

# Synthesis, X-ray structure, Conformational Analysis and DFT Studies of a giant *s*-triazine *bis*-Schiff base

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## CIF data

**Table S1.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **4**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
O(1)	5182(1)	3182(1)	7066(1)	28(1)
O(2)	865(1)	3145(1)	5234(1)	30(1)
N(1)	3837(1)	2927(1)	6542(1)	21(1)
N(2)	3515(1)	3237(1)	6259(1)	23(1)
N(3)	4740(1)	5091(1)	6321(1)	21(1)
N(4)	4501(1)	6461(1)	5921(1)	25(1)
N(5)	3419(1)	4488(1)	5875(1)	23(1)
N(6)	5775(1)	7012(1)	6349(1)	26(1)
N(7)	3474(1)	5820(1)	5489(1)	27(1)
N(8)	2728(1)	5003(1)	5314(1)	25(1)
C(1)	4510(1)	2108(1)	7128(1)	23(1)
C(2)	4796(2)	1624(1)	7403(1)	30(1)
C(3)	4106(2)	542(1)	7478(1)	33(1)
C(4)	3130(2)	-79(1)	7280(1)	31(1)
C(5)	2865(2)	389(1)	7005(1)	26(1)
C(6)	3555(1)	1483(1)	6923(1)	22(1)
C(7)	3289(1)	1910(1)	6627(1)	22(1)
C(8)	3917(1)	4335(1)	6152(1)	20(1)
C(9)	5006(1)	6163(1)	6191(1)	21(1)
C(10)	6420(2)	6802(1)	6643(1)	26(1)
C(11)	5951(2)	7818(1)	6846(1)	26(1)

C(12)	6463(2)	9017(1)	6721(1)	26(1)
C(13)	5761(2)	9178(1)	6415(1)	30(1)
C(14)	6267(2)	8152(1)	6219(1)	31(1)
C(15)	3801(1)	5567(1)	5773(1)	23(1)
C(16)	2599(2)	5253(1)	5042(1)	26(1)
C(17)	1792(2)	4433(1)	4843(1)	26(1)
C(18)	1812(2)	4661(1)	4543(1)	36(1)
C(19)	1033(2)	3904(2)	4348(1)	46(1)
C(20)	191(2)	2923(1)	4452(1)	44(1)
C(21)	127(2)	2687(1)	4748(1)	35(1)
C(22)	940(2)	3426(1)	4944(1)	27(1)

**Table S2.** Bond lengths [Å] and angles [°] for **4**.

O(1)-C(1)	1.3578(14)
O(1)-H(1)	0.96(2)
O(2)-C(22)	1.3624(16)
O(2)-H(2)	0.93(2)
N(1)-C(7)	1.2882(15)
N(1)-N(2)	1.3697(13)
N(2)-C(8)	1.3691(15)
N(2)-H(2A)	0.883(17)
N(3)-C(8)	1.3291(15)
N(3)-C(9)	1.3622(15)
N(4)-C(15)	1.3394(15)
N(4)-C(9)	1.3477(15)
N(5)-C(15)	1.3379(15)
N(5)-C(8)	1.3445(15)
N(6)-C(9)	1.3493(15)
N(6)-C(10)	1.4657(15)
N(6)-C(14)	1.4707(15)
N(7)-C(15)	1.3565(15)
N(7)-N(8)	1.3622(14)
N(7)-H(7)	0.926(18)
N(8)-C(16)	1.2831(16)
C(1)-C(2)	1.3915(17)
C(1)-C(6)	1.4068(16)
C(2)-C(3)	1.3838(19)
C(2)-H(2B)	0.9500
C(3)-C(4)	1.390(2)
C(3)-H(3)	0.9500

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C(4)-C(5)	1.3840(18)
C(4)-H(4)	0.9500
C(5)-C(6)	1.4047(16)
C(5)-H(5)	0.9500
C(6)-C(7)	1.4519(16)
C(7)-H(7A)	0.9500
C(10)-C(11)	1.5223(16)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.5259(16)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.5206(17)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.5216(18)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(16)-C(17)	1.4539(16)
C(16)-H(16)	0.9500
C(17)-C(18)	1.3974(18)
C(17)-C(22)	1.4076(18)
C(18)-C(19)	1.386(2)
C(18)-H(18)	0.9500
C(19)-C(20)	1.384(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.382(2)
C(20)-H(20)	0.9500
C(21)-C(22)	1.3921(18)
C(21)-H(21)	0.9500
C(1)-O(1)-H(1)	107.1(12)
C(22)-O(2)-H(2)	108.6(13)
C(7)-N(1)-N(2)	116.50(10)
C(8)-N(2)-N(1)	121.50(10)
C(8)-N(2)-H(2A)	117.6(10)
N(1)-N(2)-H(2A)	119.4(10)
C(8)-N(3)-C(9)	113.29(10)
C(15)-N(4)-C(9)	113.93(10)
C(15)-N(5)-C(8)	112.03(10)

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C(9)-N(6)-C(10)	122.81(10)
C(9)-N(6)-C(14)	121.91(10)
C(10)-N(6)-C(14)	114.56(10)
C(15)-N(7)-N(8)	120.60(10)
C(15)-N(7)-H(7)	119.6(11)
N(8)-N(7)-H(7)	119.8(11)
C(16)-N(8)-N(7)	117.41(10)
O(1)-C(1)-C(2)	118.15(11)
O(1)-C(1)-C(6)	121.81(11)
C(2)-C(1)-C(6)	120.03(11)
C(3)-C(2)-C(1)	120.06(12)
C(3)-C(2)-H(2B)	120.0
C(1)-C(2)-H(2B)	120.0
C(2)-C(3)-C(4)	120.87(12)
C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	119.28(12)
C(5)-C(4)-H(4)	120.4
C(3)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	121.08(12)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-C(1)	118.64(11)
C(5)-C(6)-C(7)	118.78(11)
C(1)-C(6)-C(7)	122.55(10)
N(1)-C(7)-C(6)	121.62(10)
N(1)-C(7)-H(7A)	119.2
C(6)-C(7)-H(7A)	119.2
N(3)-C(8)-N(5)	128.15(10)
N(3)-C(8)-N(2)	119.44(10)
N(5)-C(8)-N(2)	112.40(10)
N(4)-C(9)-N(6)	117.02(10)
N(4)-C(9)-N(3)	124.90(10)
N(6)-C(9)-N(3)	118.02(10)
N(6)-C(10)-C(11)	110.59(10)
N(6)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10A)	109.5
N(6)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1
C(10)-C(11)-C(12)	111.57(10)
C(10)-C(11)-H(11A)	109.3

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C(12)-C(11)-H(11A)	109.3
C(10)-C(11)-H(11B)	109.3
C(12)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
C(13)-C(12)-C(11)	110.46(10)
C(13)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12A)	109.6
C(13)-C(12)-H(12B)	109.6
C(11)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
C(12)-C(13)-C(14)	110.68(10)
C(12)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	108.1
N(6)-C(14)-C(13)	110.55(10)
N(6)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14A)	109.5
N(6)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	108.1
N(5)-C(15)-N(4)	127.31(11)
N(5)-C(15)-N(7)	118.57(10)
N(4)-C(15)-N(7)	114.12(10)
N(8)-C(16)-C(17)	120.46(11)
N(8)-C(16)-H(16)	119.8
C(17)-C(16)-H(16)	119.8
C(18)-C(17)-C(22)	118.65(12)
C(18)-C(17)-C(16)	119.61(12)
C(22)-C(17)-C(16)	121.71(11)
C(19)-C(18)-C(17)	120.94(14)
C(19)-C(18)-H(18)	119.5
C(17)-C(18)-H(18)	119.5
C(20)-C(19)-C(18)	119.66(14)
C(20)-C(19)-H(19)	120.2
C(18)-C(19)-H(19)	120.2
C(21)-C(20)-C(19)	120.61(13)
C(21)-C(20)-H(20)	119.7
C(19)-C(20)-H(20)	119.7
C(20)-C(21)-C(22)	120.11(14)
C(20)-C(21)-H(21)	119.9

C(22)-C(21)-H(21)	119.9
O(2)-C(22)-C(21)	117.92(12)
O(2)-C(22)-C(17)	122.06(11)
C(21)-C(22)-C(17)	120.01(12)

**Table S3.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **4**. The anisotropic

displacement factor exponent takes the form:  $-2p^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
O(1)	34(1)	24(1)	28(1)	-2(1)	-1(1)	-7(1)
O(2)	40(1)	19(1)	33(1)	3(1)	-3(1)	-3(1)
N(1)	24(1)	18(1)	22(1)	1(1)	1(1)	1(1)
N(2)	29(1)	17(1)	22(1)	1(1)	-2(1)	-4(1)
N(3)	25(1)	16(1)	23(1)	-1(1)	0(1)	1(1)
N(4)	34(1)	16(1)	24(1)	0(1)	-4(1)	-3(1)
N(5)	29(1)	16(1)	23(1)	0(1)	-3(1)	-1(1)
N(6)	38(1)	18(1)	22(1)	0(1)	-4(1)	-6(1)
N(7)	41(1)	16(1)	25(1)	2(1)	-9(1)	-5(1)
N(8)	32(1)	17(1)	26(1)	-1(1)	-7(1)	-1(1)
C(1)	22(1)	21(1)	27(1)	-2(1)	2(1)	1(1)
C(2)	31(1)	35(1)	25(1)	0(1)	-2(1)	-1(1)
C(3)	34(1)	37(1)	28(1)	9(1)	1(1)	4(1)
C(4)	34(1)	24(1)	35(1)	8(1)	4(1)	0(1)
C(5)	28(1)	21(1)	30(1)	2(1)	2(1)	-1(1)
C(6)	22(1)	18(1)	25(1)	1(1)	1(1)	2(1)
C(7)	23(1)	17(1)	25(1)	-1(1)	-1(1)	-1(1)
C(8)	21(1)	16(1)	23(1)	-1(1)	2(1)	3(1)
C(9)	23(1)	17(1)	23(1)	-2(1)	1(1)	1(1)
C(10)	34(1)	18(1)	25(1)	0(1)	-6(1)	-1(1)
C(11)	30(1)	23(1)	25(1)	-2(1)	-2(1)	-4(1)
C(12)	28(1)	20(1)	30(1)	-3(1)	-4(1)	-2(1)
C(13)	37(1)	18(1)	35(1)	2(1)	-10(1)	-4(1)
C(14)	47(1)	21(1)	25(1)	2(1)	-4(1)	-11(1)
C(15)	27(1)	17(1)	24(1)	0(1)	-3(1)	1(1)
C(16)	34(1)	18(1)	26(1)	2(1)	-4(1)	-2(1)
C(17)	33(1)	21(1)	26(1)	-1(1)	-6(1)	2(1)
C(18)	52(1)	31(1)	27(1)	1(1)	-4(1)	0(1)

C(19)	68(1)	44(1)	26(1)	-6(1)	-12(1)	7(1)
C(20)	56(1)	32(1)	44(1)	-16(1)	-23(1)	8(1)
C(21)	36(1)	21(1)	48(1)	-5(1)	-14(1)	2(1)
C(22)	31(1)	18(1)	31(1)	-1(1)	-6(1)	3(1)

**Table S4.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **4**.

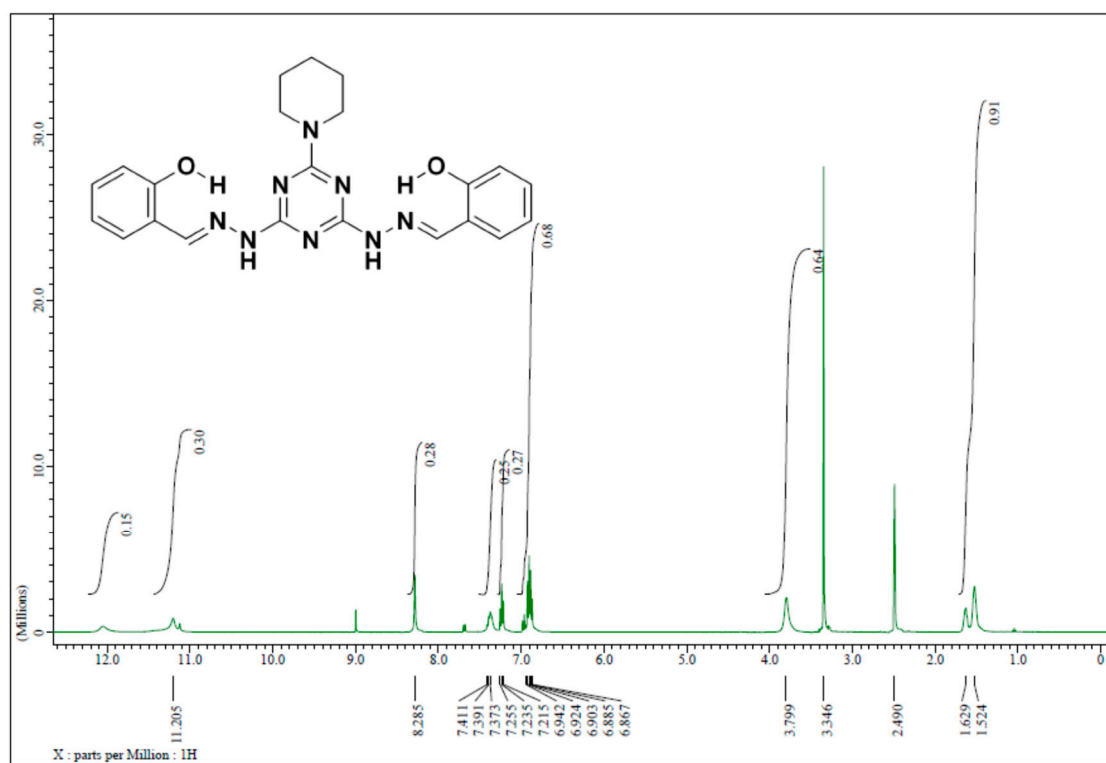
	x	y	z	U(eq)
H(2B)	5465	2037	7540	36
H(3)	4303	220	7666	39
H(4)	2650	-816	7334	37
H(5)	2205	-36	6869	32
H(7A)	2696	1429	6493	26
H(10A)	7635	6730	6635	31
H(10B)	5970	6048	6720	31
H(11A)	6492	7701	7038	31
H(11B)	4744	7811	6878	31
H(12A)	6057	9661	6849	31
H(12B)	7680	9067	6713	31
H(13A)	6168	9934	6332	36
H(13B)	4544	9220	6426	36
H(14A)	5737	8243	6025	37
H(14B)	7476	8164	6190	37
H(16)	3034	5979	4970	31
H(18)	2367	5345	4471	44
H(19)	1077	4059	4144	55
H(20)	-348	2406	4318	53
H(21)	-472	2020	4817	42
H(7)	3760(20)	6555(16)	5414(4)	37(4)
H(2A)	2840(20)	2793(15)	6153(3)	30(4)
H(2)	1460(30)	3700(20)	5338(5)	58(6)
H(1)	4890(20)	3368(17)	6868(4)	46(5)

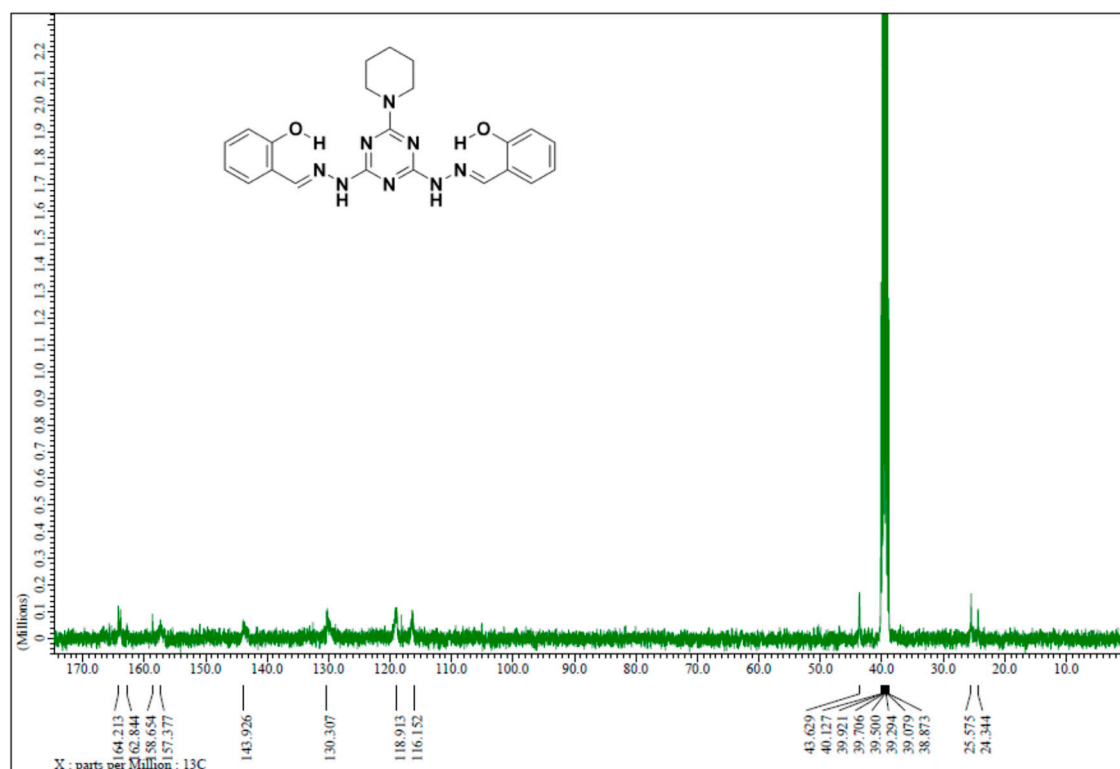
**Table S5** Torsion angles [°] for **4**.

C(7)-N(1)-N(2)-C(8)	174.48(10)
C(15)-N(7)-N(8)-C(16)	-173.37(12)
O(1)-C(1)-C(2)-C(3)	178.70(11)
C(6)-C(1)-C(2)-C(3)	-1.69(19)
C(1)-C(2)-C(3)-C(4)	0.3(2)
C(2)-C(3)-C(4)-C(5)	0.8(2)
C(3)-C(4)-C(5)-C(6)	-0.47(19)
C(4)-C(5)-C(6)-C(1)	-0.88(18)
C(4)-C(5)-C(6)-C(7)	177.68(11)
O(1)-C(1)-C(6)-C(5)	-178.44(11)
C(2)-C(1)-C(6)-C(5)	1.96(17)
O(1)-C(1)-C(6)-C(7)	3.04(17)
C(2)-C(1)-C(6)-C(7)	-176.55(11)
N(2)-N(1)-C(7)-C(6)	179.86(10)
C(5)-C(6)-C(7)-N(1)	177.31(11)
C(1)-C(6)-C(7)-N(1)	-4.18(18)
C(9)-N(3)-C(8)-N(5)	3.71(17)
C(9)-N(3)-C(8)-N(2)	-177.74(10)
C(15)-N(5)-C(8)-N(3)	-2.01(17)
C(15)-N(5)-C(8)-N(2)	179.36(10)
N(1)-N(2)-C(8)-N(3)	4.72(16)
N(1)-N(2)-C(8)-N(5)	-176.52(10)
C(15)-N(4)-C(9)-N(6)	177.74(11)
C(15)-N(4)-C(9)-N(3)	-4.97(17)
C(10)-N(6)-C(9)-N(4)	-178.59(11)
C(14)-N(6)-C(9)-N(4)	-8.87(18)
C(10)-N(6)-C(9)-N(3)	3.93(18)
C(14)-N(6)-C(9)-N(3)	173.64(11)
C(8)-N(3)-C(9)-N(4)	0.15(16)
C(8)-N(3)-C(9)-N(6)	177.42(10)
C(9)-N(6)-C(10)-C(11)	-134.52(12)
C(14)-N(6)-C(10)-C(11)	55.07(14)
N(6)-C(10)-C(11)-C(12)	-53.27(14)
C(10)-C(11)-C(12)-C(13)	54.40(14)
C(11)-C(12)-C(13)-C(14)	-55.19(14)
C(9)-N(6)-C(14)-C(13)	133.16(12)
C(10)-N(6)-C(14)-C(13)	-56.34(15)
C(12)-C(13)-C(14)-N(6)	55.32(15)
C(8)-N(5)-C(15)-N(4)	-3.99(18)
C(8)-N(5)-C(15)-N(7)	175.55(11)



C(9)-N(4)-C(15)-N(5)	7.18(18)
C(9)-N(4)-C(15)-N(7)	-172.37(11)
N(8)-N(7)-C(15)-N(5)	1.92(18)
N(8)-N(7)-C(15)-N(4)	-178.48(11)
N(7)-N(8)-C(16)-C(17)	-178.96(11)
N(8)-C(16)-C(17)-C(18)	-173.45(13)
N(8)-C(16)-C(17)-C(22)	8.56(19)
C(22)-C(17)-C(18)-C(19)	-1.0(2)
C(16)-C(17)-C(18)-C(19)	-179.07(14)
C(17)-C(18)-C(19)-C(20)	1.5(2)
C(18)-C(19)-C(20)-C(21)	-0.4(3)
C(19)-C(20)-C(21)-C(22)	-1.2(2)
C(20)-C(21)-C(22)-O(2)	-178.89(13)
C(20)-C(21)-C(22)-C(17)	1.7(2)
C(18)-C(17)-C(22)-O(2)	-179.97(12)
C(16)-C(17)-C(22)-O(2)	-1.96(19)
C(18)-C(17)-C(22)-C(21)	-0.57(19)
C(16)-C(17)-C(22)-C(21)	177.43(12)



Figure S1.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of 4**Cartesian coordinated at the optimized geometry of the studied conformers:**

4			
O	4.709758000	-0.741204000	-0.122797000
O	-4.173452000	-2.218684000	0.110491000
N	2.218360000	-1.577768000	-0.022929000
N	0.890369000	-1.338962000	-0.014031000
N	1.214766000	0.959357000	-0.195157000
N	-0.735514000	2.342734000	-0.302136000
N	-0.968876000	-0.033901000	-0.104241000
N	1.393435000	3.265208000	-0.379170000
N	-2.804060000	1.394827000	-0.206263000
N	-3.665546000	0.361140000	-0.104052000
C	5.042812000	-2.043246000	-0.046276000
C	6.404556000	-2.376762000	-0.052603000
H	7.125761000	-1.568993000	-0.118550000
C	6.806521000	-3.705084000	0.022974000
H	7.866665000	-3.941672000	0.016117000
C	5.861297000	-4.735901000	0.107162000
H	6.179228000	-5.771590000	0.165667000
C	4.511219000	-4.415362000	0.114692000
H	3.764867000	-5.203707000	0.179334000
C	4.071866000	-3.080274000	0.039336000
C	2.648249000	-2.792684000	0.048553000
H	1.955598000	-3.640767000	0.116711000
C	0.376395000	-0.068623000	-0.109666000
C	0.603820000	2.163627000	-0.291085000
C	2.856414000	3.188647000	-0.381787000
H	3.220044000	3.517901000	-1.367445000
H	3.148082000	2.149522000	-0.246809000
C	3.446540000	4.088897000	0.711829000
H	4.540042000	4.064940000	0.642331000
H	3.176088000	3.676619000	1.692103000
C	2.923872000	5.527836000	0.591926000
H	3.300229000	6.143591000	1.416533000
H	3.307507000	5.976488000	-0.335656000
C	1.388907000	5.546044000	0.564413000

H	1.015409000	6.561449000	0.386763000
H	0.996087000	5.222346000	1.536717000
C	0.842315000	4.613184000	-0.524577000
H	-0.242892000	4.543538000	-0.487332000
H	1.125976000	4.999287000	-1.516117000
C	-1.441251000	1.210717000	-0.202621000
C	-4.935630000	0.589691000	-0.096495000
H	-5.332660000	1.610049000	-0.170957000
C	-5.890002000	-0.499700000	0.011754000
C	-7.268734000	-0.215857000	0.020861000
H	-7.584578000	0.822173000	-0.054031000
C	-8.216644000	-1.224027000	0.122454000
H	-9.274595000	-0.983468000	0.127800000
C	-7.788735000	-2.554760000	0.217687000
H	-8.519491000	-3.354462000	0.297396000
C	-6.434603000	-2.867445000	0.211604000
H	-6.089462000	-3.893346000	0.285009000
C	-5.469266000	-1.855530000	0.110121000
H	-3.133138000	2.353153000	-0.275335000
H	0.215339000	-2.096507000	0.038711000
H	-3.614711000	-1.407932000	0.035644000
H	3.724113000	-0.668291000	-0.111848000
4a			
O	5.026477000	-0.854530000	-0.159388000
O	-4.027917000	-2.292136000	0.114063000
N	2.315853000	-1.367308000	-0.055465000
N	0.980442000	-1.161357000	-0.048297000
N	1.188410000	1.157235000	-0.218543000
N	-0.830812000	2.440750000	-0.296961000
N	-0.938453000	0.053245000	-0.116968000
N	1.253940000	3.464856000	-0.381576000
N	-2.846498000	1.385571000	-0.196562000
N	-3.654424000	0.310660000	-0.099022000
C	5.219177000	-2.195243000	-0.057249000
C	6.505936000	-2.744837000	-0.040998000
H	7.363160000	-2.077891000	-0.111844000
C	6.698628000	-4.120426000	0.063678000
H	7.707802000	-4.520959000	0.073959000
C	5.596981000	-4.971832000	0.153838000
H	5.732895000	-6.045160000	0.235461000
C	4.317662000	-4.427122000	0.137280000
H	3.455166000	-5.085153000	0.206659000
C	4.086836000	-3.042732000	0.033317000
C	2.697773000	-2.593804000	0.025654000
H	1.956185000	-3.403566000	0.096630000
C	0.410845000	0.083803000	-0.132799000
C	0.515477000	2.325196000	-0.298048000
C	2.717599000	3.441389000	-0.400944000
H	3.059420000	3.801653000	-1.384167000
H	3.040320000	2.407776000	-0.287169000
C	3.285675000	4.344447000	0.702025000
H	4.378922000	4.367144000	0.620918000
H	3.043196000	3.904602000	1.677651000
C	2.706209000	5.763914000	0.613446000
H	3.068316000	6.380357000	1.444127000
H	3.061324000	6.242395000	-0.310711000
C	1.170989000	5.724313000	0.603430000
H	0.758010000	6.728243000	0.448880000
H	0.803216000	5.368912000	1.574425000
C	0.646396000	4.789211000	-0.495100000
H	-0.434597000	4.673788000	-0.442529000
H	0.896661000	5.206670000	-1.483304000
C	-1.473974000	1.270603000	-0.202284000
C	-4.934566000	0.473258000	-0.091635000
H	-5.383744000	1.471958000	-0.163778000
C	-5.831483000	-0.664663000	0.013625000
C	-7.223010000	-0.453436000	0.020130000
H	-7.592331000	0.566822000	-0.054840000

C	-8.117488000	-1.509831000	0.119471000
H	-9.186602000	-1.324720000	0.122683000
C	-7.620999000	-2.816308000	0.215575000
H	-8.309119000	-3.653187000	0.293870000
C	-6.252258000	-3.057649000	0.212065000
H	-5.854049000	-4.064137000	0.285950000
C	-5.340763000	-1.996750000	0.112098000
H	-3.223163000	2.326450000	-0.261333000
H	0.322869000	-1.936698000	0.012887000
H	-3.511182000	-1.453687000	0.038826000
H	5.889803000	-0.422854000	-0.216333000
4b			
O	5.173377000	-0.706932000	-0.127718000
O	-4.411019000	-2.560904000	0.166960000
N	2.490971000	-1.357727000	-0.056996000
N	1.149690000	-1.215624000	-0.051224000
N	1.243041000	1.111018000	-0.220965000
N	-0.838104000	2.289824000	-0.273873000
N	-0.826119000	-0.099779000	-0.102814000
N	1.190098000	3.420442000	-0.376157000
N	-2.801262000	1.152457000	-0.164849000
N	-3.601132000	0.069584000	-0.073789000
C	5.433216000	-2.037407000	-0.040594000
C	6.746088000	-2.521169000	-0.022411000
H	7.568657000	-1.810659000	-0.079647000
C	7.008392000	-3.886406000	0.067251000
H	8.036588000	-4.235199000	0.079293000
C	5.950842000	-4.793327000	0.140630000
H	6.140478000	-5.859351000	0.210818000
C	4.645517000	-4.313826000	0.122632000
H	3.817163000	-5.015582000	0.179263000
C	4.344486000	-2.942048000	0.032852000
C	2.934450000	-2.563679000	0.022745000
H	2.234184000	-3.410020000	0.090323000
C	0.516776000	0.002352000	-0.129782000
C	0.509581000	2.242936000	-0.289455000
C	2.651315000	3.468592000	-0.434579000
H	2.950545000	3.840587000	-1.427722000
H	3.026700000	2.452326000	-0.325845000
C	3.205286000	4.402819000	0.649369000
H	4.293307000	4.480299000	0.536394000
H	3.013806000	3.954871000	1.632701000
C	2.553016000	5.790942000	0.574296000
H	2.907014000	6.428152000	1.392878000
H	2.857412000	6.283270000	-0.360739000
C	1.022019000	5.674456000	0.607381000
H	0.555215000	6.656355000	0.464236000
H	0.700190000	5.302926000	1.588623000
C	0.514207000	4.711507000	-0.474946000
H	-0.557600000	4.541376000	-0.390939000
H	0.713121000	5.140360000	-1.470364000
C	-1.427070000	1.087046000	-0.178987000
C	-4.867539000	0.302096000	-0.079241000
H	-5.241085000	1.334698000	-0.156575000
C	-5.913478000	-0.712462000	0.009919000
C	-7.248701000	-0.269393000	-0.024923000
H	-7.430140000	0.798546000	-0.116440000
C	-8.328150000	-1.142844000	0.052323000
H	-9.343350000	-0.761114000	0.021759000
C	-8.086756000	-2.511962000	0.169549000
H	-8.912338000	-3.214493000	0.231693000
C	-6.776918000	-2.984763000	0.207699000
H	-6.584852000	-4.052130000	0.299527000
C	-5.690026000	-2.106901000	0.129680000
H	-3.188791000	2.091657000	-0.231057000
H	0.528121000	-2.019686000	0.014288000
H	-4.426847000	-3.523946000	0.251318000
H	6.014035000	-0.231297000	-0.171501000
4c			

O	4.838565000	-0.602441000	-0.134322000
O	-4.564431000	-2.472261000	0.210302000
N	2.399984000	-1.577396000	-0.022530000
N	1.063722000	-1.406556000	-0.011099000
N	1.272054000	0.904918000	-0.193153000
N	-0.745776000	2.185423000	-0.288489000
N	-0.859089000	-0.199456000	-0.092061000
N	1.332485000	3.217711000	-0.371811000
N	-2.765765000	1.151019000	-0.189538000
N	-3.618639000	0.108449000	-0.086086000
C	5.245087000	-1.883093000	-0.053667000
C	6.623593000	-2.138825000	-0.062155000
H	7.297242000	-1.291334000	-0.133388000
C	7.101495000	-3.441564000	0.018392000
H	8.173488000	-3.616996000	0.009982000
C	6.216735000	-4.523891000	0.109430000
H	6.592958000	-5.539707000	0.171878000
C	4.850385000	-4.280346000	0.118577000
H	4.150383000	-5.109837000	0.188539000
C	4.334822000	-2.973335000	0.038559000
C	2.896710000	-2.766387000	0.050559000
H	2.252755000	-3.651843000	0.122451000
C	0.483299000	-0.161660000	-0.104059000
C	0.598404000	2.075855000	-0.283678000
C	2.796594000	3.211518000	-0.394836000
H	3.131883000	3.557723000	-1.385040000
H	3.139203000	2.187523000	-0.264152000
C	3.358644000	4.138644000	0.690783000
H	4.451082000	4.167473000	0.606244000
H	3.121879000	3.714063000	1.674515000
C	2.766256000	5.550602000	0.577836000
H	3.123758000	6.184893000	1.396940000
H	3.115713000	6.015874000	-0.355114000
C	1.231593000	5.495905000	0.570854000
H	0.808259000	6.492486000	0.397803000
H	0.868123000	5.155407000	1.548794000
C	0.714264000	4.536050000	-0.509298000
H	-0.365594000	4.412895000	-0.454266000
H	0.961217000	4.936289000	-1.505395000
C	-1.398749000	1.017657000	-0.187460000
C	-4.871450000	0.404383000	-0.104637000
H	-5.191484000	1.452933000	-0.202939000
C	-5.968459000	-0.553355000	-0.004159000
C	-7.278715000	-0.042931000	-0.062391000
H	-7.404399000	1.030475000	-0.180010000
C	-8.402163000	-0.857732000	0.024377000
H	-9.396067000	-0.425394000	-0.025123000
C	-8.232405000	-2.234283000	0.176116000
H	-9.093579000	-2.891834000	0.246738000
C	-6.949250000	-2.772820000	0.238117000
H	-6.813370000	-3.846156000	0.356701000
C	-5.817913000	-1.954006000	0.150088000
H	-3.106914000	2.107083000	-0.268644000
H	0.426082000	-2.195400000	0.045680000
H	-4.631136000	-3.430742000	0.318706000
H	3.849943000	-0.585367000	-0.119449000
4d			
O	3.896196000	-5.085360000	-0.406183000
O	-3.910385000	-2.307905000	0.150107000
N	2.373407000	-1.199589000	-0.079111000
N	1.036648000	-1.028215000	-0.059169000
N	1.180219000	1.295099000	-0.251124000
N	-0.876607000	2.520128000	-0.306734000
N	-0.913280000	0.132415000	-0.112396000
N	1.173741000	3.604844000	-0.430824000
N	-2.860088000	1.406943000	-0.175435000
N	-3.631147000	0.304794000	-0.072510000

C	4.717615000	-4.023528000	-0.129744000
C	6.080858000	-4.310588000	-0.011363000
H	6.402450000	-5.337807000	-0.146233000
C	6.988143000	-3.291126000	0.252794000
H	8.045263000	-3.524357000	0.339156000
C	6.543435000	-1.970880000	0.396165000
H	7.251337000	-1.173176000	0.597653000
C	5.188955000	-1.688061000	0.294554000
H	4.819150000	-0.676306000	0.421626000
C	4.245569000	-2.703927000	0.043513000
C	2.814235000	-2.406707000	-0.001602000
H	2.108251000	-3.246772000	0.077506000
C	0.432112000	0.203490000	-0.146566000
C	0.472295000	2.445137000	-0.327899000
C	2.637022000	3.628640000	-0.484400000
H	2.942771000	3.997579000	-1.475899000
H	2.995884000	2.606761000	-0.377797000
C	3.203141000	4.550354000	0.603778000
H	4.292590000	4.606436000	0.495265000
H	2.998900000	4.104639000	1.585530000
C	2.577490000	5.950507000	0.527675000
H	2.938965000	6.578759000	1.349582000
H	2.896239000	6.438966000	-0.404383000
C	1.044460000	5.862818000	0.553036000
H	0.596552000	6.852912000	0.407347000
H	0.710162000	5.497466000	1.532394000
C	0.523557000	4.910788000	-0.532581000
H	-0.551959000	4.763269000	-0.455849000
H	0.739284000	5.332706000	-1.526763000
C	-1.486237000	1.334094000	-0.197599000
C	-4.916052000	0.422605000	-0.062248000
H	-5.400569000	1.404433000	-0.136480000
C	-5.771410000	-0.746161000	0.048632000
C	-7.169699000	-0.584600000	0.056732000
H	-7.575400000	0.421479000	-0.021183000
C	-8.025377000	-1.672002000	0.161109000
H	-9.100412000	-1.525451000	0.165474000
C	-7.482180000	-2.959600000	0.260959000
H	-8.139846000	-3.820182000	0.343484000
C	-6.105817000	-3.152056000	0.255829000
H	-5.671920000	-4.143443000	0.332567000
C	-5.233173000	-2.059591000	0.150346000
H	-3.267852000	2.334247000	-0.247449000
H	0.399767000	-1.818131000	0.022937000
H	-3.424714000	-1.451526000	0.071081000
H	3.054727000	-4.768948000	-0.756570000
4e			
O	3.745168000	-5.004783000	0.163747000
O	-3.908837000	-2.316201000	0.121815000
N	2.387427000	-1.186001000	-0.066300000
N	1.047007000	-1.019669000	-0.055320000
N	1.181700000	1.305441000	-0.223324000
N	-0.879446000	2.522428000	-0.286990000
N	-0.908570000	0.132835000	-0.113138000
N	1.167608000	3.616528000	-0.381068000
N	-2.859455000	1.401363000	-0.182676000
N	-3.629634000	0.298424000	-0.090614000
C	4.697562000	-4.024430000	0.081677000
C	6.063206000	-4.320997000	0.075627000
H	6.386465000	-5.358200000	0.137608000
C	7.001438000	-3.294794000	-0.009254000
H	8.060012000	-3.536696000	-0.013182000
C	6.579300000	-1.964505000	-0.088707000
H	7.307914000	-1.162833000	-0.154950000
C	5.220423000	-1.671911000	-0.082758000
H	4.870743000	-0.646968000	-0.144260000
C	4.252928000	-2.687879000	0.001932000
C	2.820433000	-2.396404000	0.007744000

H	2.137537000	-3.249025000	0.076358000
C	0.438486000	0.207104000	-0.135217000
C	0.469822000	2.451728000	-0.296039000
C	2.630692000	3.645982000	-0.420678000
H	2.945808000	4.019060000	-1.407929000
H	2.991584000	2.624815000	-0.313395000
C	3.183176000	4.565919000	0.675988000
H	4.273437000	4.626904000	0.578077000
H	2.971443000	4.115702000	1.654076000
C	2.552599000	5.963814000	0.599220000
H	2.904207000	6.590853000	1.426418000
H	2.877603000	6.456712000	-0.328399000
C	1.019765000	5.869818000	0.610387000
H	0.569255000	6.858772000	0.464469000
H	0.678261000	5.499345000	1.585336000
C	0.512767000	4.919533000	-0.483348000
H	-0.562689000	4.766685000	-0.416358000
H	0.734585000	5.347297000	-1.473915000
C	-1.484212000	1.332128000	-0.193172000
C	-4.914716000	0.414726000	-0.089243000
H	-5.399669000	1.396452000	-0.162846000
C	-5.769983000	-0.755271000	0.010783000
C	-7.168361000	-0.595145000	0.008605000
H	-7.574303000	0.410879000	-0.069211000
C	-8.024080000	-1.683590000	0.102846000
H	-9.099261000	-1.537805000	0.099299000
C	-7.480639000	-2.971018000	0.202793000
H	-8.138147000	-3.832488000	0.277395000
C	-6.104071000	-3.162091000	0.207717000
H	-5.669638000	-4.153258000	0.284476000
C	-5.231401000	-2.068567000	0.112434000
H	-3.268061000	2.328656000	-0.249556000
H	0.416188000	-1.815976000	0.006126000
H	-3.422046000	-1.459977000	0.048077000
H	4.180866000	-5.865375000	0.211798000
4f			
O	4.302206000	-4.868790000	0.102965000
O	-7.627838000	0.115596000	-0.667158000
N	2.659533000	-1.160841000	-0.103125000
N	1.311368000	-1.094966000	-0.093620000
N	1.270159000	1.235901000	-0.227389000
N	-0.877344000	2.291737000	-0.247475000
N	-0.725610000	-0.094983000	-0.116920000
N	1.077196000	3.542533000	-0.345214000
N	-2.770046000	1.039693000	-0.147084000
N	-3.495471000	-0.091505000	-0.073320000
C	5.177745000	-3.817830000	0.032165000
C	6.561860000	-4.010021000	0.033245000
H	6.962228000	-5.020172000	0.091881000
C	7.420130000	-2.915167000	-0.040164000
H	8.494020000	-3.075933000	-0.038625000
C	6.898403000	-1.620490000	-0.115376000
H	7.564334000	-0.765383000	-0.172907000
C	5.521212000	-1.431773000	-0.116119000
H	5.095308000	-0.435875000	-0.173690000
C	4.632975000	-2.518563000	-0.042636000
C	3.182566000	-2.335955000	-0.040790000
H	2.565736000	-3.238392000	0.016607000
C	0.610594000	0.084327000	-0.149622000
C	0.472149000	2.325340000	-0.272524000
C	2.531918000	3.687878000	-0.409825000
H	2.797692000	4.105354000	-1.394028000
H	2.974292000	2.696451000	-0.331876000
C	3.033132000	4.625373000	0.696863000
H	4.112577000	4.776278000	0.578292000
H	2.880069000	4.138050000	1.668166000
C	2.290832000	5.969365000	0.666322000
H	2.608217000	6.603483000	1.501961000

H	2.556072000	6.508199000	-0.254827000
C	0.771151000	5.752621000	0.702991000
H	0.240776000	6.705799000	0.591198000
H	0.479612000	5.331878000	1.673799000
C	0.320622000	4.791705000	-0.405872000
H	-0.737975000	4.552575000	-0.325639000
H	0.490547000	5.259202000	-1.388851000
C	-1.391716000	1.056530000	-0.170087000
C	-4.777673000	0.024739000	-0.073055000
H	-5.241857000	1.020722000	-0.132493000
C	-5.657172000	-1.135811000	0.067464000
C	-5.156619000	-2.375821000	0.510146000
H	-4.093018000	-2.448307000	0.710692000
C	-5.995962000	-3.463947000	0.703529000
H	-5.589443000	-4.407816000	1.052762000
C	-7.368904000	-3.332224000	0.461514000
H	-8.035210000	-4.175264000	0.618740000
C	-7.886967000	-2.124378000	0.007515000
H	-8.943294000	-2.003149000	-0.207735000
C	-7.039086000	-1.033338000	-0.203090000
H	-3.214784000	1.954075000	-0.188614000
H	0.740830000	-1.935750000	-0.037311000
H	-6.959992000	0.684767000	-1.068522000
H	4.802680000	-5.693600000	0.148004000
4g			
O	4.320261000	-4.858227000	0.177856000
O	-7.536340000	0.280331000	-0.095296000
N	2.664956000	-1.157855000	-0.076933000
N	1.317657000	-1.094023000	-0.066406000
N	1.270653000	1.235027000	-0.233417000
N	-0.879788000	2.284563000	-0.269279000
N	-0.721319000	-0.099808000	-0.103714000
N	1.070710000	3.539471000	-0.383113000
N	-2.768959000	1.027549000	-0.152494000
N	-3.492312000	-0.106988000	-0.061239000
C	5.192012000	-3.804912000	0.090868000
C	6.576703000	-3.992514000	0.091911000
H	6.980456000	-5.000515000	0.163763000
C	7.431398000	-2.896032000	0.001589000
H	8.505831000	-3.053227000	0.003228000
C	6.904969000	-1.604428000	-0.090632000
H	7.567768000	-0.747850000	-0.161434000
C	5.527066000	-1.420360000	-0.091276000
H	5.097616000	-0.426821000	-0.161902000
C	4.642417000	-2.508780000	-0.000881000
C	3.191363000	-2.330647000	0.001139000
H	2.577122000	-3.233849000	0.072358000
C	0.612902000	0.083574000	-0.139153000
C	0.468352000	2.320955000	-0.294157000
C	2.524509000	3.688084000	-0.449214000
H	2.790315000	4.092938000	-1.438808000
H	2.969679000	2.699066000	-0.357309000
C	3.022601000	4.642187000	0.644755000
H	4.101652000	4.795186000	0.524605000
H	2.870690000	4.167524000	1.622512000
C	2.275909000	5.983273000	0.596057000
H	2.590931000	6.629460000	1.423405000
H	2.539998000	6.510790000	-0.332012000
C	0.756825000	5.762274000	0.634589000
H	0.223617000	6.712312000	0.509831000
H	0.466037000	5.353507000	1.610730000
C	0.310301000	4.784874000	-0.461490000
H	-0.747518000	4.543039000	-0.378666000
H	0.479078000	5.240013000	-1.450581000
C	-1.393791000	1.049051000	-0.174117000
C	-4.773975000	0.016632000	-0.063488000
H	-5.258503000	0.995413000	-0.138974000
C	-5.643861000	-1.154311000	0.035132000



C	-5.127986000	-2.456728000	0.149846000
H	-4.049410000	-2.571624000	0.163482000
C	-5.965872000	-3.562056000	0.242931000
H	-5.543818000	-4.558107000	0.330913000
C	-7.352163000	-3.384106000	0.222955000
H	-8.017564000	-4.239205000	0.294948000
C	-7.889439000	-2.103609000	0.110230000
H	-8.967907000	-1.959052000	0.094034000
C	-7.045203000	-0.994047000	0.016924000
H	-3.220174000	1.937050000	-0.217756000
H	0.748503000	-1.934750000	0.002908000
H	-8.501531000	0.246195000	-0.094463000
H	4.824348000	-5.680137000	0.233755000
4h			
O	4.487348000	-4.914553000	-0.435838000
O	-7.535502000	0.292301000	-0.077877000
N	2.656267000	-1.171756000	-0.079072000
N	1.312057000	-1.105489000	-0.061917000
N	1.270337000	1.221801000	-0.257347000
N	-0.877633000	2.276450000	-0.293454000
N	-0.723798000	-0.106129000	-0.100940000
N	1.075204000	3.524837000	-0.434897000
N	-2.769141000	1.025210000	-0.152381000
N	-3.493900000	-0.108096000	-0.044981000
C	5.221254000	-3.795360000	-0.136510000
C	6.601889000	-3.974654000	-0.010657000
H	7.005655000	-4.970758000	-0.157692000
C	7.422694000	-2.889609000	0.275650000
H	8.494478000	-3.038497000	0.367917000
C	6.872119000	-1.611765000	0.433559000
H	7.512142000	-0.762869000	0.652414000
C	5.499848000	-1.436717000	0.324622000
H	5.049135000	-0.459822000	0.463056000
C	4.643112000	-2.520948000	0.051299000
C	3.192411000	-2.339923000	-0.001493000
H	2.556476000	-3.234665000	0.074005000
C	0.608752000	0.075957000	-0.145730000
C	0.470332000	2.310474000	-0.326776000
C	2.529385000	3.669079000	-0.513458000
H	2.787273000	4.065223000	-1.508425000
H	2.973430000	2.680002000	-0.417538000
C	3.038308000	4.630997000	0.568546000
H	4.116763000	4.779617000	0.438639000
H	2.892611000	4.165289000	1.551553000
C	2.295100000	5.973757000	0.513843000
H	2.617981000	6.625829000	1.333411000
H	2.553925000	6.492729000	-0.420443000
C	0.775743000	5.757577000	0.565584000
H	0.244287000	6.707941000	0.436492000
H	0.490903000	5.358185000	1.547335000
C	0.317880000	4.772369000	-0.518723000
H	-0.740114000	4.534973000	-0.426283000
H	0.481463000	5.217463000	-1.513029000
C	-1.395294000	1.044289000	-0.181100000
C	-4.775202000	0.018886000	-0.044653000
H	-5.257129000	0.998050000	-0.130927000
C	-5.648763000	-1.147541000	0.071447000
C	-5.137489000	-2.450023000	0.204344000
H	-4.059357000	-2.568786000	0.218947000
C	-5.979336000	-3.550720000	0.314046000
H	-5.561174000	-4.547039000	0.416144000
C	-7.364999000	-3.367639000	0.292815000
H	-8.033473000	-4.219110000	0.377784000
C	-7.897767000	-2.087032000	0.162271000
H	-8.975677000	-1.938872000	0.145017000
C	-7.049522000	-0.982010000	0.052286000
H	-3.219732000	1.934350000	-0.226581000
H	0.738053000	-1.941565000	0.025324000
H	-8.500866000	0.262740000	-0.074589000

H	3.629690000	-4.656856000	-0.795149000
4I			
O	5.007092000	0.788319000	-0.229740000
O	-5.006917000	0.788054000	-0.230829000
N	3.492957000	-1.342091000	0.056298000
N	2.278352000	-1.922313000	0.139533000
N	1.198520000	0.123555000	-0.115573000
N	-1.198538000	0.123423000	-0.116005000
N	0.000051000	-1.936421000	0.141137000
N	-0.000104000	2.094582000	-0.357843000
N	-2.278246000	-1.922583000	0.138522000
N	-3.492863000	-1.342299000	0.055803000
C	6.045358000	-0.062517000	-0.132596000
C	7.340913000	0.467207000	-0.214703000
H	7.444346000	1.538246000	-0.352985000
C	8.451136000	-0.363496000	-0.120482000
H	9.445857000	0.067823000	-0.186654000
C	8.299019000	-1.744826000	0.058229000
H	9.168180000	-2.390073000	0.131435000
C	7.020685000	-2.278379000	0.140149000
H	6.885567000	-3.348688000	0.278151000
C	5.876183000	-1.464172000	0.048181000
C	4.557556000	-2.066968000	0.137132000
H	4.500496000	-3.154309000	0.273639000
C	1.115102000	-1.192787000	0.048530000
C	-0.000106000	0.748727000	-0.192727000
C	1.236088000	2.873949000	-0.469846000
H	1.282524000	3.303481000	-1.482341000
H	2.081650000	2.200275000	-0.351488000
C	1.262328000	4.002507000	0.569487000
H	2.163336000	4.607155000	0.415018000
H	1.339449000	3.559027000	1.570284000
C	-0.000238000	4.871059000	0.480825000
H	-0.000253000	5.630383000	1.270881000
H	-0.000286000	5.412938000	-0.475827000
C	-1.262717000	4.002381000	0.569514000
H	-2.163789000	4.606931000	0.415058000
H	-1.339781000	3.558881000	1.570305000
C	-1.236373000	2.873854000	-0.469856000
H	-2.081869000	2.200084000	-0.351566000
H	-1.282821000	3.303431000	-1.482334000
C	-1.114983000	-1.192992000	0.048287000
C	-4.557479000	-2.067117000	0.136983000
H	-4.500434000	-3.154458000	0.273518000
C	-5.876094000	-1.464265000	0.048261000
C	-7.020626000	-2.278351000	0.140900000
H	-6.885546000	-3.348607000	0.279340000
C	-8.298948000	-1.744741000	0.059125000
H	-9.168133000	-2.389896000	0.132869000
C	-8.451016000	-0.363483000	-0.120155000
H	-9.445723000	0.067879000	-0.186256000
C	-7.340757000	0.467104000	-0.215044000
H	-7.444164000	1.538090000	-0.353759000
C	-6.045221000	-0.062669000	-0.133049000
H	-2.178473000	-2.926159000	0.257482000
H	2.178545000	-2.926040000	0.257087000
H	-4.168091000	0.270624000	-0.157146000
H	4.168251000	0.270882000	-0.156125000
4J			
O	5.419112000	0.896623000	-0.151637000
O	-5.102827000	0.685479000	-0.195449000
N	3.511832000	-1.091396000	-0.001039000
N	2.304465000	-1.693497000	0.057547000
N	1.131065000	0.311321000	-0.171238000
N	-1.264321000	0.203118000	-0.147824000
N	0.031285000	-1.801218000	0.076885000
N	-0.149570000	2.226319000	-0.386164000

N	-2.244084000	-1.895091000	0.098649000
N	-3.485185000	-1.373901000	0.040477000
C	6.356309000	-0.082603000	-0.067735000
C	7.723330000	0.215668000	-0.088636000
H	8.033200000	1.255481000	-0.174698000
C	8.680242000	-0.792770000	-0.001227000
H	9.734627000	-0.534103000	-0.019815000
C	8.278984000	-2.124496000	0.109421000
H	9.014131000	-2.919506000	0.178161000
C	6.920882000	-2.422317000	0.131038000
H	6.601492000	-3.457869000	0.217695000
C	5.927820000	-1.428917000	0.044466000
C	4.535754000	-1.866876000	0.081298000
H	4.402445000	-2.954104000	0.189438000
C	1.116093000	-1.007684000	-0.017884000
C	-0.093521000	0.878026000	-0.231342000
C	1.059678000	3.042566000	-0.513255000
H	1.081585000	3.475065000	-1.526030000
H	1.922719000	2.387849000	-0.404484000
C	1.062709000	4.171527000	0.525858000
H	1.939904000	4.808421000	0.360406000
H	1.167530000	3.731035000	1.525496000
C	-0.229489000	4.997631000	0.454533000
H	-0.243925000	5.758348000	1.243365000
H	-0.261109000	5.537272000	-0.503008000
C	-1.461342000	4.087859000	0.562151000
H	-2.383712000	4.663243000	0.421928000
H	-1.508030000	3.642766000	1.564141000
C	-1.413202000	2.959596000	-0.477359000
H	-2.231741000	2.255676000	-0.343280000
H	-1.495696000	3.387193000	-1.488833000
C	-1.115484000	-1.109925000	0.002997000
C	-4.512975000	-2.149364000	0.128377000
H	-4.402228000	-3.234281000	0.250792000
C	-5.860184000	-1.608803000	0.066970000
C	-6.963444000	-2.476942000	0.165851000
H	-6.775898000	-3.541320000	0.287954000
C	-8.266919000	-2.003513000	0.110541000
H	-9.103340000	-2.690259000	0.188680000
C	-8.487003000	-0.629029000	-0.047509000
H	-9.501911000	-0.244394000	-0.092523000
C	-7.418456000	0.254156000	-0.148039000
H	-7.574154000	1.320803000	-0.270815000
C	-6.098261000	-0.214709000	-0.093043000
H	-2.094437000	-2.893475000	0.208416000
H	2.220549000	-2.701937000	0.169347000
H	-4.239040000	0.207553000	-0.141788000
H	5.869220000	1.749664000	-0.219763000
4K			
O	5.513418000	0.771173000	-0.165037000
O	-5.513289000	0.770980000	-0.166022000
N	3.509770000	-1.119371000	0.003742000
N	2.274989000	-1.659632000	0.058757000
N	1.199386000	0.400974000	-0.171730000
N	-1.199389000	0.400826000	-0.172318000
N	0.000058000	-1.659095000	0.056911000
N	-0.000121000	2.370820000	-0.389763000
N	-2.274869000	-1.659777000	0.058686000
N	-3.509644000	-1.119512000	0.003635000
C	6.401419000	-0.252156000	-0.070017000
C	7.781358000	-0.021479000	-0.093041000
H	8.141555000	1.001049000	-0.189994000
C	8.687997000	-1.074483000	0.006060000
H	9.753826000	-0.868123000	-0.014441000
C	8.221438000	-2.383350000	0.130951000
H	8.916467000	-3.212889000	0.209191000
C	6.850167000	-2.613963000	0.153970000
H	6.480364000	-3.631679000	0.250861000

C	5.906737000	-1.574450000	0.055471000
C	4.494706000	-1.943640000	0.091577000
H	4.308344000	-3.022690000	0.203208000
C	1.119043000	-0.917180000	-0.024498000
C	-0.000086000	1.018281000	-0.240782000
C	1.238050000	3.142187000	-0.495489000
H	1.296319000	3.574738000	-1.507222000
H	2.074861000	2.456513000	-0.371394000
C	1.262942000	4.270541000	0.544664000
H	2.162746000	4.878983000	0.393723000
H	1.337493000	3.826394000	1.545418000
C	-0.000268000	5.138862000	0.454941000
H	-0.000274000	5.900438000	1.243284000
H	-0.000367000	5.678468000	-0.503278000
C	-1.263344000	4.270361000	0.544813000
H	-2.163248000	4.878671000	0.393959000
H	-1.337731000	3.826215000	1.545578000
C	-1.238427000	3.142007000	-0.495349000
H	-2.075107000	2.456191000	-0.371157000
H	-1.296915000	3.574542000	-1.507073000
C	-1.118909000	-0.917366000	-0.024736000
C	-4.494586000	-1.943750000	0.091682000
H	-4.308235000	-3.022781000	0.203512000
C	-5.906614000	-1.574543000	0.055598000
C	-6.850053000	-2.613992000	0.154669000
H	-6.480257000	-3.631671000	0.252002000
C	-8.221323000	-2.383369000	0.131683000
H	-8.916355000	-3.212864000	0.210377000
C	-8.687875000	-1.074554000	0.006225000
H	-9.753702000	-0.868188000	-0.014289000
C	-7.781227000	-0.021611000	-0.093452000
H	-8.141417000	1.000880000	-0.190828000
C	-6.401292000	-0.252300000	-0.070451000
H	-2.140361000	-2.663171000	0.166479000
H	2.140450000	-2.663045000	0.166323000
H	-6.004925000	1.599792000	-0.244825000
H	6.005049000	1.600046000	-0.243311000
4L			
O	-3.044756000	-1.614778000	0.048421000
O	-3.044204000	1.615166000	0.051855000
N	-0.534904000	-2.492674000	-0.071618000
N	0.806360000	-2.333119000	-0.135192000
N	2.759987000	-1.192475000	-0.244388000
N	2.760147000	1.191874000	-0.246052000
N	0.675870000	-0.000088000	-0.130571000
N	4.750340000	-0.000504000	-0.347423000
N	0.806598000	2.332912000	-0.139574000
N	-0.534518000	2.492706000	-0.073550000
C	-3.385517000	-2.913258000	0.059890000
C	-4.750504000	-3.232100000	0.120714000
H	-5.460897000	-2.413064000	0.155337000
C	-5.165722000	-4.557594000	0.135118000
H	-6.227471000	-4.782323000	0.182340000
C	-4.232100000	-5.602326000	0.089449000
H	-4.560836000	-6.636275000	0.100806000
C	-2.880549000	-5.296607000	0.029239000
H	-2.142842000	-6.095031000	-0.006971000
C	-2.427454000	-3.963240000	0.012944000
C	-1.003243000	-3.696419000	-0.052589000
H	-0.330672000	-4.563557000	-0.086733000
C	1.425119000	-1.108981000	-0.170323000
C	3.390668000	-0.000352000	-0.278891000
C	5.528219000	-1.236729000	-0.432663000
H	5.985260000	-1.297012000	-1.433310000
H	4.844046000	-2.076104000	-0.325558000
C	6.629711000	-1.262005000	0.635562000
H	7.239660000	-2.162784000	0.499852000
H	6.161101000	-1.334469000	1.625247000

C	7.500691000	-0.000039000	0.565336000
H	8.241911000	0.000512000	1.372315000
H	8.063910000	-0.000791000	-0.378903000
C	6.629905000	1.262163000	0.633680000
H	7.239992000	2.162647000	0.496634000
H	6.161307000	1.336158000	1.623254000
C	5.528400000	1.235487000	-0.434494000
H	4.844359000	2.075122000	-0.328596000
H	5.985434000	1.294235000	-1.435232000
C	1.425232000	1.108638000	-0.172203000
C	-1.002719000	3.696516000	-0.055391000
H	-0.330145000	4.563549000	-0.091998000
C	-2.426792000	3.963534000	0.012373000
C	-2.879760000	5.296954000	0.027877000
H	-2.142058000	6.095277000	-0.010579000
C	-4.231178000	5.602850000	0.090130000
H	-4.559814000	6.636837000	0.100845000
C	-5.164796000	4.558244000	0.138716000
H	-6.226444000	4.783110000	0.187539000
C	-4.749700000	3.232703000	0.125175000
H	-5.460087000	2.413761000	0.162061000
C	-3.384848000	2.913683000	0.062310000
H	1.423662000	3.139050000	-0.177512000
H	1.423259000	-3.139375000	-0.173344000
H	-2.064013000	1.535113000	0.004546000
H	-2.064482000	-1.534841000	0.002570000
4M			
O	2.959989000	1.371500000	0.037112000
O	2.933558000	-1.384582000	0.037654000
N	0.493655000	2.406668000	-0.080309000
N	-0.850149000	2.305190000	-0.145004000
N	-2.832568000	1.182542000	-0.247153000
N	-2.834329000	-1.208188000	-0.247918000
N	-0.756623000	-0.014434000	-0.139518000
N	-4.822957000	-0.012418000	-0.340409000
N	-0.849736000	-2.337224000	-0.145446000
N	0.495516000	-2.394064000	-0.080077000
C	3.371199000	2.657443000	0.055406000
C	4.749480000	2.898159000	0.120519000
H	5.417131000	2.043185000	0.152685000
C	5.242656000	4.198082000	0.143154000
H	6.315289000	4.360617000	0.193910000
C	4.368939000	5.290566000	0.100961000
H	4.752873000	6.305180000	0.118443000
C	3.001613000	5.059508000	0.036058000
H	2.310630000	5.898561000	0.002692000
C	2.471288000	3.756039000	0.011769000
C	1.029555000	3.579621000	-0.056980000
H	0.414129000	4.487928000	-0.088394000
C	-1.499082000	1.089017000	-0.177669000
C	-3.461544000	-0.013852000	-0.278494000
C	-5.600059000	1.223469000	-0.426776000
H	-6.057214000	1.284553000	-1.427597000
H	-4.915584000	2.062622000	-0.319419000
C	-6.702263000	1.249844000	0.640811000
H	-7.312074000	2.150758000	0.504588000
H	-6.234028000	1.322355000	1.630698000
C	-7.573563000	-0.011941000	0.570908000
H	-8.315457000	-0.011840000	1.377395000
H	-8.136113000	-0.011485000	-0.373792000
C	-6.702942000	-1.274227000	0.640170000
H	-7.313273000	-2.174669000	0.503480000
H	-6.234808000	-1.347680000	1.630014000
C	-5.600814000	-1.248095000	-0.427352000
H	-4.916215000	-2.087176000	-0.320328000
H	-6.057689000	-1.308350000	-1.428303000
C	-1.498402000	-1.128706000	-0.177970000
C	1.061955000	-3.546685000	-0.055351000

H	0.472900000	-4.476375000	-0.085971000
C	2.511534000	-3.718148000	0.013490000
C	3.028698000	-5.024410000	0.035653000
H	2.327698000	-5.855136000	0.001427000
C	4.394960000	-5.279626000	0.099275000
H	4.760971000	-6.301038000	0.114666000
C	5.285035000	-4.204947000	0.142510000
H	6.355620000	-4.381240000	0.192168000
C	4.806373000	-2.896674000	0.122190000
H	5.498397000	-2.058328000	0.155727000
C	3.431799000	-2.635184000	0.058549000
H	-1.433904000	-3.170524000	-0.178350000
H	-1.437212000	3.133304000	-0.178427000
H	3.617025000	-0.698700000	0.069597000
H	1.974362000	1.326127000	-0.009186000
4N			
O	3.102889000	2.024241000	0.721853000
O	3.222242000	-1.970056000	-0.607953000
N	0.535553000	2.507956000	-0.132435000
N	-0.788634000	2.319203000	-0.309024000
N	-2.735426000	1.155589000	-0.341462000
N	-2.717061000	-1.222427000	-0.165031000
N	-0.643955000	-0.009437000	-0.141933000
N	-4.717618000	-0.056395000	-0.347001000
N	-0.752597000	-2.341583000	0.010072000
N	0.586504000	-2.502737000	-0.028667000
C	3.383106000	3.320028000	0.435845000
C	4.670815000	3.843985000	0.596288000
H	5.463432000	3.189713000	0.954642000
C	4.943861000	5.179532000	0.308327000
H	5.951709000	5.561381000	0.441004000
C	3.923110000	6.015924000	-0.144586000
H	4.121901000	7.058532000	-0.370071000
C	2.641929000	5.497172000	-0.301271000
H	1.841060000	6.144723000	-0.649543000
C	2.333207000	4.152407000	-0.027148000
C	0.949404000	3.724070000	-0.213450000
H	0.244491000	4.538687000	-0.440549000
C	-1.397387000	1.087027000	-0.256943000
C	-3.354285000	-0.040632000	-0.284736000
C	-5.505998000	1.163354000	-0.510995000
H	-5.968332000	1.156175000	-1.511526000
H	-4.828334000	2.013559000	-0.461368000
C	-6.604101000	1.248835000	0.558104000
H	-7.223886000	2.132963000	0.367170000
H	-6.132024000	1.389640000	1.538756000
C	-7.463267000	-0.023335000	0.575263000
H	-8.201649000	0.022104000	1.383873000
H	-8.030157000	-0.089698000	-0.364587000
C	-6.580054000	-1.270708000	0.721162000
H	-7.182827000	-2.183597000	0.646200000
H	-6.106491000	-1.275393000	1.711188000
C	-5.483036000	-1.301487000	-0.351415000
H	-4.789916000	-2.125665000	-0.194531000
H	-5.944806000	-1.430198000	-1.343883000
C	-1.379712000	-1.123130000	-0.106103000
C	1.012775000	-3.711462000	0.090682000
H	0.303036000	-4.539784000	0.240043000
C	2.415715000	-4.114989000	0.047964000
C	2.717026000	-5.455974000	0.347473000
H	1.895341000	-6.118580000	0.607788000
C	4.016210000	-5.952498000	0.323091000
H	4.208307000	-6.992941000	0.563848000
C	5.064098000	-5.096744000	-0.017783000
H	6.086619000	-5.461159000	-0.046413000
C	4.799884000	-3.764249000	-0.327384000
H	5.614241000	-3.094979000	-0.598639000
C	3.493680000	-3.262694000	-0.299798000

H	-1.377969000	-3.144107000	0.051507000
H	-1.422693000	3.107911000	-0.422072000
H	4.037209000	-1.534607000	-0.891689000
H	3.891454000	1.604060000	1.090509000
4O			
O	2.009137000	6.302152000	-0.018641000
O	2.009286000	-6.302113000	-0.019415000
N	0.606793000	2.489560000	-0.069335000
N	-0.731309000	2.333686000	-0.135869000
N	-2.689463000	1.192550000	-0.241302000
N	-2.689442000	-1.192607000	-0.241195000
N	-0.606926000	-0.000005000	-0.128202000
N	-4.680401000	-0.000049000	-0.338516000
N	-0.731271000	-2.333700000	-0.135600000
N	0.606838000	-2.489549000	-0.069156000
C	2.947401000	5.304387000	0.032891000
C	4.315204000	5.582465000	0.097821000
H	4.651664000	6.617408000	0.107924000
C	5.238980000	4.540788000	0.148916000
H	6.299633000	4.768137000	0.199110000
C	4.799055000	3.214094000	0.135487000
H	5.515909000	2.400140000	0.175210000
C	3.437744000	2.939543000	0.070803000
H	3.074088000	1.917546000	0.059206000
C	2.485247000	3.971838000	0.018010000
C	1.050900000	3.697760000	-0.051908000
H	0.377510000	4.560331000	-0.089324000
C	-1.352380000	1.108112000	-0.168437000
C	-3.317690000	-0.000035000	-0.273602000
C	-5.456579000	1.235488000	-0.429290000
H	-5.908607000	1.297760000	-1.432576000
H	-4.772085000	2.074188000	-0.317874000
C	-6.564640000	1.262102000	0.632203000
H	-7.174226000	2.162722000	0.492610000
H	-6.101786000	1.334902000	1.624597000
C	-7.435191000	-0.000038000	0.557963000
H	-8.181811000	-0.000013000	1.360194000
H	-7.992303000	-0.000079000	-0.390019000
C	-6.564620000	-1.262159000	0.632299000
H	-7.174191000	-2.162799000	0.492774000
H	-6.101765000	-1.334876000	1.624700000
C	-5.456559000	-1.235607000	-0.429195000
H	-4.772051000	-2.074287000	-0.317715000
H	-5.908586000	-1.297962000	-1.432476000
C	-1.352362000	-1.108139000	-0.168307000
C	1.050960000	-3.697741000	-0.051665000
H	0.377579000	-4.560322000	-0.089011000
C	2.485310000	-3.971798000	0.018267000
C	3.437765000	-2.939493000	0.071611000
H	3.074073000	-1.917504000	0.060426000
C	4.799080000	-3.214023000	0.136310000
H	5.515900000	-2.400062000	0.176473000
C	5.239049000	-4.540709000	0.149219000
H	6.299705000	-4.768040000	0.199432000
C	4.315316000	-5.582397000	0.097593000
H	4.651811000	-6.617331000	0.107303000
C	2.947511000	-5.304338000	0.032632000
H	-1.353160000	-3.138137000	-0.172544000
H	-1.353213000	3.138111000	-0.172821000
H	2.458993000	-7.156629000	-0.003081000
H	2.458799000	7.156677000	-0.001562000
4P			
O	2.183235000	6.301628000	0.542380000
O	2.247299000	-6.283241000	-0.583205000
N	0.595187000	2.483174000	-0.084517000
N	-0.742549000	2.334068000	-0.134808000
N	-2.700910000	1.191566000	-0.241052000

N	-2.698011000	-1.193988000	-0.243614000
N	-0.618050000	0.001177000	-0.127013000
N	-4.690346000	-0.003581000	-0.342877000
N	-0.737375000	-2.332054000	-0.134911000
N	0.598990000	-2.479153000	-0.051725000
C	2.990025000	5.249259000	0.189831000
C	4.358112000	5.519762000	0.096375000
H	4.698187000	6.527916000	0.308165000
C	5.247373000	4.505420000	-0.240686000
H	6.308965000	4.724532000	-0.307354000
C	4.778900000	3.207840000	-0.481401000
H	5.472639000	2.414016000	-0.739437000
C	3.419001000	2.942584000	-0.404555000
H	3.031133000	1.949748000	-0.606202000
C	2.494486000	3.955723000	-0.082532000
C	1.057045000	3.684312000	-0.069492000
H	0.368037000	4.542246000	-0.095864000
C	-1.365435000	1.107375000	-0.167749000
C	-3.329702000	-0.001955000	-0.275642000
C	-5.469195000	1.231442000	-0.431632000
H	-5.922750000	1.291581000	-1.434013000
H	-4.786211000	2.071515000	-0.322099000
C	-6.574835000	1.256055000	0.632296000
H	-7.185460000	2.156015000	0.493903000
H	-6.110123000	1.329376000	1.623773000
C	-7.444051000	-0.006996000	0.559416000
H	-8.188519000	-0.008066000	1.363446000
H	-8.003477000	-0.007420000	-0.387090000
C	-6.571873000	-1.268018000	0.631766000
H	-7.180363000	-2.169358000	0.492995000
H	-6.107000000	-1.340759000	1.623197000
C	-5.466218000	-1.240452000	-0.432106000
H	-4.781247000	-2.078912000	-0.322568000
H	-5.919527000	-1.301440000	-1.434560000
C	-1.362815000	-1.106710000	-0.168411000
C	1.061763000	-3.679930000	-0.033566000
H	0.374954000	-4.538329000	-0.086854000
C	2.490784000	-3.951925000	0.120737000
C	3.376489000	-2.946732000	0.556398000
H	2.969125000	-1.957932000	0.738704000
C	4.722015000	-3.215022000	0.765074000
H	5.385053000	-2.427579000	1.109081000
C	5.214046000	-4.507573000	0.545579000
H	6.263679000	-4.729001000	0.714937000
C	4.364829000	-5.513692000	0.098361000
H	4.725934000	-6.517318000	-0.099647000
C	3.013037000	-5.239782000	-0.127511000
H	-1.358544000	-3.137669000	-0.164790000
H	-1.364327000	3.138370000	-0.182308000
H	1.449114000	-5.941821000	-1.004294000
H	1.345239000	5.968818000	0.885793000