

Design of C₂-chiral bases with dual basic sites that predicted to exceed the range of superbasicity: A Computational Study

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Table S1. Proton affinity calculated for Cyclopropeneimine and Tetramethylcyclopropeneimine scaffold at B3LYP/6-311+G(d,p) and CBS-QB3 reported values in (kcal/mol)

System	PA calculated at B3LYP/6-311+G(d,p) (kcal/mol)	PA reported at CBS-QB3(in kcal/mol)
Cyclopropeneimine	255.2	250.0
Tetramethylcyclopropeneimine	260.9	255.9

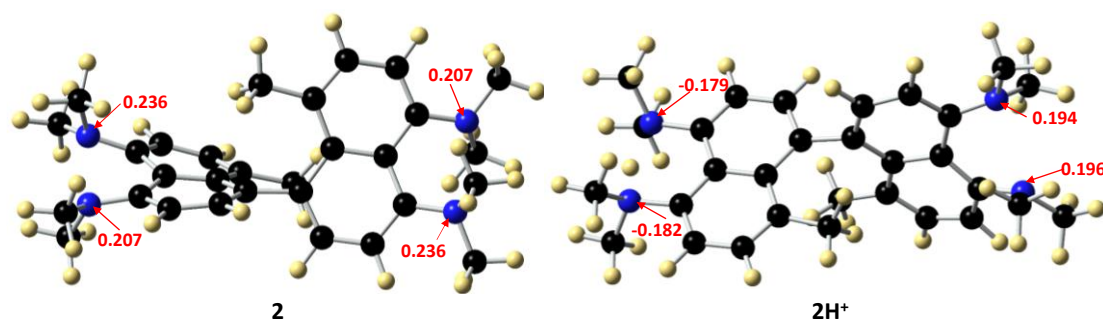
Calculation for Average proton affinity:

$$PA_{\text{avg}}(\text{B}) = \frac{(E_{\text{el}})_{\text{ZPVE}}}{2}$$

$$(\Delta E_{\text{el}})_{\text{ZPVE}} = [E(\text{B})_{\text{ZPVE}} - E(\text{BH}_2^{2+})_{\text{ZPVE}}]$$

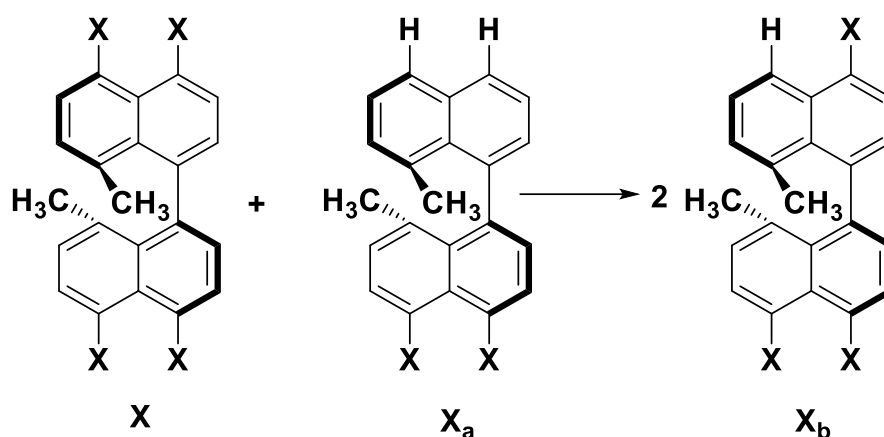
ΔE_{el} is the electronic energy and ΔZPVE is the zero-point vibrational energy contribution to the proton affinity. Here B denotes the base and BH_2^{2+} is the bisprotonated conjugate acid.

Figure S1. Mulliken charges of nitrogen atoms at the basic sites of **2** and the protonated **2H⁺** calculated at B3LYP/6-311+G(d,p) level of theory. The charges are in a.u. blue=nitrogen, black= carbon, yellow= hydrogen.



Isodesmic reactions for strain energy calculation:

The strain energy of the unprotonated designed bases (**1-9**) may be estimated by isodesmic reaction such as



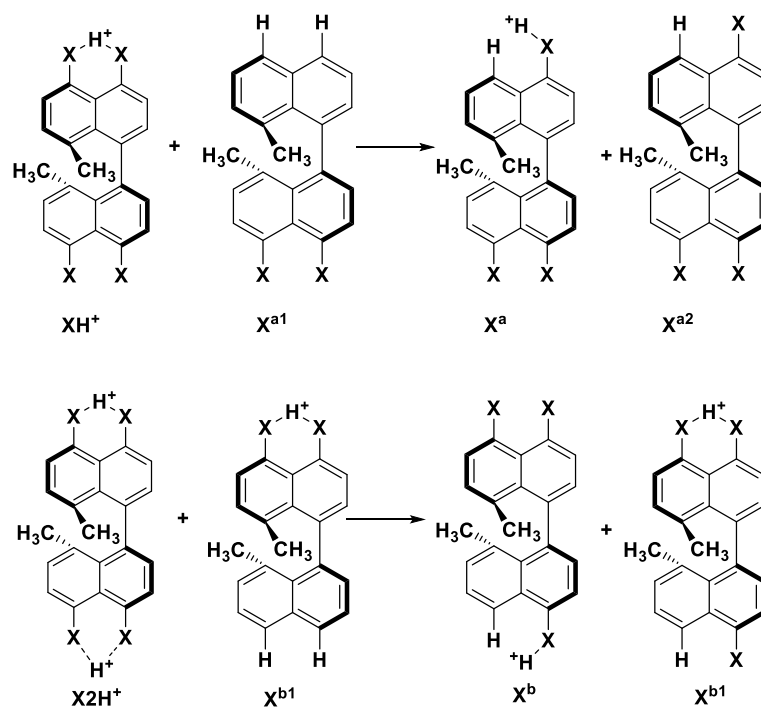
The strain energy (SE) is being calculated by the equation:

$$SE(X) = E(X) + (X_a) - 2E(X_b),$$

where X, X_a, X_b are the corresponding optimized geometries and X=1-9 of scheme 2 in the main text.

Isodesmic reactions for hydrogen bonding and cationic strain energy calculations:

The intramolecular hydrogen bonding energy and the cationic strain can be calculated by isodesmic reaction:



The cationic strain and hydrogen bonding energy can be calculated by equation:

for 1st protonation: $\{[\text{HB}(\text{XH}^+) + \text{SE}(\text{XH}^+)] = \text{E}(\text{XH}^+) + \text{E}(\text{X}^{\text{a1}}) - \text{E}(\text{X}^{\text{a}}) - \text{E}(\text{X}^{\text{a2}})\}$ and

for 2nd protonation: $\{[\text{HB}(\text{XH}^+) + \text{SE}(\text{XH}^+)] = \text{E}(\text{X2H}^+) + \text{E}(\text{X}^{\text{b1}}) - \text{E}(\text{X}^{\text{b}}) - \text{E}(\text{X}^{\text{b1}})\}$

Where X^{a1} , X^{a} , X^{a2} , X^{b1} , X^{b} , X^{b1} are the corresponding optimized structure and $\text{X}=\mathbf{1-9}$ of scheme 2 of main text.

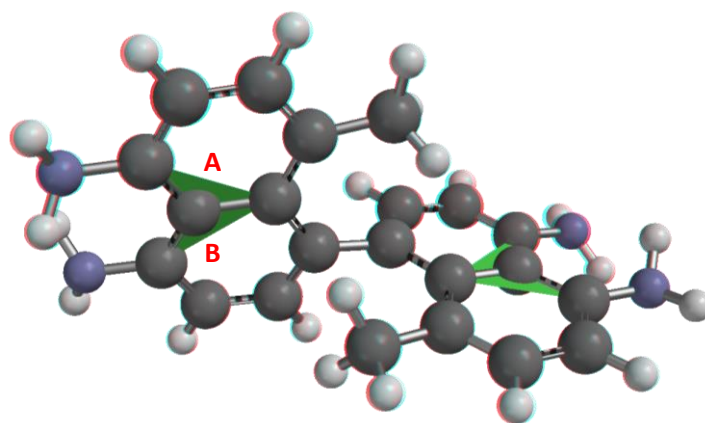


Figure S2. The nonplanarity of 8,8'-dimethyl-1,1'-binaphthalene with different substituents (**1-9**) is measured by the angle (α) between plane A (indicated by green) and plane B (indicated by green). Sky blue=nitrogen, grey=carbon, white = hydrogen

Table S2. The N...H⁺...N bond angle and angle x for measuring nonplanarity in unprotonated and bisprotonated bases for the optimized geometry of **1-9** at B3LYP/6-311+G(d,p)

System	N...H ⁺ ...N bond angle for 1 st protonation	N...H ⁺ ...N bond angle for 2 nd protonation	Angle x in unpeotonated Base	Angle x in bispeotonated Base
1	152.7°	151.8°	0.29°	0.06°
2	158.4°	157.5°	0.24°	0.04°
3	144.1°	133.9°	0.20°	1.67°
4	143.4°	144.1°	0.12°	1.12°
5	141.5°	143.3°	0.04°	0.14°
6	144.9°	144.7°	1.18°	0.04°
7	141.5°	142.3°	1.41°	0.62°
8	140.2°	140.3°	1.14°	1.31°
9	140.7°	140.7°	0.99°	1.30°

Table S3.The kinetics of protonation calculated for 1,8-bis(dimethylamino)naphthalene (DMAN) and **2** at B3LYP/6-311+G(d,p) level.

System	G _B (Hartree)	G _{HCl} (Hartree)	G _{TS} (Hartree)	ΔG (TS) (kcal/mol)
DMAN:HCl	-653.43250	-460.83839	-1114.25592	9.4
2:HCl	-1384.19869	-460.83839	-1845.02369	8.4

Cartesian Coordinates:

1	C	-1.48332700	1.43564000	-1.01461900			
	C	-0.58594300	4.13089600	-0.74551800			
	H	2.06755900	2.72484200	2.79254400			
Electronic energy = -1070.89678 a.u	C	-1.55006000	3.78645500	-1.66710200			
C	1.06372700	1.12814700	1.75474000	C	-1.99854000	2.46642200	-1.77238800
C	0.15675900	0.73690200	0.78995700	C	-1.99854000	2.46642200	-1.77238800
C	-0.47623600	1.73979400	-0.02707300	H	-1.94661100	4.54469700	-2.33538600
C	-0.07347300	3.12992000	0.15243000	H	-2.76305200	2.24045300	-2.50825100
C	0.82175700	3.47021400	1.22676100	C	-0.15675900	-0.73690200	0.78995700
C	1.38668000	2.46627000	1.98743600	C	0.47623600	-1.73979400	-0.02707300

C	-1.06372700	-1.12814700	1.75474000	H	2.80666700	-0.13501100	-2.07158100
C	1.48332700	-1.43564000	-1.01461900	1H⁺			
C	0.07347300	-3.12992000	0.15243000	Electronic energy = -1071.27789 a.u			
C	-1.38668000	-2.46627000	1.98743600	C	0.88796600	1.39259000	-1.26016200
C	1.99854000	-2.46642200	-1.77238800	C	0.67057700	0.28757100	-0.45599600
C	0.58594300	-4.13089600	-0.74551800	C	1.79508200	-0.36275900	0.16800900
C	-0.82175700	-3.47021400	1.22676100	C	3.13067400	0.09054000	-0.18336200
H	-2.06755900	-2.72484200	2.79254400	C	3.27640900	1.24495600	-1.01054500
C	1.55006000	-3.78645500	-1.66710200	C	2.17157900	1.88513000	-1.51522600
H	2.76305200	-2.24045300	-2.50825100	C	1.65675000	-1.41077100	1.15149600
H	1.94661100	-4.54469700	-2.33538600	C	4.23273700	-0.64988500	0.33652400
H	-1.52730400	-0.36442700	2.36936800	H	2.29768400	2.76113300	-2.14336300
H	1.52730400	0.36442700	2.36936800	C	4.07726600	-1.69600600	1.20138000
N	-1.16881300	-4.80236100	1.52142800	C	2.78951500	-2.04455400	1.62897600
H	-0.41890300	-5.47259900	1.41274500	H	4.93890100	-2.23949600	1.57594100
H	-1.62156400	-4.89242100	2.42050100	H	2.68327500	-2.83043900	2.36652900
N	0.15675900	-5.47661900	-0.69392800	C	-0.71956700	-0.25990200	-0.45068300
H	-0.84092100	-5.59273700	-0.56862800	C	-1.87490900	0.40371600	0.09298600
H	0.48044200	-6.00510800	-1.49300900	C	-0.88000800	-1.40488800	-1.21113500
N	1.16881300	4.80236100	1.52142800	C	-1.78654200	1.53571000	0.97535000
H	0.41890300	5.47259900	1.41274500	C	-3.18845600	-0.13189600	-0.23523200
H	1.62156400	4.89242100	2.42050100	C	-2.13439200	-1.89780800	-1.55806100
N	-0.15675900	5.47661900	-0.69392800	C	-2.95749100	2.11723600	1.42170000
H	0.84092100	5.59273700	-0.56862800	C	-4.35542000	0.46570000	0.35437800
H	-0.48044200	6.00510800	-1.49300900	C	-3.28796800	-1.24746200	-1.14426600
C	-2.03480600	0.05400200	-1.30278300	H	-2.21310000	-2.75559300	-2.21709200
H	-1.27395600	-0.63449100	-1.67481800	C	-4.21973900	1.60496100	1.12302900
H	-2.48571100	-0.41359300	-0.42702400	H	-2.89596600	2.97897100	2.07771900
H	-2.80666700	0.13501100	-2.07158100	H	-5.10180600	2.06717300	1.55346200
C	2.03480600	-0.05400200	-1.30278300	H	-0.00132600	-1.89685100	-1.61510900
H	1.27395600	0.63449100	-1.67481800	H	0.03585400	1.86900000	-1.72935200
H	2.48571100	0.41359300	-0.42702400	N	-4.50879500	-1.71913300	-1.60976800

H	-5.25704900	-1.04447700	-1.69199100	C	-1.94567500	2.88230000	-1.60923100
H	-4.44262400	-2.34657700	-2.39777500	H	-1.98784300	5.03799000	-1.65585400
N	-5.64642000	-0.05964400	0.15449100	H	-2.74912200	2.80291400	-2.33085600
H	-5.71794800	-1.06410900	0.25931200	C	-0.28121400	-0.69935500	0.52548700
H	-6.34334500	0.40592000	0.72061800	C	0.31875800	-1.83499300	-0.12566000
N	4.61710500	1.75518300	-1.31135300	C	-1.35712000	-0.87829200	1.37097900
H	4.73736800	1.89146300	-2.31285400	C	1.38913400	-1.73036900	-1.08899000
H	4.76314400	2.66329500	-0.87366500	C	-0.20558100	-3.15325600	0.19622700
N	5.60624700	-0.28702200	-0.09204400	C	-1.90312000	-2.14475100	1.61948200
H	6.22549200	-0.12832800	0.70417400	C	1.94567500	-2.88230000	-1.60923100
H	6.02471600	-1.01330400	-0.67619700	C	0.45509900	-4.28210800	-0.37521300
C	0.34493300	-1.84231700	1.76755300	C	-1.34439000	-3.26258100	1.05739800
H	-0.30885000	-0.99965000	1.98595800	H	-2.76213000	-2.24080100	2.27459500
H	-0.21480300	-2.51539900	1.11590200	C	1.50450900	-4.15975100	-1.24062500
H	0.54652500	-2.36883800	2.70204800	H	2.74912200	-2.80291400	-2.33085600
C	-0.49827300	2.12427200	1.51515600	H	1.98784300	-5.03799000	-1.65585400
H	0.21321900	1.36293600	1.83993300	H	-1.78656000	-0.01817000	1.87066100
H	0.02112500	2.75964100	0.79252400	H	1.78656000	0.01817000	1.87066100
H	-0.72630900	2.74336800	2.38471300	N	-1.91545500	-4.57867800	1.33550400
H	5.47452200	0.64965700	-0.68193700	H	-2.01701900	-4.72904500	2.33747400
1H₂²⁺				H	-2.84738800	-4.66209200	0.93185900
Electronic energy = -1071.58232 a.u				N	0.01055400	-5.64864300	-0.00899700
C	1.35712000	0.87829200	1.37097900	H	-0.22624400	-6.20786100	-0.83130800
C	0.28121400	0.69935500	0.52548700	H	0.72902400	-6.15283200	0.51575100
C	-0.31875800	1.83499300	-0.12566000	N	1.91545500	4.57867800	1.33550400
C	0.20558100	3.15325600	0.19622700	H	2.01701900	4.72904500	2.33747400
C	1.34439000	3.26258100	1.05739800	H	2.84738800	4.66209200	0.93185900
C	1.90312000	2.14475100	1.61948200	N	-0.01055400	5.64864300	-0.00899700
C	-1.38913400	1.73036900	-1.08899000	H	0.22624400	6.20786100	-0.83130800
C	-0.45509900	4.28210800	-0.37521300	H	-0.72902400	6.15283200	0.51575100
H	2.76213000	2.24080100	2.27459500	C	-1.94567500	0.42729100	-1.61755200
C	-1.50450900	4.15975100	-1.24062500	H	-1.16534600	-0.27789900	-1.90227000

H	-2.58749600	-0.07126400	-0.88893600	C	-0.34271000	-3.57232500	1.24847900
H	-2.54800200	0.62624400	-2.50418700	H	-1.38647100	-3.03534400	3.04219700
C	1.94567500	-0.42729100	-1.61755200	C	1.51535800	-3.38895100	-2.02316200
H	1.16534600	0.27789900	-1.90227000	H	2.74833700	-1.75621300	-2.65643100
H	2.58749600	0.07126400	-0.88893600	H	1.80526500	-3.99075600	-2.87359800
H	2.54800200	-0.62624400	-2.50418700	H	-1.28256400	-0.62904900	2.64885600
H	0.88384700	5.49544100	0.62372200	H	1.28256400	0.62904900	2.64885600
H	-0.88384700	-5.49544100	0.62372200	N	-0.38537900	-4.95674900	1.51275600

2

Electronic energy = -1385.37355 a.u

C	0.79120500	1.29638000	1.94935400	C	-2.15830400	-0.20979500	-1.04498200
C	0.04457900	0.75023000	0.92613700	H	-1.45208300	-0.95929600	-1.40628900
C	-0.60746700	1.63502900	-0.00713000	H	-2.51697900	-0.54939800	-0.07298500
C	-0.29320900	3.05385000	0.05382200	H	-3.00845800	-0.20117600	-1.73095300
C	0.34271000	3.57232500	1.24847900	C	2.15830400	0.20979500	-1.04498200
C	0.89626600	2.67742900	2.14728100	H	1.45208300	0.95929600	-1.40628900
C	-1.56242600	1.18156500	-0.98911500	H	2.51697900	0.54939800	-0.07298500
C	-0.63512000	3.88783800	-1.08220900	H	3.00845800	0.20117600	-1.73095300
H	1.38647100	3.03534400	3.04219700	C	1.32346600	5.43438800	2.51245600
C	-1.51535800	3.38895100	-2.02316200	H	2.31762000	5.02130600	2.33205700
C	-2.01611900	2.08368800	-1.92544800	H	1.38840500	6.52294100	2.43443800
H	-1.80526500	3.99075600	-2.87359800	H	1.02808500	5.19431300	3.54888100
H	-2.74833700	1.75621300	-2.65643100	C	-0.89626600	5.65431400	1.59232400
C	-0.04457900	-0.75023000	0.92613700	H	-0.75509700	6.71588200	1.37098700
C	0.60746700	-1.63502900	-0.00713000	H	-1.60199300	5.24845800	0.87345200
C	-0.79120500	-1.29638000	1.94935400	H	-1.33587700	5.56360000	2.59990800
C	1.56242600	-1.18156500	-0.98911500	C	-0.71074700	6.08013800	-2.18273900
C	0.29320900	-3.05385000	0.05382200	H	-1.78720700	6.12413300	-2.00673000
C	-0.89626600	-2.67742900	2.14728100	H	-0.30011700	7.08202400	-2.03168900
C	2.01611900	-2.08368800	-1.92544800	H	-0.54107400	5.80898300	-3.23969400
C	0.63512000	-3.88783800	-1.08220900	C	1.37944200	5.25740500	-1.30464500

H	1.70693200	6.26059100	-1.01750000	C	-2.23921300	-2.26205400	1.73955600
H	1.83600200	4.54411200	-0.62453100	H	-4.32334900	-2.75608400	1.90617900
H	1.74641500	5.04981700	-2.32407400	H	-1.94179200	-3.12197900	2.32669400
C	-1.37944200	-5.25740500	-1.30464500	C	0.77652600	0.67383500	0.15727000
H	-1.74641500	-5.04981700	-2.32407400	C	1.76249600	-0.01157200	-0.63584400
H	-1.70693200	-6.26059100	-1.01750000	C	1.18438100	1.48558000	1.19659100
H	-1.83600200	-4.54411200	-0.62453100	C	1.43823300	-0.80622100	-1.79335400
C	0.71074700	-6.08013800	-2.18273900	C	3.15361300	0.09352700	-0.22720200
H	1.78720700	-6.12413300	-2.00673000	C	2.53202400	1.74907200	1.45493800
H	0.30011700	-7.08202400	-2.03168900	C	2.45038200	-1.51398800	-2.40509900
H	0.54107400	-5.80898300	-3.23969400	C	4.11211500	-0.84925000	-0.77136600
C	0.89626600	-5.65431400	1.59232400	C	3.53147200	1.13572100	0.71171300
H	0.75509700	-6.71588200	1.37098700	H	2.77877000	2.50177800	2.18998000
H	1.60199300	-5.24845800	0.87345200	C	3.74689500	-1.58706500	-1.88420900
H	1.33587700	-5.56360000	2.59990800	H	2.22016600	-2.09852700	-3.28967800
C	-1.32346600	-5.43438800	2.51245600	H	4.44522000	-2.27816400	-2.33470800
H	-1.02808500	-5.19431300	3.54888100	H	0.43508300	1.99301000	1.79539700
H	-2.31762000	-5.02130600	2.33205700	H	-0.45433300	2.48229900	-1.16875700
H	-1.38840500	-6.52294100	2.43443800	N	4.86106600	1.52736100	0.87092500

2H⁺

Electronic energy = -1385.78697 a.u

C	-1.17519100	1.77287100	-0.78150700	C	0.16016800	-1.79378000	1.58030100
C	-0.70999800	0.67926600	-0.07690900	H	0.74795000	-1.99624400	0.68445700
C	-1.65518800	-0.26278000	0.46907700	H	0.67865500	-1.00833500	2.12939100
C	-3.07485500	-0.03588700	0.22114300	H	0.15895400	-2.69641200	2.19285500
C	-3.47606700	1.11132900	-0.53939300	C	0.06243200	-0.91550100	-2.41883700
C	-2.53652200	1.98812800	-1.01739400	H	-0.67076300	-1.39131000	-1.76310400
C	-1.26397300	-1.41553100	1.24937400	H	-0.34460400	0.05329600	-2.71435000
C	-4.00516200	-0.97828400	0.76270400	H	0.13107700	-1.52821300	-3.31954700
H	-2.84336200	2.86041900	-1.58289400	C	-5.23096800	1.33262200	-2.24281400
C	-3.60239100	-2.05521800	1.50143200	H	-4.87778500	0.39810300	-2.67988800

H	-6.31503600	1.39548500	-2.35957900	Electronic energy = -1386.13127 a.u			
H	-4.77559900	2.16425800	-2.79087200	C	1.21918300	1.04806800	1.21244600
C	-5.37755000	2.61720700	-0.16759000	C	0.18809400	0.73029300	0.35300000
H	-6.46141600	2.68347500	-0.28483800	C	-0.53737900	1.77848300	-0.31567900
H	-5.13242700	2.60900400	0.89498200	C	-0.18137900	3.15795700	-0.00813400
H	-4.92558500	3.50636300	-0.61963000	C	0.91621700	3.41526300	0.88076700
C	-6.24608900	-0.55867600	1.76163200	C	1.59569200	2.37373200	1.45972700
H	-5.79177300	0.25987600	2.31678800	C	-1.57872700	1.52697700	-1.28323100
H	-7.26887700	-0.30019500	1.48567900	C	-0.95747700	4.19530400	-0.61739700
H	-6.25198700	-1.45540800	2.38010100	H	2.42220000	2.57033900	2.13190300
C	-6.04986600	-1.88040100	-0.32455600	C	-1.97394600	3.92111600	-1.48916200
H	-7.07498700	-1.60859500	-0.57841500	C	-2.26201400	2.59379700	-1.82976900
H	-5.45731300	-1.98748600	-1.23129200	H	-2.55473400	4.71849500	-1.93707100
H	-6.04706200	-2.82232700	0.22272900	H	-3.04500200	2.40517400	-2.55388600
C	5.42260100	-1.39681300	1.22670200	C	-0.18809400	-0.73029300	0.35300000
H	5.35042900	-2.48940800	1.34845400	C	0.53737900	-1.77848300	-0.31567900
H	6.36460200	-1.06243700	1.66892700	C	-1.21918300	-1.04806800	1.21244600
H	4.60636000	-0.93705700	1.77662000	C	1.57872700	-1.52697700	-1.28323100
C	6.40410100	-1.70309500	-0.96191300	C	0.18137900	-3.15795700	-0.00813400
H	6.47120300	-1.27646200	-1.96400200	C	-1.59569200	-2.37373200	1.45972700
H	7.36586800	-1.55495400	-0.46544900	C	2.26201400	-2.59379700	-1.82976900
H	6.24114100	-2.78983300	-1.05213100	C	0.95747700	-4.19530400	-0.61739700
C	5.63149800	1.89963700	-0.31655500	C	-0.91621700	-3.41526300	0.88076700
H	6.67830900	1.61112600	-0.19441900	H	-2.42220000	-2.57033900	2.13190300
H	5.24186300	1.40939600	-1.20350500	C	1.97394600	-3.92111600	-1.48916200
H	5.58439600	2.98754600	-0.47631500	H	3.04500200	-2.40517400	-2.55388600
C	5.22393700	2.32087800	2.03401600	H	2.55473400	-4.71849500	-1.93707100
H	4.88495300	3.36772100	1.97148800	H	-1.74581600	-0.25058300	1.72336100
H	4.81929300	1.87592200	2.94461800	H	1.74581600	0.25058300	1.72336100
H	6.31270800	2.33110400	2.11865900	N	-1.32309200	-4.78965000	1.16763700
H	-5.45619700	0.14369700	-0.07927700	N	0.67239300	-5.61255700	-0.28874700
2H₂²⁺				N	1.32309200	4.78965000	1.16763700

N	-0.67239300	5.61255700	-0.28874700	H	2.66497400	-6.35691500	-0.11922800
C	-1.97394600	0.15709500	-1.78918700	C	-1.25514500	-5.13119600	2.60930200
H	-1.11525700	-0.44084000	-2.09424100	H	-1.43133700	-6.20187000	2.72708900
H	-2.52119200	-0.41718800	-1.04003600	H	-0.26664200	-4.88801800	3.00010400
H	-2.62213300	0.26863300	-2.65878200	H	-2.00555500	-4.59395700	3.19845100
C	1.97394600	-0.15709500	-1.78918700	C	-2.65603900	-5.11404300	0.60214700
H	1.11525700	0.44084000	-2.09424100	H	-3.45711300	-4.55340900	1.09564500
H	2.52119200	0.41718800	-1.04003600	H	-2.67325400	-4.87861600	-0.46266500
H	2.62213300	-0.26863300	-2.65878200	H	-2.84891900	-6.18026000	0.73446600
C	2.65603900	5.11404300	0.60214700	H	-0.20616800	-5.51176400	0.36772300
H	2.67325400	4.87861600	-0.46266500	H	0.20616800	5.51176400	0.36772300
H	2.84891900	6.18026000	0.73446600	3			
H	3.45711300	4.55340900	1.09564500	Electronic energy =	-1537.88235	a.u	
C	1.25514500	5.13119600	2.60930200	C	1.24521800	-1.00259200	1.27039400
H	1.43133700	6.20187000	2.72708900	C	0.22282100	-0.71922300	0.38815000
H	0.26664200	4.88801800	3.00010400	C	-0.41326500	-1.79449200	-0.32686300
H	2.00555500	4.59395700	3.19845100	C	0.03601900	-3.15622200	-0.06724800
C	-1.77214100	6.26067300	0.49723500	C	1.10639500	-3.37981300	0.86492700
H	-1.99489800	5.64503400	1.36683600	C	1.69744300	-2.30490700	1.49969300
H	-1.43869300	7.24867600	0.81475600	C	-1.45786600	-1.58236900	-1.29955000
H	-2.66497400	6.35691500	-0.11922800	C	-0.59756700	-4.24973100	-0.75187800
C	-0.27874200	6.43613500	-1.47697800	H	2.52129300	-2.48441100	2.18066100
H	0.04424700	7.41688700	-1.12802900	C	-1.62399900	-3.99383400	-1.63664100
H	0.53703600	5.93843800	-1.99790300	C	-2.02773000	-2.68188900	-1.90675300
H	-1.12586900	6.55233500	-2.15123600	H	-2.11893000	-4.82677100	-2.12251400
C	0.27874200	-6.43613500	-1.47697800	H	-2.81827600	-2.52506500	-2.63335800
H	1.12586900	-6.55233500	-2.15123600	C	-0.22282100	0.71922300	0.38815000
H	-0.04424700	-7.41688700	-1.12802900	C	0.41326500	1.79449200	-0.32686300
H	-0.53703600	-5.93843800	-1.99790300	C	-1.24521800	1.00259200	1.27039400
C	1.77214100	-6.26067300	0.49723500	C	1.45786600	1.58236900	-1.29955000
H	1.99489800	-5.64503400	1.36683600	C	-0.03601900	3.15622200	-0.06724800
H	1.43869300	-7.24867600	0.81475600	C	-1.69744300	2.30490700	1.49969300

C	2.02773000	2.68188900	-1.90675300	H	0.01238800	8.03810200	-0.03154100
C	0.59756700	4.24973100	-0.75187800	C	-0.59756700	4.91301300	3.30832400
C	-1.10639500	3.37981300	0.86492700	H	0.12694500	5.71770000	3.47265300
H	-2.52129300	2.48441100	2.18066100	H	-1.16519800	4.80232800	4.23813500
C	1.62399900	3.99383400	-1.63664100	H	-0.05866700	3.98770700	3.11320400
H	2.81827600	2.52506500	-2.63335800	C	-2.25790400	6.59663300	2.34275000
H	2.11893000	4.82677100	-2.12251400	H	-2.85904000	6.57765400	3.25825200
H	-1.70906000	0.18331900	1.80902800	H	-1.55249100	7.42868000	2.44387900
H	1.70906000	-0.18331900	1.80902800	H	-2.90967900	6.77934500	1.48934900
N	-1.66928300	4.65195600	1.08242000	C	0.49993600	-7.80042700	-0.96295300
N	0.29435300	5.59814500	-0.47565400	H	0.10122100	-8.43118200	-1.76490400
N	1.66928300	-4.65195600	1.08242000	H	1.56270600	-8.04715900	-0.86464300
N	-0.29435300	-5.59814500	-0.47565400	H	-0.01238800	-8.03810200	-0.03154100
C	-1.97332200	-0.22858200	-1.74337100	C	0.97703600	-5.89048600	-2.59013400
H	-2.51554100	0.29802000	-0.95652300	H	0.55900800	-6.43559600	-3.44284400
H	-1.17623400	0.43745100	-2.07699700	H	0.85709100	-4.82256300	-2.76262100
H	-2.65764500	-0.36855600	-2.58319900	H	2.04581500	-6.12701300	-2.55552100
C	1.97332200	0.22858200	-1.74337100	C	0.59756700	-4.91301300	3.30832400
H	2.51554100	-0.29802000	-0.95652300	H	1.16519800	-4.80232800	4.23813500
H	1.17623400	-0.43745100	-2.07699700	H	0.05866700	-3.98770700	3.11320400
H	2.65764500	0.36855600	-2.58319900	H	-0.12694500	-5.71770000	3.47265300
C	-1.51388200	5.29710300	2.16927500	C	2.25790400	-6.59663300	2.34275000
C	-0.32887400	6.34128200	-1.30109900	H	2.85904000	-6.57765400	3.25825200
C	1.51388200	-5.29710300	2.16927500	H	1.55249100	-7.42868000	2.44387900
C	0.32887400	-6.34128200	-1.30109900	H	2.90967900	-6.77934500	1.48934900
C	-0.97703600	5.89048600	-2.59013400	3H⁺			
H	-2.04581500	6.12701300	-2.55552100	Electronic energy = -1538.29231 a.u			
H	-0.55900800	6.43559600	-3.44284400	C	-1.03939800	0.63345400	1.43577100
H	-0.85709100	4.82256300	-2.76262100	C	-0.71149100	0.04121900	0.22925200
C	-0.49993600	7.80042700	-0.96295300	C	-1.75441900	-0.40174200	-0.65853200
H	-0.10122100	8.43118200	-1.76490400	C	-3.13150300	-0.10966600	-0.29510900
H	-1.56270600	8.04715900	-0.86464300	C	-3.40815700	0.52877500	0.96422300

C	-2.36226700	0.85890300	1.81293800	H	-0.38992800	-1.67494300	2.44832900
C	-1.49243900	-1.15749500	-1.85318900	H	-0.35297400	-2.41528000	0.86377500
C	-4.18876100	-0.47939900	-1.19543800	H	0.39663500	-3.23891800	2.23202600
H	-2.58733100	1.31196400	2.77069200	C	5.05098900	2.82283800	-0.77258100
C	-3.87452900	-1.13171700	-2.37436000	C	6.46580000	-1.45571600	0.24888900
C	-2.55665600	-1.48448100	-2.67106100	C	-5.28566900	1.84661300	1.52633400
H	-4.67174400	-1.38065300	-3.06431000	C	-6.46126500	-0.92268100	-0.74595700
H	-2.36632400	-2.05388300	-3.57499300	C	6.24394000	-2.94426400	0.16928300
C	0.73329100	0.13431200	-0.13031400	H	6.80940300	-3.34567100	-0.67554300
C	1.80041900	-0.52935100	0.57804400	H	6.63319800	-3.43913300	1.06539400
C	1.04046500	1.05402300	-1.12211700	H	5.19357500	-3.20966700	0.06305700
C	1.57055000	-1.61502100	1.49828800	C	7.86504800	-1.00102400	-0.06280600
C	3.16698300	-0.11737200	0.31170300	H	8.58245100	-1.53821400	0.56568700
C	2.34080400	1.50840700	-1.32659500	H	8.12256000	-1.24068100	-1.10012100
C	2.65650700	-2.15972900	2.15758300	H	7.98792100	0.06781600	0.10667400
C	4.25173600	-0.84777200	0.90619800	C	4.12619100	3.97439400	-0.98884900
C	3.37585200	1.00507300	-0.56264200	H	4.59386500	4.88778000	-0.61790800
H	2.52155000	2.27523500	-2.06591400	H	3.93678400	4.12612500	-2.05751900
C	3.97398700	-1.79182400	1.87274000	H	3.16474500	3.82441600	-0.49665700
H	2.48636200	-2.94763400	2.88224700	C	6.51763800	3.11241400	-0.73377400
H	4.78842400	-2.28008400	2.39251700	H	6.82456800	3.58408100	-1.67337900
H	0.23126600	1.49880100	-1.68796300	H	6.73188900	3.83349200	0.06144700
H	-0.24436000	0.97164200	2.09238000	H	7.11903400	2.21787900	-0.57811300
N	4.66884300	1.59177600	-0.59195300	C	-7.87414900	-0.40392800	-0.69512200
N	5.58369900	-0.55807300	0.52234900	H	-8.50633900	-0.94980200	-1.40328500
N	-4.70618400	0.71513600	1.44386900	H	-8.30550100	-0.56331700	0.29865000
N	-5.52136700	-0.09647600	-0.99150900	H	-7.90236700	0.65761100	-0.93656200
C	-0.13370800	-1.68763600	-2.26447500	C	-6.29247400	-2.39371400	-0.44821800
H	0.49623300	-0.93371300	-2.74492800	H	-6.85157100	-2.99761300	-1.16999400
H	0.43455400	-2.08953200	-1.42378900	H	-5.24981200	-2.70606400	-0.46079700
H	-0.26979900	-2.49995200	-2.98091900	H	-6.71638500	-2.61014000	0.53773900
C	0.23088400	-2.26366600	1.77100800	C	-4.76116300	3.14477400	0.96147800

H	-4.75792900	3.92584400	1.72766800	H	2.79271500	-2.11007800	2.23079900
H	-3.75864100	3.04486100	0.54876700	C	-1.41090000	-4.22043300	-1.24549200
H	-5.43501500	3.48207700	0.16674200	H	-2.75870100	-2.92084900	-2.27392300
C	-6.63574000	1.91615800	2.18833000	H	-1.94765500	-5.10338600	-1.55825400
H	-6.61188800	2.61786400	3.02866600	H	1.75931400	0.05892100	1.77589200
H	-7.38663700	2.29197800	1.48562400	H	-1.75931400	-0.05892100	1.77589200
H	-6.93758400	0.93473900	2.55100500	N	2.04046000	-4.46284300	1.31804200
H	5.38838900	0.89519300	-0.24124200	N	0.22584300	-5.60662800	-0.11148100
3H₂²⁺				N	-2.04046000	4.46284300	1.31804200
Electronic energy = -1538.63559 a.u				N	-0.22584300	5.60662800	-0.11148100
C	-1.38686400	0.81710300	1.25757300	C	1.92098400	0.51431600	-1.72880400
C	-0.31654100	0.68322200	0.39722900	H	2.57054500	0.01266500	-1.00905100
C	0.22584300	1.85149200	-0.24343100	H	1.16058500	-0.20424600	-2.03278700
C	-0.35828800	3.14592200	0.06805700	H	2.52232200	0.75144700	-2.60734300
C	-1.51168100	3.21084600	0.92968200	C	-1.92098400	-0.51431600	-1.72880400
C	-1.98457500	2.05273500	1.51375100	H	-2.57054500	-0.01266500	-1.00905100
C	1.32859300	1.79005800	-1.17329800	H	-1.16058500	0.20424600	-2.03278700
C	0.27408300	4.31895800	-0.47740600	H	-2.52232200	-0.75144700	-2.60734300
H	-2.79271500	2.11007800	2.23079900	C	3.29762100	-4.73110300	1.39738200
C	1.41090000	4.22043300	-1.24549200	C	0.21965100	-6.74438800	-0.74356300
C	1.89946000	2.96552100	-1.61561600	C	-3.29762100	4.73110300	1.39738200
H	1.94765500	5.10338600	-1.55825400	C	-0.21965100	6.74438800	-0.74356300
H	2.75870100	2.92084900	-2.27392300	C	-0.28600900	-6.93871900	-2.13313200
C	0.31654100	-0.68322200	0.39722900	H	0.28638400	-7.73481900	-2.61239300
C	-0.22584300	-1.85149200	-0.24343100	H	-1.32964400	-7.27351100	-2.11625900
C	1.38686400	-0.81710300	1.25757300	H	-0.22864400	-6.02980000	-2.73122800
C	-1.32859300	-1.79005800	-1.17329800	C	0.77435300	-7.93814400	-0.03794300
C	0.35828800	-3.14592200	0.06805700	H	0.01549600	-8.72766100	-0.01647100
C	1.98457500	-2.05273500	1.51375100	H	1.62127600	-8.34220300	-0.60154300
C	-1.89946000	-2.96552100	-1.61561600	H	1.08375000	-7.72260500	0.98368700
C	-0.27408300	-4.31895800	-0.47740600	C	4.43281300	-3.85325100	0.93842700
C	1.51168100	-3.21084600	0.92968200	H	5.17670700	-4.46968700	0.42709600

H	4.11105900	-3.05110100	0.27674400	C	1.62401200	1.42166600	-1.32559200
H	4.94410300	-3.40951600	1.79933200	C	1.11696000	4.16940100	-0.70548200
C	3.70298900	-6.05734500	1.97592600	H	-2.28301200	2.73354500	2.10169300
H	4.20827700	-6.66859500	1.22047500	C	2.10481300	3.79853400	-1.59636300
H	4.42967800	-5.90558900	2.78043600	C	2.32984200	2.45275300	-1.90891100
H	2.84857600	-6.59843300	2.37982700	H	2.71649900	4.57154300	-2.04780100
C	-0.77435300	7.93814400	-0.03794300	H	3.09426900	2.21322300	-2.64117600
H	-0.01549600	8.72766100	-0.01647100	C	0.14725900	-0.73839100	0.34924300
H	-1.62127600	8.34220300	-0.60154300	C	-0.61023900	-1.74349400	-0.34991100
H	-1.08375000	7.72260500	0.98368700	C	1.14439100	-1.12565800	1.22066500
C	0.28600900	6.93871900	-2.13313200	C	-1.62401200	-1.42166600	-1.32559200
H	1.32964400	7.27351100	-2.11625900	C	-0.32242500	-3.14524500	-0.07271100
H	0.22864400	6.02980000	-2.73122800	C	1.46358800	-2.46883600	1.44299000
H	-0.28638400	7.73481900	-2.61239300	C	-2.32984200	-2.45275300	-1.90891100
C	-4.43281300	3.85325100	0.93842700	C	-1.11696000	-4.16940100	-0.70548200
H	-5.17670700	4.46968700	0.42709600	C	0.75275700	-3.48249100	0.82670600
H	-4.11105900	3.05110100	0.27674400	H	2.28301200	-2.73354500	2.10169300
H	-4.94410300	3.40951600	1.79933200	C	-2.10481300	-3.79853400	-1.59636300
C	-3.70298900	6.05734500	1.97592600	H	-3.09426900	-2.21322300	-2.64117600
H	-4.20827700	6.66859500	1.22047500	H	-2.71649900	-4.57154300	-2.04780100
H	-4.42967800	5.90558900	2.78043600	H	1.69985100	-0.35864500	1.74984300
H	-2.84857600	6.59843300	2.37982700	H	-1.69985100	0.35864500	1.74984300
H	0.79807100	-5.54529900	0.76298700	N	1.17754800	-4.80591100	1.03172400
H	-0.79807100	5.54529900	0.76298700	N	-0.99303800	-5.53052700	-0.37651200
4				N	-1.17754800	4.80591100	1.03172400
Electronic energy = -1666.35341 a.u				N	0.99303800	5.53052700	-0.37651200
C	-1.14439100	1.12565800	1.22066500	C	1.96277400	0.02330400	-1.80197000
C	-0.14725900	0.73839100	0.34924300	H	2.45536700	-0.57911900	-1.03692400
C	0.61023900	1.74349400	-0.34991100	H	1.08444600	-0.53653900	-2.12595100
C	0.32242500	3.14524500	-0.07271100	H	2.64028300	0.09578400	-2.65596300
C	-0.75275700	3.48249100	0.82670600	C	-1.96277400	-0.02330400	-1.80197000
C	-1.46358800	2.46883600	1.44299000	H	-2.45536700	0.57911900	-1.03692400

H	-1.08444600	0.53653900	-2.12595100	C	1.07976800	1.18664300	-1.06256900
H	-2.64028300	-0.09578400	-2.65596300	C	0.75377600	0.25069300	-0.09947700
C	0.88103000	-5.43797500	2.10128200	C	1.80508500	-0.46337900	0.58179200
C	-0.42700900	-6.35263400	-1.17401300	C	3.18476500	-0.09689200	0.30271300
C	-0.88103000	5.43797500	2.10128200	C	3.42752400	0.99484800	-0.59282700
C	0.42700900	6.35263400	-1.17401300	C	2.40329300	1.56054000	-1.31873500
N	-0.05288100	6.08287900	-2.45026700	C	1.54961200	-1.54574700	1.49999600
H	-0.05364100	5.10180500	-2.69415800	C	4.26105700	-0.84488100	0.90146100
H	-0.91586300	6.55293500	-2.68636000	H	2.61362400	2.31152800	-2.07125500
N	0.21187100	7.67088400	-0.77741100	C	3.95483700	-1.80089200	1.84835300
H	0.64663500	7.87396100	0.11253900	C	2.62567000	-2.14030600	2.12833400
H	0.40646400	8.36653000	-1.48532400	H	4.75728200	-2.31785300	2.36139600
N	-1.21210100	6.78534300	2.22816500	H	2.43809600	-2.93223200	2.84476200
H	-1.78025200	7.10926400	1.45711900	C	-0.70041000	0.18810300	0.26193700
H	-1.57826500	7.05086300	3.13281700	C	-1.74371000	-0.33478200	-0.57786500
N	-0.21187100	4.93469100	3.21043300	C	-1.02544400	0.85757000	1.42620600
H	0.17692700	4.01108600	3.07754600	C	-1.47634000	-1.14439400	-1.73988000
H	0.43461200	5.57961600	3.64357800	C	-3.12658000	-0.06023100	-0.20860800
N	1.21210100	-6.78534300	2.22816500	C	-2.34835700	1.06206600	1.81736500
H	1.78025200	-7.10926400	1.45711900	C	-2.54004200	-1.54979600	-2.51878400
H	1.57826500	-7.05086300	3.13281700	C	-4.19139800	-0.51458100	-1.07391200
N	0.21187100	-4.93469100	3.21043300	C	-3.40448900	0.64380400	1.02197900
H	-0.17692700	-4.01108600	3.07754600	H	-2.57330000	1.56768300	2.74870300
H	-0.43461200	-5.57961600	3.64357800	C	-3.86620700	-1.22500500	-2.21717400
N	-0.21187100	-7.67088400	-0.77741100	H	-2.34414200	-2.15381000	-3.39900600
H	-0.64663500	-7.87396100	0.11253900	H	-4.66203900	-1.53049900	-2.88659300
H	-0.40646400	-8.36653000	-1.48532400	H	-0.22800800	1.25291000	2.04761200
N	0.05288100	-6.08287900	-2.45026700	H	0.27926900	1.68252700	-1.59833100
H	0.05364100	-5.10180500	-2.69415800	N	-4.69245400	0.85055200	1.52256400
H	0.91586300	-6.55293500	-2.68636000	N	-5.52363000	-0.17088200	-0.84029700
4H⁺				N	4.76128600	1.49159200	-0.72611800
Electronic energy = -1666.77567 a.u				N	5.60627200	-0.57838400	0.54848700

H	-3.13344600	-2.21408900	-2.57456700	N	1.35351600	-6.58210100	2.69094800
H	-2.61928100	-4.56737500	-2.14987300	H	1.91869300	-6.97997100	1.95634100
H	1.68769400	-0.37312600	1.80105100	H	1.59041100	-6.89595500	3.61997900
H	-1.68769400	0.37312600	1.80105100	N	0.69491300	-4.56360500	3.62434700
N	0.90445800	-4.83853100	1.27295800	H	0.22695400	-3.67608500	3.53030500
N	-0.59693600	-5.50869200	-0.69442800	H	0.62417400	-5.02261300	4.51834900
N	-0.90445800	4.83853100	1.27295800	N	-0.19495000	-7.68444900	-1.29733500
N	0.59693600	5.50869200	-0.69442800	H	-0.31197900	-7.97425200	-0.33952900
C	2.00489100	0.02505800	-1.73080600	H	0.04131000	-8.38891500	-1.97755700
H	2.48277400	-0.54999600	-0.93671400	N	-0.63268300	-6.13886400	-2.96056200
H	1.14183900	-0.54932400	-2.06941600	H	-0.70515000	-5.17979500	-3.26418100
H	2.70655600	0.08642700	-2.56382800	H	-0.67699100	-6.86520100	-3.65726400
C	-2.00489100	-0.02505800	-1.73080600	H	-0.01818600	5.63244500	0.15608500
H	-2.48277400	0.54999600	-0.93671400	H	0.01818600	-5.63244500	0.15608500
H	-1.14183900	0.54932400	-2.06941600	5			
H	-2.70655600	-0.08642700	-2.56382800	Electronic energy = -2295.34408 a.u			
C	0.98673900	-5.27343700	2.50273000	C	-1.03570400	1.17833800	1.21922200
C	-0.48802500	-6.42042100	-1.65951700	C	-0.11536800	0.74494100	0.28505800
C	-0.98673900	5.27343700	2.50273000	C	0.62177600	1.71889800	-0.47703600
C	0.48802500	6.42042100	-1.65951700	C	0.34802700	3.13030700	-0.24240300
N	0.63268300	6.13886400	-2.96056200	C	-0.56868300	3.51740900	0.79812200
H	0.70515000	5.17979500	-3.26418100	C	-1.26063200	2.53170400	1.48322300
H	0.67699100	6.86520100	-3.65726400	C	1.60640500	1.36135200	-1.46950700
N	0.19495000	7.68444900	-1.29733500	C	0.99736800	4.12836300	-1.05281200
H	0.31197900	7.97425200	-0.33952900	H	-1.93200300	2.82058700	2.28435000
H	-0.04131000	8.38891500	-1.97755700	C	1.94950200	3.72606800	-1.97210600
N	-1.35351600	6.58210100	2.69094800	C	2.24705000	2.37184400	-2.15689600
H	-1.91869300	6.97997100	1.95634100	H	2.42309200	4.47314300	-2.59951300
H	-1.59041100	6.89595500	3.61997900	H	2.98835400	2.10423400	-2.90358300
N	-0.69491300	4.56360500	3.62434700	C	0.11536800	-0.74494100	0.28505800
H	-0.22695400	3.67608500	3.53030500	C	-0.62177600	-1.71889800	-0.47703600
H	-0.62417400	5.02261300	4.51834900	C	1.03570400	-1.17833800	1.21922200

C	-1.60640500	-1.36135200	-1.46950700	N	2.94097100	-5.25892000	0.67907100
C	-0.34802700	-3.13030700	-0.24240300	N	-1.03570400	-7.69570800	-1.47367900
C	1.26063200	-2.53170400	1.48322300	N	-2.59729300	-6.46122900	-0.24044300
C	-2.24705000	-2.37184400	-2.15689600	C	2.84579400	5.49769400	0.82268100
C	-0.99736800	-4.12836300	-1.05281200	H	1.90103600	5.20328700	1.27700500
C	0.56868300	-3.51740900	0.79812200	H	3.36625100	4.60027900	0.46511700
H	1.93200300	-2.82058700	2.28435000	H	3.46812500	5.97687700	1.58697500
C	-1.94950200	-3.72606800	-1.97210600	C	3.79097500	7.05445900	-0.82732400
H	-2.98835400	-2.10423400	-2.90358300	H	3.52021200	7.68883300	-1.66921300
H	1.57655000	-0.43497000	1.79553700	H	4.32950500	7.66047300	-0.08880400
H	-1.57655000	0.43497000	1.79553700	H	4.47604500	6.27284700	-1.18627500
N	0.65478800	-4.83619500	1.25661000	C	-0.07251900	7.72781000	-2.41639900
N	-0.57732800	-5.46414100	-1.06120100	H	-1.04890500	7.72386300	-1.91216200
N	-0.65478800	4.83619500	1.25661000	H	0.00437400	8.63792600	-3.01875800
N	0.57732800	5.46414100	-1.06120100	H	-0.02835000	6.85821100	-3.06901500
C	1.98674500	-0.05545900	-1.84868600	C	1.16641900	8.91224000	-0.67837400
H	2.43463100	-0.60891900	-1.02177200	H	1.44319800	9.75529300	-1.31934100
H	1.13538800	-0.64342900	-2.19585000	H	0.21915300	9.16290200	-0.17805600
H	2.71559900	-0.02084000	-2.66212600	H	1.93132500	8.78493300	0.08394400
C	-1.98674500	0.05545900	-1.84868600	C	-2.46274000	7.76673900	1.99713700
H	-2.43463100	0.60891900	-1.02177200	H	-3.00413600	8.17904100	2.85466900
H	-1.13538800	0.64342900	-2.19585000	H	-1.69883300	8.49826300	1.69487500
H	-2.71559900	0.02084000	-2.66212600	H	-3.15867200	7.63934400	1.17134100
C	1.76936500	-5.46410700	1.40482000	C	-0.78599300	6.59527700	3.33144400
C	-1.38314700	-6.45878000	-0.92618400	H	-0.47262700	5.60205400	3.64624400
C	-1.76936500	5.46410700	1.40482000	H	0.09453800	7.11921800	2.93436800
C	1.38314700	6.45878000	-0.92618400	H	-1.15868000	7.14983600	4.19796200
N	2.59729300	6.46122900	-0.24044300	C	-2.88981300	4.68206600	-0.65681900
N	1.03570400	7.69570800	-1.47367900	H	-1.92808300	4.90709500	-1.11539000
N	-1.85437200	6.48806400	2.34930600	H	-3.03897300	3.59504200	-0.65193200
N	-2.94097100	5.25892000	0.67907100	H	-3.68216800	5.13651700	-1.26227900
N	1.85437200	-6.48806400	2.34930600	C	-4.23498700	5.17249300	1.34141000

H	-4.98748600	5.76791400	0.81030500	H	-3.52021200	-7.68883300	-1.66921300
H	-4.58665800	4.13120200	1.36820300	H	-4.32950500	-7.66047300	-0.08880400
H	-4.15908200	5.53696700	2.36407500	H	-4.47604500	-6.27284700	-1.18627500
C	0.78599300	-6.59527700	3.33144400	H	-2.42309200	-4.47314300	-2.59951300
H	0.47262700	-5.60205400	3.64624400	5H⁺			
H	-0.09453800	-7.11921800	2.93436800	Electronic energy = -2295.78624 a.u			
H	1.15868000	-7.14983600	4.19796200	C	-0.95769100	-1.18801500	0.60390300
C	2.46274000	-7.76673900	1.99713700	C	-0.64875800	-0.03652100	-0.09771600
H	3.00413600	-8.17904100	2.85466900	C	-1.71125100	0.79383800	-0.60106700
H	1.69883300	-8.49826300	1.69487500	C	-3.08110200	0.41463000	-0.29121100
H	3.15867200	-7.63934400	1.17134100	C	-3.33635600	-0.72836400	0.55096000
C	0.07251900	-7.72781000	-2.41639900	C	-2.26855900	-1.53577400	0.92774200
H	1.04890500	-7.72386300	-1.91216200	C	-1.48132400	1.94832600	-1.42936000
H	-0.00437400	-8.63792600	-3.01875800	C	-4.17545200	1.17623100	-0.83784000
H	0.02835000	-6.85821100	-3.06901500	H	-2.45675100	-2.39243500	1.56470100
C	-1.16641900	-8.91224000	-0.67837400	C	-3.88932400	2.32197700	-1.56638100
H	-1.44319800	-9.75529300	-1.31934100	C	-2.57176800	2.68552100	-1.84984600
H	-0.21915300	-9.16290200	-0.17805600	H	-4.70763500	2.88869900	-1.99551900
H	-1.93132500	-8.78493300	0.08394400	H	-2.40185400	3.55767500	-2.47395600
C	4.23498700	-5.17249300	1.34141000	C	0.80618200	0.31833500	-0.08786900
H	4.98748600	-5.76791400	0.81030500	C	1.82542500	-0.43212700	-0.78033700
H	4.58665800	-4.13120200	1.36820300	C	1.18036600	1.31491500	0.79415400
H	4.15908200	-5.53696700	2.36407500	C	1.53098100	-1.38071100	-1.82502000
C	2.88981300	-4.68206600	-0.65681900	C	3.21338600	-0.20102100	-0.42634200
H	1.92808300	-4.90709500	-1.11539000	C	2.52027000	1.64637700	1.01865900
H	3.03897300	-3.59504200	-0.65193200	C	2.57419300	-2.11401400	-2.35517100
H	3.68216800	-5.13651700	-1.26227900	C	4.23321400	-1.09922300	-0.90982900
C	-2.84579400	-5.49769400	0.82268100	C	3.52065400	0.92186300	0.40896100
H	-1.90103600	-5.20328700	1.27700500	H	2.76914600	2.45182700	1.70047200
H	-3.36625100	-4.60027900	0.46511700	C	3.89018700	-2.01363600	-1.88701700
H	-3.46812500	-5.97687700	1.58697500	H	2.36658100	-2.80500800	-3.16508000
C	-3.79097500	-7.05445900	-0.82732400	H	0.40715100	1.84355700	1.33895400

H	-0.14714300	-1.80626700	0.97710000	H	-6.52041400	4.51653500	0.01566100
N	4.88518200	1.27403800	0.61130400	C	-7.82177900	0.23851500	-2.14170300
N	5.55399300	-1.00229500	-0.42874100	H	-7.77181700	-0.82359100	-1.86602700
N	-4.58031600	-0.94391300	1.12653300	H	-8.76706000	0.41797300	-2.66144200
N	-5.48249000	0.69906200	-0.81139100	H	-6.99521200	0.45324700	-2.81563900
C	-0.12692600	2.40279400	-1.93545300	C	-8.92649000	1.03998800	-0.11228000
H	0.46963900	2.90157800	-1.16574300	H	-9.80172600	1.45860600	-0.61822000
H	0.48013700	1.58248400	-2.32290400	H	-9.15285900	-0.00283000	0.15122500
H	-0.27187200	3.11404600	-2.75163900	H	-8.75378800	1.59465900	0.80658800
C	0.16625900	-1.58927400	-2.44630700	C	-7.38037400	-2.94051900	1.91463200
H	-0.49345300	-2.18928600	-1.81701400	H	-7.64150600	-3.67951400	2.67809000
H	-0.35545300	-0.65250700	-2.64145100	H	-8.14972300	-2.15601500	1.92294700
H	0.28714700	-2.10985200	-3.39886100	H	-7.39571900	-3.42254400	0.94035000
C	5.39914300	2.49590300	0.79933700	C	-6.01240600	-1.53138000	3.37182000
C	6.29411700	-2.06361500	-0.19867700	H	-4.98129300	-1.26570000	3.59530700
C	-5.18684200	-2.08541200	1.14434300	H	-6.58553500	-0.60307400	3.24576100
C	-6.50118300	1.40979500	-0.45572300	H	-6.43284100	-2.08755400	4.21426900
N	-6.48793300	2.45630600	0.45927100	C	-4.69713800	-2.74774800	-1.18818300
N	-7.75320200	1.11196500	-0.97896700	H	-4.94421200	-1.70841900	-1.39947400
N	-6.06139000	-2.37272200	2.18413000	H	-3.62629400	-2.90815800	-1.36799600
N	-5.08421400	-3.07603900	0.17656300	H	-5.26051300	-3.38830600	-1.87519800
N	6.54111000	2.59696300	1.52667700	C	-4.99351100	-4.48740300	0.52752700
N	4.85074900	3.61725300	0.27443900	H	-5.72318100	-5.08386700	-0.03260000
N	7.65829200	-1.95002600	-0.32116000	H	-3.99208800	-4.87253000	0.29153500
N	5.82998400	-3.29374000	0.21214500	H	-5.17345100	-4.62387600	1.59179900
C	-5.46155900	2.53015500	1.48880000	C	6.90963200	1.58492100	2.51820700
H	-5.07614800	1.53245900	1.69342200	H	6.02545000	1.03821300	2.83852700
H	-4.62894200	3.18629400	1.20440300	H	7.64186500	0.87676600	2.11637100
H	-5.91336600	2.92593100	2.40502900	H	7.35247400	2.08445400	3.38313000
C	-7.21942500	3.69389700	0.21976900	C	7.57296700	3.59431600	1.23298000
H	-7.87902500	3.58247800	-0.63835300	H	7.67575000	4.31667400	2.04770600
H	-7.82146300	3.97266200	1.09261300	H	8.53184000	3.08509100	1.10250500

H	2.57749600	-0.39771900	-2.99016300	H	4.72570300	7.56633400	0.95258600
C	-1.92906200	0.35317600	-2.11328200	C	-1.83168700	8.05433600	1.40869600
H	-2.31594600	1.06265400	-1.37866000	H	-2.47872200	8.28038500	2.26023000
H	-0.94533000	0.71237700	-2.41672300	H	-1.14397100	8.89197900	1.26846200
H	-2.57749600	0.39771900	-2.99016300	H	-2.43761400	7.95288200	0.51167800
C	1.23185100	-5.70432300	0.91662100	C	0.07532400	6.97940300	2.56816600
C	-3.31939500	-5.80062600	-0.32255700	H	0.44493700	5.99997600	2.86270800
C	-1.23185100	5.70432300	0.91662100	H	0.89306600	7.55278500	2.12065300
C	3.31939500	5.80062600	-0.32255700	H	-0.27284200	7.51067300	3.45655300
N	4.48866700	5.22554900	0.11199600	C	-2.66870100	4.67060500	-0.79621500
N	3.36334300	7.13973100	-0.59498300	H	-1.75540400	4.67422400	-1.38639700
N	-1.04779300	6.83519200	1.63664700	H	-2.96785500	3.63533800	-0.61100000
N	-2.46747500	5.39989900	0.45704100	H	-3.45683000	5.17144000	-1.36357900
N	1.04779300	-6.83519200	1.63664700	C	-3.68469000	5.66348600	1.23092800
N	2.46747500	-5.39989900	0.45704100	H	-4.31920100	6.40702900	0.74145400
N	-3.36334300	-7.13973100	-0.59498300	H	-4.25222600	4.73258200	1.31900800
N	-4.48866700	-5.22554900	0.11199600	H	-3.43194900	6.00872700	2.23069700
C	4.48466900	4.05633900	0.98306900	C	-0.07532400	-6.97940300	2.56816600
H	3.53171600	3.97888500	1.50307300	H	-0.44493700	-5.99997600	2.86270800
H	4.65667000	3.12859400	0.42673000	H	-0.89306600	-7.55278500	2.12065300
H	5.27904900	4.17127200	1.72582700	H	0.27284200	-7.51067300	3.45655300
C	5.79103800	5.55450100	-0.46970600	C	1.83168700	-8.05433600	1.40869600
H	5.67968600	6.29277600	-1.26059800	H	2.47872200	-8.28038500	2.26023000
H	6.48292600	5.94190400	0.28447000	H	1.14397100	-8.89197900	1.26846200
H	6.23139100	4.65030700	-0.90428100	H	2.43761400	-7.95288200	0.51167800
C	2.35401600	7.75718100	-1.44876700	C	-2.35401600	-7.75718100	-1.44876700
H	1.55657100	8.22703100	-0.85932700	H	-1.55657100	-8.22703100	-0.85932700
H	2.82704200	8.53253000	-2.05674400	H	-2.82704200	-8.53253000	-2.05674400
H	1.91170100	7.00836800	-2.10094100	H	-1.91170100	-7.00836800	-2.10094100
C	4.20985000	8.07741400	0.14327600	C	-4.20985000	-8.07741400	0.14327600
H	4.95005100	8.55195400	-0.50771800	H	-4.95005100	-8.55195400	-0.50771800
H	3.58473500	8.86636300	0.57416000	H	-3.58473500	-8.86636300	0.57416000

H	-4.72570300	-7.56633400	0.95258600	C	0.90493300	4.27093000	-1.85476900
C	3.68469000	-5.66348600	1.23092800	C	1.51082900	3.05575500	-2.19067400
H	4.31920100	-6.40702900	0.74145400	H	1.23789900	5.18834200	-2.32716600
H	4.25222600	-4.73258200	1.31900800	H	2.30755700	3.06020500	-2.92773400
H	3.43194900	-6.00872700	2.23069700	C	0.36616700	-0.65718500	0.01994200
C	2.66870100	-4.67060500	-0.79621500	C	-0.06006700	-1.85056600	-0.66348800
H	1.75540400	-4.67422400	-1.38639700	C	1.44664600	-0.71524600	0.87528500
H	2.96785500	-3.63533800	-0.61100000	C	-1.13093300	-1.85394100	-1.63145700
H	3.45683000	-5.17144000	-1.36357900	C	0.63809400	-3.09867800	-0.38142800
C	-4.48466900	-4.05633900	0.98306900	C	2.16195600	-1.89575700	1.09327600
H	-3.53171600	-3.97888500	1.50307300	C	-1.51082900	-3.05575500	-2.19067400
H	-4.65667000	-3.12859400	0.42673000	C	0.15168800	-4.31985800	-0.96809500
H	-5.27904900	-4.17127200	1.72582700	C	1.77899900	-3.08167100	0.49578900
C	-5.79103800	-5.55450100	-0.46970600	H	3.04002600	-1.88848000	1.72949200
H	-5.67968600	-6.29277600	-1.26059800	C	-0.90493300	-4.27093000	-1.85476900
H	-6.48292600	-5.94190400	0.28447000	H	-2.30755700	-3.06020500	-2.92773400
H	-6.23139100	-4.65030700	-0.90428100	H	1.75061500	0.18943900	1.39123200
H	-3.69349100	-3.90265000	-2.19979100	H	-1.75061500	-0.18943900	1.39123200
H	0.75542200	5.41422600	0.37522200	C	1.85910400	0.62190300	-2.13089100
H	-0.75542200	-5.41422600	0.37522200	H	2.51905800	0.18343900	-1.38036800
6				H	1.18200500	-0.16986400	-2.45314100
Electronic energy = -1527.77681 a.u				H	2.47232800	0.89896200	-2.99155300
C	-1.44664600	0.71524600	0.87528500	C	-1.85910400	-0.62190300	-2.13089100
C	-0.36616700	0.65718500	0.01994200	H	-2.51905800	-0.18343900	-1.38036800
C	0.06006700	1.85056600	-0.66348800	H	-1.18200500	0.16986400	-2.45314100
C	-0.63809400	3.09867800	-0.38142800	H	-2.47232800	-0.89896200	-2.99155300
C	-1.77899900	3.08167100	0.49578900	H	-1.23789900	-5.18834200	-2.32716600
C	-2.16195600	1.89575700	1.09327600	C	2.80910400	-4.66142800	1.83761900
C	1.13093300	1.85394100	-1.63145700	C	2.60875000	-4.75597000	3.26443500
C	-0.15168800	4.31985800	-0.96809500	C	3.46989900	-5.59457500	2.69123100
H	-3.04002600	1.88848000	1.72949200	N	2.59530900	-4.21470400	0.68083200
				N	0.77216700	-5.56199300	-0.72051900

C	0.07257800	-6.53611800	-0.33374200	H	4.78154500	2.21772600	2.27135600
C	-1.13093300	-7.18084400	0.13679200	H	2.47273700	2.82844500	2.83281800
C	-0.02651100	-7.91545700	0.01902600	C	-0.72707100	0.25918000	-0.26123500
N	-2.59530900	4.21470400	0.68083200	C	-1.77607300	-0.54522200	0.30687300
C	-2.80910400	4.66142800	1.83761900	C	-1.06266100	1.38782400	-0.98349600
C	-3.46989900	5.59457500	2.69123100	C	-1.51801000	-1.67501900	1.16919200
C	-2.60875000	4.75597000	3.26443500	C	-3.15359300	-0.18475300	0.02167400
N	-0.77216700	5.56199300	-0.72051900	C	-2.38679800	1.79496200	-1.16385100
C	-0.07257800	6.53611800	-0.33374200	C	-2.57947400	-2.44736900	1.59815400
C	1.13093300	7.18084400	0.13679200	C	-4.18397900	-1.08680200	0.44826100
C	0.02651100	7.91545700	0.01902600	C	-3.43245000	1.04661100	-0.66637200
H	4.16580200	-6.40735000	2.84027600	H	-2.58834500	2.69137500	-1.73663300
H	2.14604200	-4.44188800	4.18836700	C	-3.90072600	-2.18535700	1.21917400
H	0.41510900	-8.89529600	0.12935000	H	-2.38695500	-3.28587300	2.25675200
H	-2.17677300	-7.17440000	0.40595800	H	-0.26647500	1.96742700	-1.43558700
H	-2.14604200	4.44188800	4.18836700	H	0.20495500	-1.59544300	-1.75889000
H	-4.16580200	6.40735000	2.84027600	C	0.19157000	1.90782200	1.97700000
H	2.17677300	7.17440000	0.40595800	H	-0.36727700	2.54310000	1.28546900
H	-0.41510900	8.89529600	0.12935000	H	-0.44653300	1.05338300	2.20962000
6H⁺				H	0.32543200	2.47127700	2.90254900
Electronic energy = -1528.21518 a.u.				C	-0.15517900	-2.05773700	1.70068700
C	1.01790200	-1.10832300	-1.22993100	H	0.46548400	-2.53623900	0.94154600
C	0.72098600	-0.12980700	-0.30135500	H	0.40546300	-1.19836400	2.06652900
C	1.78451100	0.53733200	0.40269900	H	-0.27859900	-2.75806800	2.52890800
C	3.15461500	0.18034300	0.06611700	H	-4.69040400	-2.83969000	1.56608300
C	3.40055500	-0.79761100	-0.96149600	C	-5.10533000	2.67494200	-0.99573900
C	2.33268200	-1.44408300	-1.55934400	C	-4.84821800	4.07205000	-1.10098300
C	1.55304000	1.50611600	1.44380300	C	-6.11031000	3.65083400	-1.18723500
C	4.24124900	0.80729500	0.77054100	N	-4.78938500	1.44869400	-0.83071300
H	2.52849500	-2.16257900	-2.34653200	N	-5.52654300	-0.82373300	0.02216700
C	3.96190600	1.76844300	1.72266800	C	-6.51134800	-1.64909800	0.01483300
C	2.64337500	2.09981200	2.04681100	C	-7.10795900	-2.90457700	0.24484700

C	-7.85613000	-1.93036100	-0.27568600	H	-3.01022100	2.36866400	2.60441000
N	4.68583100	-1.02490600	-1.47375600	C	-0.18301300	-0.73066700	-0.36087800
C	5.24826000	-2.14679300	-1.34374400	C	0.53441200	-1.77224900	0.32576700
C	6.36500700	-2.99152700	-1.59212600	C	-1.19400900	-1.06700900	-1.23747800
C	5.39250600	-3.47655200	-0.82185300	C	1.56823600	-1.50657300	1.29808400
N	5.56974800	0.37434800	0.61341700	C	0.18301300	-3.15300400	0.03472000
C	6.46164000	1.19089300	0.24866200	C	-1.58523800	-2.39071900	-1.45606200
C	6.95131000	2.44560300	-0.25075800	C	2.24396100	-2.56728000	1.86482100
C	7.82666800	1.46251100	-0.04691000	C	0.98328300	-4.18893500	0.62611100
H	-7.14639600	3.92419000	-1.31849000	C	-0.94010500	-3.43353100	-0.82605700
H	-4.17268000	4.91330500	-1.11681600	H	-2.38856700	-2.59214500	-2.15215300
H	-8.81672800	-1.61232900	-0.64978400	C	1.97951500	-3.89695600	1.52225900
H	-7.04034200	-3.92455600	0.58816900	H	3.01022100	-2.36866400	2.60441000
H	5.04839800	-4.31265100	-0.23217100	H	-1.70101000	-0.27745500	-1.78021800
H	7.32988400	-3.17249200	-2.04197700	H	1.70101000	0.27745500	-1.78021800
H	6.80544900	3.46268900	-0.58169200	C	-1.95999900	0.13033400	1.78988900
H	8.86014100	1.15419700	-0.10235700	H	-2.48795700	-0.44730200	1.02967500
H	-5.59964800	0.16084900	-0.40593700	H	-1.10229200	-0.46310300	2.10673500
6H₂²⁺				H	-2.62371600	0.23251300	2.64942600
Electronic energy = -1528.58475 a.u				C	1.95999900	-0.13033400	1.78988900
C	1.19400900	1.06700900	-1.23747800	H	2.48795700	0.44730200	1.02967500
C	0.18301300	0.73066700	-0.36087800	H	1.10229200	0.46310300	2.10673500
C	-0.53441200	1.77224900	0.32576700	H	2.62371600	-0.23251300	2.64942600
C	-0.18301300	3.15300400	0.03472000	H	2.55658000	-4.68464300	1.98792800
C	0.94010500	3.43353100	-0.82605700	C	-2.50263200	-5.09873600	-1.42755900
C	1.58523800	2.39071900	-1.45606200	C	-3.84306400	-4.84867600	-1.82888700
C	-1.56823600	1.50657300	1.29808400	C	-3.41774600	-6.11257600	-1.78045300
C	-0.98328300	4.18893500	0.62611100	N	-1.32994600	-4.78373200	-1.02068800
H	2.38856700	2.59214500	-2.15215300	N	0.73303400	-5.54482000	0.24134300
C	-1.97951500	3.89695600	1.52225900	C	1.48125300	-6.56981300	0.46549100
C	-2.24396100	2.56728000	1.86482100	C	2.61927400	-7.21596800	0.97954500
H	-2.55658000	4.68464300	1.98792800	C	1.71434300	-7.94441800	0.32128400

N	1.32994600	4.78373200	-1.02068800	H	0.87159100	3.76319000	-3.29142900
C	2.50263200	5.09873600	-1.42755900	C	0.60449500	-0.44753800	-0.38971000
C	3.41774600	6.11257600	-1.78045300	C	0.70050200	-1.71990500	-1.05781000
C	3.84306400	4.84867600	-1.82888700	C	1.62459600	-0.04909200	0.44972400
N	-0.73303400	5.54482000	0.24134300	C	-0.28017500	-2.16612800	-2.01908200
C	-1.48125300	6.56981300	0.46549100	C	1.84232000	-2.57742900	-0.76382400
C	-2.61927400	7.21596800	0.97954500	C	2.77183300	-0.82161500	0.64854700
C	-1.71434300	7.94441800	0.32128400	C	-0.15142300	-3.43324700	-2.54815700
H	-3.66039600	-7.15422500	-1.92831800	C	1.86175900	-3.92555800	-1.28076500
H	-4.66282700	-4.18057000	-2.04424400	C	2.91182900	-2.07078500	0.06176400
H	1.40715900	-8.91098400	-0.04763800	H	3.59192600	-0.42925000	1.24117500
H	3.55475800	-7.18481100	1.51588400	C	0.87113500	-4.31038200	-2.17111700
H	4.66282700	4.18057000	-2.04424400	H	-0.87159100	-3.76319000	-3.29142900
H	3.66039600	7.15422500	-1.92831800	H	1.53621600	0.90817100	0.95386400
H	-3.55475800	7.18481100	1.51588400	H	-1.53621600	-0.90817100	0.95386400
H	-1.40715900	8.91098400	-0.04763800	C	1.42838100	1.32853000	-2.54725400
H	0.15995700	5.61139800	-0.34966100	H	2.22401800	1.18137200	-1.81439900
H	-0.15995700	-5.61139800	-0.34966100	H	1.11701800	0.33454000	-2.87061800
7				H	1.86342100	1.83358000	-3.41368600
Electronic energy = -1970.86558 a.u				C	-1.42838100	-1.32853000	-2.54725400
C	-1.62459600	0.04909200	0.44972400	H	-2.22401800	-1.18137200	-1.81439900
C	-0.60449500	0.44753800	-0.38971000	H	-1.11701800	-0.33454000	-2.87061800
C	-0.70050200	1.71990500	-1.05781000	H	-1.86342100	-1.83358000	-3.41368600
C	-1.84232000	2.57742900	-0.76382400	H	0.92512600	-5.29686300	-2.61957800
C	-2.91182900	2.07078500	0.06176400	C	4.61044500	-2.94314600	1.35712200
C	-2.77183300	0.82161500	0.64854700	C	4.55433100	-2.97053500	2.78529700
C	0.28017500	2.16612800	-2.01908200	C	5.66873500	-3.41585100	2.16966000
C	-1.86175900	3.92555800	-1.28076500	N	4.13060800	-2.74772000	0.19493600
H	-3.59192600	0.42925000	1.24117500	N	2.86793500	-4.83648400	-0.92995400
C	-0.87113500	4.31038200	-2.17111700	C	2.51126100	-6.02048400	-0.61274900
C	0.15142300	3.43324700	-2.54815700	C	1.55523200	-7.02570900	-0.27231900
H	-0.92512600	5.29686300	-2.61957800	C	2.86793500	-7.33965700	-0.24815100

N	-4.13060800	2.74772000	0.19493600	7H⁺		
C	-4.61044500	2.94314600	1.35712200	Electronic energy =	-1971.33402	a.u
C	-5.66873500	3.41585100	2.16966000	C	-1.06915900	1.18102600 0.90948600
C	-4.55433100	2.97053500	2.78529700	C	-0.77327200	0.22197100 -0.03935100
N	-2.86793500	4.83648400	-0.92995400	C	-1.85650700	-0.45168100 -0.70662300
C	-2.51126100	6.02048400	-0.61274900	C	-3.21879400	-0.07997600 -0.35673100
C	-1.55523200	7.02570900	-0.27231900	C	-3.45836800	1.00172700 0.56494000
C	-2.86793500	7.33965700	-0.24815100	C	-2.37810900	1.56739800 1.21604600
N	0.25918700	-7.36860200	-0.03738800	C	-1.65298200	-1.48993900 -1.69354600
H	-0.43691200	-6.75925200	-0.44176700	C	-4.29749800	-0.80583200 -0.95711200
H	0.01585000	-8.34824300	-0.03002200	H	-2.54637600	2.31966400 1.97832700
N	3.85660200	-8.23697900	0.03552400	C	-4.06888600	-1.73398400 -1.94259100
H	3.61679100	-9.21722200	0.03014200	C	-2.75376500	-2.06311300 -2.29753700
H	4.76313800	-8.02867000	-0.35562900	H	-4.90019600	-2.20175600 -2.45841800
N	3.83539700	-2.79002000	3.92913400	H	-2.59649300	-2.80891300 -3.06847900
H	4.33820600	-2.73326400	4.80267600	C	0.68600000	0.07919100 -0.37485100
H	3.04422100	-2.16750000	3.85680800	C	1.63751800	-0.74521800 0.32478400
N	6.89535600	-4.01341300	2.24313200	C	1.11996400	0.91561700 -1.38517700
H	7.47550900	-3.91593900	1.42299700	C	1.26197800	-1.65629500 1.37817500
H	7.39890900	-3.93789000	3.11471000	C	3.03826800	-0.65617700 -0.06377400
N	-0.25918700	7.36860200	-0.03738800	C	2.44403000	0.92444500 -1.82658200
H	0.43691200	6.75925200	-0.44176700	C	2.25899800	-2.35794100 2.02595600
H	-0.01585000	8.34824300	-0.03002200	C	4.03975900	-1.33201300 0.73094300
N	-3.85660200	8.23697900	0.03552400	C	3.40865400	0.12751600 -1.22101200
H	-3.61679100	9.21722200	0.03014200	H	2.71946600	1.50636500 -2.69953100
H	-4.76313800	8.02867000	-0.35562900	C	3.61467000	-2.19179100 1.73653700
N	-3.83539700	2.79002000	3.92913400	H	1.97831000	-3.06539100 2.80084700
H	-4.33820600	2.73326400	4.80267600	H	0.39449200	1.54979700 -1.88619800
H	-3.04422100	2.16750000	3.85680800	H	-0.24509300	1.66062700 1.42579000
N	-6.89535600	4.01341300	2.24313200	C	-0.30485800	-2.02391900 -2.12306400
H	-7.47550900	3.91593900	1.42299700	H	0.30997000	-1.26686400 -2.60965900
H	-7.39890900	3.93789000	3.11471000	H	0.27721900	-2.40446500 -1.28293700

H	-0.45258000	-2.84590700	-2.82642000	H	7.74251300	0.44310900	-3.88706100
C	-0.15858700	-1.94337800	1.82486800	H	8.15377800	2.09046400	-3.81701000
H	-0.63904600	-1.09007100	2.30865100	N	-6.60424400	-4.08704700	-1.02122200
H	-0.81034300	-2.25345000	1.00539300	H	-5.64375900	-4.31317900	-1.22850200
H	-0.14127100	-2.76082800	2.54952000	H	-7.25692500	-4.84775200	-0.92286100
H	4.35336800	-2.76962700	2.28088200	N	-9.03322600	-1.68122800	0.36922500
C	5.35185600	1.02595700	-2.11954900	H	-9.75607000	-2.38235100	0.37578200
C	5.69882200	2.40792500	-2.07117600	H	-9.30259200	-0.73029500	0.56020400
C	6.51360200	1.55201000	-2.72636200	N	-3.47343400	4.94259200	1.01183000
N	4.65682800	0.00049700	-1.81738900	H	-3.65352100	5.93384500	1.02619700
N	5.39763400	-1.15065400	0.48577500	H	-2.60281700	4.64132800	0.60332000
C	6.19654000	-1.07297300	1.48578700	N	-7.04459300	4.25060000	1.60158800
C	6.52050400	-0.92056500	2.86378000	H	-7.72175200	3.58697300	1.94357100
C	7.52216400	-0.96696800	1.95486600	H	-7.15104200	5.19041100	1.95223600
N	-4.77770500	1.46638700	0.78513200	H	-5.70517500	0.30717200	0.07471400
C	-4.94554300	2.73293400	1.01653800	7H₂²⁺			
C	-5.79873200	3.79751200	1.33152000	Electronic energy = -1971.74603 a.u			
C	-4.49009700	4.06620300	1.07873700	C	-1.12486800	1.14717700	1.15809500
N	-5.62843000	-0.58208400	-0.49241600	C	-0.13555900	0.74087400	0.28478600
C	-6.53225600	-1.53178000	-0.42896500	C	0.62242700	1.73587600	-0.42617900
C	-6.91339700	-2.85702500	-0.60631700	C	0.32857500	3.13897200	-0.16978400
C	-7.81592700	-1.95488900	-0.11063000	C	-0.66919500	3.50189700	0.81196100
N	6.11382300	-0.73778800	4.14685600	C	-1.40426700	2.49214000	1.41163900
H	5.16305600	-1.00014800	4.35967900	C	1.64379800	1.40409800	-1.39258200
H	6.77903200	-0.88585000	4.89125600	C	1.06126500	4.13174100	-0.90331900
N	8.84446900	-0.86423200	1.66353100	H	-2.21514200	2.74589200	2.08363900
H	9.51541200	-1.00223100	2.40366300	C	2.09082100	3.77517700	-1.74099000
H	9.13545300	-1.18943400	0.75440700	C	2.35998400	2.42345500	-1.98368100
N	5.46281500	3.65881800	-1.58960000	H	2.70712600	4.53472300	-2.20688900
H	5.94525700	4.43557700	-2.01666200	H	3.15662700	2.17142600	-2.67445000
H	4.52069000	3.85597400	-1.28881700	C	0.13555900	-0.74087400	0.28478600
N	7.68285000	1.31290100	-3.37958900	C	-0.62242700	-1.73587600	-0.42617900

C	1.12486800	-1.14717700	1.15809500	C	-1.67024400	4.90516800	3.64209400
C	-1.64379800	-1.40409800	-1.39258200	N	0.70860100	5.50147800	-0.76386500
C	-0.32857500	-3.13897200	-0.16978400	C	0.92096400	6.41967000	-1.68372500
C	1.40426700	-2.49214000	1.41163900	C	1.35016100	6.81027000	-2.94618400
C	-2.35998400	-2.42345500	-1.98368100	C	0.84108800	7.74612000	-2.08262000
C	-1.06126500	-4.13174100	-0.90331900	N	-1.90151200	-6.50182600	-4.11970800
C	0.66919500	-3.50189700	0.81196100	H	-2.03140500	-5.53691500	-4.37962100
H	2.21514200	-2.74589200	2.08363900	H	-2.04025000	-7.20345700	-4.82944400
C	-2.09082100	-3.77517700	-1.74099000	N	-0.49458200	-9.00794300	-1.82633300
H	-3.15662700	-2.17142600	-2.67445000	H	-0.67558100	-9.74054500	-2.49412800
H	1.70360100	-0.38895500	1.67491100	H	-0.20478800	-9.28182100	-0.90166400
H	-1.70360100	0.38895500	1.67491100	N	1.79903300	-4.03176100	4.65385100
C	1.99421700	0.00046200	-1.84006400	H	2.02723900	-4.35695500	5.58023800
H	2.47067200	-0.58803200	-1.05491300	H	1.35197800	-3.13202000	4.58330400
H	1.12085700	-0.56085100	-2.17397700	N	2.16190400	-7.45489600	3.37288300
H	2.68906400	0.05709400	-2.67985200	H	2.34184100	-8.04937800	2.57952500
C	-1.99421700	-0.00046200	-1.84006400	H	2.63218800	-7.70950900	4.22792300
H	-2.47067200	0.58803200	-1.05491300	N	1.90151200	6.50182600	-4.11970800
H	-1.12085700	0.56085100	-2.17397700	H	2.03140500	5.53691500	-4.37962100
H	-2.68906400	-0.05709400	-2.67985200	H	2.04025000	7.20345700	-4.82944400
H	-2.70712600	-4.53472300	-2.20688900	N	0.49458200	9.00794300	-1.82633300
C	1.35016100	-5.17452000	2.29857400	H	0.67558100	9.74054500	-2.49412800
C	1.67024400	-4.90516800	3.64209400	H	0.20478800	9.28182100	-0.90166400
C	1.83424600	-6.16757200	3.15538900	N	-1.79903300	4.03176100	4.65385100
N	0.88985600	-4.85509700	1.12161000	H	-2.02723900	4.35695500	5.58023800
N	-0.70860100	-5.50147800	-0.76386500	H	-1.35197800	3.13202000	4.58330400
C	-0.92096400	-6.41967000	-1.68372500	N	-2.16190400	7.45489600	3.37288300
C	-1.35016100	-6.81027000	-2.94618400	H	-2.34184100	8.04937800	2.57952500
C	-0.84108800	-7.74612000	-2.08262000	H	-2.63218800	7.70950900	4.22792300
N	-0.88985600	4.85509700	1.12161000	H	0.03487300	5.65599700	0.03586300
C	-1.35016100	5.17452000	2.29857400	H	-0.03487300	-5.65599700	0.03586300
C	-1.83424600	6.16757200	3.15538900	8			

Electronic energy = -2599.91967 a.u

C	0.00099800	1.60999300	-0.01135000	C	-1.37809300	1.37934800	-3.03294300
C	0.42395100	0.62218100	-0.87729700	H	-1.27471800	2.15470300	-2.27182700
C	1.67285400	0.78747300	-1.57574100	H	-0.36884200	1.13462800	-3.36671500
C	2.47414100	1.97600200	-1.30098500	H	-1.90722600	1.81651700	-3.88361600
C	1.95013400	2.99540100	-0.42332200	H	-5.16602000	-1.24684000	-3.27354300
C	0.72714300	2.78556900	0.19436100	C	-2.91653600	-4.66498100	0.88519400
C	2.14996500	-0.16825000	-2.54734600	C	-3.19670200	-4.56740600	2.28753300
C	3.78529400	2.09513600	-1.89402100	C	-3.45450500	-5.73476500	1.63785800
H	0.32519800	3.56825000	0.82915300	N	-2.57241900	-4.23837300	-0.26583300
C	4.20052400	1.12856400	-2.79347500	N	-4.63152400	-3.18490900	-1.64509700
C	3.38619900	0.04039000	-3.12262300	C	-5.79243800	-2.98698900	-1.15205000
H	5.16602000	1.24684000	-3.27354300	C	-6.82968300	-2.23072800	-0.51221200
H	3.74121800	-0.66759400	-3.86588500	C	-7.02967600	-3.55270500	-0.76522200
C	-0.42395100	-0.62218100	-0.87729700	N	2.57241900	4.23837300	-0.26583300
C	-1.67285400	-0.78747300	-1.57574100	C	2.91653600	4.66498100	0.88519400
C	-0.00099800	-1.60999300	-0.01135000	C	3.45450500	5.73476500	1.63785800
C	-2.14996500	0.16825000	-2.54734600	C	3.19670200	4.56740600	2.28753300
C	-2.47414100	-1.97600200	-1.30098500	N	4.63152400	3.18490900	-1.64509700
C	-0.72714300	-2.78556900	0.19436100	C	5.79243800	2.98698900	-1.15205000
C	-3.38619900	-0.04039000	-3.12262300	C	6.82968300	2.23072800	-0.51221200
C	-3.78529400	-2.09513600	-1.89402100	C	7.02967600	3.55270500	-0.76522200
C	-1.95013400	-2.99540100	-0.42332200	N	-7.24461800	-1.07379700	0.06957100
H	-0.32519800	-3.56825000	0.82915300	N	-7.75171700	-4.70081900	-0.65897600
C	-4.20052400	-1.12856400	-2.79347500	N	-3.28633200	-3.80471900	3.41058400
H	-3.74121800	0.66759400	-3.86588500	N	-3.96651400	-6.99324200	1.58450000
H	0.93812200	-1.47015000	0.51482800	N	7.24461800	1.07379700	0.06957100
H	-0.93812200	1.47015000	0.51482800	N	7.75171700	4.70081900	-0.65897600
C	1.37809300	-1.37934800	-3.03294300	N	3.28633200	3.80471900	3.41058400
H	1.27471800	-2.15470300	-2.27182700	N	3.96651400	6.99324200	1.58450000
H	0.36884200	-1.13462800	-3.36671500	C	4.20052400	7.71906000	2.82239600
H	1.90722600	-1.81651700	-3.88361600	H	4.72884000	7.08360400	3.53422400
				H	4.82867800	8.58814700	2.61461200

H	3.26713900	8.07005100	3.28939700	H	-2.95164300	-1.87025800	4.13855400
C	3.57197500	7.79847400	0.42913200	C	-3.56412900	-4.46270200	4.67761400
H	3.45957000	7.14803500	-0.43772200	H	-4.39224100	-5.16307400	4.56085100
H	2.62051000	8.32326800	0.59865100	H	-2.69269900	-5.00973900	5.07003100
H	4.34654800	8.54133700	0.22172000	H	-3.85853400	-3.71164000	5.41386700
C	3.56412900	4.46270200	4.67761400	C	-4.20052400	-7.71906000	2.82239600
H	4.39224100	5.16307400	4.56085100	H	-4.72884000	-7.08360400	3.53422400
H	2.69269900	5.00973900	5.07003100	H	-4.82867800	-8.58814700	2.61461200
H	3.85853400	3.71164000	5.41386700	H	-3.26713900	-8.07005100	3.28939700
C	2.46491500	2.59909200	3.48516600	C	-3.57197500	-7.79847400	0.42913200
H	1.46114000	2.80943800	3.88213900	H	-3.45957000	-7.14803500	-0.43772200
H	2.35554300	2.16917700	2.49088000	H	-2.62051000	-8.32326800	0.59865100
H	2.95164300	1.87025800	4.13855400	H	-4.34654800	-8.54133700	0.22172000
C	6.58172500	-0.16921100	-0.31883200	C	-7.36154900	-5.78833000	-1.55526000
H	5.53768800	0.03026600	-0.55373900	H	-7.85195000	-5.70935600	-2.53651000
H	7.05127400	-0.62670100	-1.20142800	H	-6.28264200	-5.75848800	-1.70338500
H	6.63355200	-0.87995200	0.51011800	H	-7.63484000	-6.74628100	-1.10531100
C	8.64066400	0.95332900	0.46013300	C	-9.16499200	-4.62251000	-0.32591600
H	9.30920200	0.80534700	-0.40207400	H	-9.31142500	-3.96749600	0.53388200
H	8.95673700	1.84843900	0.99745900	H	-9.77642400	-4.24803400	-1.16165300
H	8.75199400	0.09923700	1.13156300	H	-9.52407000	-5.61819200	-0.05652300
C	7.36154900	5.78833000	-1.55526000	C	-8.64066400	-0.95332900	0.46013300
H	7.85195000	5.70935600	-2.53651000	H	-9.30920200	-0.80534700	-0.40207400
H	6.28264200	5.75848800	-1.70338500	H	-8.95673700	-1.84843900	0.99745900
H	7.63484000	6.74628100	-1.10531100	H	-8.75199400	-0.09923700	1.13156300
C	9.16499200	4.62251000	-0.32591600	C	-6.58172500	0.16921100	-0.31883200
H	9.31142500	3.96749600	0.53388200	H	-5.53768800	-0.03026600	-0.55373900
H	9.77642400	4.24803400	-1.16165300	H	-7.05127400	0.62670100	-1.20142800
H	9.52407000	5.61819200	-0.05652300	H	-6.63355200	0.87995200	0.51011800
C	-2.46491500	-2.59909200	3.48516600	8H⁺			
H	-1.46114000	-2.80943800	3.88213900	Electronic energy =	-2600.39252	a.u	
H	-2.35554300	-2.16917700	2.49088000	C	1.07672800	1.21960900	-0.14160100

C	0.78416600	-0.07944900	-0.50498800	H	0.60241500	-0.19259700	-3.15438800
C	1.86612300	-0.96248200	-0.85276200	H	-0.17982100	0.94070500	-4.24477800
C	3.23014900	-0.46792100	-0.73449200	H	-4.64451800	0.65043400	-3.75353100
C	3.47065500	0.90458900	-0.35660100	C	-5.21779500	-1.50301300	1.64450400
C	2.38149100	1.71806200	-0.09868500	C	-5.54954200	-0.73421800	2.80213800
C	1.65193500	-2.30531600	-1.34785000	C	-6.34819900	-1.77917300	2.44507100
C	4.30544800	-1.36913100	-1.03158300	N	-4.56981400	-1.78967300	0.58150300
H	2.54098500	2.76873000	0.11494000	N	-5.48410200	-0.46399500	-1.56025200
C	4.06333800	-2.63206200	-1.51282300	C	-6.38913700	0.43946400	-1.64575100
C	2.74628000	-3.08262200	-1.66570800	C	-6.90322800	1.77231200	-1.71559600
H	4.88854600	-3.26583100	-1.81674900	C	-7.76975100	0.72657100	-1.59217900
H	2.58264100	-4.07414700	-2.07243500	N	4.78142600	1.42841800	-0.36188700
C	-0.65826200	-0.48273400	-0.37113700	C	5.08441500	2.42346400	0.42246000
C	-1.70237500	-0.20649900	-1.32425200	C	6.00726400	3.42949800	0.73549100
C	-0.97655100	-1.06337000	0.84100600	C	4.90157600	3.27894200	1.53668100
C	-1.44281600	0.37368300	-2.61902800	N	5.65190900	-0.93295000	-0.87618200
C	-3.07408300	-0.54919100	-0.96392100	C	6.66067300	-1.71430200	-0.53940000
C	-2.27721000	-1.45234800	1.16139600	C	7.19389200	-2.91864800	-0.07716800
C	-2.51731200	0.66071700	-3.43703900	C	8.03323300	-1.86044900	-0.38171400
C	-4.15451800	-0.17756200	-1.85111800	N	-6.68697600	3.11305400	-1.72774400
C	-3.33264000	-1.23282700	0.28422700	N	-9.01180500	0.21404300	-1.41444100
H	-2.47482400	-1.97509400	2.09071900	N	-5.31956700	0.35158000	3.58708000
C	-3.83994200	0.41692200	-3.06524500	N	-7.46633600	-2.53293800	2.57897300
H	-2.32576800	1.08667800	-4.41757700	N	7.02695500	-4.18349100	0.31055300
H	-0.18112500	-1.24595400	1.55764500	N	9.24571100	-1.30897100	-0.45797500
H	0.25271400	1.88192500	0.09994700	N	4.15841500	3.69511200	2.57662800
C	0.29761900	-2.92683600	-1.61085200	N	7.16220200	4.04511900	0.41319900
H	-0.26829900	-3.10132600	-0.69518600	C	7.60879700	5.20215200	1.18120400
H	-0.33009200	-2.30688700	-2.25089900	H	7.43654100	5.03078400	2.24372800
H	0.43781500	-3.88759600	-2.11073300	H	8.68112100	5.33814400	1.02882500
C	-0.06976900	0.66665500	-3.19299200	H	7.09722500	6.12545000	0.87735200
H	0.44168700	1.49158800	-2.69226800	C	7.61053100	3.96997100	-0.97774500

H	7.24069900	3.04896000	-1.42738800	H	-7.10159500	0.25542900	4.68642800
H	7.23756800	4.81594000	-1.56899600	H	-5.65703800	-0.20042400	5.62146700
H	8.70253800	3.97612400	-1.01260800	H	-5.96332500	1.50111300	5.20504300
C	4.61168200	4.82838900	3.37671000	C	-8.23716000	-2.46767000	3.81124400
H	5.04963000	5.58971100	2.73162300	H	-8.38485000	-1.42787700	4.10485300
H	3.75278000	5.26933700	3.88562400	H	-9.21960900	-2.91285200	3.64165300
H	5.34745700	4.53100000	4.13628700	H	-7.75237900	-3.00405100	4.64060400
C	3.24289400	2.76142500	3.23676000	C	-7.48457800	-3.80924000	1.86454300
H	2.34671200	3.29566800	3.55971500	H	-6.91616400	-3.70995000	0.94038600
H	2.94973700	1.97997900	2.53929100	H	-7.04509300	-4.62011400	2.46239000
H	3.71348200	2.30224900	4.11595100	H	-8.51615000	-4.07640900	1.62247300
C	5.74499700	-4.64385000	0.85657100	C	-9.17793900	-1.21011700	-1.70491600
H	4.96243800	-3.92665400	0.62142200	H	-9.42451100	-1.38562000	-2.76144600
H	5.48234600	-5.60798900	0.41610700	H	-8.25084800	-1.73273800	-1.47229200
H	5.81463600	-4.75925600	1.94402600	H	-9.98280800	-1.61605700	-1.08722300
C	8.18881700	-5.02975400	0.57681500	C	-10.17728100	1.05811900	-1.63171300
H	7.92175600	-6.06869200	0.37649500	H	-10.04697100	2.01400500	-1.12323900
H	9.01008900	-4.75875800	-0.08527200	H	-10.36759200	1.24774900	-2.69851500
H	8.51821400	-4.95149300	1.62006300	H	-11.05594200	0.56803600	-1.20766300
C	9.43820800	-0.08896400	-1.24276700	C	-7.81689200	4.00385800	-1.95217200
H	9.84863800	-0.31530600	-2.23309200	H	-8.13176900	4.02704100	-3.00602300
H	8.48378600	0.42028900	-1.36869100	H	-8.66418600	3.69345500	-1.34025300
H	10.12724400	0.57726700	-0.71924800	H	-7.53798600	5.01654400	-1.65394600
C	10.44106800	-2.06699800	-0.09606400	C	-5.38812400	3.60370400	-2.18013500
H	10.20674500	-2.77391800	0.69862400	H	-4.61356400	2.88548100	-1.91629900
H	10.85491700	-2.60939700	-0.95444300	H	-5.36209100	3.75571600	-3.26842200
H	11.20025000	-1.37691300	0.27633700	H	-5.17366700	4.55808000	-1.69211800
C	-3.98655000	0.94557200	3.55833400	H	5.71832000	0.11204700	-0.79367600
H	-3.30598700	0.46570500	4.27687000	8H₂²⁺			
H	-3.56187500	0.84133900	2.56092200	Electronic energy =	-2600.81550	a.u	
H	-4.05924500	2.00796700	3.80521700	C	-0.56629500	1.48558700	0.71775400
C	-6.04500900	0.47408100	4.84320500	C	0.16060200	0.73610500	-0.18596300

C	1.19841600	1.37705000	-0.95021300	H	-2.50115900	1.00826200	-3.14403400
C	1.44581200	2.79459400	-0.72402400	H	-3.90964100	-3.26052600	-3.06255000
C	0.62970300	3.53460600	0.21544600	C	-0.41783100	-5.52934500	1.44196500
C	-0.36268200	2.85415100	0.90392500	C	-0.13638000	-5.60424600	2.82331500
C	1.98091700	0.68390700	-1.94905100	C	-0.11341000	-6.74863500	2.05688600
C	2.49231800	3.43061600	-1.47456900	N	-0.77282700	-4.92406300	0.33745300
H	-1.02183100	3.40136000	1.56721600	N	-2.78104500	-4.80265000	-1.25791400
C	3.18748700	2.74448300	-2.44141100	C	-3.96030200	-5.37398200	-1.45638300
C	2.92991500	1.38704300	-2.66067000	C	-5.33636500	-5.33200900	-1.67400100
H	3.90964100	3.26052600	-3.06255000	C	-4.68674300	-6.55286800	-1.55430900
H	3.48977900	0.87484200	-3.43506300	N	0.77282700	4.92406300	0.33745300
C	-0.16060200	-0.73610500	-0.18596300	C	0.41783100	5.52934500	1.44196500
C	-1.19841600	-1.37705000	-0.95021300	C	0.11341000	6.74863500	2.05688600
C	0.56629500	-1.48558700	0.71775400	C	0.13638000	5.60424600	2.82331500
C	-1.98091700	-0.68390700	-1.94905100	N	2.78104500	4.80265000	-1.25791400
C	-1.44581200	-2.79459400	-0.72402400	C	3.96030200	5.37398200	-1.45638300
C	0.36268200	-2.85415100	0.90392500	C	5.33636500	5.33200900	-1.67400100
C	-2.92991500	-1.38704300	-2.66067000	C	4.68674300	6.55286800	-1.55430900
C	-2.49231800	-3.43061600	-1.47456900	N	-6.45323600	-4.64295500	-1.89904800
C	-0.62970300	-3.53460600	0.21544600	N	-4.69777500	-7.88242300	-1.51696000
H	1.02183100	-3.40136000	1.56721600	N	0.04790700	-5.00389300	4.01041800
C	-3.18748700	-2.74448300	-2.44141100	N	0.05657300	-8.07278500	1.92247200
H	-3.48977900	-0.87484200	-3.43506300	N	6.45323600	4.64295500	-1.89904800
H	1.35019100	-0.99439200	1.28450000	N	4.69777500	7.88242300	-1.51696000
H	-1.35019100	0.99439200	1.28450000	N	-0.04790700	5.00389300	4.01041800
C	1.82032100	-0.77456700	-2.32362800	N	-0.05657300	8.07278500	1.92247200
H	2.05067300	-1.44905600	-1.49838900	C	-0.44845700	8.89063600	3.06707100
H	0.81058700	-1.01450500	-2.65897900	H	0.05650000	8.53817000	3.96592400
H	2.50115900	-1.00826200	-3.14403400	H	-0.14156600	9.92264100	2.88844500
C	-1.82032100	0.77456700	-2.32362800	H	-1.53344000	8.87642300	3.23167100
H	-2.05067300	1.44905600	-1.49838900	C	-0.36268200	8.60639700	0.59439800
H	-0.81058700	1.01450500	-2.65897900	H	0.00412500	7.91783500	-0.16599600

H	-1.44288300	8.73333200	0.45381900	H	0.92358200	-5.15082200	5.90066600
H	0.12018500	9.57803000	0.46665000	H	-0.41917800	-6.28412000	5.65070900
C	-0.44163900	5.80185900	5.16941800	C	0.44845700	-8.89063600	3.06707100
H	-1.16098900	6.56345200	4.87029900	H	-0.05650000	-8.53817000	3.96592400
H	-0.92358200	5.15082200	5.90066600	H	0.14156600	-9.92264100	2.88844500
H	0.41917800	6.28412000	5.65070900	H	1.53344000	-8.87642300	3.23167100
C	0.62525000	3.73484800	4.29564300	C	0.36268200	-8.60639700	0.59439800
H	-0.02585200	3.10583200	4.90664600	H	-0.00412500	-7.91783500	-0.16599600
H	0.83934900	3.21572300	3.36372100	H	1.44288300	-8.73333200	0.45381900
H	1.56379600	3.89986600	4.83989800	H	-0.12018500	-9.57803000	0.46665000
C	6.57523600	3.23941100	-1.48940400	C	-3.44299200	-8.62793200	-1.63191500
H	5.59619100	2.83994500	-1.23649600	H	-3.32534600	-9.04478600	-2.63767100
H	6.99730200	2.65072200	-2.30675300	H	-2.60270700	-7.96600700	-1.42770700
H	7.23405200	3.15596600	-0.61823200	H	-3.43501200	-9.44578400	-0.90815300
C	7.70162400	5.33818100	-2.21635100	C	-5.94032300	-8.63821500	-1.67376400
H	8.30907300	4.69702300	-2.85709200	H	-6.78111800	-8.05373700	-1.30392500
H	7.49166700	6.25720400	-2.76121400	H	-6.11721300	-8.91050900	-2.72023600
H	8.27592600	5.56986300	-1.31191700	H	-5.87655300	-9.55363600	-1.08294500
C	3.44299200	8.62793200	-1.63191500	C	-7.70162400	-5.33818100	-2.21635100
H	3.32534600	9.04478600	-2.63767100	H	-8.30907300	-4.69702300	-2.85709200
H	2.60270700	7.96600700	-1.42770700	H	-7.49166700	-6.25720400	-2.76121400
H	3.43501200	9.44578400	-0.90815300	H	-8.27592600	-5.56986300	-1.31191700
C	5.94032300	8.63821500	-1.67376400	C	-6.57523600	-3.23941100	-1.48940400
H	6.78111800	8.05373700	-1.30392500	H	-5.59619100	-2.83994500	-1.23649600
H	6.11721300	8.91050900	-2.72023600	H	-6.99730200	-2.65072200	-2.30675300
H	5.87655300	9.55363600	-1.08294500	H	-7.23405200	-3.15596600	-0.61823200
C	-0.62525000	-3.73484800	4.29564300	H	-2.02686500	-5.28188300	-0.70875700
H	0.02585200	-3.10583200	4.90664600	H	2.02686500	5.28188300	-0.70875700
H	-0.83934900	-3.21572300	3.36372100	9			
H	-1.56379600	-3.89986600	4.83989800	Electronic energy =	-3219.44029	a.u	
C	0.44163900	-5.80185900	5.16941800	C	-1.32376300	0.93175100	-0.29182900
H	1.16098900	-6.56345200	4.87029900	C	-0.26247900	0.70541000	-1.14494600

C	0.33622600	1.82078300	-1.83197800	H	-2.57416000	-0.50836800	-4.16135300
C	-0.16305000	3.16349200	-1.55165100	H	-2.04244700	-4.93592300	-3.46856400
C	-1.32376300	3.32307300	-0.70873800	C	2.07252200	-5.11461900	0.56191000
C	-1.86864400	2.20339200	-0.09842300	C	1.71045600	-5.31130500	1.93270900
C	1.39575100	1.65657100	-2.79974800	C	2.57938100	-6.17886900	1.34508200
C	0.52949300	4.30475800	-2.10745900	N	2.00030700	-4.54199400	-0.57415400
H	-2.75375400	2.32933700	0.51641400	N	-0.15730300	-5.61781600	-1.80134600
C	1.56105900	4.08144200	-3.00504200	C	-1.06247000	-6.46607500	-1.48297900
C	1.95667700	2.78736400	-3.35636800	C	-2.37652300	-6.87830300	-1.08528200
H	2.04244700	4.93592300	-3.46856400	C	-1.38152900	-7.80640000	-1.16915300
H	2.73813100	2.66771400	-4.10159500	N	-2.00030700	4.54199400	-0.57415400
C	0.26247900	-0.70541000	-1.14494600	C	-2.07252200	5.11461900	0.56191000
C	-0.33622600	-1.82078300	-1.83197800	C	-2.57938100	6.17886900	1.34508200
C	1.32376300	-0.93175100	-0.29182900	C	-1.71045600	5.31130500	1.93270900
C	-1.39575100	-1.65657100	-2.79974800	N	0.15730300	5.61781600	-1.80134600
C	0.16305000	-3.16349200	-1.55165100	C	1.06247000	6.46607500	-1.48297900
C	1.86864400	-2.20339200	-0.09842300	C	2.37652300	6.87830300	-1.08528200
C	-1.95667700	-2.78736400	-3.35636800	C	1.38152900	7.80640000	-1.16915300
C	-0.52949300	-4.30475800	-2.10745900	C	4.24378000	5.25470700	-0.82584500
C	1.32376300	-3.32307300	-0.70873800	C	4.61219200	7.62472200	-0.34323600
H	2.75375400	-2.32933700	0.51641400	C	5.50145900	5.40942700	0.03625900
C	-1.56105900	-4.08144200	-3.00504200	H	4.49890200	4.95490700	-1.84914400
H	-2.73813100	-2.66771400	-4.10159500	H	3.53180000	4.52414300	-0.43818000
H	1.75935600	-0.08408700	0.22814900	C	5.94023600	6.85915800	-0.23764800
H	-1.75935600	0.08408700	0.22814900	H	4.30190500	8.03095000	0.63058000
C	1.92073300	0.32657100	-3.30392500	H	4.66773900	8.46146300	-1.04898800
H	2.49830600	-0.21801600	-2.55466800	H	5.24845900	5.28523300	1.09390800
H	1.12833600	-0.34666500	-3.63384200	H	6.27070300	4.67657400	-0.21355300
H	2.57416000	0.50836800	-4.16135300	H	6.59266400	7.26566500	0.53746800
C	-1.92073300	-0.32657100	-3.30392500	H	6.47822500	6.91313000	-1.18883600
H	-2.49830600	0.21801600	-2.55466800	N	3.66477600	6.60701400	-0.80404900
H	-1.12833600	0.34666500	-3.63384200	C	-4.24378000	-5.25470700	-0.82584500

C	-4.61219200	-7.62472200	-0.34323600	H	0.39171000	-2.98132100	2.48833300
C	-5.50145900	-5.40942700	0.03625900	H	-1.05649500	-5.63261400	4.90798800
H	-4.49890200	-4.95490700	-1.84914400	H	0.05212300	-5.05616100	6.15415800
H	-3.53180000	-4.52414300	-0.43818000	H	-1.27230700	-3.21346600	4.65819700
C	-5.94023600	-6.85915800	-0.23764800	H	0.46098400	-2.97469500	4.91502500
H	-4.30190500	-8.03095000	0.63058000	N	1.01707100	-4.92968900	3.02275100
H	-4.66773900	-8.46146300	-1.04898800	C	-4.30975700	7.62905400	0.35806100
H	-5.24845900	-5.28523300	1.09390800	C	-3.61781900	7.99671500	2.66981400
H	-6.27070300	-4.67657400	-0.21355300	C	-4.82053300	8.99919500	0.81045300
H	-6.59266400	-7.26566500	0.53746800	H	-5.13072900	6.89955400	0.30682300
H	-6.47822500	-6.91313000	-1.18883600	H	-3.81209500	7.63983900	-0.61333400
N	-3.66477600	-6.60701400	-0.80404900	C	-4.84439600	8.87078900	2.34527400
C	-1.02055800	5.68046000	4.28066500	H	-2.74707400	8.60194900	2.95548100
C	-0.00478900	3.86564700	2.99655200	H	-3.81835000	7.29893200	3.49217000
C	0.13968000	5.06048200	5.07945300	H	-4.11736000	9.77987100	0.50435800
H	-1.98221300	5.55780700	4.79808700	H	-5.79820200	9.24173700	0.39000900
H	-0.87467700	6.75287600	4.10373300	H	-4.81451700	9.83461600	2.85690600
C	0.28623100	3.64797500	4.48390700	H	-5.75854000	8.35831000	2.65897000
H	0.89671000	4.19337600	2.45972600	N	-3.35454100	7.28260500	1.41726000
H	-0.39171000	2.98132100	2.48833300	C	4.30975700	-7.62905400	0.35806100
H	1.05649500	5.63261400	4.90798800	C	3.61781900	-7.99671500	2.66981400
H	-0.05212300	5.05616100	6.15415800	C	4.82053300	-8.99919500	0.81045300
H	1.27230700	3.21346600	4.65819700	H	5.13072900	-6.89955400	0.30682300
H	-0.46098400	2.97469500	4.91502500	H	3.81209500	-7.63983900	-0.61333400
N	-1.01707100	4.92968900	3.02275100	C	4.84439600	-8.87078900	2.34527400
C	1.02055800	-5.68046000	4.28066500	H	2.74707400	-8.60194900	2.95548100
C	0.00478900	-3.86564700	2.99655200	H	3.81835000	-7.29893200	3.49217000
C	-0.13968000	-5.06048200	5.07945300	H	4.11736000	-9.77987100	0.50435800
H	1.98221300	-5.55780700	4.79808700	H	5.79820200	-9.24173700	0.39000900
H	0.87467700	-6.75287600	4.10373300	H	4.81451700	-9.83461600	2.85690600
C	-0.28623100	-3.64797500	4.48390700	H	5.75854000	-8.35831000	2.65897000
H	-0.89671000	-4.19337600	2.45972600	N	3.35454100	-7.28260500	1.41726000

C	1.85991400	10.20590400	-0.77503900	C	3.30788700	1.43638600	-0.16517700
C	-0.38084100	9.50883300	-1.46713400	C	2.24843100	1.77535200	0.67050600
C	0.91728100	11.41868100	-0.77379200	C	1.43516400	-0.53881600	-2.83453300
H	2.62610500	10.29505500	-1.55973600	C	4.14908000	-0.00731900	-2.05238900
H	2.37774400	10.07540300	0.18156000	H	2.43654500	2.44559100	1.50236800
C	-0.19817400	11.00526400	-1.75024600	C	3.83996800	-0.71548100	-3.20726200
H	-1.10700700	9.33931500	-0.66176500	C	2.51753700	-0.94157400	-3.59189200
H	-0.71043700	8.93932500	-2.33823200	H	4.64903200	-1.07056200	-3.83549900
H	0.50377400	11.56840300	0.22831400	H	2.33265200	-1.46258300	-4.52718100
H	1.42534100	12.33931500	-1.06658100	C	-0.80188200	0.17071000	-0.80200200
H	-1.11966500	11.57378900	-1.61071700	C	-1.88723400	1.01676800	-1.22296500
H	0.13374300	11.15258800	-2.78252400	C	-1.09244100	-1.08912000	-0.31775700
N	0.96330700	9.08218700	-1.04800700	C	-1.67465000	2.29583300	-1.86526400
C	-1.85991400	-10.20590400	-0.77503900	C	-3.25127400	0.54618400	-1.02922300
C	0.38084100	-9.50883300	-1.46713400	C	-2.39773000	-1.57323800	-0.20525900
C	-0.91728100	-11.41868100	-0.77379200	C	-2.77074800	3.04354100	-2.24126400
H	-2.62610500	-10.29505500	-1.55973600	C	-4.32818600	1.41931100	-1.39873300
H	-2.37774400	-10.07540300	0.18156000	C	-3.49049100	-0.77965900	-0.50987600
C	0.19817400	-11.00526400	-1.75024600	H	-2.55960400	-2.59826300	0.10811500
H	1.10700700	-9.33931500	-0.66176500	C	-4.08658600	2.62313800	-2.01173400
H	0.71043700	-8.93932500	-2.33823200	H	-2.60972500	3.98304100	-2.75837000
H	-0.50377400	-11.56840300	0.22831400	H	-0.26580200	-1.72859800	-0.02724900
H	-1.42534100	-12.33931500	-1.06658100	H	0.15199400	1.61202400	1.08976500
H	1.11966500	-11.57378900	-1.61071700	C	0.06434400	-0.85974200	-3.39878300
H	-0.13374300	-11.15258800	-2.78252400	H	-0.46568500	-1.63232300	-2.83665500
N	-0.96330700	-9.08218700	-1.04800700	H	-0.59684700	0.00781300	-3.44106200
9H⁺				H	0.18216200	-1.22415300	-4.42222000
Electronic energy = -3219.92284 a.u				C	-0.32159300	2.86988900	-2.22650300
C	0.95162100	1.33173800	0.40998900	H	0.26158500	3.15190900	-1.34928900
C	0.63834600	0.58934900	-0.71288900	H	0.29177400	2.16994500	-2.79392900
C	1.68793400	0.18349400	-1.61153500	H	-0.46540900	3.76195300	-2.84021500
C	3.05909900	0.54475700	-1.27599500	H	-4.91349900	3.22635700	-2.36571500

C	-5.08485600	-2.20412500	0.46053200	H	-5.44045000	5.39440200	-1.34674800
C	-4.87535300	-2.92842700	1.65983700	H	-5.08876600	4.51091900	0.14545900
C	-5.98492800	-3.18773300	0.88891500	C	-7.66872000	6.65577400	-0.06954100
N	-4.80092000	-1.29225500	-0.42856600	H	-8.75133000	4.93230000	0.73373200
N	-5.67188000	1.00974400	-1.17360800	H	-9.01968100	5.18722200	-1.00337800
C	-6.68164600	1.82533100	-0.93017000	H	-6.23949500	6.17010100	1.49681900
C	-7.22287700	3.08593800	-0.66883500	H	-5.55931000	7.21649300	0.24608400
C	-8.04647600	1.97421000	-0.71864400	H	-8.24260000	7.28838300	0.60836400
N	4.52779000	2.07579100	0.00398100	H	-7.64411000	7.14772700	-1.04572500
C	5.16537700	2.04051700	1.11131200	N	-7.11098900	4.39740100	-0.49688000
C	6.26039800	2.51067800	1.87117100	C	6.09750200	0.56017200	4.59513600
C	5.48164500	1.52544300	2.40336400	C	4.26699100	-0.42452000	3.31228600
N	5.47324100	0.18893800	-1.68211500	C	5.66020300	-0.76634600	5.24187800
C	6.31993400	-0.77328500	-1.79702800	H	5.95904100	1.41147300	5.27388800
C	6.72784600	-2.13422800	-1.95633800	H	7.15169600	0.54327800	4.29464400
C	7.66725800	-1.17584800	-1.69879300	C	4.21767400	-0.96805400	4.74254600
C	5.10886600	-3.98305600	-2.34731500	H	4.63810800	-1.18621700	2.61151000
C	7.49434700	-4.47650900	-2.12323000	H	3.30436400	-0.06950600	2.94128100
C	5.29203700	-5.46469400	-2.00001000	H	6.29421300	-1.58207500	4.88236700
H	4.77190100	-3.86052200	-3.38361600	H	5.73797400	-0.74241900	6.33018300
H	4.39606400	-3.46384000	-1.70434700	H	3.89752400	-2.01087700	4.78301600
C	6.72676200	-5.76099300	-2.47142500	H	3.52084200	-0.37551000	5.34318800
H	7.93926200	-4.53184500	-1.11976700	N	5.21520300	0.69138200	3.42851200
H	8.30014100	-4.26556500	-2.83443000	C	-4.54459200	-4.28749100	3.69061400
H	5.21281300	-5.60837900	-0.91786400	C	-3.07650700	-2.36971900	3.28429900
H	4.54622100	-6.10087900	-2.47986800	C	-3.65485400	-4.03515400	4.91955900
H	7.16157900	-6.64338700	-1.99885400	H	-4.35303700	-5.26951700	3.24256600
H	6.73953200	-5.92232400	-3.55335000	H	-5.61041600	-4.22707500	3.93254800
N	6.46186500	-3.43486500	-2.16955600	C	-2.44889200	-3.26408500	4.35457800
C	-5.83071900	5.13033300	-0.35942000	H	-3.49719500	-1.45776100	3.72820600
C	-8.27907700	5.25416800	-0.20222400	H	-2.38665400	-2.07715800	2.49490800
C	-6.23824900	6.38189500	0.42367800	H	-4.18791200	-3.41452300	5.64526400

H	-3.37395100	-4.96255000	5.42010900	C	11.29029000	-0.91580900	-1.24771100
H	-1.91802300	-2.69001400	5.11510500	H	10.14135700	-2.18629700	-2.61173900
H	-1.73648000	-3.95365400	3.89258300	H	9.93827700	-2.61905700	-0.90441500
N	-4.15634600	-3.22242800	2.74684500	C	10.88195000	0.49053000	-1.72124700
C	7.58450800	4.38481400	0.96260100	H	9.23213100	0.93288300	-0.35253200
C	8.15436500	3.46544200	3.15840400	H	8.81859200	1.20302800	-2.05134900
C	8.97145900	4.88814300	1.37395100	H	11.45381900	-0.91666400	-0.16582100
H	6.83895400	5.18945200	1.01505800	H	12.20232000	-1.28014700	-1.72324600
H	7.55017800	3.96134100	-0.04289800	H	11.46183000	1.28441100	-1.24720200
C	8.95228900	4.75656800	2.90789400	H	11.01825100	0.57662300	-2.80340300
H	8.81362800	2.59153600	3.25126700	N	8.95058800	-0.83567900	-1.49032700
H	7.54861500	3.52298800	4.06964700	C	-10.48092300	2.19831900	-0.33471700
H	9.74590500	4.24330000	0.94748400	C	-9.53028800	0.00997000	-0.92485100
H	9.16160600	5.90868900	1.03763800	C	-11.54664100	1.10546400	-0.17875000
H	9.95006000	4.71959000	3.34827400	H	-10.71768200	2.87599600	-1.16333600
H	8.42651600	5.60920000	3.34741900	H	-10.34949800	2.79483300	0.57156500
N	7.30827400	3.34722600	1.96674800	C	-11.05249800	-0.01759200	-1.10695300
C	-7.78428300	-3.88331500	-0.64384600	H	-9.21425600	-0.61162300	-0.07909500
C	-7.55692700	-4.99694600	1.52497100	H	-8.98636800	-0.31089700	-1.81546200
C	-9.04159800	-4.71261800	-0.37166700	H	-11.57456600	0.75619300	0.85717500
H	-7.15845800	-4.35022600	-1.41461200	H	-12.54320300	1.46432700	-0.43738900
H	-7.99440400	-2.85867400	-0.95719500	H	-11.48047900	-0.99024300	-0.86173800
C	-8.55291600	-5.76476000	0.63960100	H	-11.30825600	0.20918600	-2.14562400
H	-8.03530300	-4.59692800	2.42678300	N	-9.25650100	1.43255600	-0.63714800
H	-6.71597500	-5.62300000	1.83758900	H	-5.73892400	-0.01747900	-0.96298500
H	-9.81639400	-4.08500900	0.07928100	9H₂²⁺			
H	-9.45224000	-5.15590200	-1.27978400	Electronic energy = -3220.35633 a.u			
H	-9.36281600	-6.20901800	1.21939300	C	-0.82690100	1.36679300	0.48840300
H	-8.03763900	-6.57369600	0.11463100	C	0.02942800	0.75263700	-0.40423500
N	-7.10034600	-3.89324700	0.66092200	C	0.94724300	1.56338900	-1.16088900
C	10.06825100	-1.77810200	-1.59348300	C	0.94410700	3.00320600	-0.93648100
C	9.38952700	0.56494800	-1.37401200	C	0.00038000	3.59275400	-0.00920600

C	-0.86667300	2.74945300	0.67015400	C	0.86933600	-5.56058000	2.58237500
C	1.84610300	1.01519200	-2.15219100	C	1.14491100	-6.65879200	1.79379600
C	1.87539800	3.80972700	-1.67642200	N	0.10753600	-4.98291500	0.10502600
H	-1.62002600	3.17737300	1.32067700	N	-1.91846800	-5.20971500	-1.45977400
C	2.69548400	3.25031200	-2.62572000	C	-2.96749600	-5.99240000	-1.67220500
C	2.67399200	1.86982500	-2.84822100	C	-4.31213200	-6.21777400	-1.96757100
H	3.32886300	3.88199700	-3.23444400	C	-3.46863900	-7.28634200	-1.69907500
H	3.32270900	1.45988500	-3.61432200	N	-0.10753600	4.98291500	0.10502600
C	-0.02942800	-0.75263700	-0.40423500	C	-0.58434100	5.52378400	1.19968700
C	-0.94724300	-1.56338900	-1.16088900	C	-1.14491100	6.65879200	1.79379600
C	0.82690100	-1.36679300	0.48840300	C	-0.86933600	5.56058000	2.58237500
C	-1.84610300	-1.01519200	-2.15219100	N	1.91846800	5.20971500	-1.45977400
C	-0.94410700	-3.00320600	-0.93648100	C	2.96749600	5.99240000	-1.67220500
C	0.86667300	-2.74945300	0.67015400	C	4.31213200	6.21777400	-1.96757100
C	-2.67399200	-1.86982500	-2.84822100	C	3.46863900	7.28634200	-1.69907500
C	-1.87539800	-3.80972700	-1.67642200	C	5.98081100	4.39567000	-2.30161400
C	-0.00038000	-3.59275400	-0.00920600	C	6.65652300	6.75131600	-2.47849800
H	1.62002600	-3.17737300	1.32067700	C	7.49577900	4.51646200	-2.11296300
C	-2.69548400	-3.25031200	-2.62572000	H	5.74151900	3.93809000	-3.26653700
H	-3.32270900	-1.45988500	-3.61432200	H	5.47968700	3.82625600	-1.51777900
H	1.52022100	-0.74639500	1.04684400	C	7.83623700	5.83478800	-2.82798700
H	-1.52022100	0.74639500	1.04684400	H	6.84022500	7.30637900	-1.55137200
C	1.93178600	-0.44712900	-2.53694000	H	6.42538700	7.46696400	-3.27118800
H	2.27263900	-1.08022000	-1.71719300	H	7.73801200	4.58624400	-1.04862600
H	0.97545100	-0.84927700	-2.87321300	H	8.03035600	3.65966700	-2.52417500
H	2.64066000	-0.55735100	-3.35982700	H	8.78957800	6.25911200	-2.51239100
C	-1.93178600	0.44712900	-2.53694000	H	7.88184100	5.67779100	-3.90895800
H	-2.27263900	1.08022000	-1.71719300	N	5.53263900	5.80720000	-2.28348100
H	-0.97545100	0.84927700	-2.87321300	C	-5.98081100	-4.39567000	-2.30161400
H	-2.64066000	0.55735100	-3.35982700	C	-6.65652300	-6.75131600	-2.47849800
H	-3.32886300	-3.88199700	-3.23444400	C	-7.49577900	-4.51646200	-2.11296300
C	0.58434100	-5.52378400	1.19968700	H	-5.74151900	-3.93809000	-3.26653700

H	-5.47968700	-3.82625600	-1.51777900	H	0.03065200	-2.85497600	6.14525300
C	-7.83623700	-5.83478800	-2.82798700	H	1.66784900	-2.92437900	5.48186800
H	-6.84022500	-7.30637900	-1.55137200	N	0.90428400	-5.00197200	3.79358500
H	-6.42538700	-7.46696400	-3.27118800	C	-1.90928400	8.51023600	0.35521200
H	-7.73801200	-4.58624400	-1.04862600	C	-2.22913700	8.65744500	2.78227200
H	-8.03035600	-3.65966700	-2.52417500	C	-2.32101500	9.93708000	0.72840100
H	-8.78957800	-6.25911200	-2.51239100	H	-2.72246800	7.98059300	-0.15526300
H	-7.88184100	-5.67779100	-3.90895800	H	-1.02373300	8.46327100	-0.28179000
N	-5.53263900	-5.80720000	-2.28348100	C	-3.04101700	9.75376400	2.07591300
C	-1.44872400	5.69940000	4.97675700	H	-1.43814800	9.07877800	3.41336200
C	-0.17708400	3.76923700	4.16018000	H	-2.85528700	8.01257300	3.40456200
C	-0.94410700	4.86111600	6.16177500	H	-1.43394100	10.56479600	0.85590600
H	-2.54331500	5.71682200	4.92672000	H	-2.95325300	10.39813500	-0.03119300
H	-1.09265800	6.73274000	5.01816900	H	-3.09090800	10.67192000	2.66199600
C	-0.71930400	3.46399800	5.55809900	H	-4.06527600	9.40992900	1.90822600
H	0.90352300	3.96017100	4.18815700	N	-1.63492700	7.89362800	1.66746700
H	-0.36566300	2.98060200	3.43338400	C	1.90928400	-8.51023600	0.35521200
H	0.00242400	5.26605300	6.53031200	C	2.22913700	-8.65744500	2.78227200
H	-1.64963000	4.85961300	6.99319900	C	2.32101500	-9.93708000	0.72840100
H	-0.03065200	2.85497600	6.14525300	H	2.72246800	-7.98059300	-0.15526300
H	-1.66784900	2.92437900	5.48186800	H	1.02373300	-8.46327100	-0.28179000
N	-0.90428400	5.00197200	3.79358500	C	3.04101700	-9.75376400	2.07591300
C	1.44872400	-5.69940000	4.97675700	H	1.43814800	-9.07877800	3.41336200
C	0.17708400	-3.76923700	4.16018000	H	2.85528700	-8.01257300	3.40456200
C	0.94410700	-4.86111600	6.16177500	H	1.43394100	-10.56479600	0.85590600
H	2.54331500	-5.71682200	4.92672000	H	2.95325300	-10.39813500	-0.03119300
H	1.09265800	-6.73274000	5.01816900	H	3.09090800	-10.67192000	2.66199600
C	0.71930400	-3.46399800	5.55809900	H	4.06527600	-9.40992900	1.90822600
H	-0.90352300	-3.96017100	4.18815700	N	1.63492700	-7.89362800	1.66746700
H	0.36566300	-2.98060200	3.43338400	C	4.34520900	9.59994300	-1.72869500
H	-0.00242400	-5.26605300	6.53031200	C	1.95218100	9.20091100	-1.32737200
H	1.64963000	-4.85961300	6.99319900	C	3.66258300	10.90293000	-1.29464400

H	4.66756200	9.64362900	-2.77512200	C	-4.56638000	0.83269500	0.65277200
H	5.20910200	9.34561500	-1.11022200	C	-5.09813900	-0.28716900	1.22834100
C	2.18573200	10.67875800	-1.66327500	H	-4.98030300	-2.40809800	1.41048600
H	1.66541100	9.06670500	-0.27814500	C	-1.15342700	-0.35436200	-0.36438800
H	1.19610300	8.73165800	-1.96000600	C	-2.77540300	1.92994300	-0.61846500
H	3.76845100	11.03927400	-0.21486800	H	-5.09728400	1.77788500	0.67255500
H	4.09548500	11.77501400	-1.78498800	H	-6.05188600	-0.24971000	1.74173900
H	1.50799000	11.33792800	-1.12001400	C	-1.53065100	1.90728700	-1.19160800
H	2.03235500	10.84715400	-2.73260000	C	-0.70546300	0.77825400	-1.02351700
N	3.27697600	8.59105500	-1.56940500	H	-3.38605000	2.82533800	-0.64879300
C	-4.34520900	-9.59994300	-1.72869500	H	-1.14450300	2.78006000	-1.70617200
C	-1.95218100	-9.20091100	-1.32737200	H	0.32506400	0.83046500	-1.34993500
C	-3.66258300	-10.90293000	-1.29464400	N	-0.27007000	-1.39141200	0.02038000
H	-4.66756200	-9.64362900	-2.77512200	N	-2.75093300	-2.98412000	0.05660200
H	-5.20910200	-9.34561500	-1.11022200	C	0.03825900	-1.34544300	1.46024100
C	-2.18573200	-10.67875800	-1.66327500	H	0.58787800	-2.24332400	1.73676500
H	-1.66541100	-9.06670500	-0.27814500	H	0.63791900	-0.45462400	1.70807700
H	-1.19610300	-8.73165800	-1.96000600	H	-0.88034400	-1.31644900	2.04587100
H	-3.76845100	-11.03927400	-0.21486800	C	0.94092700	-1.56922400	-0.77187100
H	-4.09548500	-11.77501400	-1.78498800	H	1.69443000	-0.78149400	-0.60429700
H	-1.50799000	-11.33792800	-1.12001400	H	1.38567100	-2.52836300	-0.50043600
H	-2.03235500	-10.84715400	-2.73260000	H	0.69563700	-1.59293600	-1.83561700
N	-3.27697600	-8.59105500	-1.56940500	C	-3.65658300	-4.08985800	0.45527900
H	-1.09161800	-5.54935400	-0.91122700	H	-4.64277500	-3.99165200	-0.00752900
H	1.09161800	5.54935400	-0.91122700	H	-3.19462400	-5.02040100	0.13240600
DMAN:HCl				H	-3.74903700	-4.12451800	1.53975500
Free energy = -1114.55645 a.u				C	-2.52613400	-3.08272500	-1.41291500
Negative vibration = -497.62 cm-1				H	-2.06556500	-4.04889200	-1.61948200
C	-4.45224100	-1.53162100	1.06984300	H	-3.47853600	-3.00207000	-1.94681100
C	-3.22923100	-1.65030900	0.43563400	H	-1.85521700	-2.29781700	-1.74275900
C	-2.53690100	-0.44491800	0.03248100	Cl	-0.55031500	-4.58365000	0.98382600
C	-3.29615700	0.77574600	0.02326500	H	-1.55754800	-3.56118300	0.58081000

2:HCl

Free energy = -1845.65162 a.u

Negative frequency = -305.72 cm⁻¹

C	-1.12485200	1.55455000	-0.97500400	N	5.37422400	1.00790800	0.78704100
C	-0.75653700	0.30779000	-0.51233000	N	-4.78240200	1.16227400	-1.48325300
C	-1.78096200	-0.64427800	-0.16736000	N	-5.46106700	-0.41555800	0.85226100
C	-3.16542000	-0.21071900	-0.24325800	C	-0.12885700	-2.62398600	0.32642100
C	-3.47056500	0.98366400	-0.99009900	H	0.54695000	-2.09700600	1.00220700
C	-2.45677100	1.87845500	-1.26712300	H	0.35998100	-2.65313600	-0.64767900
C	-1.50221500	-1.99152300	0.26812500	H	-0.22491800	-3.65016400	0.68738400
C	-4.17972800	-0.99011500	0.43204000	C	-0.18884900	0.83425100	2.31895900
H	-2.66930600	2.80226900	-1.78875300	H	-0.70193100	-0.12486500	2.22970100
C	-3.86178900	-2.27378100	0.81442500	H	-0.79034600	1.56959700	1.78215300
C	-2.55935100	-2.77639000	0.66531200	H	-0.19167100	1.11037000	3.37568400
H	-4.58685600	-2.91113400	1.29578100	C	-5.18278500	2.51620400	-1.84375700
H	-2.37057400	-3.80118600	0.96594300	H	-4.94814700	3.20831500	-1.03253400
C	0.72504600	0.03947800	-0.53866600	H	-6.26335000	2.52167300	-1.99550000
C	1.65547800	0.34351300	0.51792700	H	-4.70163400	2.88243900	-2.76626500
C	1.20915800	-0.41278800	-1.74757100	C	-5.12541700	0.20361200	-2.54660300
C	1.24346500	0.77897100	1.83080000	H	-6.18629500	0.29007100	-2.77616000
C	3.07693800	0.20749000	0.24250800	H	-4.92996900	-0.81724700	-2.21979900
C	2.55380200	-0.75220100	-1.93462700	H	-4.53797900	0.39651000	-3.45888300
C	2.21570700	1.15497500	2.73085000	C	-6.29064200	-1.33409000	1.66675400
C	4.02386100	0.81901800	1.15317000	H	-6.56567900	-2.21070900	1.08170900
C	3.49001500	-0.52267400	-0.94052900	H	-7.20759900	-0.80739600	1.92349500
H	2.83829900	-1.25017400	-2.85117700	H	-5.77808600	-1.63940900	2.58449000
C	3.57244300	1.23421800	2.39149300	C	-5.27513400	0.84089300	1.62600200
H	1.91525900	1.46913700	3.72509500	H	-6.25891300	1.26882200	1.82087100
H	4.25641800	1.67794300	3.10180600	H	-4.69205700	1.55424200	1.05436800
H	0.50878000	-0.59107300	-2.55647200	H	-4.76835200	0.63343800	2.57492300
H	-0.34653500	2.27164400	-1.21085500	C	6.33163900	1.28911800	1.84196200
N	4.80854600	-0.98982200	-1.08674200	H	6.24114500	2.30555700	2.26332300
				H	7.33964800	1.19387200	1.42978500
				H	6.22749300	0.56775400	2.65455600
				C	5.62239900	1.82307200	-0.40076800

H	4.87004000	1.63639300	-1.16182600
H	6.60171000	1.57674900	-0.82038300
H	5.60858600	2.89850100	-0.15644000
C	5.24550200	-1.41306200	-2.40501000
H	6.33043800	-1.54272400	-2.38467200
H	5.00958800	-0.65111700	-3.15021800
H	4.80237600	-2.37010200	-2.73069900
C	5.33220800	-1.85730200	-0.03337400
H	5.06419100	-2.91045400	-0.22031700
H	4.93592400	-1.57117800	0.93636000
H	6.42209600	-1.77885300	0.00557800
H	-6.53901400	-0.03382500	-0.08895700
Cl	-7.86508800	0.28067700	-0.61119900