
38.6550	36.1830	28.0680	C	0	37.2270	37.3960	35.8800	H	0	44.7880	40.8410	43.1110	C	0
39.6280	35.4600	28.2230	O	0	35.7740	36.7970	33.8830	C	0	45.1160	40.3180	42.0680	O	0
37.4390	35.7380	28.3300	N	0	36.6430	37.4190	33.6660	H	0	45.5190	41.8470	43.6550	N	0
36.5980	36.2850	28.2110	H	0	36.0640	35.7710	33.6560	H	0	45.3520	42.0960	44.6200	H	0
37.1630	34.4040	28.8240	C	0	35.0780	37.1330	33.1140	H	0	46.6470	42.5620	42.9600	C	0
37.9610	33.6760	28.6790	H	0	33.2390	36.1210	36.8650	C	0	46.8920	41.8870	42.1400	H	0
36.9700	34.5570	30.3980	C	0	32.9080	37.2580	37.1600	O	0	46.2730	43.7660	42.1190	C	0
36.1410	35.2510	30.5370	H	0	33.0510	35.0360	37.6040	N	0	45.3960	43.5070	41.5260	H	0
36.6080	33.6430	30.8690	H	0	33.5040	34.1700	37.3480	H	0	45.6820	44.9630	42.9350	C	0
38.2030	35.0950	31.2250	C	0	32.3050	35.0330	38.8620	C	0	45.0220	44.5620	43.7040	H	0
38.5490	36.0050	30.7360	H	0	31.8570	36.0250	38.9240	H	0	46.4560	45.5390	43.4420	H	0
37.9760	35.3090	32.2690	H	0	31.1920	33.9150	38.8320	C	0	45.0780	45.5670	42.2580	H	0
39.3550	34.1110	31.3410	C	0	30.8950	33.7290	37.8000	H	0	47.3800	44.2860	41.2570	C	0
39.1290	32.9280	30.9370	O	0	31.7490	33.0080	39.0680	H	0	47.8610	43.4930	40.6830	H	0
40.5360	34.3490	31.6840	O	0	30.0110	34.2290	39.6230	C	0	46.8370	44.9050	40.5440	H	0
35.9850	33.7260	28.1060	C	0	29.8750	34.0890	40.9750	C	0	48.0400	44.7410	41.9950	H	0
35.0880	34.4040	27.6600	O	0	30.6080	33.6080	41.6060	H	0	47.7880	42.8190	43.9640	C	0
36.0240	32.4020	27.9920	N	0	28.6330	34.5160	41.3810	N	0	47.5810	43.3190	45.0880	O	0
36.8920	31.9230	28.1810	H	0	28.1760	34.4170	42.2760	H	0	49.0690	42.5510	43.5510	N	0
34.8160	31.7090	27.3390	C	0	27.9740	35.1120	40.3570	C	0	49.1720	42.3170	42.5740	H	0
34.6230	32.1240	26.3500	H	0	26.7690	35.8010	40.2870	C	0	50.3000	42.5240	44.3320	C	0
35.2300	30.2770	27.2470	C	0	26.2020	36.0700	41.1670	H	0	50.0400	42.8070	45.3520	H	0
35.6690	29.9320	28.1840	H	0	26.2900	36.2230	39.0330	C	0	51.0700	41.2600	44.2790	C	0
34.4050	29.5820	27.0930	H	0	25.2990	36.6330	38.9120	H	0	51.9510	41.4370	44.8950	H	0
36.1900	30.0100	26.1280	C	0	27.0240	35.8710	37.8700	C	0	50.3990	39.9990	44.7590	C	0
37.4200	29.3520	26.2340	N	0	26.5670	36.1140	36.9220	H	0	51.0770	39.1630	44.5870	H	0
37.8870	29.3380	24.9690	C	0	28.3040	35.2820	37.9380	C	0	50.2300	40.2420	45.8080	H	0
38.8560	28.9320	24.7190	H	0	28.7720	35.1020	36.9820	H	0	49.4660	39.9330	44.2000	H	0
36.9450	29.9210	24.1360	N	0	28.7870	34.8340	39.1910	C	0	51.5760	41.0790	43.0090	O	0
37.0010	29.9460	23.1280	H	0	33.2610	35.0530	40.0740	C	0	50.8330	41.2390	42.4230	H	0
35.9520	30.4450	24.8820	C	0	32.8000	34.9510	41.2020	O	0	51.3350	43.6120	43.9510	C	0
34.9860	30.8090	24.5660	H	0	34.5420	35.3850	39.8930	N	0	51.4620	43.9780	42.7880	O	0
33.5890	31.7080	28.3030	C	0	34.9160	35.4240	38.9550	H	0	52.0170	44.1310	45.0290	N	0
32.4630	31.5260	27.7730	O	0	35.5130	35.5280	40.9810	C	0	51.7340	43.8240	45.9490	H	0
33.7420	32.0110	29.6010	N	0	35.0050	35.2980	41.9170	H	0	53.1750	45.0950	44.7870	C	0
34.6920	32.0460	29.9410	H	0	36.6540	34.5290	40.7770	C	0	52.7110	46.0090	44.4140	H	0
32.6320	32.1900	30.5430	C	0	36.2860	33.5410	41.0550	H	0	53.7960	45.3160	46.1050	C	0
31.7080	32.0490	29.9820	H	0	36.9030	34.6280	39.7200	H	0	54.5310	46.0940	45.9010	H	0
32.7950	31.0250	31.5360	C	0	37.7960	34.7680	41.5770	O	0	53.0150	45.6150	46.8040	H	0
33.7260	31.1320	32.0930	H	0	37.6090	34.2400	42.3570	H	0	54.2380	44.4140	46.5270	H	0
32.0450	31.0690	32.3260	H	0	36.0310	36.9560	41.0500	C	0	54.2390	44.5160	43.8450	C	0
32.7900	29.6520	30.8340	C	0	36.1950	37.6730	40.0770	O	0	54.8960	45.2530	43.1290	O	0
31.6540	29.1070	30.3720	C	0	36.3310	37.4450	42.2820	N	0	54.3490	43.1280	43.8180	N	0
30.7030	29.6150	30.4270	H	0	36.1550	36.7910	43.0320	H	0	53.8060	42.6500	44.5220	H	0
31.7090	27.8830	29.8320	C	0	36.8260	38.8580	42.5810	C	0	55.1710	42.1750	43.0580	C	0
30.8300	27.4140	29.4150	H	0	36.4910	39.6370	41.8970	H	0	56.2060	42.5070	43.1380	H	0
32.9450	27.2170	29.6360	C	0	36.4750	39.1020	43.5840	H	0	54.9810	41.1950	43.4970	H	0

54.8480	42.1960	41.5760	C	0	41.3590	34.0780	38.9470	C	0	46.5430	25.1610	34.3810	H	0
55.5640	41.5150	40.8210	O	0	42.0760	33.2810	38.3560	O	0	44.4530	25.9950	34.3200	C	0
53.9120	42.9970	41.1080	N	0	40.1240	33.6710	39.2480	N	0	44.6740	26.7550	35.0540	H	0
53.2850	43.4180	41.7790	H	0	39.5380	34.2580	39.8240	H	0	43.2620	26.0610	33.5950	C	0
53.5070	43.1050	39.6990	C	0	39.6110	32.3030	38.9100	C	0	41.7720	28.7630	36.9550	C	0
52.9500	44.0060	39.4400	H	0	40.4040	31.6660	38.5260	H	0	41.1010	29.8140	36.7640	O	0
54.3650	43.2970	39.0550	H	0	39.2380	31.8350	39.8210	H	0	42.4530	28.6850	38.0350	N	0
52.5550	42.0400	39.1660	C	0	38.4370	32.2920	37.8700	C	0	42.9320	27.8080	38.1800	H	0
52.5620	41.9240	37.9230	O	0	37.7110	33.2920	37.6690	O	0	43.0300	29.7780	38.7170	C	0
51.8700	41.2690	40.0130	N	0	38.2760	31.1400	37.2040	N	0	42.2370	30.5240	38.7840	H	0
51.8830	41.5190	40.9920	H	0	39.0010	30.4870	37.4670	H	0	43.3240	29.3270	40.1640	C	0
50.9620	40.1870	39.6480	C	0	37.3250	30.9500	36.1390	C	0	42.3890	28.9610	40.5880	H	0
51.0050	40.0760	38.5640	H	0	36.8370	31.9190	36.0340	H	0	44.0010	28.4790	40.2610	H	0
51.3830	38.9140	40.2500	C	0	38.1080	30.6900	34.8790	C	0	43.8090	30.4270	41.1270	C	0
51.3080	38.9700	41.3360	H	0	37.4200	30.5880	34.0400	H	0	43.2230	31.6470	41.1790	C	0
50.7170	38.0960	39.9750	H	0	39.0360	31.7900	34.4530	C	0	42.5020	31.9100	40.4190	H	0
52.7810	38.5060	39.8990	C	0	38.5480	32.7310	34.7080	H	0	43.5600	32.6530	42.0810	C	0
53.5090	39.3090	40.0060	H	0	39.9190	31.6970	35.0860	H	0	42.9820	33.5660	42.0850	H	0
53.2870	37.3110	40.6870	C	0	39.3300	31.6530	33.4130	H	0	44.5240	32.3590	43.1230	C	0
54.2180	36.9320	40.2650	H	0	38.8120	29.4920	35.0030	O	0	44.7810	33.1210	43.8450	H	0
53.5770	37.7790	41.6280	H	0	39.6460	29.6280	35.4580	H	0	45.1150	31.0550	43.1280	C	0
52.4220	36.6650	40.8380	H	0	36.2680	29.8740	36.3600	C	0	45.7390	30.7390	43.9510	H	0
52.7470	38.0020	38.4040	C	0	36.5480	28.8090	36.9270	O	0	44.7650	30.1210	42.1160	C	0
52.5470	38.7650	37.6520	H	0	35.1290	30.1640	35.7090	N	0	45.1900	29.1300	42.1830	H	0
53.7760	37.7530	38.1480	H	0	35.0870	30.9390	35.0630	H	0	44.2630	30.1740	37.9070	C	0
52.0850	37.1740	38.1520	H	0	34.1640	29.0410	35.6790	C	0	45.1640	29.3910	37.5910	O	0
49.5250	40.5310	40.1400	C	0	34.0250	28.6340	36.6800	H	0	44.2410	31.4970	37.5440	N	0
49.2610	41.1820	41.1460	O	0	32.8720	29.5370	35.0540	C	0	43.4970	32.0820	37.8970	H	0
48.5880	40.0430	39.3360	N	0	33.1100	30.2230	34.2410	H	0	45.0750	32.2030	36.5050	C	0
48.8830	39.5420	38.5100	H	0	32.3850	28.6310	34.6940	H	0	45.8590	31.5760	36.0820	H	0
47.1040	40.0040	39.5040	C	0	32.0050	30.3440	36.0450	C	0	44.2540	32.8140	35.3670	C	0
46.9700	40.1780	40.5720	H	0	32.5980	30.5180	36.9430	H	0	43.3930	33.2320	35.8890	H	0
46.3030	41.0220	38.6340	C	0	31.8170	31.3110	35.5780	H	0	44.8340	33.4710	34.7200	H	0
45.3330	41.1430	39.1160	H	0	30.3660	29.5730	36.4050	S	0	43.7810	31.7370	34.4010	C	0
46.9330	41.9090	38.6950	H	0	29.9300	30.6230	37.8270	C	0	44.7020	31.3010	34.0140	H	0
46.2340	40.7670	37.5770	H	0	30.6840	30.6570	38.6140	H	0	43.1000	31.0850	34.9470	H	0
46.6930	38.5070	39.3760	C	0	29.7300	31.5810	37.3480	H	0	42.9530	32.2890	33.2530	C	0
47.1250	37.7320	38.4980	O	0	28.9740	30.2520	38.1970	H	0	42.1270	32.8690	33.6670	H	0
45.7450	38.0750	40.2310	N	0	34.7590	27.9190	34.9090	C	0	43.6170	32.9090	32.6500	H	0
45.6030	38.6600	41.0420	H	0	34.2140	26.8360	35.0270	O	0	42.3230	31.1180	32.4010	C	0
45.2930	36.6770	40.4180	C	0	35.8010	28.1040	34.1160	N	0	43.0090	30.3530	33.0380	H	0
45.6640	36.0150	39.6360	H	0	36.1110	29.0620	34.0340	H	0	41.6320	30.5390	33.0130	H	0
45.9100	36.1710	41.7370	C	0	36.5510	27.0710	33.3950	C	0	41.7170	31.7600	31.2490	N	0
45.7970	36.9100	42.5310	H	0	35.9290	26.3820	32.8240	H	0	41.4470	31.0940	30.5400	H	0
45.3610	35.3000	42.0930	H	0	37.5120	27.7250	32.3610	C	0	40.8470	32.2110	31.4930	H	0
47.4560	35.9480	41.7130	C	0	37.1030	28.6460	31.9440	H	0	42.3210	32.4070	30.7610	H	0
48.3540	36.9560	42.1680	C	0	38.4440	27.9910	32.8590	H	0	45.7830	33.3520	37.2940	C	0
47.9410	37.9020	42.4880	H	0	37.8950	26.8150	31.1680	C	0	45.2500	33.9390	38.2880	O	0
49.7300	36.6860	42.3920	C	0	37.2940	25.6900	31.0330	O	0	46.9700	33.6790	36.8370	N	0
50.3270	37.4540	42.8620	H	0	38.8520	27.2050	30.4430	O	0	47.3740	33.1140	36.1040	H	0
50.2580	35.3920	42.3200	C	0	37.4390	26.2370	34.2740	C	0	47.8200	34.7640	37.3290	C	0
51.2880	35.1440	42.5290	H	0	38.1910	25.3960	33.8420	O	0	47.1980	35.3780	37.9810	H	0
49.4140	34.3890	41.9200	C	0	37.3550	26.3720	35.5770	N	0	48.7970	34.0860	38.3020	C	0
49.8330	33.4000	41.8010	H	0	36.7750	27.1370	35.8920	H	0	48.3650	33.2330	38.8250	H	0
48.0700	34.7050	41.6290	C	0	38.2390	25.6830	36.5660	C	0	49.6030	33.6270	37.7290	H	0
47.4030	33.9020	41.3540	H	0	37.7690	25.8340	37.5380	H	0	49.2350	34.7570	39.0410	H	0
43.7610	36.6110	40.3530	C	0	38.2970	24.6130	36.3680	H	0	48.5260	35.5550	36.2050	C	0
43.1110	37.4460	41.0020	O	0	39.6430	26.2270	36.7210	C	0	49.1620	34.9590	35.3560	O	0
43.1710	35.6540	39.6290	N	0	40.3370	25.7150	37.6030	O	0	48.5880	36.9080	36.3000	N	0
43.6910	35.0350	39.0230	H	0	40.1250	27.1880	35.9980	N	0	48.1710	37.2530	37.1530	H	0
41.7340	35.4990	39.5470	C	0	39.6220	27.5780	35.2130	H	0	48.8390	37.8560	35.2250	C	0
41.2350	35.6330	40.5070	H	0	41.5160	27.5540	36.0530	C	0	49.1830	37.3380	34.3300	H	0
41.0900	36.4180	38.5030	C	0	42.1370	26.7860	36.5160	H	0	47.5130	38.5760	34.7740	C	0
40.0050	36.3220	38.5460	H	0	41.9660	28.0330	34.6780	C	0	46.9870	39.0020	35.6280	H	0
41.2730	37.4880	38.5990	H	0	41.2760	28.7750	34.2760	H	0	47.7380	39.6600	33.7620	C	0
41.5130	36.2440	37.0480	C	0	42.8860	28.5990	34.8250	H	0	46.8780	40.2880	33.5310	H	0
42.8040	36.5970	36.5940	C	0	42.1610	26.9390	33.6850	C	0	48.4570	40.4230	34.0610	H	0
43.4440	37.3050	37.1000	H	0	41.2210	26.4750	32.7840	C	0	48.0790	39.2790	32.7990	H	0
43.2510	36.1800	35.3260	C	0	40.2080	26.8280	32.6600	H	0	46.5870	37.4710	34.1470	C	0
44.2430	36.4010	34.9610	H	0	41.8580	25.4970	31.9780	N	0	46.3880	36.5980	34.7680	H	0
42.3260	35.5950	34.3850	C	0	41.3000	24.8330	31.4590	H	0	45.6250	37.9170	33.8940	H	0
42.6990	35.3170	33.1580	O	0	43.1280	25.2120	32.4330	C	0	47.0840	37.0630	33.2670	H	0
41.9600	34.9840	32.6440	H	0	44.1720	24.3920	31.9790	C	0	49.9590	38.8780	35.5830	C	0
41.0290	35.2730	34.7860	C	0	44.2270	23.8630	31.0400	H	0	49.9450	39.4930	36.6480	O	0
40.2520	34.8470	34.1680	H	0	45.4000	24.4830	32.6650	C	0	50.8410	39.1450	34.6010	N	0
40.6660	35.5810	36.1240	C	0	46.2310	23.9070	32.2860	H	0	50.6390	38.6250	33.7590	H	0
39.7050	35.2390	36.4800	H	0	45.5950	25.2320	33.8680	C	0	51.8360	40.1720	34.7360	C	0

52.3420	40.2120	35.7000	H	0	52.0520	37.0140	29.4680	H	0	47.5980	28.7730	35.5250	C	0
53.0090	39.8400	33.8490	C	0	52.1490	38.9190	28.4130	C	0	47.1150	29.3480	36.3140	H	0
53.5610	39.0740	34.3950	H	0	52.0050	39.9860	28.5840	H	0	46.8670	29.1890	34.2440	C	0
52.6910	39.3740	32.9160	H	0	53.2260	38.7730	28.3300	H	0	45.8010	29.0520	34.4240	H	0
53.9560	41.0030	33.7450	C	0	51.3800	38.6830	27.0710	C	0	47.0460	30.2350	33.9930	H	0
53.8820	42.0280	34.4910	O	0	51.5820	37.6890	26.6730	H	0	47.2190	28.3560	32.9630	C	0
54.7360	40.9360	32.7910	O	0	50.3050	38.8000	27.2120	H	0	48.2220	28.6040	32.6160	H	0
51.1540	41.5370	34.4700	C	0	51.7230	39.7760	26.0990	C	0	47.2760	27.2870	33.1690	H	0
50.6950	41.7880	33.3700	O	0	51.0950	40.6600	26.2120	H	0	46.2500	28.6520	31.8200	C	0
50.9620	42.4580	35.4970	N	0	52.7640	40.0820	26.2050	H	0	45.5260	29.5870	31.7840	O	0
51.5700	42.3520	36.2960	H	0	51.4610	39.3110	24.7100	N	0	46.0750	27.7800	30.8250	N	0
50.1070	43.6500	35.3530	C	0	50.5880	38.8050	24.6650	H	0	45.2360	27.9350	30.2850	H	0
49.1090	43.3360	35.0450	H	0	51.4630	40.0440	24.0150	H	0	46.5130	26.8730	30.9080	H	0
49.8710	44.2460	36.7450	C	0	52.0980	38.5380	24.5750	H	0	47.5160	27.2950	35.9290	C	0
49.1370	45.0130	36.4970	H	0	49.9280	37.2220	31.1820	C	0	48.3680	26.4780	35.5090	O	0
49.0390	43.2510	37.5860	C	0	50.3960	37.4770	32.2520	O	0	46.5860	26.9470	36.8600	N	0
48.5950	43.7430	38.4520	H	0	49.1810	36.1360	30.9560	N	0	46.1220	27.6670	37.3940	H	0
48.2200	42.8250	37.0060	H	0	48.8370	35.8900	30.0380	H	0	46.3610	25.5270	37.2770	C	0
49.6120	42.4020	37.9600	H	0	49.0520	35.0000	31.9610	C	0	46.8430	24.8850	36.5400	H	0
51.1210	44.9560	37.3280	C	0	48.8760	35.5940	32.8570	H	0	47.0720	25.2150	38.5850	C	0
51.9340	44.2430	37.4640	H	0	47.7970	34.0900	31.6620	C	0	48.0270	25.7380	38.5250	H	0
51.4500	45.7270	36.6330	H	0	47.8530	33.7910	30.6160	H	0	46.6080	25.7490	39.4140	H	0
50.8950	45.7070	38.6290	C	0	47.8000	32.9730	32.7120	C	0	47.3480	23.7160	38.9530	C	0
50.1140	46.4660	38.6690	H	0	46.8300	32.4760	32.6900	H	0	46.3780	23.2390	39.0960	H	0
50.6370	44.9150	39.3320	H	0	48.5180	32.2020	32.4310	H	0	47.8970	23.1860	38.1750	H	0
51.8250	46.2000	38.9140	H	0	48.0000	33.3620	33.7110	H	0	48.2710	23.4920	40.1090	C	0
50.5920	44.6790	34.3660	C	0	46.4770	34.7890	31.9600	C	0	49.2470	24.1130	40.4020	O	0
49.7420	45.3170	33.7720	O	0	46.2450	34.8610	33.0230	H	0	48.0600	22.3970	40.8350	N	0
51.9230	44.8120	34.1430	N	0	46.4220	35.8090	31.5780	H	0	48.6780	22.3250	41.6300	H	0
52.5600	44.2380	34.6760	H	0	45.6740	34.2820	31.4250	H	0	47.1220	22.0240	40.8180	H	0
52.4340	45.8070	33.1780	C	0	50.4100	34.2340	32.0820	C	0	44.8600	25.3290	37.3590	C	0
51.6980	46.6100	33.2090	H	0	50.5490	33.3660	31.2690	O	0	44.0770	26.2230	37.5650	O	0
53.8010	46.3690	33.6990	C	0	51.2120	34.5110	33.1000	N	0	44.4270	24.0980	37.0490	N	0
54.4050	45.4640	33.7590	H	0	50.9100	35.1980	33.7760	H	0	45.1240	23.3670	37.0500	H	0
54.2320	47.0000	32.9210	H	0	52.4250	33.7080	33.4070	C	0	43.0100	23.6340	36.9330	C	0
53.7730	47.1130	35.0490	C	0	53.0250	33.6570	32.4990	H	0	42.3770	24.5130	36.8080	H	0
53.0220	47.9020	35.0030	H	0	53.2850	34.4800	34.4350	C	0	42.9630	22.8200	35.6800	C	0
53.5460	46.4690	35.8990	H	0	52.8230	34.2080	35.3840	H	0	43.4240	23.4120	34.8890	H	0
55.0810	47.8620	35.3610	C	0	54.3110	34.1120	34.4260	H	0	43.5600	21.9400	35.9200	H	0
55.2250	48.7170	34.7010	H	0	53.3780	36.0180	34.3880	C	0	41.5490	22.3380	35.2810	C	0
54.7400	48.1790	36.3470	H	0	52.3980	36.4840	34.4930	H	0	41.7300	21.4030	34.7510	H	0
56.3240	46.9810	35.3330	C	0	54.4240	36.5100	35.3830	C	0	40.8900	22.2160	36.1400	H	0
56.5670	46.5510	34.3610	H	0	54.0840	37.4740	35.7610	H	0	40.7400	23.2690	34.2920	C	0
57.1230	47.6780	35.5840	H	0	54.6070	35.8110	36.1990	H	0	40.6390	24.2580	34.7390	H	0
56.4160	45.8750	36.3030	N	0	55.4070	36.7920	35.0060	H	0	41.2970	23.2340	33.3560	H	0
56.4330	46.3200	37.2090	H	0	53.6800	36.4670	32.9080	C	0	39.4720	22.5200	34.0530	C	0
55.5770	45.3200	36.3940	H	0	52.8600	36.2130	32.2360	H	0	39.6800	21.4570	33.9360	H	0
57.1930	45.2450	36.1610	H	0	53.9720	37.5160	32.8560	H	0	39.0010	22.6500	35.0270	H	0
52.4810	45.2460	31.7340	C	0	54.5340	35.8630	32.6000	H	0	38.7370	23.0300	32.8860	N	0
52.9400	45.9460	30.8500	O	0	52.1700	32.3260	33.9380	C	0	38.5250	24.0070	33.0240	H	0
52.0090	44.0010	31.4870	N	0	52.7870	31.3150	33.5760	O	0	39.3300	22.9170	32.0760	H	0
51.6950	43.4650	32.2830	H	0	51.1690	32.1730	34.8200	N	0	37.8170	22.6470	32.7230	H	0
51.9020	43.3810	30.1730	C	0	50.5290	32.9370	34.9860	H	0	42.5810	22.9310	38.2640	C	0
51.9830	44.2010	29.4600	H	0	50.7530	30.9180	35.5040	C	0	43.1520	21.9530	38.7590	O	0
52.9850	42.2990	29.8830	C	0	51.1870	30.0720	34.9710	H	0	41.6090	23.5050	38.9370	N	0
52.7780	41.8140	28.9290	H	0	51.3730	30.9720	36.9620	C	0	41.1760	24.2580	38.4210	H	0
54.3700	42.9230	29.6530	C	0	52.4450	31.1610	36.9060	H	0	40.8960	23.0300	40.1560	C	0
54.5460	43.7610	30.3280	H	0	50.8960	31.8690	37.3570	H	0	41.5050	22.3600	40.7630	H	0
55.0770	42.1360	29.9150	H	0	51.1010	29.8290	37.8750	C	0	40.4340	24.2460	40.9470	C	0
54.5810	43.1160	28.6010	H	0	51.8060	28.7490	37.9460	C	0	39.8930	24.9800	40.3500	H	0
52.7650	41.2920	30.8810	O	0	52.7550	28.6450	37.4400	H	0	39.7000	23.9220	41.6840	H	0
53.5120	41.3400	31.4830	H	0	51.2240	27.7940	38.8020	N	0	41.5440	24.9630	41.6910	C	0
50.6170	42.6480	29.8810	C	0	51.5700	26.8670	39.0050	H	0	42.0800	24.2270	42.2900	H	0
50.3930	42.4140	28.7420	O	0	50.0410	28.2870	39.3010	C	0	42.5380	25.7190	40.7760	C	0
49.7610	42.3920	30.8410	N	0	48.9980	27.7540	39.9830	C	0	43.2230	24.9560	40.4080	H	0
50.0430	42.5640	31.7950	H	0	49.1500	26.7770	40.4170	H	0	41.9780	26.0500	39.9010	H	0
48.5200	41.6590	30.5880	C	0	47.8610	28.5590	40.3180	C	0	42.9020	26.5980	41.3070	H	0
47.8940	41.6040	31.4790	H	0	47.2180	27.9950	40.9780	H	0	40.8270	25.9430	42.6410	C	0
48.0480	42.1650	29.7460	H	0	47.7200	29.8150	39.7250	C	0	41.5760	26.6980	42.8810	H	0
48.6650	40.1780	30.1970	C	0	46.7870	30.3490	39.8300	H	0	40.0800	26.4910	42.0680	H	0
47.7150	39.6470	29.5990	O	0	48.7590	30.3300	38.9220	C	0	40.2560	25.4110	43.4020	H	0
49.8900	39.5700	30.3950	N	0	48.7310	31.3040	38.4560	H	0	39.7870	22.0870	39.6970	C	0
50.6860	40.0050	30.8380	H	0	49.8990	29.5250	38.6610	C	0	39.3330	22.2010	38.5250	O	0
50.1980	38.1500	30.0050	C	0	49.2640	30.6340	35.4520	C	0	39.2250	21.2880	40.6310	N	0
49.6330	37.8520	29.1220	H	0	48.3260	31.4510	35.5620	O	0	39.7000	21.0880	41.5000	H	0
51.7130	38.0340	29.6490	C	0	48.9700	29.3050	35.3610	N	0	38.3270	20.2760	40.2100	C	0
52.2890	38.3380	30.5230	H	0	49.7080	28.6160	35.3580	H	0	38.5680	19.8330	39.2440	H	0

38.3580	19.4710	40.9440	H	0	34.9290	38.1220	47.8360	H	0	53.6850	37.4530	54.8230	C	0
36.8340	20.7500	40.0900	C	0	38.7420	35.3480	46.3660	C	0	52.8560	38.0320	54.4150	H	0
36.0840	20.0000	39.4550	O	0	38.8570	35.1560	47.5890	O	0	54.6030	38.4990	55.6120	C	0
36.5040	21.9410	40.6380	N	0	39.9020	35.3420	45.6210	N	0	55.1280	39.0860	54.8580	H	0
37.2280	22.4060	41.1680	H	0	39.9680	35.1650	44.1490	C	0	54.1350	39.2380	56.2630	H	0
35.2020	22.5140	40.4720	C	0	39.2470	35.7350	43.5630	H	0	55.4340	37.9730	56.0810	H	0
34.6800	22.0430	39.6390	H	0	39.8260	34.1030	43.9510	H	0	54.3570	36.7700	53.6950	C	0
34.3260	22.4250	41.6730	C	0	41.3980	35.4630	43.7650	C	0	54.9470	37.4180	53.0460	H	0
34.1970	21.3640	41.8860	H	0	41.6580	36.5190	43.8470	H	0	54.9550	35.9270	54.0400	H	0
34.7540	22.9540	42.5250	H	0	41.5560	35.0650	42.7620	H	0	53.6450	36.2590	53.0470	H	0
33.0670	22.8990	41.3970	O	0	42.0720	34.6470	44.9090	C	0	51.9050	34.2890	56.3590	C	0
32.5560	22.2910	40.8580	H	0	43.1210	34.9110	45.0460	H	0	50.8820	34.3950	57.0510	O	0
35.2420	23.9870	40.0740	C	0	41.9460	33.5700	44.8010	H	0	52.7280	33.2170	56.5180	N	0
35.9960	24.6940	40.6800	O	0	41.2430	35.0340	46.1350	C	0	53.3800	32.9950	55.7790	H	0
34.3770	24.4540	39.1240	N	0	41.1870	34.1240	46.7330	H	0	52.5990	32.1610	57.4840	C	0
33.8400	23.7390	38.6530	H	0	41.9740	35.9800	47.1150	C	0	51.6090	32.0790	57.9320	H	0
34.3740	25.8670	38.5810	C	0	41.7860	37.1910	47.1710	O	0	52.7280	31.2290	56.9320	H	0
35.1130	25.9710	37.7860	H	0	42.9060	35.4490	47.9440	N	0	53.6070	32.3670	58.5670	C	0
33.4220	26.1910	38.1590	H	0	43.0290	34.4510	47.8430	H	0	54.4820	33.2400	58.5030	O	0
34.5630	26.8820	39.7450	C	0	43.6200	36.1900	49.0160	C	0	53.5830	31.6490	59.7410	N	0
33.8510	26.8980	40.7790	O	0	43.4230	37.2600	48.9510	H	0	52.5890	30.6120	60.1300	C	0
35.5180	27.8410	39.6500	N	0	43.2050	35.7730	50.4540	C	0	52.3770	29.8400	59.3910	H	0
35.9720	28.0050	38.7630	H	0	43.5020	36.6080	51.0890	H	0	51.7140	31.1850	60.4340	H	0
35.7850	28.9530	40.6230	C	0	41.6760	35.8320	50.4130	C	0	53.1490	29.8440	61.3100	C	0
35.6620	28.5200	41.6150	H	0	41.3700	36.6670	49.7840	H	0	53.5560	28.9310	60.8760	H	0
37.2600	29.4760	40.6130	C	0	41.2260	34.9340	49.9900	H	0	52.3770	29.6530	62.0560	H	0
37.3500	29.9860	39.6540	H	0	41.2050	35.9550	51.3880	H	0	54.2810	30.6980	61.8550	C	0
37.5680	30.5020	41.7660	C	0	43.6540	34.4860	51.1420	C	0	55.1580	30.0780	62.0430	H	0
37.5830	30.0190	42.7430	H	0	42.9040	33.7060	51.0080	H	0	53.9720	31.1330	62.8060	H	0
38.5090	30.9950	41.5220	H	0	44.6790	34.2050	50.9010	H	0	54.6500	31.7420	60.8350	C	0
36.7660	31.2260	41.9120	H	0	43.5900	34.7270	52.6980	C	0	54.6050	32.7060	61.3420	H	0
38.1920	28.2890	40.6570	C	0	42.5530	34.7820	53.0280	H	0	56.0690	31.4620	60.3020	C	0
38.2310	27.9920	41.7050	H	0	44.0410	33.9290	53.2880	H	0	57.0400	32.0470	60.8370	O	0
37.8210	27.4820	40.0250	H	0	44.1360	35.6330	52.9610	H	0	56.2620	30.7970	59.1500	N	0
39.6640	28.5140	40.2940	C	0	45.0920	35.8670	48.8770	C	0	55.5050	30.3820	58.6270	H	0
40.1160	29.0380	41.1360	H	0	45.4440	34.8020	48.3530	O	0	57.5420	30.7350	58.4660	C	0
40.3660	27.6840	40.2280	H	0	45.9470	36.6140	49.4920	N	0	58.2870	30.4300	59.2010	H	0
39.8030	29.0960	39.3830	H	0	45.6000	37.5170	49.7830	H	0	57.5530	29.5850	57.3600	C	0
34.7560	30.0340	40.5150	C	0	47.3250	36.2570	49.8280	C	0	56.7850	29.6990	56.5950	H	0
34.7960	31.0620	39.8030	O	0	47.3190	35.1700	49.9060	H	0	58.4410	29.6120	56.7280	H	0
33.7020	29.8240	41.3440	N	0	48.3470	36.6350	48.6560	C	0	57.5120	28.1650	57.8730	C	0
33.5000	28.8670	41.5940	H	0	48.0020	36.2190	47.7090	H	0	58.1770	27.8090	58.8920	O	0
33.1740	30.8570	42.2750	C	0	48.3250	38.1680	48.4440	C	0	56.8420	27.3550	57.2300	O	0
33.1930	31.8590	41.8470	H	0	48.8750	38.6880	49.2280	H	0	57.9310	32.0180	57.6750	C	0
31.7360	30.4530	42.7020	C	0	48.7540	38.3650	47.4610	H	0	59.1090	32.1570	57.3330	O	0
31.3710	31.3410	43.2180	H	0	47.3610	38.6740	48.4140	H	0	57.0640	32.9970	57.6340	N	0
30.8580	30.1790	41.4700	C	0	49.7160	36.3050	48.9970	O	0	56.2630	32.7300	58.1880	H	0
29.8980	29.8760	41.8890	H	0	49.6890	35.3800	49.2530	H	0	57.0040	34.1260	56.7230	C	0
30.7160	31.1020	40.9070	H	0	47.8710	36.8050	51.1930	C	0	56.0310	34.5930	56.8750	H	0
31.1840	29.3320	40.8660	H	0	47.3190	37.8470	51.6210	O	0	58.1270	35.1910	56.9420	C	0
31.6460	29.2260	43.6800	C	0	48.8470	36.1440	51.7910	N	0	59.1210	34.8060	57.1700	H	0
32.1380	28.3770	43.2060	H	0	49.3880	35.4290	51.3260	H	0	58.3170	35.8370	56.0850	H	0
32.3180	29.4970	44.4940	H	0	49.1360	36.1880	53.2390	C	0	57.7510	36.1940	58.0310	C	0
30.2630	28.9160	44.2550	C	0	49.0940	37.2020	53.6360	H	0	58.5210	36.9650	58.0000	H	0
29.7230	29.8310	44.5000	H	0	48.0240	35.4870	53.9770	C	0	56.7690	36.6600	57.9540	H	0
29.6770	28.3920	43.5000	H	0	48.1230	35.8650	54.9950	H	0	57.8020	35.6340	59.4810	C	0
30.4350	28.3550	45.1740	H	0	47.1120	35.9980	53.6700	H	0	56.8760	35.1230	59.7450	H	0
34.1280	30.9810	43.4880	C	0	47.8130	33.9610	53.9460	C	0	58.5670	34.8990	59.7300	H	0
34.9180	30.0700	43.8060	O	0	47.0860	33.4010	52.8700	C	0	57.9730	36.6760	60.5590	C	0
34.0810	32.1400	44.1500	N	0	46.6190	34.0630	52.1560	H	0	58.8910	37.2600	60.4900	H	0
33.3100	32.7240	43.8580	H	0	46.8270	32.0380	52.8460	C	0	57.1420	37.3720	60.4450	H	0
34.8680	32.6360	45.3140	C	0	46.3640	31.5610	51.9950	H	0	57.8340	36.1470	61.9420	N	0
34.2460	33.1760	46.0280	H	0	47.2430	31.1920	53.9280	C	0	57.5740	36.8340	62.6360	H	0
35.3700	31.8530	45.8830	H	0	46.9020	30.1840	54.1100	H	0	57.1140	35.4390	61.9840	H	0
35.9390	33.6650	44.9010	C	0	48.1190	31.7620	54.9260	C	0	58.7050	35.7650	62.2820	H	0
36.2840	33.7390	43.7170	O	0	48.5010	31.2210	55.7800	H	0	56.8590	33.7510	55.2370	C	0
36.4170	34.4150	45.8690	N	0	48.4110	33.1800	54.9440	C	0	57.1290	34.6090	54.3840	O	0
35.9340	34.1260	46.7070	H	0	48.8910	33.5980	55.8160	H	0	56.4780	32.4930	54.9140	N	0
37.3270	35.5630	45.8200	C	0	50.5220	35.6120	53.5490	C	0	55.8600	32.0210	55.5570	H	0
37.5210	35.8150	44.7770	H	0	51.2330	34.9330	52.8030	O	0	56.3360	32.0120	53.5300	C	0
36.6040	36.7300	46.6160	C	0	51.0170	35.9510	54.7170	N	0	57.1660	32.4850	53.0070	H	0
36.4530	36.3310	47.6190	H	0	50.5120	36.5760	55.3300	H	0	56.3430	30.5390	53.5510	C	0
37.2280	37.6100	46.7680	H	0	52.1850	35.3630	55.2980	C	0	57.3130	30.3680	54.0160	H	0
35.2570	37.1550	46.1250	C	0	52.7970	34.8530	54.5540	H	0	55.5900	30.1820	54.2540	H	0
34.9270	36.9600	44.9650	O	0	53.0650	36.4860	55.8720	C	0	56.3250	30.0460	52.1170	C	0
34.5590	37.8410	46.9390	N	0	52.4140	37.0380	56.5500	H	0	55.3930	30.2720	51.6000	H	0
33.5880	38.0670	46.7760	H	0	53.8650	36.0240	56.4490	H	0	57.1820	30.5860	51.7160	H	0

56.6190	28.5280	52.0190	C	0	42.4620	29.3160	47.4020	H	0	25.1850	28.9740	41.3190	N	0
57.6070	28.2880	52.4110	H	0	40.7370	30.3610	46.7570	C	0	24.7500	28.6520	42.1710	H	0
55.9460	27.9140	52.6170	H	0	40.2240	31.1910	47.2430	H	0	24.6680	30.2450	40.7670	C	0
56.6010	27.8470	50.5970	C	0	41.0790	30.5710	45.2500	C	0	23.9110	30.6610	41.4320	H	0
57.1570	26.9090	50.6050	H	0	41.8450	31.3360	45.1230	H	0	25.4640	30.9890	40.7370	H	0
55.5880	27.5600	50.3170	H	0	41.4580	29.2330	44.5530	C	0	23.9290	30.1650	39.3930	C	0
57.2030	28.6500	49.5040	N	0	42.2350	28.7040	45.1050	H	0	23.8350	29.0770	38.7510	O	0
58.1220	28.9810	49.7600	H	0	40.6350	28.5300	44.4220	H	0	23.4240	31.2780	38.9740	N	0
57.3360	28.1820	48.6190	H	0	41.8670	29.4640	43.5690	H	0	23.6750	32.1100	39.4880	H	0
56.6550	29.4880	49.3730	H	0	39.8430	31.1380	44.6340	C	0	22.5530	31.4210	37.6810	C	0
54.9800	32.5860	52.9880	C	0	39.0670	30.4420	44.3150	H	0	21.6890	30.7590	37.7350	H	0
53.9600	32.4640	53.6790	O	0	39.5590	32.0160	45.2140	H	0	22.0740	32.8720	37.7320	C	0
55.0020	33.2930	51.8660	N	0	40.1620	31.4910	43.6540	H	0	21.6800	33.1930	38.6960	H	0
55.9010	33.5050	51.4570	H	0	39.8840	29.1480	47.0900	C	0	22.8190	33.5810	37.3710	H	0
53.7910	33.8530	51.2290	C	0	40.4250	28.1040	47.4430	O	0	20.9190	33.2470	36.8890	C	0
53.2520	34.3880	52.0110	H	0	38.5890	29.2780	46.8990	N	0	20.1270	32.4060	36.1290	C	0
54.1430	34.8320	50.0930	C	0	38.1740	30.1500	46.6040	H	0	20.3100	31.3540	35.9700	H	0
54.6030	35.7240	50.5170	H	0	37.5910	28.1740	46.8430	C	0	19.2340	33.1390	35.2740	N	0
54.9440	34.5270	49.4190	H	0	37.9370	27.3550	47.4740	H	0	18.8120	32.7810	34.4280	H	0
52.8590	35.3810	49.4100	C	0	36.1970	28.7150	47.3270	C	0	19.2590	34.4380	35.6630	C	0
52.1620	34.6990	48.9230	H	0	35.8540	29.4720	46.6210	H	0	18.4680	35.6000	35.2940	C	0
52.1970	35.7380	50.1990	H	0	35.4030	27.9840	47.1730	H	0	17.5900	35.6270	34.6660	H	0
53.1610	36.5900	48.4340	C	0	36.1700	29.1850	48.7410	C	0	18.8040	36.8540	35.8380	C	0
54.3080	37.0450	48.1960	O	0	36.7590	28.5520	49.8140	C	0	18.1120	37.6430	35.5810	H	0
52.1620	37.3190	47.8990	N	0	37.1850	27.5610	49.7490	H	0	19.9740	37.0290	36.5460	C	0
52.3580	38.1560	47.3690	H	0	36.7570	29.1640	51.0400	C	0	20.2140	38.0200	36.9020	H	0
51.2720	36.9870	48.2420	H	0	37.3640	28.7100	51.8100	H	0	20.7610	35.8420	36.9500	C	0
52.9220	32.7290	50.6180	C	0	36.1140	30.3680	51.3270	C	0	21.5410	36.0210	37.6760	H	0
53.4060	31.8270	49.8870	O	0	36.2150	31.0960	52.4970	O	0	20.3660	34.5340	36.5440	C	0
51.6150	32.7640	50.9620	N	0	35.5740	31.8090	52.4630	H	0	23.1600	31.0170	36.3360	C	0
51.2420	33.5080	51.5340	H	0	35.4350	30.9450	50.2590	C	0	22.5140	30.2520	35.6310	O	0
50.6300	31.8850	50.4580	C	0	35.0800	31.9560	50.3940	H	0	24.4040	31.4420	36.0820	N	0
51.0320	31.1620	49.7480	H	0	35.5060	30.4470	48.9830	C	0	25.0530	31.9430	36.6710	H	0
50.0560	31.1680	51.6810	C	0	35.0710	31.0810	48.2250	H	0	25.1700	30.9190	34.9150	C	0
49.9230	31.8710	52.5040	H	0	37.4230	27.5700	45.3830	C	0	24.5340	30.9820	34.0320	H	0
49.0710	30.7210	51.5520	H	0	37.9400	28.1250	44.3960	O	0	26.3530	31.8370	34.5900	C	0
50.8720	30.0340	52.2860	C	0	36.6190	26.4380	45.3040	N	0	26.0070	32.8700	34.5660	H	0
51.6820	30.3530	53.4120	C	0	36.3730	25.9390	46.1470	H	0	27.0530	31.7810	35.4240	H	0
51.7050	31.2990	53.9310	H	0	36.3180	25.8320	44.0300	C	0	27.0440	31.3710	33.2960	C	0
52.5310	29.3660	53.9710	C	0	36.0560	26.6440	43.3520	H	0	26.6010	31.9590	32.0630	C	0
53.1250	29.4860	54.8640	H	0	37.6300	25.1390	43.5840	C	0	25.8420	32.7240	31.9950	H	0
52.4750	28.0620	53.4970	C	0	38.2070	25.8990	43.0570	H	0	27.2080	31.4640	30.8410	C	0
53.2730	27.0790	54.0470	O	0	38.1680	24.8750	44.4940	H	0	26.9760	31.8390	29.8550	H	0
52.9850	26.2020	53.7830	H	0	37.4380	24.0200	42.7610	O	0	28.1880	30.4820	30.8940	C	0
51.5940	27.7140	52.4670	C	0	36.9520	24.2740	41.9730	H	0	28.6180	30.1240	29.9700	H	0
51.5570	26.7280	52.0260	H	0	35.1380	24.9260	44.2190	C	0	28.5960	29.8890	32.1220	C	0
50.8490	28.7440	51.8450	C	0	35.1850	23.9540	45.0230	O	0	29.2830	29.0580	32.1770	H	0
50.3140	28.5130	50.9360	H	0	33.9960	25.2480	43.6690	N	0	27.9960	30.3240	33.3260	C	0
49.5400	32.6540	49.7230	C	0	34.0180	25.9460	42.9400	H	0	28.3700	29.9030	34.2470	H	0
49.5350	33.8810	49.8170	O	0	32.6870	24.7590	44.1120	C	0	25.5080	29.4910	35.1140	C	0
48.8670	31.9270	48.8310	N	0	32.6710	23.6690	44.0960	H	0	25.5610	28.7480	34.1950	O	0
49.2290	30.9890	48.7410	H	0	32.6490	25.0870	45.1510	H	0	25.6760	29.0150	36.3680	N	0
47.7240	32.3750	47.9970	C	0	31.4990	25.2550	43.3490	C	0	25.4300	29.6080	37.1480	H	0
47.3800	33.3540	48.3280	H	0	30.6480	25.9030	43.9420	O	0	26.1120	27.6030	36.6950	C	0
48.2610	32.5580	46.6060	C	0	31.4750	25.0680	42.0220	N	0	26.9660	27.3420	36.0700	H	0
48.6900	31.5860	46.3620	H	0	32.2090	24.4770	41.6590	H	0	26.5390	27.6290	37.6970	H	0
47.0860	32.9190	45.6550	C	0	30.5540	25.8740	41.1630	C	0	25.0160	26.6240	36.5940	C	0
47.5710	33.0040	44.6830	H	0	30.9170	26.8900	41.3160	H	0	25.1340	25.4680	36.8000	O	0
46.5710	31.9820	45.4430	H	0	30.7920	25.5950	39.6640	C	0	23.7930	27.0440	36.2590	N	0
46.4630	33.7650	45.9460	H	0	31.8720	25.5240	39.5350	H	0	23.6650	28.0130	36.0020	H	0
49.2970	33.6540	46.3350	C	0	30.1780	24.2050	39.2300	C	0	22.4790	26.2830	36.1870	C	0
48.7950	34.6180	46.2560	H	0	29.0970	24.1050	39.3360	H	0	22.2510	26.0520	37.2270	H	0
49.9360	33.7460	47.2140	H	0	30.4640	23.9410	38.2120	H	0	21.4100	27.1550	35.5920	C	0
49.8900	33.3720	45.4660	H	0	30.5080	23.4390	39.9310	H	0	21.4730	28.1340	36.0660	H	0
46.5520	31.3560	48.0630	C	0	30.2790	26.7350	38.7160	C	0	21.6390	27.4720	34.1090	C	0
46.7730	30.1900	48.2220	O	0	30.6820	27.6700	39.1040	H	0	22.6690	27.7650	33.9080	H	0
45.3090	31.7840	48.1700	N	0	30.7640	26.5500	37.7570	H	0	21.3590	26.6130	33.4990	H	0
45.1390	32.7800	48.1940	H	0	29.1950	26.7310	38.6030	H	0	20.9360	28.2240	33.7500	H	0
44.2110	30.8890	48.4360	C	0	29.0730	25.8130	41.4680	C	0	20.0230	26.6010	35.7890	C	0
44.3900	29.9130	47.9850	H	0	28.5650	24.7270	41.6740	O	0	19.8470	25.5940	35.4120	H	0
44.1180	30.7360	49.9580	C	0	28.4440	26.9760	41.4210	N	0	19.8850	26.4320	36.8570	H	0
45.0820	30.3470	50.2850	H	0	29.0350	27.7850	41.2890	H	0	18.9070	27.4380	35.1890	C	0
43.8860	31.6950	50.4210	H	0	26.9670	27.2820	41.8010	C	0	19.0290	28.4850	35.4630	H	0
43.3800	29.9830	50.2340	H	0	26.3720	26.3690	41.7730	H	0	18.9720	27.3750	34.1030	H	0
42.8410	31.2570	47.8060	C	0	27.0220	27.5090	42.8650	H	0	17.9550	27.1250	35.6180	H	0
42.5120	32.4500	47.7540	O	0	26.3750	28.4320	40.9680	C	0	22.5810	24.9660	35.5230	C	0
42.0560	30.2400	47.4430	N	0	27.0470	28.9240	40.0720	O	0	22.1110	24.0060	36.0820	O	0

23.3970	24.8770	34.4300	N	0	16.7680	24.4160	36.5480	H	0	15.0370	29.3640	27.4430	C	0
23.7440	25.7230	34.0020	H	0	17.3220	25.1500	35.1670	H	0	15.6730	30.1060	26.9600	H	0
23.4970	23.6250	33.6610	C	0	15.9120	24.0190	35.0440	H	0	13.7030	29.6430	26.8470	C	0
22.4810	23.2320	33.6870	H	0	17.1880	21.8350	35.8630	C	0	13.0250	28.8980	27.2640	H	0
23.9390	24.0090	32.2090	C	0	16.4330	21.4800	35.1610	H	0	13.3290	30.6030	27.2020	H	0
23.9290	23.1140	31.5880	H	0	17.9640	21.1010	36.0800	H	0	13.6970	29.3760	25.3320	C	0
23.2860	24.8000	31.8410	H	0	16.6620	22.1000	36.7800	H	0	13.2060	28.2280	24.7840	C	0
24.9440	24.4290	32.1740	H	0	19.8520	21.3440	32.3860	C	0	12.7290	27.5250	25.4520	H	0
24.4030	22.5230	34.2530	C	0	20.8670	21.8890	32.0680	O	0	13.2490	27.9520	23.4030	C	0
24.2030	21.3410	34.0030	O	0	19.2490	20.4800	31.5780	N	0	12.7290	27.0660	23.0700	H	0
25.2900	22.9080	35.1760	N	0	17.9200	19.8750	31.7250	C	0	13.7560	28.9120	22.5380	C	0
25.4670	23.8910	35.3230	H	0	17.1400	20.6370	31.7170	H	0	13.7200	28.6070	21.1380	O	0
26.0260	21.9290	35.9760	C	0	17.8880	19.3410	32.6750	H	0	14.2420	29.1830	20.5760	H	0
25.8540	20.9140	35.6160	H	0	17.5950	18.9910	30.5060	C	0	14.3230	30.1070	23.0370	C	0
27.5700	22.1740	35.9610	C	0	16.8340	19.4310	29.8620	H	0	14.7470	30.7590	22.2870	H	0
27.9810	21.3880	36.5950	H	0	17.2920	17.9950	30.8310	H	0	14.3610	30.2990	24.4730	C	0
28.2430	21.9910	34.6020	C	0	19.0640	18.9850	29.8740	C	0	14.6960	31.2100	24.9460	H	0
27.7940	22.6670	33.8740	H	0	18.9370	18.9230	28.7930	H	0	14.9600	29.3970	29.0690	C	0
29.2960	22.2680	34.5460	H	0	19.7090	18.1840	30.2330	H	0	14.6530	30.4370	29.6000	O	0
28.0900	20.9400	34.3580	H	0	19.6960	20.2260	30.2090	C	0	15.2220	28.3070	29.7890	N	0
27.9980	23.5060	36.5620	C	0	20.7750	20.0690	30.2250	H	0	15.5050	27.4800	29.2830	H	0
27.3840	24.3010	36.1370	H	0	19.2910	21.3280	29.2090	C	0	15.0460	28.1290	31.2620	C	0
27.8960	23.4250	37.6440	H	0	18.2920	22.0080	29.4210	O	0	14.0630	28.4860	31.5690	H	0
29.0660	23.6610	36.4140	H	0	19.9400	21.4320	28.0380	N	0	15.1710	26.6340	31.5060	C	0
25.6320	21.8500	37.4510	C	0	21.0780	20.6390	27.6660	C	0	16.1070	26.2810	31.0740	H	0
25.7890	20.7570	38.0090	O	0	21.0110	19.5520	27.6900	H	0	15.1680	26.4660	32.5830	H	0
25.0470	22.9260	38.0090	N	0	21.9420	20.9340	28.2620	H	0	14.3120	26.1490	31.0430	H	0
24.9030	23.7820	37.4930	H	0	21.3710	20.9920	26.1950	C	0	16.1090	28.9870	31.9820	C	0
24.7620	22.9760	39.4860	C	0	20.8070	20.3660	25.5030	H	0	17.2760	28.9300	31.6150	O	0
25.4050	22.2540	39.9890	H	0	22.4380	20.9230	25.9850	H	0	15.7000	29.6780	33.0110	N	0
25.3080	24.2660	39.9460	C	0	20.8350	22.4680	26.0190	C	0	14.7710	29.4280	33.3190	H	0
25.0130	25.0990	39.3080	H	0	20.6140	22.6050	24.9600	H	0	16.4040	30.7510	33.6510	C	0
24.9750	24.4850	40.9600	H	0	21.5200	23.1990	26.4480	H	0	16.0450	30.9410	34.6630	H	0
26.3960	24.2610	39.8870	H	0	19.5950	22.3730	26.8900	C	0	17.4260	30.4860	33.9210	H	0
23.3210	22.7080	39.9040	C	0	19.2770	23.3080	27.3520	H	0	16.6730	31.9910	32.8170	C	0
23.1430	21.9800	40.8990	O	0	18.3600	21.8500	26.1240	C	0	17.7740	32.5710	32.8920	O	0
22.2580	23.1910	39.1690	N	0	17.8930	22.5210	25.2380	O	0	15.7220	32.3590	31.8890	N	0
22.4260	23.8580	38.4300	H	0	17.7750	20.7460	26.4850	N	0	14.8020	31.9460	31.9500	H	0
20.9220	22.4770	39.2730	C	0	18.2190	20.1980	27.2080	H	0	15.7480	33.5220	30.9850	C	0
20.8770	21.8960	40.1940	H	0	16.4910	20.2180	25.9510	C	0	14.7610	33.5140	30.5240	H	0
19.7000	23.4350	39.2640	C	0	16.6740	19.9230	24.9170	H	0	15.9930	34.8750	31.6440	C	0
19.8180	24.0260	38.3560	H	0	16.0860	18.9440	26.6670	C	0	16.9520	34.9590	32.1550	H	0
18.7330	22.9320	39.2430	H	0	15.4830	19.1690	27.5470	H	0	16.0890	35.5410	30.7860	H	0
19.7570	24.4360	40.4640	C	0	15.4560	18.3620	25.9950	H	0	14.9490	35.5320	32.5680	C	0
19.6980	23.7990	41.3470	H	0	17.2290	17.8930	26.9330	C	0	14.0380	35.6270	31.9770	H	0
20.7000	24.9790	40.5400	H	0	18.2240	17.9000	26.1920	O	0	14.7130	34.7380	33.8150	C	0
18.6410	25.4160	40.6010	C	0	16.9020	16.9510	27.6930	O	0	14.2650	33.7970	33.4960	H	0
17.7930	25.6000	39.7460	O	0	15.2610	21.1630	25.9990	C	0	15.5780	34.5840	34.4600	H	0
18.5110	26.0380	41.7550	N	0	14.3150	20.8630	25.3050	O	0	14.0410	35.3320	34.4330	H	0
17.8480	26.7950	41.8430	H	0	15.3640	22.2110	26.8580	N	0	15.5250	36.8760	32.9450	C	0
19.0600	25.8280	42.5750	H	0	16.1850	22.3630	27.4260	H	0	16.4890	36.7990	33.4480	H	0
20.7810	21.4450	38.1880	C	0	14.5210	23.4950	26.7730	C	0	15.6680	37.5910	32.1340	H	0
19.7360	20.7980	38.1490	O	0	14.0120	23.5190	25.8100	H	0	14.8020	37.3660	33.5960	H	0
21.8520	21.2610	37.3620	N	0	13.4580	23.5110	27.9150	C	0	16.6460	33.1970	29.8230	C	0
22.4940	22.0360	37.4430	H	0	12.8380	22.6200	27.8210	H	0	16.9230	34.0580	29.0170	O	0
22.0080	20.3040	36.3160	C	0	13.9900	23.4470	28.8640	H	0	17.0630	31.9360	29.6020	N	0
22.9420	20.5220	35.7970	H	0	12.6890	24.8200	27.8580	C	0	16.5800	31.2150	30.1190	H	0
22.2130	18.9910	37.0140	C	0	12.0480	25.2800	28.8600	O	0	18.1910	31.6850	28.5920	C	0
22.5180	19.0430	38.0590	H	0	12.4210	25.2290	26.7080	O	0	17.8280	30.8580	27.9820	H	0
21.2340	18.5110	36.9900	H	0	15.5830	24.6810	26.8980	C	0	18.2670	32.4410	27.8110	H	0
23.0880	18.1260	36.2420	C	0	16.0150	25.0510	27.9930	O	0	19.4860	31.3240	29.2140	C	0
24.3190	18.4390	36.1660	O	0	15.9140	25.3580	25.7580	N	0	20.3750	30.9900	28.4450	O	0
22.6610	17.0790	35.6240	N	0	15.5300	24.8200	24.4110	C	0	19.6320	31.2320	30.5350	N	0
23.3590	16.5840	35.0870	H	0	14.5780	25.2670	24.1220	H	0	18.8060	31.5970	30.9860	H	0
21.7250	16.7060	35.6960	H	0	15.4580	23.7390	24.5300	H	0	20.8310	30.8080	31.2810	C	0
20.9620	20.3580	35.1910	C	0	16.6720	25.3760	23.5030	C	0	21.6410	31.4690	30.9740	H	0
20.5940	19.3030	34.6650	O	0	16.3000	25.4830	22.4840	H	0	20.6620	31.0870	32.7460	C	0
20.4570	21.5430	34.8300	N	0	17.4520	24.6640	23.7710	H	0	21.6010	31.1560	33.2960	H	0
20.6930	22.3800	35.3420	H	0	17.1400	26.7420	24.2370	C	0	20.2440	32.0910	32.8150	H	0
19.3160	21.5610	33.8630	C	0	16.6180	27.6620	23.9710	H	0	19.8860	30.3980	33.0810	H	0
18.6290	20.7350	34.0450	H	0	18.2090	26.9040	24.1050	H	0	21.2400	29.4010	30.8800	C	0
18.4490	22.8400	33.9790	C	0	16.9400	26.4290	25.7390	C	0	22.4090	29.2250	30.3650	O	0
18.9560	23.7330	33.6150	H	0	17.9240	26.1340	26.1020	H	0	20.3270	28.4040	30.9560	N	0
17.5990	22.5860	33.3460	H	0	16.7200	27.7340	26.5940	C	0	19.3820	28.5590	31.2770	H	0
17.8660	23.0600	35.3930	C	0	17.7190	28.4120	26.8070	O	0	20.7160	27.0360	30.3650	C	0
18.7040	23.2680	36.0580	H	0	15.5020	28.0860	26.9650	N	0	21.6510	26.7540	30.8510	H	0
16.8910	24.2020	35.4870	C	0	14.7370	27.4770	26.7120	H	0	19.6550	25.9990	30.6870	C	0

19.2620	26.3510	31.6410	H	0	25.3570	28.6700	20.1640	N	0	33.7270	21.6560	30.4130	N	0
18.5560	26.1030	29.6660	C	0	25.1030	27.9330	19.5230	H	0	32.8530	21.9670	30.0150	H	0
18.9570	25.8750	28.6780	H	0	25.3380	29.6430	19.8950	H	0	34.6530	22.5600	31.1000	C	0
17.7500	25.4120	29.9120	H	0	27.7640	27.3290	24.3540	C	0	35.6390	22.5470	30.6350	H	0
18.1750	27.1240	29.6850	H	0	28.4810	27.0350	23.4340	O	0	34.0340	23.9560	31.0720	C	0
20.2710	24.6090	30.9320	C	0	28.1970	27.7640	25.5360	N	0	33.9060	24.3940	30.0820	H	0
21.0390	24.3350	30.2090	H	0	27.4920	28.0940	26.1800	H	0	33.0320	23.9680	31.5020	H	0
20.7830	24.6100	31.8950	H	0	29.5890	27.7590	26.0590	C	0	34.5550	24.6730	31.7080	H	0
19.4700	23.8720	31.0020	H	0	30.2110	28.2940	25.3400	H	0	34.8680	22.1090	32.5750	C	0
21.1260	27.0060	28.8920	C	0	29.6670	28.7130	27.2830	C	0	36.0660	22.0600	33.0210	O	0
21.8030	26.0560	28.4360	O	0	29.1550	29.6560	27.0930	H	0	33.8730	21.8540	33.4720	N	0
20.6400	28.0560	28.2130	N	0	29.0890	28.1190	27.9920	H	0	32.9490	21.9640	33.0790	H	0
20.2140	28.8420	28.6810	H	0	30.6680	28.8690	27.6850	H	0	34.0670	21.5670	34.9080	C	0
21.0610	28.3600	26.8640	C	0	30.2320	26.3640	26.5190	C	0	35.0330	21.0630	34.9570	H	0
20.9200	27.5680	26.1280	H	0	31.3360	26.3920	27.0320	O	0	34.3360	22.9250	35.5880	C	0
20.5180	29.2430	26.5260	H	0	29.5310	25.2560	26.3820	N	0	35.1250	23.4590	35.0590	H	0
22.4970	28.7710	26.7360	C	0	28.6460	25.3180	25.8990	H	0	33.0650	23.7630	35.7270	C	0
23.2020	28.0210	26.1020	O	0	30.0190	23.9090	26.7440	C	0	32.2340	23.3610	36.3080	H	0
22.8860	29.9020	27.2880	N	0	29.3960	23.1090	26.3420	H	0	33.4030	24.6910	36.1890	H	0
22.2420	30.4880	27.7990	H	0	30.9860	23.8290	26.2470	H	0	32.7170	23.9890	34.7190	H	0
24.3250	30.3500	27.1910	C	0	30.1990	23.6890	28.2560	C	0	34.7450	22.6650	36.9430	O	0
24.6420	30.3030	26.1490	H	0	31.1000	22.9140	28.6190	O	0	35.6300	22.2950	36.9380	H	0
24.5700	31.7980	27.6860	C	0	29.4820	24.3360	29.2170	N	0	32.9720	20.6750	35.5910	C	0
25.6340	32.0210	27.7610	H	0	28.8520	25.0950	29.0020	H	0	32.1790	20.0500	34.9060	O	0
23.8780	32.7380	26.7070	C	0	29.9510	24.1580	30.6280	C	0	32.8560	20.5920	36.9010	N	0
24.0670	33.7720	26.9960	H	0	30.9400	24.6130	30.5730	H	0	33.4400	21.1960	37.4610	H	0
24.1260	32.4930	25.6740	H	0	29.0020	25.0250	31.5180	C	0	31.7730	19.8540	37.7220	C	0
22.7880	32.7460	26.6980	H	0	28.6420	25.9220	31.0140	H	0	30.8520	19.8390	37.1390	H	0
23.8110	32.0080	29.0770	C	0	28.1200	24.4790	31.8530	H	0	32.1550	18.3660	37.8380	C	0
22.7420	31.8040	29.0220	H	0	29.6150	25.4350	32.8770	C	0	32.4570	17.8610	36.9210	H	0
24.1930	31.3740	29.8770	H	0	29.9130	24.5520	33.4420	H	0	32.9850	17.9980	39.0550	C	0
23.9950	33.0320	29.4010	H	0	30.8130	26.3770	32.9140	C	0	33.7950	17.3720	38.6820	H	0
25.3280	29.4050	27.9870	C	0	30.8840	27.0270	33.7860	H	0	33.5080	18.8600	39.4710	H	0
26.3600	29.0600	27.4560	O	0	31.8240	25.9710	32.9030	H	0	32.3470	17.5990	39.8440	H	0
24.8740	28.7420	29.1060	N	0	30.7400	26.9910	32.0160	H	0	30.9210	17.7270	38.0370	O	0
24.0060	29.0500	29.5190	H	0	28.5090	25.9670	33.8530	C	0	30.4610	17.5330	37.2180	H	0
25.8100	27.7950	29.8040	C	0	28.9380	26.3110	34.7940	H	0	31.4940	20.5430	39.1120	C	0
26.7970	28.1880	30.0510	H	0	27.8490	26.5950	33.2540	H	0	32.1030	21.5500	39.4150	O	0
25.2670	27.5950	31.2430	C	0	27.8890	25.1230	34.1550	H	0	30.5170	20.0940	39.8820	N	0
25.2650	28.5990	31.6680	H	0	30.0250	22.7120	31.2440	C	0	29.8620	19.4280	39.4990	H	0
24.3120	27.0740	31.3180	H	0	31.0560	22.4560	31.9150	O	0	30.4000	20.6840	41.2200	C	0
25.9710	27.0560	31.8770	H	0	29.1690	21.7100	31.0120	N	0	30.4090	21.7440	40.9630	H	0
26.1420	26.5170	29.0220	C	0	27.8580	21.8400	30.3650	C	0	28.9460	20.4140	41.8490	C	0
27.3250	26.1480	28.8170	O	0	27.8120	22.0070	29.2890	H	0	28.9480	20.9440	42.8010	H	0
25.1090	26.0050	28.3300	N	0	27.2670	22.5090	30.9900	H	0	27.7580	20.9860	41.1100	C	0
24.2030	26.4450	28.4060	H	0	27.0850	20.5210	30.5610	C	0	26.8980	20.9300	41.7780	H	0
25.3760	24.8720	27.3970	C	0	26.5520	20.3450	29.6270	H	0	27.9300	22.0590	41.0400	H	0
26.1160	24.2320	27.8790	H	0	26.3570	20.5790	31.3700	H	0	27.5610	20.4420	40.1870	H	0
24.0730	24.0830	27.2050	C	0	28.2280	19.5540	30.7510	C	0	28.7710	18.8990	42.0770	C	0
23.6410	23.7880	28.1610	H	0	28.4830	19.1630	29.7660	H	0	27.8100	18.6080	42.5010	H	0
23.3590	24.7470	26.7170	H	0	27.9100	18.7000	31.3490	H	0	29.0010	18.3190	41.1830	H	0
24.3110	22.7860	26.4230	C	0	29.4410	20.2890	31.2980	C	0	29.4830	18.5900	42.8430	H	0
23.9900	22.7590	25.0830	C	0	29.3350	20.2000	32.3790	H	0	31.4600	20.3320	42.2410	C	0
23.3990	23.5290	24.6090	H	0	30.7180	19.5650	30.8750	C	0	32.2350	19.4010	42.1860	O	0
24.1890	21.5700	24.3560	C	0	31.1330	18.6740	31.5740	O	0	31.4000	21.0700	43.3770	N	0
23.9340	21.4880	23.3100	H	0	31.4350	20.0290	29.7970	N	0	30.5510	21.6130	43.4420	H	0
24.7970	20.4890	24.9690	C	0	31.1360	20.8570	29.3020	H	0	32.1780	20.9120	44.5540	C	0
25.1010	19.4330	24.1760	O	0	32.7910	19.5770	29.3840	C	0	31.8570	20.0220	45.0940	H	0
25.6750	18.8060	24.6210	H	0	32.8690	18.5070	29.5770	H	0	33.2530	20.8630	44.3770	H	0
25.0370	20.5420	26.3600	C	0	32.9250	19.9070	27.8620	C	0	31.9260	22.0130	45.6400	C	0
25.3650	19.6800	26.9220	H	0	32.1430	19.4010	27.2950	H	0	30.8530	22.5900	45.7550	O	0
24.8720	21.7380	27.1200	C	0	32.7820	20.9830	27.7600	H	0	32.9700	22.2850	46.4200	N	0
25.1030	21.8450	28.1700	H	0	34.2190	19.3880	27.2190	C	0	33.8590	21.8050	46.4110	H	0
26.0080	25.3510	26.1470	C	0	35.1470	19.6790	27.7120	H	0	32.8010	23.0770	47.6080	C	0
26.7820	24.6480	25.5090	O	0	34.2530	18.2990	27.2470	H	0	32.5640	24.1240	47.4220	H	0
25.6170	26.5180	25.6230	N	0	34.2760	19.8500	25.7570	C	0	31.9250	22.7650	48.1770	H	0
24.7890	26.9240	26.0340	H	0	33.5890	19.2200	25.1930	H	0	34.0420	22.9830	48.4980	C	0
26.1530	27.1060	24.3370	C	0	34.1780	20.9350	25.7940	H	0	33.8270	22.6550	49.6870	O	0
26.0490	26.3330	23.5760	H	0	35.6360	19.6820	25.1370	C	0	35.2640	23.0910	47.9250	N	0
25.3700	28.4060	23.9030	C	0	36.2670	20.4760	25.5350	H	0	35.3240	23.3560	46.9520	H	0
24.3500	28.0480	23.7660	H	0	36.0470	18.7030	25.3850	H	0	36.5560	22.8710	48.6250	C	0
25.4200	29.2160	24.6300	H	0	35.7100	19.6300	23.6240	N	0	36.2830	22.5340	49.6250	H	0
25.7680	29.1090	22.5930	C	0	34.9250	19.0710	23.3200	H	0	37.5250	21.7630	48.1010	C	0
25.2490	30.0660	22.5440	H	0	35.7320	20.5390	23.1850	H	0	37.5570	21.9310	47.0250	H	0
26.8290	29.3510	22.6500	H	0	36.5170	19.2600	23.1430	H	0	38.5410	21.8930	48.4740	H	0
25.5030	28.1920	21.3930	C	0	33.9110	20.4000	30.1170	C	0	37.0730	20.3000	48.2700	C	0
25.3140	26.9960	21.4890	O	0	35.0090	19.9730	30.3860	O	0	37.6750	19.7450	47.5510	H	0

37.3860	19.9000	49.2350	H	0	46.8030	25.4290	41.5780	H	0
35.5340	20.0150	47.9920	C	0	47.7610	26.4680	43.2590	C	0
34.9180	19.3840	48.8480	O	0	48.7440	26.2200	42.8860	H	0
34.9030	20.3920	46.9650	O	0	50.2620	28.2290	47.2020	C	0
37.2560	24.2450	48.8280	C	0	50.1460	29.3100	47.8120	O	0
37.1600	25.1540	48.0200	O	0	51.5190	27.7590	46.9120	N	0
38.1150	24.3600	49.8230	N	0	51.6390	26.9180	46.3660	H	0
38.2740	23.5410	50.3920	H	0	52.7840	28.4000	47.2920	C	0
39.2320	25.3720	49.9900	C	0	52.6480	29.4810	47.2570	H	0
38.9770	26.3320	49.5420	H	0	53.1310	27.9410	48.7400	C	0
39.4990	25.7010	51.4720	C	0	53.6100	26.9690	48.6150	H	0
38.6400	26.2180	51.9000	H	0	53.7100	28.6040	49.3830	H	0
39.6020	24.7270	51.9500	H	0	52.1400	27.8610	49.1860	H	0
40.7200	26.4950	51.8410	C	0	53.9290	27.9050	46.3740	C	0
41.6270	25.9160	51.6650	H	0	53.7750	26.9140	45.6880	O	0
40.8210	27.8540	51.1230	C	0	55.0750	28.6030	46.3090	N	0
40.8480	27.6150	50.0600	H	0	55.1440	29.4020	46.9230	H	0
39.9210	28.4440	51.2980	H	0	56.2400	28.1490	45.5930	C	0
41.7210	28.2930	51.5540	H	0	55.9380	27.8140	44.6010	H	0
40.6290	26.8880	53.3260	C	0	57.2320	29.3180	45.3700	C	0
41.3790	27.5360	53.7800	H	0	57.4300	29.7880	46.3340	H	0
39.6610	27.2390	53.6840	H	0	58.1670	28.8980	44.9990	H	0
40.7580	25.9090	53.7870	H	0	56.6300	30.4420	44.5110	C	0
40.5140	24.8740	49.3030	C	0	55.7060	30.8500	44.9220	H	0
40.8540	23.7100	49.5040	O	0	57.6760	31.5340	44.3410	C	0
41.2210	25.6640	48.4480	N	0	57.1390	32.4110	43.9790	H	0
40.7600	26.5510	48.3040	H	0	57.9050	31.9390	45.3270	H	0
42.5130	25.4700	47.7890	C	0	58.6270	31.1820	43.9430	H	0
42.9290	24.5320	48.1550	H	0	56.4360	29.8870	43.1160	C	0
42.2750	25.0510	46.2850	C	0	55.5920	29.1980	43.0850	H	0
41.6980	25.8770	45.8690	H	0	56.2500	30.6360	42.3470	H	0
43.2440	25.0680	45.7870	H	0	57.3340	29.4150	42.7150	H	0
41.5250	23.8800	45.8000	C	0	56.8200	26.9080	46.2820	C	0
40.1070	23.8950	45.8140	C	0	56.9030	26.8020	47.4950	O	0
39.6710	24.7250	46.3490	H	0	57.2940	26.0260	45.5570	O	0
39.3040	22.9060	45.2110	C	0	21.3290	37.4830	45.3400	N	0
38.2720	22.9650	45.5250	H	0	22.0680	36.4300	44.8540	C	0
39.8570	21.7070	44.7130	C	0	23.2080	35.7670	45.6530	C	0
39.0170	20.6490	44.4170	O	0	24.0350	35.0200	45.1380	O	0
38.1090	20.8980	44.6070	H	0	23.4490	36.2260	46.7080	O	0
41.3390	21.6260	44.7440	C	0	21.6920	36.2220	43.5480	C	0
41.7750	20.7650	44.2610	H	0	20.6940	37.0940	43.1470	C	0
42.1160	22.6720	45.2680	C	0	20.4550	37.8470	44.2930	C	0
43.1890	22.6300	45.1540	H	0	19.9380	37.1390	41.9160	C	0
43.5920	26.5950	47.9460	C	0	20.1300	36.3270	41.0650	O	0
43.2590	27.8000	47.9500	O	0	18.8970	38.2870	41.8280	C	0
44.7720	26.1270	48.1980	N	0	18.2270	38.4070	40.8190	O	0
44.8020	25.1220	48.2960	H	0	18.8480	39.1980	43.0310	C	0
45.9300	26.9180	48.8350	C	0	17.9770	40.2990	42.8840	N	0
45.7070	27.9670	48.6390	H	0	17.9110	41.2080	43.9020	C	0
46.0090	26.5680	50.3580	C	0	16.9940	42.4330	43.8380	C	0
46.2130	25.5040	50.4750	H	0	16.5640	42.8100	42.7770	O	0
47.1450	27.4690	50.9930	C	0	16.3890	42.9200	44.8140	O	0
48.1570	27.0820	50.8690	H	0	18.5710	40.9510	45.0980	C	0
47.1400	28.4540	50.5260	H	0	19.3210	39.7730	45.3560	C	0
47.0690	27.3870	52.0780	H	0	19.8350	39.5260	46.7010	C	0
44.7350	26.9490	51.0870	C	0	19.0920	39.1880	47.6090	O	0
43.8360	26.4300	50.7530	H	0	21.0100	39.6240	46.9110	O	0
44.9030	26.7110	52.1370	H	0	19.5820	38.9330	44.2360	C	0
44.5570	28.0240	51.0660	H	0	21.4540	38.0200	46.1870	H	0
47.1750	26.6480	48.0290	C	0	18.1870	41.6170	45.8670	H	0
47.4330	25.4980	47.7540	O	0	22.0970	35.4030	42.9620	H	0
47.9220	27.6270	47.6180	N	0	16.3050	43.1870	40.6690	Yb	0
47.7260	28.5400	48.0030	H	0					
49.0880	27.4530	46.6820	C	0					
49.3350	26.3920	46.6470	H	0					
48.7590	27.8430	45.1830	C	0					
48.5760	28.9050	45.0210	H	0					
49.6290	27.6790	44.5470	H	0					
47.5520	27.2650	44.4590	C	0					
46.1940	27.5730	44.8240	C	0					
45.9700	28.2430	45.6410	H	0					
45.1310	27.0350	44.0590	C	0					
44.1620	27.2810	44.4690	H	0					
45.2620	26.1030	42.9830	C	0					
44.3900	25.7260	42.4710	H	0					
46.6400	25.9380	42.5170	C	0					