Supporting Information

Gas-phase basicity of cyclic guanidine derivatives - a DFT study

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Table S1. Electronic energies (E_{SCF}), correction to Gibbs energies (G_{corr}), the gas-phase basicities (GB) and Gibbs energies of solvation (ΔG_{sol}) of all calculated structures.[a]

Molecule	E_{SCF}	G_{corr}	G_{tot}	GB	ΔG_{sol}
1	-400.78426	0.15923	-400.62503	240.8	-3.1
1H$^+$	-401.19172	0.17298	-401.01874		-43.2
2	-440.11639	0.18649	-439.92991	246.0	-2.9
2H$^+$	-440.53341	0.20144	-440.33197		-41.4
3	-479.46914	0.21525	-479.25390	247.4	-2.9
3H$^+$	-479.88943	0.23129	-479.65814		-40.5
4	-518.79942	0.24399	-518.55543	246.3	-2.7
4H$^+$	-519.21769	0.25981	-518.95788		-40.0
5	-558.11551	0.27152	-557.84400	247.9	-2.2
5H$^+$	-558.53663	0.28754	-558.24909		-39.1
6	-322.10388	0.10303	-322.00085	217.9	-3.5
6H$^+$	-322.47369	0.11566	-322.35803		-48.5
7	-361.47842	0.13207	-361.34635	235.8	-3.9
7H$^+$	-361.87740	0.14533	-361.73207		-44.9
8	-400.83111	0.16195	-400.66916	242.8	-3.3
8H$^+$	-401.24081	0.17475	-401.06606		-42.9
9	-440.14853	0.18977	-439.95877	247.8	-3.3
9H$^+$	-440.56827	0.20458	-440.36369		-41.7
10	-479.47274	0.21770	-479.25504	247.1	-3.0
10H$^+$	-479.89133	0.23249	-479.65883		-40.9
11	-361.47152	0.13297	-361.33855	238.5	-4.5
11H$^+$	-361.87493	0.14633	-361.72860		-45.0
12	-400.82881	0.16147	-400.66735	241.2	-3.2
12H$^+$	-401.23763	0.17589	-401.06174		-43.1
13	-440.15445	0.18968	-439.96477	244.2	-2.8
13H$^+$	-440.56887	0.20496	-440.36391		-41.7
14	-479.47291	0.21761	-479.25530	247.6	-2.7
14H$^+$	-479.89256	0.23260	-479.65996		-40.9
15	-320.85551	0.08551	-320.77000	225.8	-5.6
15H$^+$	-321.23693	0.09717	-321.13976		-50.7
16	-360.24198	0.11410	-360.12787	235.5	-5.7
16H$^+$	-360.64092	0.12783	-360.51310		-46.5
17	-399.58941	0.14304	-399.44637	239.9	-5.3
17H$^+$	-399.99477	0.15615	-399.83862		-44.6
18	-438.91911	0.17048	-438.74863	240.8	-5.0
18H$^+$	-439.32674	0.18435	-439.14238		-43.2
19	-360.24500	0.11421	-360.13079	234.5	-5.1
19H$^+$	-360.64151	0.12706	-360.51445		-46.5
20	-399.62485	0.14359	-399.48127	240.1	-4.5
20H$^+$	-400.03100	0.15706	-399.87394		-44.2

a) E_{SCF}, G_{corr} and G_{tot} are given in a.u, while GB and ΔG_{sol} are given in kcal mol^{-1}.

Table S1. (continued)

Molecule	E_{SCF}	G_{corr}	G_{tot}	GB	
21	-438.95833	0.17174	-438.786585	244.2	-4.1
21H$^+$	-439.37068	0.18501	-439.185675		-42.5
22	-478.27714	0.19962	-478.07752	243.4	-3.6
22H$^+$	-478.68920	0.21382	-478.47538		-41.5
23	-399.59336	0.14268	-399.45068	238.0	-4.4
23H$^+$	-399.99562	0.15559	-399.84004		-44.5
24	-438.96017	0.17149	-438.78869	244.3	-3.7
24H$^+$	-439.37294	0.18500	-439.18794		-42.4
25	-478.28205	0.19930	-478.08275	248.3	-3.3
25H$^+$	-478.70129	0.21282	-478.48848		-40.9
26	-517.60129	0.22754	-517.37375	246.5	-3.1
26H$^+$	-518.01878	0.24217	-517.77662		-40.3
27	-438.92668	0.17003	-438.75664	238.1	-4.0
27H$^+$	-439.32949	0.18347	-439.14602		-43.0
28	-478.28053	0.19894	-478.08159	245.1	-3.2
28H$^+$	-478.69266	0.21045	-478.48221		-41.3
29	-517.59731	0.22721	-517.37011	249.6	-3.3
29H$^+$	-518.01978	0.24192	-517.77786		-40.3
30	-556.92037	0.25499	-556.66538	249.3	-3.0
30H$^+$	-557.34239	0.26979	-557.07261		-39.5
31	-402.02603	0.18014	-401.84589	244.6	-2.6
31H$^+$	-402.44137	0.19576	-402.24562		-42.4

a) E_{SCF}, G_{corr} and G_{tot} are given in a.u, while GB and ΔG_{sol} are given in kcal mol^{-1}.

Calculation of the pK_a

Calculation of the pK_a is based in the thermodynamic cycle usually used in pK_a calculation as for example the Cycle 1 used by Liptak and Shields.[1]

According to them, pK_a can be written as a function of the Gibbs energy for deprotonation of the acid $\mathbf{BH}^+$ (Equation S1)

$$pK_a(\mathbf{BH}^+) = \Delta G^*(\mathbf{BH}^+)/2.303RT \quad \text{(S1)}$$

where $\Delta G^*(\mathbf{BH}^+)$ is the Gibbs energy of dissociation of the acid $\mathbf{BH}^+$ to the free base **B** and the proton ($\mathbf{H}^+$) in solution at the reference state of 1 mol dm^{-3}. $\Delta G^*(\mathbf{BH}^+)$ is then calculated using Equation S2.

$$\Delta G^*(\mathbf{BH}^+) = G^*(\mathbf{B}) - G^*(\mathbf{BH}^+) + G^*(\mathbf{H}^+) \quad \text{(S2)}$$

Gibbs energy of each species in solution can be expressed by Equations S2-S5

$$G^*(\mathbf{B}) = G^\circ_{gas}(\mathbf{B}) + \Delta G^\circ_{sol}(\mathbf{B}) + G^{\circ\rightarrow *} \quad \text{(S3)}$$

$$G^*(\mathbf{BH}^+) = G^\circ_{gas}(\mathbf{BH}^+) + \Delta G^\circ_{sol}(\mathbf{BH}^+) + G^{\circ\rightarrow *} \quad \text{(S4)}$$

$$G^*(\mathbf{H}^+) = G^\circ_{gas}(\mathbf{H}^+) + \Delta G^\circ_{sol}(\mathbf{H}^+) + G^{\circ\rightarrow *} \quad \text{(S5)}$$

where G°_{gas} represents the Gibbs energy of each species in the gas phase at the reference state of 101325 Pa and ΔG°_{sol} is the Gibbs energy of solvation for the corresponding species. These energies are clculated in the gas phase using standard computational approach where G°_{gas} was calculated at B3LYP/6-311+G(2df,p)//B3LYP/6-31G(d) level of theory and ΔG°_{sol} was calculated at IPCM/B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level of theory. The third contribution to the G^* ($G^{\circ\rightarrow *}$) is the conversion factor for the change in reference state on going from the gas-phase to the solution[2] and it amounts 1.89 kcal mol^{-1}.

By combining equations S2-S5, we can write:

$$\Delta G^*(\mathbf{BH}^+) = G^\circ_{gas}(\mathbf{B}) + \Delta G^\circ_{sol}(\mathbf{B}) + G^{\circ\rightarrow *} - G^\circ_{gas}(\mathbf{BH}^+) - \Delta G^\circ_{sol}(\mathbf{BH}^+) - G^{\circ\rightarrow *} + G^*(\mathbf{H}^+) \quad \text{(S6)}$$

or

$$\Delta G^*(\mathbf{BH}^+) = [G^\circ_{gas}(\mathbf{B}) - G^\circ_{gas}(\mathbf{BH}^+)] + [\Delta G^\circ_{sol}(\mathbf{B}) - \Delta G^\circ_{sol}(\mathbf{BH}^+)] - G^{\circ\rightarrow *} + G^*(\mathbf{H}^+) \quad \text{(S7)}$$

We further simplified Equation S7 by defining the reduced gas-phase basicity (GB') and Δ (ΔG_{sol}) as

$$GB' = G^\circ_{gas}(\mathbf{B}) - G^\circ_{gas}(\mathbf{BH}^+) \quad \text{(S8)}$$

$$\Delta\,(\Delta G_{sol}) = \Delta G^\circ_{sol}(\mathbf{B}) - \Delta G^\circ_{sol}(\mathbf{BH}^+) \quad \text{(S9)}$$

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[1] M. D. Liptak, G. C. Shields, *J. Am. Chem. Soc.* **2001,** *123,* 7314-7319.
[2] A. Ben-Naim, *J. Phys. Chem*. **1978**, *82,* 792.

Having in mind that the $G°\rightarrow*$ and $G*(\mathbf{H}^+)$ are the constant for the given solvent and can be denoted as C.

Now, we can write:

$$\Delta G*(\mathbf{BH}^+) = GB' + \Delta(\Delta G_{sol}) + C \quad \text{(S10)}$$

Using the "reduced basicity" notation we can now define:

$$\Delta G_a'(\mathbf{BH}^+) = GB' + \Delta(\Delta G_{sol}) \quad \text{(S11)}$$

what leads us to:

$$pK_a(\mathbf{BH}^+) = (1/2.303RT) \times \Delta G_a'(\mathbf{BH}^+) + (C/2.303RT) \quad \text{(S12)}$$

or, finally, to:

$$pK_a(\mathbf{BH}^+) = a \times \Delta G_a'(\mathbf{BH}^+) + b \quad \text{(S13)}$$

Advantage of this approach is the cancellation of some systematic errors present in the continuum solvation models and avoiding usage of the reference base.

For a given computational model, values of the slope and intercept are a = 0.545 and b = -133.5, respectively.

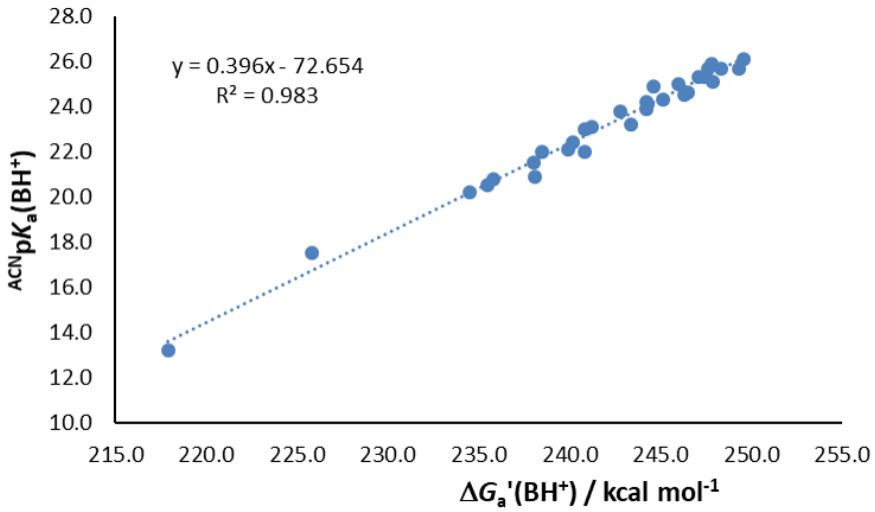

Figure S1. Correlation of calculated $^{ACN}pK_a(\mathbf{B}H^+)$ against $\Delta G_a'(\mathbf{BH}^+)$

Table S2. Electronic energies (E_{SCF}), protonation energies (ΔE_p) and sum of degrees of pyramidalization (ΣDP) within one structure calculated for the deformed guanidine (**GU**$_{def}$) and its conjugate acid (**GUH**$^+_{def}$).[a]

Angle	E_{SCF}(**GU**$_{def}$)	E_{SCF}(**GUH**$^+_{def}$)	ΔE_p	ΣDP(**GU**$_{def}$)	ΣDP(**GUH**$^+_{def}$)
α_1					
120	-205.45473	-205.84553	245.2	31.8	0.0
115	-205.45545	-205.84562	244.8	37.4	0.0
110	-205.45530	-205.84440	244.2	43.2	1.4
105	-205.45422	-205.84187	243.3	49.3	10.4
100	-205.45210	-205.83896	242.8	55.6	17.7
95	-205.44887	-205.83479	242.2	62.0	26.0
90	-205.44446	-205.82951	241.6	68.4	34.6
α_2					
120	-205.45203	-205.84550	246.9	48.2	0.3
115	-205.45472	-205.84399	244.3	49.0	1.3
110	-205.45477	-205.83932	241.3	50.0	4.9
105	-205.45189	-205.83128	238.1	51.4	10.1
100	-205.44566	-205.81954	234.6	53.3	15.8
95	-205.43558	-205.80363	231.0	55.8	21.9
90	-205.42107	-205.78302	227.1	59.2	28.8
α_3					
120	-205.45507	-205.84550	245.0	49.8	0.3
115	-205.45347	-205.84399	245.1	49.0	1.3
110	-205.44871	-205.83932	245.1	48.6	4.9
105	-205.44041	-205.83128	245.3	47.6	10.1
100	-205.42806	-205.81954	245.7	46.7	15.8
95	-205.41109	-205.80363	246.3	46.2	21.9
90	-205.38903	-205.78302	247.2	47.3	28.8
α_4					
120	-205.45375	-205.84545	245.8	50.0	0.0
115	-205.45491	-205.84431	244.3	50.0	1.9
110	-205.45499	-205.84195	242.8	49.7	10.6
105	-205.45387	-205.83857	241.4	49.4	19.6
100	-205.45154	-205.83406	240.0	49.1	28.6
95	-205.44800	-205.82827	238.6	48.9	37.1
90	-205.44333	-205.82112	237.1	49.9	45.9
α_5					
120	-205.45463	-205.84545	245.2	42.7	0.0
115	-205.45509	-205.84431	244.2	48.6	1.9
110	-205.45458	-205.84195	243.1	54.8	10.6
105	-205.45300	-205.83857	242.0	60.8	19.6
100	-205.45022	-205.83406	240.9	67.1	28.6
95	-205.44612	-205.82827	239.8	73.6	37.1
90	-205.44060	-205.82112	238.8	80.2	45.9

a) angle α is given in degrees, E_{SCF} is given in a.u., ΔE_p is given in kcal mol^{-1} and ΣDP is given in %.

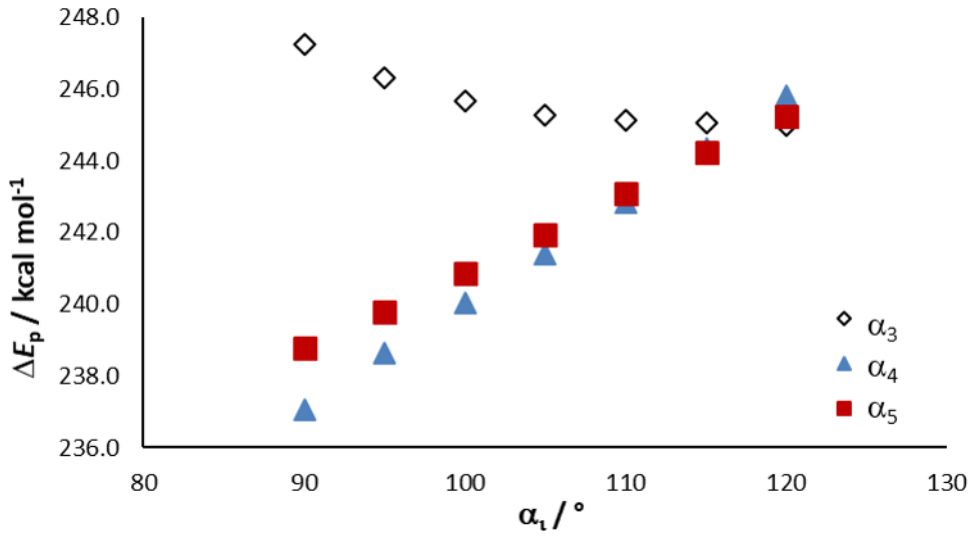

Figure S2. Changes in ΔEp of the unsubstituted guanidine as the function of the angles α_3, α_4 and α_5

Table S3. Selected parameters of geometrical and electronic structure of modeled guanidines and their protonated forms.

Parameter	**16**	**16H$^+$**	**17**	**17H$^+$**
	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)
C1-N2	24.0-26.6 (1.392)	29.1-28.4 (1.345)	30.2-27.6 (1.397)	30.1-32.1 (1.340)
C1-N3	37.9-34.3 (1.305)	33.8-30.8 (1.367)	36.4-34.5 (1.306)	31.6-30.9 (1.379)
C1-N4	32.8-33.7 (1.366)	37.0-34.9 (1.315)	33.2-33.4 (1.368)	37.2-35.7 (1.314)
N3-X	44.9	28.6	44.5	26.6
HOMA	0.84	0.95	0.82	0.92
	DP / %	DP / %	DP / %	DP / %
N2	51.7	26.8	36.1	5.7
N3	-	20.5	-	28.7
N4	12.7	0.1	14.2	0.9
	18	**18H$^+$**	**19**	**19H$^+$**
	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)
C1-N2	30.6-28.2 (1.407)	30.9-34.0 (1.356)	28.8-27.0 (1.398)	29.4-31.7 (1.352)
C1-N3	36.0-34.2 (1.307)	30.7-31.4 (1.375)	40.6-38.3 (1.275)	36.1-35.9 (1.323)
C1-N4	33.3-34.3 (1.362)	37.2-35.7 (1.317)	30.7-29.1 (1.410)	34.4-35.7 (1.345)
N3-X	44.3	26.5	37.5	31.9
HOMA	0.79	0.92	0.58	0.98
	DP / %	DP / %	DP / %	DP / %
N2	37.1	13.3	38.3	30.1
N3	-	27.8	-	0.2
N4	6.7	0.9	24.4	4.9
	20	**20H$^+$**	**21**	**21H$^+$**
	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)
C1-N2	29.9-29.1 (1.402)	30.7-30.7 (1.348)	31.1-30.8 (1.407)	32.0-34.2 (1.344)
C1-N3	38.7-38.0 (1.283)	34.2-35.4 (1.337)	36.9-37.2 (1.291)	32.2-34.7 (1.355)
C1-N4	31.3-33.4 (1.375)	34.8-35.1 (1.328)	31.7-33.7 (1.380)	35.2-35.6 (1.330)
N3-X	36.2	29.0	35.6	27.2
HOMA	0.72	0.99	0.71	0.98
	DP / %	DP / %	DP / %	DP / %
N2	7.9	1.7	17.2	3.2
N3	-	5.1	-	10.3
N4	22.8	12.6	9.3	0.2
	22	**22H$^+$**	**23**	**23H$^+$**
	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)
C1-N2	31.3-31.3 (1.410)	33.5-35.7 (1.351)	30.2-27.7 (1.414)	30.9-32.6 (1.343)
C1-N3	36.8-37.8 (1.290)	31.7-37.3 (1.355)	40.6-40.1 (1.266)	36.1-36.5 (1.320)
C1-N4	31.7-33.2 (1.386)	34.4-35.5 (1.340)	29.1-30.3 (1.407)	32.7-34.2 (1.361)
N3-X	35.1	28.9	31.6	29.3
HOMA	0.68	0.98	0.49	0.97
	DP / %	DP / %	DP / %	DP / %
N2	21.3	11.2	34.4	9.4
N3	-	11.3	-	0.2
N4	13.4	3.5	30.0	15.0

Table S3 (continued)

Parameter	**24**	**24H$^+$**	**25**	**25H$^+$**
	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)
C1-N2	31.3-31.3 (1.399)	32.5-34.2 (1.343)	32.1-32.8 (1.406)	33.8-35.2 (1.346)
C1-N3	39.0-39.1 (1.280)	34.0-37.0 (1.334)	37.6-38.8 (1.288)	32.6-36.8 (1.351)
C1-N4	29.6-32.7 (1.394)	33.0-34.9 (1.346)	30.2-33.2 (1.401)	33.5-35.1 (1.351)
N3-X	31.1	28.0	29.9	27.7
HOMA	0.67	0.99	0.63	0.98
	DP / %	DP / %	DP / %	DP / %
N2	11.4	3.0	8.9	0.2
N3	-	0.6	-	0.9
N4	10.5	4.5	9.0	0.0
	26	**26H$^+$**	**27**	**27H$^+$**
	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)
C1-N2	32.1-34.3 (1.396)	33.5-35.8 (1.344)	30.2-28.5 (1.421)	31.7-30.6 (1.358)
C1-N3	37.8-38.5 (1.289)	33.3-37.1 (1.347)	40.9-39.9 (1.265)	36.4-37.3 (1.321)
C1-N4	30.0-32.7 (1.404)	33.0-35.3 (1.356)	28.5-30.4 (1.407)	31.7-31.4 (1.359)
N3-X	31.5	27.8	29.9	27.0
HOMA	0.66	0.98	0.45	0.96
	DP / %	DP / %	DP / %	DP / %
N2	5.7	1.8	28.5	16.4
N3	-	3.4	-	0.7
N4	15.0	4.2	23.3	13.9
	28	**28H$^+$**	**29**	**29H$^+$**
	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)
C1-N2	31.6-31.3 (1.415)	32.6-34.9 (1.347)	31.9-31.6 (1.412)	33.4-34.3 (1.350)
C1-N3	39.2-39.9 (1.277)	34.3-37.5 (1.342)	37.7-39.0 (1.287)	33.0-36.6 (1.353)
C1-N4	29.1-32.0 (1.404)	33.1-34.9 (1.344)	30.1-34.7 (1.393)	33.4-36.3 (1.346)
N3-X	27.6	26.1	29.6	26.7
HOMA	0.54	0.99	0.63	0.98
	DP / %	DP / %	DP / %	DP / %
N2	18.7	6.0	15.1	4.6
N3	-	4.4	-	3.7
N4	14.0	0.0	5.9	0.2
	30	**30H$^+$**		
	s-char. / % (*d* / Å)	s-char. / % (*d* / Å)		
C1-N2	32.0-34.1 (1.402)	33.0-35.0 (1.349)		
C1-N3	37.6-39.3 (1.287)	33.1-37.8 (1.347)		
C1-N4	30.3-33.8 (1.397)	33.8-36.0 (1.348)		
N3-X	29.8	26.5		
HOMA	0.66	0.98		
	DP / %	DP / %		
N2	10.1	1.1		
N3	-	1.4		
N4	1.8	0.0		

Cartesian coordinates of all optimized structures

1

0 1

C	0.020133	0.312835	0.087178
N	-0.874071	-0.734616	0.441279
N	-0.279488	1.556370	0.045812
N	1.326725	-0.105742	-0.204954
C	-2.054098	-0.975488	-0.390990
C	-1.639409	1.990612	0.308590
H	-2.165204	1.381557	1.057782
H	-1.606551	3.022921	0.674369
H	-2.252388	1.999188	-0.605553
C	-0.937339	-1.958242	-0.356590
C	2.248744	0.955189	-0.595105
H	2.509613	1.616190	0.245637
H	3.162341	0.490497	-0.981248
H	1.793525	1.569880	-1.371696
H	-1.037902	-2.880845	0.211859
H	-0.292326	-2.020569	-1.231041
H	-2.978593	-1.165522	0.149779
H	-2.164834	-0.382358	-1.296579
C	1.942563	-1.089977	0.684930
H	1.233191	-1.872677	0.951475
H	2.794857	-1.551882	0.174990
H	2.308546	-0.628044	1.617186

1H$^+$

1 1

C	0.055623	0.261129	-0.088140
N	-0.810106	-0.745968	-0.396497
N	-0.407987	1.516757	0.019185
N	1.370872	0.013800	0.024095
C	-1.790780	1.941803	-0.236325
H	-2.195536	1.429680	-1.111988
H	-2.434486	1.764342	0.628886
H	-1.771980	3.013610	-0.436521
C	2.306234	1.075704	0.414081
H	3.238418	0.608520	0.733480
H	2.527540	1.752252	-0.421846
H	1.914515	1.642479	1.263653

C	1.970200	-1.250976	-0.435777
H	1.294659	-1.768579	-1.114379
H	2.884904	-1.014130	-0.984648
H	2.222588	-1.899422	0.409191
C	-2.052779	-1.069200	0.319455
C	-0.916485	-2.031699	0.301615
H	-0.955095	-2.900869	-0.348376
H	-0.343517	-2.152354	1.218018
H	-2.249062	-0.547286	1.252529
H	-2.915386	-1.235189	-0.318754
H	0.280909	2.254260	0.053819

2

0 1

C	1.794782	0.904932	-0.508948
C	3.029105	-0.007857	-0.300736
C	2.053716	-1.070915	0.268618
H	1.859001	1.925646	-0.115536
H	1.451805	0.947288	-1.552352
H	3.730790	0.383110	0.440451
H	3.577383	-0.288923	-1.202407
H	2.299175	-1.513809	1.239796
H	1.802795	-1.872793	-0.433853
N	1.005452	-0.033190	0.326697
C	-0.339474	-0.337716	0.122575
N	-0.678384	-1.570440	-0.003785
N	-1.190301	0.779000	0.133372
C	-2.208233	0.943952	-0.889199
H	-3.196592	1.137462	-0.448777
H	-1.963753	1.791538	-1.550411
H	-2.272799	0.045909	-1.503488
C	-0.862332	1.982091	0.876203
H	-0.446868	2.779631	0.237234
H	-1.769651	2.379460	1.352008
H	-0.136323	1.744787	1.654974
C	-2.062604	-1.973754	0.130179
H	-2.689166	-1.247905	0.672551
H	-2.533407	-2.155747	-0.848018
H	-2.099521	-2.927647	0.671696

$2H^+$

1 1

N	-1.002616	0.103896	-0.083918
C	0.326968	0.225273	0.028156
N	0.852145	1.458871	0.178268
N	1.123909	-0.861441	-0.029532
C	2.150148	1.915734	-0.332495
H	2.894540	2.002810	0.464219
H	2.510703	1.218924	-1.090745
H	2.015616	2.894767	-0.798431
C	-2.051827	1.143542	-0.219369
C	-3.111192	0.067571	0.141079
C	-1.956992	-0.941211	0.378302
C	0.735385	-2.069201	-0.765672
H	1.626831	-2.472541	-1.254551
H	0.326136	-2.838877	-0.101118
H	0.004995	-1.819041	-1.535649
H	-3.767038	-0.199686	-0.688182
H	-3.713317	0.294350	1.020968
H	-1.786428	-1.225457	1.421542
H	-1.970439	-1.836875	-0.246374
H	-2.104527	1.571269	-1.224701
H	-1.968505	1.950503	0.518520
C	2.378279	-0.952186	0.730526
H	2.382569	-1.898715	1.280278
H	3.249919	-0.928682	0.068290
H	2.442769	-0.137320	1.450978
H	0.217498	2.178160	0.498066

3

0 1

H	0.497201	0.190937	-0.351226
C	0.179904	0.497229	0.652166
N	1.194233	1.357239	1.295265
C	2.123384	2.082533	0.557383
N	1.594876	2.710859	-0.582938
C	0.287136	3.335607	-0.590695
N	3.339191	2.142059	0.975328
C	4.243773	3.148147	0.460476
C	1.599004	0.811229	2.599106
C	2.292264	2.675384	-1.852988
H	3.739658	4.013823	0.001681

H	4.865251	3.518495	1.286074
H	4.938127	2.734247	-0.286777
H	-0.774774	1.030796	0.544360
C	0.027697	-0.696441	1.612215
H	-0.437357	2.793440	-1.220369
H	-0.101523	3.380730	0.428030
H	1.772072	1.622112	3.313684
C	0.431180	-0.106168	2.973181
H	2.539176	0.250493	2.511710
H	1.650195	2.230716	-2.629985
H	2.588702	3.677347	-2.198395
H	3.189262	2.061029	-1.764854
H	0.359631	4.362731	-0.978384
H	-0.982641	-1.117583	1.597714
H	0.726614	-1.494228	1.333037
H	0.714899	-0.866952	3.706991
H	-0.396429	0.478085	3.394911

3H$^+$

1 1

H	0.296540	0.099653	-0.323252
C	0.106674	0.454890	0.693149
N	1.295630	1.196773	1.201989
C	2.092775	1.966238	0.442814
N	1.609732	2.622890	-0.636154
C	0.250487	3.172902	-0.676727
N	3.396160	2.084259	0.772700
C	4.247450	3.255182	0.538237
C	1.656198	0.755460	2.575553
C	2.407212	2.807251	-1.856247
H	3.622358	4.132245	0.363600
H	4.849485	3.431436	1.432768
H	4.917283	3.111715	-0.314717
H	-0.770540	1.108578	0.675218
C	-0.075840	-0.668620	1.721483
H	-0.424858	2.552641	-1.276357
H	-0.143498	3.274994	0.334681
H	1.891728	1.621224	3.200746
C	0.420184	-0.029294	3.027857
H	2.531173	0.090858	2.548626
H	1.794865	2.518628	-2.716537
H	2.716413	3.850130	-1.983537
H	3.287350	2.164838	-1.831580

H	0.298739	4.168723	-1.127844
H	-1.114325	-1.004091	1.773151
H	0.545167	-1.531768	1.457320
H	0.664648	-0.760981	3.801242
H	-0.333473	0.654341	3.433900
H	3.780368	1.360152	1.364282

4

0 1

C	-4.195889	2.151426	1.363612
C	-4.599649	0.818059	0.727168
H	-4.450377	-0.005871	1.428024
H	-5.677809	0.842567	0.480851
N	-3.818605	0.558287	-0.490638
C	-3.983021	1.605621	-1.502793
H	-3.381933	1.331499	-2.371176
H	-5.030342	1.648182	-1.847929
C	-3.559914	2.965093	-0.934279
H	-2.481822	2.943094	-0.724225
H	-3.725371	3.739875	-1.693630
C	-4.326559	3.298989	0.352935
C	-3.752931	-0.765896	-0.955661
N	-4.072317	-1.023498	-2.173055
N	-3.287019	-1.686593	-0.003193
C	-2.236985	-1.365645	0.944158
C	-3.927432	-2.974700	0.175342
H	-1.812966	-0.391117	0.699671
H	-1.437830	-2.120596	0.898270
H	-2.604274	-1.336347	1.983545
H	-4.267320	-3.089978	1.217054
H	-3.253694	-3.814803	-0.050490
H	-4.801203	-3.048017	-0.473566
C	-3.676308	-2.273460	-2.789679
H	-3.386305	-2.074762	-3.829186
H	-4.510747	-2.989198	-2.832243
H	-2.832157	-2.773304	-2.289132
H	-3.155909	2.080438	1.710107
H	-4.821366	2.336188	2.246281
H	-5.389791	3.448601	0.113294
H	-3.966165	4.239775	0.787172

4H$^+$

1 1

C	-2.328352	-1.080508	0.910424
C	-3.301263	-0.049176	0.322497
C	-2.563583	1.241081	-0.064843
C	-1.383562	0.922228	-0.989087
H	-2.838788	-2.031366	1.100533
H	-3.788310	-0.468949	-0.568551
H	-4.097611	0.168913	1.041150
H	-3.235986	1.937510	-0.577647
H	-2.201794	1.752407	0.838880
H	-1.756443	0.483322	-1.924066
H	-0.806668	1.809552	-1.256633
H	-1.943722	-0.725568	1.875780
N	-0.473435	-0.079128	-0.386970
C	-1.140414	-1.352106	-0.026034
H	-1.479643	-1.838866	-0.949088
H	-0.414495	-2.006231	0.456852
C	0.797976	0.201876	-0.041710
N	1.748140	-0.758797	-0.040582
N	1.125962	1.465634	0.304192
C	1.749474	-1.863907	-1.005822
H	1.540124	-2.822357	-0.518653
H	1.009373	-1.682889	-1.785119
H	2.740118	-1.920264	-1.468996
C	2.851370	-0.766428	0.928395
H	2.932628	-1.771990	1.353417
H	3.805552	-0.511580	0.454923
H	2.645262	-0.065014	1.736697
C	2.406861	2.133567	0.049248
H	2.208488	3.137138	-0.335190
H	3.012159	2.216689	0.956786
H	2.964060	1.578472	-0.706756
H	0.369978	2.047345	0.640782

5

0 1

H	-0.150664	0.330578	3.587946
C	-0.165241	-0.685456	3.171249
H	-0.133093	-1.358393	4.038964
C	-1.512095	-0.951999	2.475105
H	-1.652726	-2.032117	2.379351

H	-2.312916	-0.590120	3.140857
N	-1.653887	-0.382741	1.132784
C	-0.993472	0.885436	0.818739
H	-1.556624	1.340648	-0.000099
H	-1.087098	1.543368	1.693962
C	0.477926	0.759287	0.384803
H	0.504536	0.032340	-0.432966
H	0.790149	1.724085	-0.040472
C	1.466966	0.367891	1.490830
H	1.582218	1.206714	2.194727
H	2.455792	0.216801	1.037048
C	1.089194	-0.883104	2.301691
H	0.949970	-1.741719	1.629769
H	1.932877	-1.137056	2.956644
C	-2.158494	-1.138366	0.076170
N	-1.749298	-0.897968	-1.122568
N	-3.105175	-2.107259	0.451565
C	-3.084152	-3.440506	-0.116241
C	-4.226092	-1.799203	1.319394
H	-2.150191	-3.593667	-0.659741
H	-3.922039	-3.626832	-0.805734
H	-3.139346	-4.191474	0.686726
H	-4.217716	-2.402990	2.240631
H	-5.179281	-1.990635	0.802847
H	-4.196485	-0.744190	1.597129
C	-2.509554	-1.370070	-2.261128
H	-2.490407	-0.598431	-3.041368
H	-3.564501	-1.595694	-2.037921
H	-2.065372	-2.272869	-2.707881

5H$^+$

1 1

H	-0.284507	0.449046	3.560967
C	-0.182181	-0.586011	3.211922
H	-0.171977	-1.199308	4.121055
C	-1.450755	-1.016229	2.462684
H	-1.484439	-2.107140	2.397407
H	-2.322523	-0.692357	3.042163
N	-1.556710	-0.509093	1.068099
C	-0.930400	0.789461	0.724669
H	-1.489316	1.201620	-0.119976
H	-1.097741	1.461956	1.571438
C	0.570954	0.716698	0.389906

H	0.746125	-0.064862	-0.364873
H	0.844115	1.665243	-0.088759
C	1.502170	0.470970	1.584795
H	1.506482	1.366887	2.220905
H	2.524965	0.363705	1.205584
C	1.149908	-0.743802	2.457184
H	1.140312	-1.664219	1.855341
H	1.949728	-0.874699	3.194207
C	-2.151641	-1.254938	0.114336
N	-1.773380	-1.113840	-1.173941
N	-3.120748	-2.147438	0.423841
C	-3.244858	-3.432506	-0.276617
C	-4.146368	-1.880146	1.438938
H	-2.334121	-3.643567	-0.837179
H	-4.104907	-3.443766	-0.954964
H	-3.381747	-4.221272	0.469987
H	-3.990424	-2.477909	2.343299
H	-5.122786	-2.137851	1.016142
H	-4.154786	-0.821032	1.696662
C	-2.632131	-1.283952	-2.350293
H	-2.414595	-0.480897	-3.058562
H	-3.679622	-1.209193	-2.054208
H	-2.464097	-2.245048	-2.845597
H	-0.853073	-0.728618	-1.336857

6

0 1

C	0.217649	0.282792	-0.174084
N	-1.127808	0.314354	-0.479930
N	-0.481721	-0.726743	0.490393
N	1.300457	0.878341	-0.377071
C	2.510136	0.312048	0.211412
H	3.216014	0.061037	-0.588931
H	2.989228	1.072717	0.838019
H	2.338110	-0.584470	0.824711
C	-1.969009	1.285151	0.228120
H	-1.989340	2.199639	-0.373818
H	-2.984919	0.887668	0.300116
H	-1.592097	1.518510	1.231391
C	-0.485053	-2.072336	-0.097392
H	0.317700	-2.646186	0.378315
H	-1.439774	-2.553940	0.131759
H	-0.333761	-2.062562	-1.183641

6H$^+$

1 1

C	0.152162	-0.264759	-0.121808
N	-0.480749	0.767192	0.451532
N	1.310073	-0.825688	-0.253109
N	-1.139570	-0.373233	-0.460769
C	-0.526129	2.124418	-0.126201
H	0.334923	2.674255	0.266098
H	-0.502068	2.097939	-1.219672
H	-1.440126	2.603419	0.224675
C	2.586326	-0.241683	0.207645
H	2.379966	0.681804	0.748940
H	3.078559	-0.951960	0.874660
H	3.222351	-0.036125	-0.656274
C	-2.089109	-1.262784	0.234888
H	-3.087156	-0.841179	0.116543
H	-2.051658	-2.233192	-0.270077
H	-1.839778	-1.369151	1.294984
H	1.337208	-1.734855	-0.710593

7

0 1

C	0.072831	-0.344380	-0.095861
N	0.313930	0.986211	0.371062
N	0.724918	-1.421130	-0.214963
N	-1.290173	-0.093426	-0.334525
C	1.324140	1.866660	-0.198679
H	2.308425	1.404475	-0.096502
H	1.150709	2.087714	-1.264749
H	1.336494	2.811280	0.355218
C	2.127303	-1.445166	0.163676
H	2.377080	-0.747984	0.978728
H	2.389147	-2.455646	0.497016
H	2.779877	-1.213498	-0.691474
C	-1.123354	1.270315	0.180917
H	-1.340714	2.058975	-0.553439
H	-1.656241	1.474960	1.120990
C	-2.352456	-1.006432	0.038362
H	-3.285376	-0.727842	-0.462546
H	-2.062853	-2.006738	-0.291263
H	-2.528053	-1.033261	1.126510

7H$^+$

1 1

C	0.009686	-0.270405	-0.072480
N	0.295352	1.019128	0.254582
N	0.755326	-1.359620	-0.157221
N	-1.324718	-0.094653	-0.249336
C	1.408392	1.885961	-0.132368
H	2.354431	1.407350	0.123008
H	1.391875	2.116373	-1.204329
H	1.332572	2.812571	0.440139
C	2.190688	-1.430539	0.150184
H	2.406850	-0.842320	1.044767
H	2.439817	-2.471987	0.355604
H	2.797514	-1.078462	-0.689266
C	-1.147402	1.333056	0.102528
H	-1.374825	2.021463	-0.716180
H	-1.631111	1.631283	1.036963
C	-2.442633	-0.975087	0.073472
H	-3.353154	-0.549402	-0.352603
H	-2.281997	-1.950201	-0.393280
H	-2.567815	-1.102766	1.155506
H	0.291733	-2.205805	-0.464521

8

0 1

C	-0.156610	-0.359075	0.058218
N	-0.485571	0.985432	-0.235796
N	-0.866310	-1.420952	0.091392
N	1.227781	-0.410927	0.283452
C	1.919044	-1.676352	0.140382
H	1.311050	-2.456946	0.597850
H	2.087837	-1.943264	-0.916531
H	2.888488	-1.618526	0.647094
C	-1.685025	1.608643	0.308200
H	-2.567299	0.999767	0.124183
H	-1.602686	1.790316	1.393220
H	-1.832568	2.574441	-0.187470
C	-2.272953	-1.432477	-0.245269
H	-2.525542	-0.800033	-1.111348
H	-2.559151	-2.459820	-0.499453
H	-2.919531	-1.127996	0.593449
C	0.720854	1.805602	-0.097166

H	0.765870	2.267783	0.903408
C	1.843939	0.784161	-0.267145
H	2.754063	1.057598	0.277739
H	2.107068	0.654364	-1.332396
H	0.745604	2.604432	-0.846405

8H$^+$

1 1

C	0.106517	-0.278708	-0.036643
N	0.406427	1.025973	0.144153
N	0.957694	-1.309486	-0.089157
N	-1.227886	-0.468154	-0.153523
C	2.407610	-1.328853	0.142900
H	2.656449	-0.927982	1.129005
H	2.722507	-2.372222	0.109846
H	2.948783	-0.785682	-0.634623
C	-0.828727	1.823340	-0.020986
H	-0.851671	2.263000	-1.026442
C	-1.934166	0.781104	0.173656
H	-2.784345	0.929940	-0.495402
H	-2.295385	0.751185	1.209816
H	-0.860901	2.625974	0.718626
C	1.680845	1.697623	-0.127998
H	1.594371	2.720222	0.243842
H	2.503304	1.224261	0.403939
H	1.899578	1.731999	-1.202243
C	-1.891818	-1.762518	-0.043601
H	-1.789744	-2.198262	0.958820
H	-2.952387	-1.617738	-0.255046
H	-1.508811	-2.460351	-0.795471
H	0.523038	-2.214610	-0.198950

9

0 1

C	-0.489862	0.331534	-0.036505
N	-0.342125	-1.045604	-0.324793
N	-1.597073	0.957000	0.156250
N	0.696687	1.061677	-0.086379
C	-2.864710	0.332451	-0.155241
H	-2.793850	-0.489993	-0.884915
H	-3.364681	-0.060993	0.744574
H	-3.539062	1.093979	-0.567930

C	0.979699	-1.448833	-0.808738
H	1.160194	-0.985256	-1.785622
C	1.991497	0.515614	0.327297
H	0.975477	-2.533949	-0.953935
C	2.051302	-1.014006	0.192870
H	2.751302	0.977358	-0.317859
H	2.232337	0.822852	1.358873
H	3.053441	-1.329070	-0.120029
H	1.853568	-1.495255	1.157826
C	-0.946882	-2.005014	0.598319
H	-1.165556	-2.937352	0.065301
H	-0.291820	-2.244544	1.452481
H	-1.880830	-1.614109	0.997399
C	0.605456	2.509495	-0.012782
H	1.511692	2.943189	-0.452703
H	-0.274264	2.842697	-0.562752
H	0.510623	2.871493	1.022433

9H$^+$

1 1

C	-0.373032	0.271129	0.055026
N	-0.278716	-1.053339	-0.181703
N	-1.576138	0.841903	0.290183
N	0.730725	1.042102	0.021197
C	-2.859049	0.426335	-0.291977
H	-2.680146	-0.265823	-1.115964
H	-3.508096	-0.050218	0.448229
H	-3.366408	1.309725	-0.688008
C	1.014295	-1.553718	-0.684935
H	1.156316	-1.214317	-1.717385
C	2.102394	0.498555	0.166253
H	0.968848	-2.643313	-0.696428
C	2.119090	-1.027301	0.228935
H	2.671528	0.851054	-0.701342
H	2.556054	0.940223	1.060877
H	3.102527	-1.393067	-0.080705
H	1.943396	-1.382677	1.250489
C	-1.175890	-2.032653	0.452937
H	-1.741989	-2.589417	-0.299418
H	-0.575694	-2.738109	1.036488
H	-1.865214	-1.533090	1.131653
C	0.646948	2.503098	-0.080615
H	1.551814	2.865397	-0.573828

H	-0.211604	2.795003	-0.688972
H	0.583281	2.978229	0.906249
H	-1.564244	1.743082	0.746577

10

0 1

C	2.550158	0.242727	0.036371
C	1.447065	1.024415	0.762968
C	2.186823	-1.222125	-0.226557
C	-0.782613	0.300569	-0.004998
C	0.822516	-1.380224	-0.917023
H	2.760847	0.750034	-0.914946
H	1.184369	0.515893	1.702035
H	2.174169	-1.777743	0.721874
H	0.684891	-2.424024	-1.229142
H	3.470043	0.292146	0.634762
H	1.835777	2.008784	1.042753
H	2.959966	-1.690440	-0.850550
H	0.797656	-0.770147	-1.826746
N	0.241941	1.250282	-0.051979
N	-0.326991	-1.022591	-0.089429
N	-2.005087	0.692527	0.074045
C	-3.086317	-0.221433	-0.233118
H	-3.555604	-0.623555	0.677702
H	-3.871477	0.328969	-0.767074
H	-2.786017	-1.077566	-0.858038
C	-0.157502	2.641968	-0.225725
H	-0.947998	2.696876	-0.974636
H	-0.547469	3.091419	0.699730
H	0.708281	3.220466	-0.566168
C	-0.855527	-2.053264	0.788064
H	-1.556573	-1.607821	1.495290
H	-1.378266	-2.847025	0.234730
H	-0.049267	-2.523590	1.370066

10H$^+$

1 1

C	2.602590	0.177811	-0.047351
C	1.588762	0.984756	0.767537
C	2.194336	-1.287286	-0.214182
C	-0.672469	0.279454	0.096838
C	0.811779	-1.441872	-0.853418

H	2.740274	0.648908	-1.029366
H	1.384960	0.482935	1.720240
H	2.209971	-1.799823	0.756782
H	0.621042	-2.488009	-1.107474
H	3.567682	0.235800	0.468537
H	1.990629	1.972896	1.003853
H	2.920054	-1.802951	-0.853170
H	0.762014	-0.868521	-1.785427
N	0.288501	1.226405	0.088346
N	-0.325901	-1.020286	-0.000027
N	-1.965792	0.644783	0.195948
C	-3.118453	-0.067389	-0.365838
H	-3.658034	-0.637272	0.396310
H	-3.799362	0.664706	-0.806498
H	-2.781116	-0.743817	-1.152450
C	0.007593	2.604798	-0.334665
H	-0.825565	2.618560	-1.039435
H	-0.221512	3.255309	0.518901
H	0.890787	3.001531	-0.841292
C	-1.065197	-2.080864	0.699199
H	-1.707060	-1.645723	1.465644
H	-1.670966	-2.677615	0.009251
H	-0.344850	-2.741040	1.191168
H	-2.150245	1.551363	0.605838

11

0 1

C	0.055116	-0.363557	-0.070384
N	0.485721	-1.594271	-0.087379
N	-1.191242	0.144822	0.169955
N	1.237462	0.363086	-0.350974
C	-2.239697	-0.831735	0.435857
H	-1.815628	-1.662566	1.002089
H	-3.034227	-0.356498	1.021459
H	-2.676016	-1.231953	-0.492146
C	1.838041	-1.010392	-0.267834
H	2.350135	-1.320884	-1.185559
H	2.499111	-1.132598	0.599737
C	1.722025	1.399291	0.557574
H	2.736014	1.682480	0.257429
H	1.091910	2.290785	0.484042
H	1.744299	1.079481	1.612666
C	-1.615025	1.348977	-0.533354

H	-2.297598	1.928831	0.098211
H	-0.749157	1.965546	-0.776596
H	-2.135189	1.106408	-1.473707

11H$^+$

1 1

C	0.018372	-0.321793	-0.056724
N	0.524020	-1.593171	0.049060
N	-1.227179	0.104204	-0.015773
N	1.218802	0.300980	-0.212064
C	-2.320438	-0.830388	0.294303
H	-1.918454	-1.732406	0.758732
H	-2.999848	-0.350394	1.003149
H	-2.872503	-1.090566	-0.614539
C	1.879629	-1.024606	-0.151313
H	2.365164	-1.319603	-1.084828
H	2.537466	-1.155986	0.711677
C	1.752821	1.545667	0.341091
H	2.697349	1.764428	-0.161234
H	1.065940	2.368955	0.145101
H	1.923739	1.463339	1.421023
C	-1.583463	1.500809	-0.306998
H	-1.671083	2.084598	0.614929
H	-0.839805	1.947961	-0.967976
H	-2.545065	1.505806	-0.824825
H	0.166078	-2.388353	-0.471921

12

0 1

C	-0.061561	-0.279377	0.004048
N	0.879236	0.754623	-0.179985
N	-1.401034	0.060973	0.188356
N	0.375773	-1.488851	-0.016415
C	0.774058	1.993470	0.581072
H	-0.264075	2.320676	0.638232
H	1.151411	1.875627	1.611555
H	1.360658	2.779169	0.092250
C	-2.008007	0.896722	-0.851445
H	-1.307067	1.661208	-1.187995
H	-2.305355	0.299291	-1.729472
H	-2.902026	1.386819	-0.450519
C	2.194032	0.094547	-0.130634

H	2.696591	0.334949	0.820151
C	1.825414	-1.411122	-0.217329
H	2.361708	-2.014335	0.525106
H	2.071718	-1.827384	-1.203575
H	2.842888	0.433993	-0.945836
C	-2.261666	-1.050512	0.582630
H	-3.226054	-0.643486	0.905448
H	-2.430387	-1.763446	-0.238781
H	-1.801456	-1.592668	1.409688

12H$^+$

1 1

C	-0.068449	-0.240452	-0.000113
N	0.831066	0.759508	-0.058079
N	-1.400037	-0.106999	0.034538
N	0.544371	-1.447874	0.050050
H	0.056376	-2.269947	-0.281495
C	0.626403	2.137154	0.399701
H	-0.320199	2.227964	0.932376
H	1.432068	2.395318	1.093408
H	0.648080	2.841120	-0.437379
C	-2.110626	1.036685	-0.560661
H	-1.425143	1.662264	-1.130413
H	-2.866857	0.648909	-1.250225
H	-2.609211	1.635005	0.207915
C	2.203904	0.209038	-0.057766
H	2.686557	0.459844	0.893647
C	1.988243	-1.310385	-0.212627
H	2.572278	-1.894052	0.501618
H	2.220008	-1.654849	-1.225530
H	2.794584	0.639235	-0.870514
C	-2.241744	-1.252884	0.405843
H	-3.160115	-0.869559	0.856002
H	-2.510126	-1.858339	-0.469399
H	-1.732487	-1.870291	1.148153

13

0 1

C	-0.239011	-0.244731	-0.114989
N	0.241784	-1.438306	-0.125783
N	-1.638931	-0.057894	-0.123508
N	0.499282	0.939850	-0.085710

C	-2.414265	-1.247461	-0.460651
H	-2.005532	-1.709597	-1.359931
H	-2.402095	-2.001846	0.340171
H	-3.449791	-0.940554	-0.647032
C	1.690375	-1.561326	-0.222786
H	2.016622	-1.486696	-1.273909
C	1.946245	0.885463	0.112204
H	1.974063	-2.563539	0.119057
C	2.392200	-0.486066	0.612056
H	2.451566	1.115382	-0.841490
H	2.237852	1.676374	0.819415
H	3.484304	-0.561715	0.549885
H	2.110820	-0.614541	1.664547
C	0.023147	2.170026	-0.696559
H	0.640535	2.428879	-1.571468
H	-1.006918	2.042163	-1.027434
H	0.074471	3.013448	0.007052
C	-2.196981	0.648844	1.031693
H	-2.250760	-0.000837	1.922064
H	-1.589223	1.519189	1.283078
H	-3.211108	0.989843	0.795196

13H$^+$

1 1

C	-0.249935	-0.213951	-0.055925
N	0.407755	-1.389831	-0.103025
N	-1.602480	-0.224104	0.019061
N	0.444030	0.936001	-0.131196
C	-2.364777	-1.409672	-0.389450
H	-1.861681	-1.917188	-1.214404
H	-2.515626	-2.110362	0.443255
H	-3.347279	-1.080861	-0.737436
C	1.868974	-1.452489	-0.252969
H	2.134232	-1.348167	-1.311439
C	1.903544	0.999729	0.120324
H	2.192682	-2.440857	0.077601
C	2.480083	-0.333403	0.587762
H	2.380106	1.312581	-0.816654
H	2.082565	1.788571	0.859483
H	3.568376	-0.309880	0.479708
H	2.256469	-0.508034	1.645985
H	-0.064978	-2.195463	0.283644
C	-0.137320	2.177807	-0.657879

H	0.554239	2.592321	-1.397869
H	-1.086709	1.971574	-1.150272
H	-0.285166	2.920038	0.132953
C	-2.351937	0.750062	0.827719
H	-2.940357	0.206740	1.574959
H	-1.670146	1.417423	1.353192
H	-3.033662	1.338605	0.205923

14

1 1

C	-0.249935	-0.213951	-0.055925
N	0.407755	-1.389831	-0.103025
N	-1.602480	-0.224104	0.019061
N	0.444030	0.936001	-0.131196
C	-2.364777	-1.409672	-0.389450
H	-1.861681	-1.917188	-1.214404
H	-2.515626	-2.110362	0.443255
H	-3.347279	-1.080861	-0.737436
C	1.868974	-1.452489	-0.252969
H	2.134232	-1.348167	-1.311439
C	1.903544	0.999729	0.120324
H	2.192682	-2.440857	0.077601
C	2.480083	-0.333403	0.587762
H	2.380106	1.312581	-0.816654
H	2.082565	1.788571	0.859483
H	3.568376	-0.309880	0.479708
H	2.256469	-0.508034	1.645985
H	-0.064978	-2.195463	0.283644
C	-0.137320	2.177807	-0.657879
H	0.554239	2.592321	-1.397869
H	-1.086709	1.971574	-1.150272
H	-0.285166	2.920038	0.132953
C	-2.351937	0.750062	0.827719
H	-2.940357	0.206740	1.574959
H	-1.670146	1.417423	1.353192
H	-3.033662	1.338605	0.205923

14H$^+$

1 1

C	2.632616	0.632703	0.015886
C	1.380303	1.242478	0.654404
C	2.694878	-0.888750	0.166654

C	-0.528916	-0.204197	0.075143
C	1.490550	-1.603340	-0.448380
H	2.681052	0.915947	-1.044030
H	1.268356	0.880721	1.682370
H	2.775616	-1.160938	1.226823
H	1.625834	-2.686330	-0.398133
H	3.506327	1.082990	0.500601
H	1.469008	2.330834	0.703412
H	3.594604	-1.271507	-0.328384
H	1.389315	-1.334353	-1.506644
N	0.109549	0.975711	-0.063572
N	0.199963	-1.329086	0.223621
N	-1.875566	-0.279679	0.071481
C	-2.583656	-1.511246	-0.299839
H	-2.873248	-2.091547	0.585083
H	-3.492943	-1.239122	-0.842968
H	-1.961826	-2.123440	-0.954761
C	-0.414568	2.056973	-0.909216
H	-1.207399	1.677337	-1.554340
H	-0.798578	2.891014	-0.312460
H	0.396903	2.426721	-1.542981
H	-0.266467	-2.117401	0.652513
C	-2.723217	0.790469	0.615346
H	-3.427931	0.349055	1.327158
H	-2.112769	1.522346	1.142974
H	-3.291411	1.288524	-0.176927

15

0 1

C	-0.227654	-0.366359	-0.487850
N	-0.941312	0.835952	-0.361676
N	-0.980282	-1.319651	-0.030590
N	1.072494	0.152407	-0.440017
C	2.125159	-0.582424	0.248099
H	2.416660	-1.438722	-0.366027
H	2.998064	0.066088	0.363942
H	1.807906	-0.952818	1.235473
C	0.366833	1.319332	0.222978
H	0.419842	1.253806	1.318428
H	0.668471	2.304451	-0.139566
C	-1.866592	-0.161952	0.355930
H	-2.878277	-0.141095	-0.061218
H	-1.875444	-0.024238	1.440005

15H$^+$

1 1

C	0.191025	-0.381048	0.352763
N	0.848563	0.811662	0.398554
N	1.215366	-1.216147	0.083879
N	-1.051124	0.025166	0.109756
C	-0.455159	1.385955	-0.138769
H	-0.426110	1.622498	-1.204184
H	-0.844997	2.200062	0.473050
C	1.967859	0.043476	-0.298378
H	2.932262	0.171879	0.190008
H	2.002235	0.187972	-1.380058
C	-2.353231	-0.582388	-0.128514
H	-2.605178	-0.553596	-1.193034
H	-2.318987	-1.619536	0.211065
H	-3.114661	-0.049122	0.445814
H	1.182838	-2.100899	-0.410592

16

0 1

C	-0.235003	-0.535473	0.288347
N	1.083737	-0.181403	0.319086
N	-1.014813	-1.530574	-0.033381
N	-1.091578	0.557239	0.392273
C	1.098138	1.286848	0.101420
C	-0.372422	1.633375	-0.305012
H	1.813304	1.546714	-0.686714
H	1.389875	1.810351	1.019192
H	-0.490981	1.577059	-1.399311
H	-0.673037	2.630147	0.030134
C	2.114702	-1.045906	-0.224689
H	1.794560	-2.083009	-0.101729
H	2.290433	-0.861676	-1.295900
H	3.057821	-0.905631	0.313819
C	-2.061959	-0.468056	-0.169206
H	-2.323490	-0.268325	-1.215098
H	-2.960647	-0.587193	0.444601

16H$^+$

1 1

C	0.196748	-0.492905	-0.154545
N	-1.080815	-0.210829	-0.021920
N	1.153562	-1.428805	0.121187
N	1.012779	0.565463	-0.304438
C	-1.173049	1.284246	-0.089864
C	0.291768	1.754926	0.190816
H	-1.881509	1.639068	0.661480
H	-1.514899	1.588769	-1.084314
H	0.471836	1.915351	1.260773
H	0.554652	2.654102	-0.366622
C	-2.221030	-1.115705	0.078560
H	-1.859748	-2.127307	0.275145
H	-2.859970	-0.801434	0.907863
H	-2.801603	-1.111204	-0.849363
C	2.161272	-0.324523	0.070579
H	2.588227	-0.117974	1.054571
H	2.920986	-0.404216	-0.708274
H	1.249092	-2.352191	-0.288334

17

0 1

C	0.185189	-0.697160	-0.178995
N	-1.131120	-0.337478	-0.271459
N	0.816757	-1.809026	0.084717
N	1.235336	0.205829	-0.362498
C	-1.414326	1.035147	0.179913
H	-1.567141	1.041945	1.274271
C	1.088450	1.512333	0.267466
H	-2.357175	1.357297	-0.277240
C	-0.290822	2.021375	-0.185422
H	1.133031	1.458097	1.370607
H	1.882435	2.189502	-0.066320
H	-0.511869	2.989720	0.276902
H	-0.269903	2.164431	-1.271536
C	-2.113681	-1.349340	0.088686
H	-2.249131	-1.429838	1.178922
H	-3.076726	-1.098634	-0.368365
H	-1.778199	-2.317064	-0.288625
C	2.051901	-0.967488	0.087578
H	2.828749	-1.254219	-0.629909

H	2.478855	-0.845711	1.090620

17H$^+$

1 1

C	0.782624	1.778585	0.248540
C	-0.645748	1.960480	-0.303544
C	-1.619527	0.848276	0.134605
C	0.255246	-0.608499	-0.071476
H	-1.051446	2.918550	0.033084
H	0.832854	1.941176	1.332780
H	1.477304	2.466326	-0.239179
H	-1.896355	0.955330	1.190672
H	-2.535455	0.905251	-0.459914
H	-0.596907	1.991936	-1.396818
N	-1.055194	-0.517304	-0.042131
N	1.132124	0.403997	-0.088152
N	1.186763	-1.619091	0.038858
C	-1.939491	-1.681433	0.048618
H	-1.344546	-2.591522	0.145404
H	-2.576775	-1.586184	0.932940
H	-2.567355	-1.749493	-0.844642
C	2.248182	-0.563122	0.014076
H	2.811722	-0.513992	0.948560
H	2.902354	-0.582390	-0.860873
H	1.211038	-2.433932	-0.566946

18

0 1

C	-1.953000	-0.978957	-0.236885
C	-0.720726	-1.585664	0.455788
C	-2.257331	0.491551	0.091034
C	0.922221	0.168966	0.043901
C	-1.178059	1.484443	-0.349318
H	-1.835732	-1.105054	-1.321669
H	-0.768876	-1.401082	1.541241
H	-2.408090	0.601478	1.173053
H	-1.500130	2.503823	-0.106619
H	-2.822218	-1.581539	0.058827
H	-0.746636	-2.670879	0.316441
H	-3.202059	0.769511	-0.393950
H	-1.045033	1.435635	-1.445767
N	0.559469	-1.136490	-0.096847

N	0.072086	1.242886	0.365416
N	2.078026	0.768038	-0.075626
C	1.319364	2.032961	0.101043
C	1.647305	-2.101432	-0.204434
H	2.489139	-1.617228	-0.703081
H	1.987882	-2.457096	0.779475
H	1.319548	-2.961287	-0.797846
H	1.254142	2.642481	-0.809464
H	1.632345	2.649001	0.951983

18H$^+$

1 1

C	2.016578	0.851160	-0.316216
C	0.877751	1.620843	0.364333
C	2.251539	-0.578262	0.195297
C	-0.845585	-0.085601	0.044376
C	1.204701	-1.593253	-0.262268
H	1.866243	0.854643	-1.403736
H	0.981972	1.574391	1.456260
H	2.309881	-0.580799	1.291004
H	1.425396	-2.580780	0.152196
H	2.923994	1.436267	-0.128616
H	0.929490	2.672922	0.076437
H	3.220752	-0.931732	-0.172427
H	1.203040	-1.677842	-1.358498
N	-0.495508	1.183384	0.006718
N	-0.137201	-1.231544	0.202012
N	-2.070738	-0.689817	-0.116127
C	-1.396664	-2.000342	0.068291
C	-1.531967	2.213453	-0.167569
H	-2.415582	1.772360	-0.632878
H	-1.803269	2.662419	0.793817
H	-1.146469	2.990399	-0.831195
H	-1.443045	-2.637058	-0.818852
H	-1.682362	-2.540407	0.974285
H	-2.904025	-0.416937	0.396515

19

0 1

C	-0.032612	-0.466605	0.018191
N	-1.333021	-0.058044	-0.343422
N	0.807115	-1.404844	-0.182240

N	0.394380	0.807152	0.405777
C	1.786178	0.840964	-0.059961
H	1.862667	1.166396	-1.110126
H	2.424185	1.474290	0.562011
C	-2.574402	-0.619294	0.156744
H	-2.550363	-1.701229	0.002523
H	-2.740428	-0.419560	1.227888
H	-3.418028	-0.213069	-0.410474
C	2.096598	-0.695232	0.082255
H	2.855698	-1.029418	-0.630679
H	2.461126	-0.916347	1.095216
C	-0.891678	1.342161	-0.112062
H	-0.813927	1.915216	-1.045835
H	-1.464756	1.901909	0.637663

19H$^+$

1 1

C	0.088528	-0.379494	0.110139
N	1.359517	-0.015580	-0.137788
N	-0.825681	-1.321929	-0.055160
N	-0.419129	0.851117	0.346247
C	-1.801291	0.855352	-0.174647
C	-2.158003	-0.650030	0.054531
H	-2.447730	1.524882	0.392980
H	-1.832473	1.121329	-1.238673
H	-2.581257	-0.816927	1.049230
H	-2.836764	-1.040227	-0.705159
C	2.661084	-0.653659	0.000660
H	2.555698	-1.718665	-0.218302
H	3.349780	-0.217744	-0.726260
H	3.063866	-0.527316	1.011379
C	0.921601	1.408495	-0.032141
H	1.391934	1.991167	0.762235
H	0.940263	1.920779	-0.997537
H	-0.677775	-2.316510	-0.154235

20

0 1

C	-0.052989	-0.457068	0.010932
N	1.297524	-0.280724	-0.176970
N	-0.810503	-1.485502	-0.109374
N	-0.646137	0.778968	0.302210

C	-2.043617	0.606943	-0.089975
C	1.628292	1.114744	0.108285
C	0.273248	1.823329	-0.125406
C	-2.172751	-0.940514	0.080401
H	-2.725461	1.177209	0.548293
H	-2.202805	0.912014	-1.139107
H	-2.545146	-1.184922	1.086437
H	-2.870208	-1.376820	-0.642406
H	2.416753	1.479746	-0.558985
H	1.966888	1.247488	1.149500
H	0.143728	2.077562	-1.192008
H	0.172961	2.738048	0.466721
C	2.248069	-1.353700	0.015333
H	1.757202	-2.293860	-0.245138
H	3.115742	-1.211337	-0.638755
H	2.602644	-1.416727	1.056971

20H^{+}

1 1

C	0.012398	-0.390165	0.033456
N	-1.308367	-0.300150	-0.069509
N	0.888915	-1.391275	-0.092420
N	0.617475	0.801859	0.203640
C	2.043122	0.666742	-0.128123
H	2.225154	0.944597	-1.174822
H	2.666397	1.283192	0.521715
C	-2.271862	-1.393872	-0.044523
H	-1.798773	-2.310811	-0.403845
H	-2.664303	-1.556635	0.965734
H	-3.099537	-1.154374	-0.716526
C	-1.685847	1.123110	0.126602
H	-2.066388	1.269530	1.144187
C	-0.345259	1.868349	-0.104576
H	-0.222085	2.723975	0.561352
H	-0.235339	2.201180	-1.145232
H	-2.460364	1.408663	-0.588514
C	2.257114	-0.851581	0.111220
H	2.954400	-1.296061	-0.600433
H	2.597587	-1.056339	1.131629
H	0.659088	-2.365453	0.048446

21

0 1

C	-0.259188	-0.517539	-0.096178
N	-0.703598	0.809656	-0.242868
N	1.093335	-0.776530	-0.179499
C	0.142574	1.911088	0.1838360
H	0.112629	2.038210	1.2834570
C	2.032378	0.268111	0.2231590
H	-0.234751	2.841807	-0.2564750
C	1.574526	1.638168	-0.2752520
H	2.153551	0.289172	1.3221470
H	3.012660	0.018524	-0.1994060
H	2.247805	2.414124	0.1053410
H	1.614921	1.660360	-1.3701500
C	1.519453	-2.146322	0.0625590
H	1.602381	-2.375286	1.1369970
H	0.787751	-2.825631	-0.3742680
H	2.497687	-2.303044	-0.4052130
C	-2.110988	0.783491	0.1594580
N	-1.172219	-1.421822	0.0255020
C	-2.452571	-0.708835	-0.0661270
H	-2.896899	-0.858570	-1.0619600
H	-3.167957	-1.090088	0.6704740
H	-2.217759	1.069126	1.2214220
H	-2.711750	1.473200	-0.4430490

21H$^+$

1 1

C	0.214330	0.448861	-0.002007
N	0.645506	-0.824457	-0.005010
N	-1.069791	0.795402	0.024798
C	-0.258192	-1.950472	0.219792
H	-0.347054	-2.159170	1.295073
C	-2.118875	-0.247502	0.104608
H	0.172872	-2.833590	-0.259866
C	-1.611709	-1.598307	-0.401928
H	-2.460295	-0.314819	1.145229
H	-2.962448	0.089935	-0.503709
H	-2.346878	-2.369168	-0.154778
H	-1.512849	-1.573417	-1.492433
C	-1.477685	2.203305	0.081137
H	-0.791814	2.776150	0.711375

H	-1.527832	2.647339	-0.919573
H	-2.468206	2.256369	0.536172
C	2.103901	-0.864125	0.184020
N	1.258871	1.312160	0.007271
C	2.516430	0.568811	-0.209247
H	2.823039	0.628353	-1.259642
H	3.312960	0.966407	0.421491
H	2.344067	-1.088216	1.231101
H	2.556306	-1.626182	-0.454623
H	1.156823	2.254845	-0.343474

22

0 1

C	-0.406348	-1.724452	-0.546850
C	-1.792531	-1.711281	0.100049
C	0.634676	0.487656	-0.000783
C	-2.513480	-0.364936	0.006449
C	-1.724789	0.805711	0.601133
H	-0.476221	-1.424968	-1.606916
H	-1.682105	-2.001067	1.153500
H	-2.737704	-0.131696	-1.042925
H	-0.029142	-2.752092	-0.530458
H	-2.405356	-2.484038	-0.382729
H	-3.475544	-0.434483	0.531958
H	-2.376023	1.684032	0.633135
H	-1.442723	0.582379	1.641752
N	-0.543126	1.193052	-0.189162
N	0.585529	-0.911259	0.165604
N	1.797831	1.044721	0.036231
C	-0.364517	2.633036	-0.372639
H	0.443420	2.805132	-1.084093
H	-1.294422	3.054161	-0.767077
H	-0.100480	3.148937	0.562555
C	2.768010	-0.034095	0.240761
C	1.986247	-1.347667	0.013479
H	3.624852	0.063845	-0.436177
H	3.161762	0.020637	1.266424
H	2.232964	-2.141507	0.726753
H	2.151482	-1.738693	-1.004010

22H$^+$

1 1

C	-0.481611	-1.801130	-0.476735
C	-1.862037	-1.677034	0.159580
C	0.563495	0.435992	-0.001875
C	-2.537031	-0.328959	-0.090065
C	-1.807477	0.844600	0.561043
H	-0.539640	-1.628754	-1.561165
H	-1.785824	-1.869360	1.237293
H	-2.646579	-0.143594	-1.166161
H	-0.104848	-2.815576	-0.325914
H	-2.480596	-2.477403	-0.261707
H	-3.548299	-0.350210	0.332091
H	-2.430136	1.739041	0.508351
H	-1.627267	0.637153	1.623823
N	-0.515480	1.227426	-0.069368
N	0.557779	-0.912345	0.090003
N	1.828240	0.920725	-0.042765
C	-0.320476	2.657605	-0.357189
H	0.472475	2.784817	-1.097164
H	-1.243554	3.050983	-0.785396
H	-0.083327	3.231498	0.548352
C	2.799340	-0.146448	0.249817
C	1.954496	-1.403638	-0.005680
H	3.668878	-0.077636	-0.406415
H	3.131170	-0.080578	1.291850
H	2.131522	-2.195049	0.725605
H	2.124187	-1.806678	-1.011651
H	2.015871	1.864766	0.269749

23

0 1

C	1.764227	-1.284210	0.112981
C	2.335582	0.146145	-0.072925
C	1.350847	1.234113	0.394762
C	-0.297164	-0.359784	-0.322095
H	1.178743	1.161347	1.483534
H	3.283873	0.238690	0.469073
H	2.546407	0.324485	-1.133770
H	1.966801	-1.631686	1.136265
H	2.303598	-1.973199	-0.549245
H	1.739448	2.235767	0.181306

N	0.133565	0.986183	-0.366202
N	0.319295	-1.445847	-0.115396
N	-1.659160	-0.011560	-0.382316
C	-1.252560	1.370489	-0.019979
H	-1.393349	1.592827	1.051218
H	-1.685460	2.164814	-0.637084
C	-2.676808	-0.759519	0.329891
H	-2.528606	-0.758208	1.422491
H	-3.664192	-0.344464	0.104593
H	-2.647897	-1.795211	-0.016793

23H$^+$

1 1

C	1.861453	-1.213491	0.235152
C	2.300067	0.122931	-0.394381
C	1.493305	1.330347	0.131380
C	-0.342700	-0.342615	0.014619
H	1.863746	1.675294	1.101586
H	3.361897	0.280084	-0.185604
H	2.186554	0.051403	-1.481622
H	2.063343	-1.237000	1.311849
H	2.392375	-2.045416	-0.230763
H	1.547788	2.168309	-0.570717
N	0.100237	0.896556	0.283074
N	0.410083	-1.427340	0.008290
N	-1.626099	-0.001646	-0.283309
C	-1.256024	1.419680	-0.011400
H	-1.756193	1.863743	0.853338
H	-1.317026	2.057703	-0.896803
C	-2.881214	-0.679857	0.024903
H	-3.109972	-0.661887	1.097297
H	-3.685502	-0.191672	-0.528922
H	-2.818755	-1.715847	-0.316938
H	0.032881	-2.339670	-0.210730

24

0 1

C	1.980003	-1.325657	0.145610
C	2.506861	0.019874	-0.388945
C	1.677808	1.183920	0.166893
C	-0.164697	-0.400780	0.063637
H	1.838512	1.294477	1.254552

H	3.563630	0.148599	-0.126529
H	2.433644	0.038326	-1.483128
H	2.341907	-1.475996	1.175530
H	2.415966	-2.142863	-0.443938
H	1.963518	2.132163	-0.304379
N	0.285593	0.908040	-0.137690
N	0.526613	-1.475558	0.139696
N	-1.552164	-0.349398	0.185485
C	-2.020350	0.980826	-0.173722
C	-0.789621	1.841613	0.154055
H	-2.274581	1.051280	-1.246079
H	-2.904290	1.263891	0.408125
H	-0.721473	2.741697	-0.466642
H	-0.795222	2.148901	1.214260
C	-2.356492	-1.517084	-0.099584
H	-2.602079	-1.604261	-1.171469
H	-1.788287	-2.399013	0.200852
H	-3.292607	-1.475062	0.468746

24H$^+$

1 1

C	-2.051353	-1.279520	-0.203025
C	-2.515731	0.043256	0.411170
C	-1.696856	1.220953	-0.127949
C	0.209134	-0.335337	-0.051748
H	-1.924737	1.419427	-1.184514
H	-3.573269	0.196521	0.179292
H	-2.417295	-0.001656	1.500926
H	-2.325339	-1.341994	-1.263128
H	-2.505590	-2.126938	0.315295
H	-1.911670	2.131752	0.438133
N	-0.273981	0.915484	0.027966
N	-0.586397	-1.406276	-0.069269
N	1.554108	-0.351364	-0.106036
C	2.058308	1.013051	0.149111
C	0.819947	1.882728	-0.144215
H	2.387095	1.105331	1.192069
H	2.900036	1.236166	-0.509871
H	0.712138	2.715933	0.553872
H	0.823694	2.275083	-1.169130
C	2.390801	-1.528536	0.088529
H	2.464265	-1.813843	1.145570
H	2.005597	-2.370058	-0.494699

H	3.390879	-1.305621	-0.288557
H	-0.167421	-2.324580	-0.115131

25

0 1

C	-2.343668	-0.102760	0.192438
C	-2.014880	-1.504243	-0.303321
C	-0.646234	-1.903370	0.227816
C	0.056851	0.477781	-0.019866
H	-2.773911	-2.217693	0.036976
H	-2.498743	-0.117569	1.288281
H	-3.280153	0.251188	-0.253593
H	-0.701389	-2.060753	1.321690
H	-0.321773	-2.855299	-0.211258
H	-2.003424	-1.511390	-1.399110
N	0.351570	-0.894351	-0.107622
N	-1.288839	0.827516	-0.189525
N	0.920250	1.425487	0.106875
C	2.337942	1.115463	0.170167
C	2.698575	-0.266491	-0.382127
C	1.725352	-1.288108	0.193731
C	-1.621379	2.236148	-0.033240
H	-2.616789	2.405236	-0.458010
H	-1.627280	2.556570	1.020829
H	-0.886252	2.842374	-0.560258
H	2.886901	1.893610	-0.377365
H	2.676062	1.193130	1.216630
H	3.730308	-0.540408	-0.130356
H	2.610810	-0.267634	-1.475630
H	1.879723	-1.387699	1.283726
H	1.889697	-2.280749	-0.244232

25H$^+$

1 1

C	-2.403060	-0.118768	0.175401
C	-2.028249	-1.465721	-0.425416
C	-0.707610	-1.938072	0.163808
C	-0.000454	0.412964	-0.037868
H	-2.814153	-2.195458	-0.211344
H	-2.683330	-0.221486	1.232063
H	-3.255093	0.312836	-0.356563
H	-0.814907	-2.205894	1.223217

H	-0.343282	-2.821771	-0.367717
H	-1.941661	-1.379600	-1.514358
N	0.320741	-0.892694	0.026268
N	-1.280878	0.832048	0.058879
N	0.974014	1.336787	-0.182743
C	2.400176	1.019635	-0.326168
C	2.690999	-0.275381	0.420469
C	1.721562	-1.355576	-0.044023
H	1.942838	-1.671610	-1.071950
H	1.798149	-2.237893	0.597918
H	2.658731	0.927424	-1.388784
H	2.969287	1.855061	0.089395
H	2.586973	-0.115257	1.499216
H	3.718051	-0.597433	0.227707
C	-1.593588	2.261297	0.158220
H	-2.647740	2.362217	0.416373
H	-1.009875	2.742131	0.950590
H	-1.430837	2.782192	-0.793992
H	0.691067	2.289290	-0.355144

26

0 1

C	1.951928	-1.774568	0.018013
C	0.690595	-1.553128	-0.825677
C	2.739745	-0.484140	0.255946
C	-0.397349	0.571431	-0.120183
C	1.878279	0.661532	0.798153
H	1.654545	-2.217388	0.978419
H	0.953338	-1.031320	-1.755655
H	3.198424	-0.152361	-0.685278
H	2.530439	1.504581	1.047221
H	2.592886	-2.509271	-0.487947
H	0.274253	-2.525783	-1.110043
H	3.559327	-0.675327	0.961827
H	1.389046	0.354606	1.734425
N	-0.375508	-0.824312	-0.127506
N	0.877264	1.158657	-0.166710
N	-1.440627	1.325696	-0.061759
C	0.884873	2.607314	-0.356677
H	0.207090	2.869154	-1.169494
H	0.556361	3.157049	0.537569
H	1.901807	2.917571	-0.618842
C	-2.738753	0.668550	-0.110631

C	-2.718435	-0.667576	0.637491
C	-1.638894	-1.552648	0.023228
H	-3.481895	1.344302	0.329754
H	-3.053392	0.503101	-1.155189
H	-3.685595	-1.182291	0.588102
H	-2.494939	-0.481406	1.695408
H	-1.461056	-2.441435	0.644413
H	-1.980484	-1.914671	-0.960844

26H$^+$

1 1

C	1.974612	-1.777899	0.019185
C	0.714311	-1.576982	-0.824019
C	2.777615	-0.489132	0.194615
C	-0.333300	0.527650	-0.083839
C	1.954016	0.635450	0.820688
H	1.698996	-2.195435	0.996378
H	0.964759	-1.069256	-1.762913
H	3.175032	-0.154478	-0.772159
H	2.595592	1.489590	1.048565
H	2.592250	-2.531251	-0.482843
H	0.280258	-2.545415	-1.082729
H	3.639836	-0.675379	0.845130
H	1.516423	0.300028	1.769002
N	-0.379518	-0.812803	-0.169430
N	0.861425	1.167910	-0.039032
N	-1.472888	1.246571	-0.073460
C	0.944773	2.588836	-0.401264
H	0.247250	2.809726	-1.211595
H	0.741924	3.251820	0.451451
H	1.955838	2.794196	-0.759249
C	-2.794323	0.608473	-0.168525
C	-2.749195	-0.694837	0.626649
C	-1.631985	-1.570484	0.069065
H	-3.529439	1.309698	0.230344
H	-3.039656	0.425841	-1.221142
H	-3.698120	-1.233715	0.549970
H	-2.579611	-0.471047	1.685763
H	-1.399652	-2.393920	0.752565
H	-1.940776	-2.010517	-0.886948
H	-1.423188	2.181321	0.308534

27

0 1

C	0.552803	-0.386732	0.049206
N	0.172729	0.923246	-0.351759
N	1.871231	0.003546	0.348385
N	-0.005853	-1.519375	0.122298
C	-1.015583	1.581753	0.175115
C	-1.405028	-1.632765	-0.273310
C	-2.384526	-0.610244	0.339227
C	-2.286583	0.821485	-0.215499
H	-1.488958	-1.582918	-1.372378
H	-1.739298	-2.637034	0.012408
H	-3.404337	-0.976396	0.157790
H	-2.246853	-0.598055	1.429753
H	-2.357075	0.795022	-1.311332
H	-3.143960	1.404880	0.144658
H	-1.051390	2.595359	-0.241755
H	-0.964348	1.679812	1.274742
C	1.549065	1.376524	-0.064844
H	2.087289	1.729444	-0.956327
H	1.632910	2.116530	0.743333
C	3.048250	-0.739694	-0.054411
H	3.258432	-0.654838	-1.133457
H	3.925141	-0.393951	0.502943
H	2.875309	-1.791738	0.184239

27H$^+$

1 1

C	-0.598758	-0.306399	-0.049920
N	-0.171827	0.951517	0.231684
N	-1.904033	0.011178	-0.252744
N	0.054818	-1.452395	-0.121523
C	1.072105	1.614239	-0.176230
C	1.474852	-1.633665	0.259568
C	2.427782	-0.584015	-0.323724
C	2.304856	0.827867	0.274292
H	1.545171	-1.648292	1.354428
H	1.749639	-2.626021	-0.103811
H	3.440182	-0.953181	-0.124478
H	2.317862	-0.553166	-1.415520
H	2.322474	0.774893	1.370117
H	3.180331	1.413723	-0.025874

H	1.066995	2.604182	0.287928
H	1.079329	1.751020	-1.267400
C	-1.565705	1.425242	0.035911
H	-2.024026	1.825127	0.944695
H	-1.700934	2.092165	-0.820049
C	-3.120038	-0.718342	0.088648
H	-3.286690	-0.759665	1.171949
H	-3.967766	-0.226616	-0.392611
H	-3.055055	-1.734230	-0.309262
H	-0.490772	-2.281608	-0.323308

28

0 1

C	0.414221	0.379092	0.033049
N	0.008494	-0.948178	-0.241502
N	1.796641	0.353299	0.277130
N	-0.231234	1.480876	0.049598
C	-1.620310	1.617096	-0.336944
C	-1.246527	-1.482734	0.289515
C	-2.646987	0.664434	0.292456
C	-2.513888	-0.780687	-0.190864
H	-2.546734	-0.810283	-1.288674
H	-3.366577	-1.371555	0.169452
H	-2.554770	0.703139	1.387250
H	-3.651945	1.034277	0.046386
H	-1.705159	1.529835	-1.434775
H	-1.916614	2.645717	-0.095384
H	-1.285461	-2.532903	-0.023587
H	-1.224242	-1.481276	1.394913
C	2.347035	-0.896897	-0.215145
C	1.157711	-1.837112	-0.034746
H	2.640621	-0.824021	-1.277943
H	3.226204	-1.206929	0.360458
H	1.148712	-2.665994	-0.750514
H	1.150555	-2.258179	0.984403
C	2.569734	1.567314	0.113082
H	2.798103	1.777284	-0.945631
H	1.991172	2.400686	0.511866
H	3.512889	1.475187	0.662784

28H$^+$

1 1

C	-0.466657	-0.311764	0.048735
N	-0.015534	0.948446	-0.101073
N	-1.809163	-0.375411	0.022498
N	0.308493	-1.395048	0.215203
C	-2.622021	-1.583419	0.028070
H	-2.112770	-2.389210	-0.509054
H	-2.859562	-1.911691	1.047030
H	-3.557024	-1.377465	-0.498045
C	1.664508	-1.593454	-0.347598
C	1.278847	1.474971	0.376000
C	2.725038	-0.639544	0.195455
C	2.516966	0.815774	-0.229409
H	2.473488	0.891748	-1.323542
H	3.379203	1.409978	0.093867
H	2.764047	-0.718256	1.289308
H	3.692745	-0.988731	-0.182640
H	1.610908	-1.519362	-1.441467
H	1.928245	-2.623899	-0.099683
H	1.273378	2.535074	0.111949
H	1.309023	1.409299	1.473120
C	-2.398276	0.971576	0.007062
C	-1.166271	1.874429	-0.218324
H	-2.911168	1.179454	0.953077
H	-3.126066	1.047898	-0.805551
H	-1.164953	2.347486	-1.204903
H	-1.088064	2.655839	0.542001
H	-0.190808	-2.245485	0.438189

29

0 1

C	-0.199634	0.541192	-0.132177
N	0.147648	-0.791342	-0.445453
N	-1.569261	0.786672	-0.065151
N	0.621044	1.520321	0.019939
C	1.153686	-1.420254	0.431764
C	1.999186	1.403042	-0.427726
C	2.896725	0.458700	0.388411
C	2.598845	-1.018167	0.126372
H	2.037247	1.083273	-1.483908
H	2.431989	2.410349	-0.388557

H	3.947147	0.662834	0.140000
H	2.771673	0.686885	1.456121
H	2.811535	-1.256680	-0.924603
H	3.258559	-1.648027	0.739129
H	1.056991	-2.502767	0.297921
H	0.936317	-1.207343	1.491048
C	-2.528521	-0.195754	0.449727
C	-0.976610	-1.648374	-0.833237
C	-2.002568	2.167356	0.065522
H	-3.040578	2.245637	-0.279958
H	-1.950826	2.525435	1.105072
H	-1.357632	2.805571	-0.537683
C	-2.041303	-1.642119	0.264847
H	-3.465454	-0.043081	-0.102616
H	-2.756410	0.004474	1.509986
H	-2.884991	-2.297757	0.019568
H	-1.596292	-2.024560	1.191137
H	-1.398678	-1.272187	-1.772508
H	-0.595457	-2.655347	-1.026518

29H$^+$

1 1

C	0.274136	0.435772	-0.047679
N	-0.092496	-0.843019	0.179309
N	1.571762	0.792716	-0.012704
N	-0.677305	1.365578	-0.292912
C	-1.284817	-1.416015	-0.502943
C	-1.995444	1.421383	0.382931
C	-3.021739	0.423366	-0.150320
C	-2.632081	-1.031448	0.114361
H	-1.841956	1.270721	1.458470
H	-2.353899	2.443875	0.242783
H	-3.980963	0.641721	0.332834
H	-3.161520	0.588118	-1.226178
H	-2.609093	-1.235585	1.192383
H	-3.391214	-1.693946	-0.317242
H	-1.157784	-2.499089	-0.462628
H	-1.258893	-1.121527	-1.559385
C	2.682212	-0.177584	-0.164678
C	0.964607	-1.753040	0.662740
C	1.984191	2.197234	0.083789
H	2.954660	2.236410	0.583998
H	2.090832	2.659620	-0.905294

H	1.270860	2.765836	0.683915
C	2.182813	-1.617717	-0.249276
H	3.333720	-0.048352	0.707088
H	3.260831	0.098385	-1.053684
H	2.984470	-2.297920	0.053518
H	1.899407	-1.878686	-1.274800
H	1.217937	-1.490157	1.696541
H	0.563639	-2.766450	0.667869
H	-0.358027	2.228401	-0.709603

30

0 1

C	-2.032358	-1.879232	0.215559
C	-0.778011	-1.468005	1.002518
C	-2.920644	-0.687302	-0.151546
C	0.098756	0.689910	0.105861
C	-2.161258	0.447397	-0.851490
H	-1.723032	-2.409239	-0.696736
H	-1.070639	-0.876640	1.877178
H	-3.388501	-0.279442	0.754810
H	-2.882894	1.186739	-1.212871
H	-2.607717	-2.598893	0.813861
H	-0.272646	-2.364464	1.382805
H	-3.735069	-1.022993	-0.807756
H	-1.644171	0.059450	-1.741565
N	0.212409	-0.699801	0.247520
N	-1.213564	1.160139	0.022776
N	1.076383	1.526202	0.069538
C	-1.400574	2.604154	0.114517
H	-0.758176	2.999312	0.901746
H	-1.137950	3.125193	-0.818053
H	-2.448166	2.812587	0.357987
C	2.395713	1.123243	0.535229
C	1.138122	-1.420334	-0.630711
C	3.157826	0.119928	-0.348092
C	2.617518	-1.308065	-0.243326
H	2.744424	-1.676985	0.784077
H	3.194613	-1.976339	-0.897772
H	3.115620	0.462856	-1.391509
H	4.216290	0.126867	-0.054751
H	2.330986	0.700208	1.553036
H	2.995952	2.038027	0.612863
H	0.838141	-2.474054	-0.621355

H	1.015798	-1.068131	-1.665961

30H$^+$

1 1

C	-2.057815	-1.905325	0.223610
C	-0.720711	-1.527220	0.866818
C	-2.980189	-0.698833	0.032809
C	0.014799	0.617912	-0.084363
C	-2.334609	0.420656	-0.788650
H	-1.874793	-2.400886	-0.738970
H	-0.896693	-0.969037	1.792890
H	-3.294098	-0.301826	1.007109
H	-3.076166	1.182289	-1.041035
H	-2.546262	-2.643444	0.869953
H	-0.156081	-2.423476	1.135685
H	-3.892153	-1.010620	-0.488763
N	0.181168	-0.717119	0.012428
N	-1.227104	1.140919	-0.107288
N	1.093715	1.421269	-0.161164
C	-1.489464	2.527885	0.298546
H	-0.726135	2.864368	1.002334
H	-1.518927	3.205839	-0.563612
H	-2.459020	2.568450	0.801247
C	2.385803	1.180153	0.519225
C	1.282523	-1.397582	-0.710092
C	3.260904	0.106105	-0.130271
C	2.659788	-1.298803	-0.045335
H	0.977651	-2.442674	-0.804870
H	1.327110	-0.984017	-1.723669
H	-1.948001	0.020639	-1.732818
H	2.904250	2.141871	0.518965
H	2.178806	0.919981	1.564159
H	4.232082	0.121580	0.377364
H	3.446254	0.374896	-1.178151
H	2.587351	-1.623252	1.001222
H	3.325459	-2.009025	-0.549176
H	0.948737	2.343177	-0.551481

31

0 1

C	0.027203	-0.324198	-0.011926
N	1.371115	0.069096	-0.115961

N	-0.252349	-1.570062	0.128852
N	-0.891012	0.731997	-0.125729
C	-0.693894	1.841931	-1.038388
H	0.164909	1.637597	-1.678790
H	-1.583474	1.976022	-1.671664
H	-0.517538	2.794139	-0.510728
C	-2.027790	0.841375	0.767265
H	-2.002482	0.035407	1.501882
H	-1.996317	1.798936	1.311752
H	-2.987418	0.794136	0.231116
C	1.850445	1.124728	0.771453
H	2.149419	0.726020	1.755802
H	2.722009	1.618888	0.326612
H	1.072616	1.872670	0.930164
C	2.345392	-0.995936	-0.312180
H	1.977846	-1.692937	-1.065901
H	3.287482	-0.549611	-0.651789
H	2.534988	-1.567474	0.609051
C	-1.592484	-2.056702	-0.128275
H	-1.522289	-3.027251	-0.635500
H	-2.146386	-2.234660	0.805573
H	-2.200873	-1.386286	-0.755409

31H^{+}

1 1

C	0.010987	-0.229657	0.089490
N	1.356546	-0.134994	0.053464
N	-0.553114	-1.442312	0.259408
N	-0.764241	0.866410	-0.049107
C	-0.388946	1.990037	-0.916741
H	0.450784	1.709730	-1.552463
H	-1.243673	2.233724	-1.555857
H	-0.127292	2.879174	-0.333469
C	-2.044857	1.012924	0.656214
H	-2.894354	0.925409	-0.029251
H	-2.129043	0.263180	1.442712
H	-2.073025	2.004488	1.118985
C	2.076336	1.028635	0.590757
H	1.388244	1.686958	1.119929
H	2.831082	0.674609	1.300287
H	2.578787	1.586176	-0.206079
C	2.203890	-1.269874	-0.334407
H	1.651928	-1.949160	-0.985735

H	3.065566	-0.885471	-0.886941
H	2.574682	-1.815298	0.542541
C	-1.838920	-1.890751	-0.287594
H	-1.715596	-2.902344	-0.681636
H	-2.625004	-1.901395	0.472978
H	-2.135909	-1.234258	-1.106665
H	0.017550	-2.147136	0.707997