Electronic Supplementary Information

Rational Design of a new class of polycyclic organic bases bearing two superbasic sites and their applications in CO_2 capture and activation process

Rabindranath Lo, Ajeet Singh, Manoj K. Kesharwani and Bishwajit Ganguly*

Analytical Science Discipline, Central Salt & Marine Chemicals Research Institute (Council of Scientific and Industrial Research), Bhavnagar, Gujarat, India-364002.

E-mail: ganguly@csmcri.org.

Table of content

Computational Section

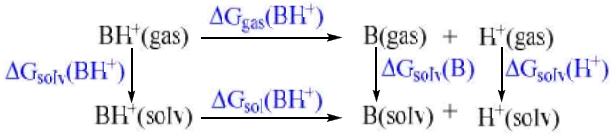
Calculations were performed for compound **1-5** with the density functional theory using Becke's three-parameter hybrid functional with correlation formula of Lee, Yang, and Parr (B3LYP).[1]All these species were fully optimized with 6-31+G* basis set,[2] and harmonic vibrational frequency calculations were used to confirm that the optimized structures were minima, as characterized by positive vibrational frequencies. Zero-point vibrational energies (ZPVE) computed at B3LYP/6-31+G* level used in the proton affinity calculations are unscaled. Proton affinities calculated at B3LYP/6-311+G**//B3LYP/6-31+G* level employing the general equation: PA(B) = (ΔEel) + (ΔZPVE), where (ΔEel) = [E(B) – E(BH^+)] and (ΔZPVE) = [ZPVE(B) – ZPVE(BH^+)] are the electronic and the Zero-point vibrational energy contributions to the proton affinity, respectively. Here, B and BH^+, denote the base in question and its conjugate acid, respectively.

The MESP was calculated using equation 1 where Z_A was the charge on nucleus A, situated at R_A and ρ(r') is the electron density.[3]

$$V(r) = \sum_A^N \frac{Z_A}{|r-R_A|} - \int \frac{\rho(r')d^3r'}{|r-r'|} \qquad (1)$$

In general, electron rich regions are shown by highly negative MESP whereas electron deficient regions are characterized by positive MESP.[4] The most negative valued point (V_{min}) in electron rich regions can be determined from the MESP topography calculation.[5] Molecular electrostatic potential (MESP) calculations have been performed at the B3LYP/6-311+G** level of theory. Solvent effects are taken into account by means of the polarizable continuum model (PCM)[6-10] through single-point energy calculations at the B3LYP/6-311+G** level of theory (using the gas-phase optimized geometries).

The p*K*a calculations have been performed using the standard thermodynamical cycle[11] depicted in Scheme 1,



Scheme 1

The p*K*a value of the acid BH^+ is calculated using the following relation,

$$\mathbf{pKa = \Delta G_{sol}/2.303RT}$$

Where, $\Delta G_{sol} = \Delta G_{gas} + \Delta\Delta G_{solv} + \Delta G_{corr}$

ΔG_{gas} is the Gibbs free energy change of the reaction in the gas phase and $\Delta\Delta G_{solv}$ is the difference in solvation free energies (ΔG_{solv}) between products and reactants. ΔG_{corr} is the correction associated to the

change in standard state from gas phase (1 atm) to solution (1 mol/L) and its value at 298.15 K is 1.89 kcal/mol.[12]

Now ΔG_{sol} can be expressed as:

$\Delta G_{sol} = G_{gas}(B) + \Delta G_{solv}(B) + G_{gas}(H^+) + \Delta G_{solv}(H^+) - G_{gas}(BH)^+ - \Delta G_{solv}(BH)^+ + 1.89$

Here, the value of Gibbs free energy of the proton in the gas phase is set to -6.28 kcal/mol using translational entropy calculated according to the well-known Sackur-Tetrode equation[13] and the value of Gibbs free energy of proton in acetonitrile solvent phase taken as -250.76 kcal/mol.[14]

The ΔG_{solv} values in B3LYP/6-31+G* optimized geometry with UAHF radii and 'scfvac' keyword using acetonitrile (ε = 36.64) as a solvent.[15] Both electrostatic and nonelectrostatic (i.e., cavitation, repulsion and dispersion) terms were included in the calculation of ΔG_{solv} values. The calculation of absolute p*K*a is complicated from first principle study, partly because of the difficulty in computing accurate gas-phase deprotonation free energies for charged species.[16] It has been noted that the accuracy of solvation energy depends upon the shape and size of the dielectric cavity of the molecule in which the solute is embedded.[17] Here, we have employed 'UAHF' radii for solvation energy calculation in solution to calculate the p*K*a of these superbases. The solvent cavity 'UFF' model has been found to be more suitable for the predictions of p*K*a for these acyclic amines (Table S2). All quantum chemical calculations were performed using Gaussian 03, Revision E.01 program.[18]

References:

1 *(a)* A. D. Becke, *J. Chem. Phys*., 1993, ***98***, 5648; *(b)* C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.

2 W. J. Hehre, L. Radom, P. v. R Schleyer and J. A. Pople, *Ab initio Molecular Orbital Theory*, Wiley, New York, **1988**.

3 P. Politzer, J. S. Murray, in *Reviews in Computational Chemistry, vol 2.* (Eds: K. B. Lipkowitz, D. B. Boyd) VCH Publishers, New York (ch 7) 1991, **2**, 273.

4 *(a)* J. Tomasi, R. Bonaccorsi and R. Cammi, *Theoretical Models of Chemical Bonding* (Ed: R. Maksic) Springer, Berlin, 1990, 230; *(b)* R. K. Pathak and S. R. Gadre, *J. Chem. Phys.*, 1990, **93**, 1770; *(c)* E. Scrocco and J. Tomasi, *Adv. Quantum Chem.*, 1979, **11**, 115; *(d)* J. S. Murray and P. Politzer, *J. Mol. Struct.: THEOCHEM,* 1998, **425**, 107; *(e)* T. Brinck, J. S. Murray and P. Politzer, *Mol. Phys.*, 1992, **76**, 609.

5 *(a)* J. S. Murray and P. Politzer, *Chem. Phys. Lett.,* 1988, **152**, 364; *(b)* M. Haeberlein, J. S. Murray, T. Brinck and P. Politzer, *Can. J. Chem*., 1992, **70**, 2209; *(c)* C. H. Suresh, *Inorg. Chem*., 2006, **45**, 4982.

6 J. Tomasi and M. Persico, *Chem. Rev*., 1994, **94**, 2027.

7 M. Cossi, V. Barone, R. Cammi and J. Tomasi, *Chem. Phys. Lett*., 1996, **255**, 327.

8 V. Barone, M. Cossi and J. Tomasi, *J. Chem. Phys*., 1997, **107**, 3210.

9 V. Barone, M. Cossi and J. Tomasi, *J. Comput. Chem*., 1998, **19**, 404.

10 M. Cossi and V. Barone, *J. Chem. Phys*., 1998, **109**, 6246.

11 G. I. Almerindo, D. W. Tondo and J. R. Pliego Jr., *J. Phys. Chem. A*., 2004, **108**, 166.

12 D. M. Camaioni and C. A. Schwerdtfeger, *J. Phys. Chem. A*., 2005, **109**, 10795.

13 I. A. Topol, G. J. Tawa, S. K. Burt and A. A. Rashin, *J. Phys. Chem. A*., 1997, **101**, 10075.

14 A. A. Magill, K. J. Cavell and B. F. Yates, *J. Am. Chem. Soc*., 2004, **126**, 8717.

15 (*a*) T. N. Brown and N. Mora-Diez, *J. Phys. Chem. B.*, **2006**, *110*, 9270-9279; *(b)* A. Trummal, A. Rummel, E. Lippmaa, P. Burk and I. A. Koppel, *J. Phys. Chem. A.*, 2009, **113***,* 6206.

16 *(a)* J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev*., 2005, **105**, 2999; *(b)* V. P. Kumar, B. Ganguly and S. Bhattacharya, *J. Org. Chem.,* 2004, **69**, 8634.

17 R. B. Ardakani, M. A. Karimi and A. Ebady, *J. Mol. Struct.: THEOCHEM,* 2009, **910**, 99.

18 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian 03, Revision E.01, Gaussian, Inc., Wallingford CT, **2004**.

Table S1 Experimental and calculated (B3LYP/6-311+G**//B3LYP/6-31+G*) proton affinities of amine and imine bases.

	Proton Affinity (kcal/mol)	
Compound	Experimental	Calculated[d]
CH_2=NH	205.5[a]	206.1
CH_3-NH_2	214.9[b]	213.1
$(CH_3)_2NH$	222.2[b]	220.1
H_2N-$(CH_2)_2$-NH_2	227.1[c]	225.5
H_2N-$(CH_2)_3$-NH_2	233.0[c]	233.1

[a] S. Hammerum and T. I. Sølling, *J. Am. Chem. Soc*., 1999, **121**, 6002 and references therein.
[b] C. Wesdemiotis, *J. Mass Spectrom*., **2004**, *39*, 998.
[c] R. Yamdagni and P. Kebarle, *J. Am. Chem. Soc*., **1973**, *95*, 3504.
[d] Zero point vibrational energy corrected.

Table S2 Experimental and calculated (B3LYP/6-311+G**//B3LYP/6-31+G*) p*K*a(MeCN) of amino bases.

Compounds	Experimental	Calculated	
		UFF	UAHF
CH_3-NH_2	18.4[a]	16.6	10.5
$(CH_3)_2NH$	18.7[a]	17.2	12.0
H_2N-$(CH_2)_2$-NH_2	18.5[b]	17.2	14.9
H_2N-$(CH_2)_3$-NH_2	19.7[b]	20.1	18.1

[a] J. –N. Li, Y. Fu, L.Liu and Q. –X. Guo, *Tetrahedron*, 2006, **62**, 11801 and references therein..
[b] E. Rõõm, A. Kütt, I. Kaljurand, I. Koppel, I. Leito, I. A. Koppel, M. Mishima, K. Goto and Y. Miyahara, *Chem. Eur. J*., 2007, **13**, 7631.

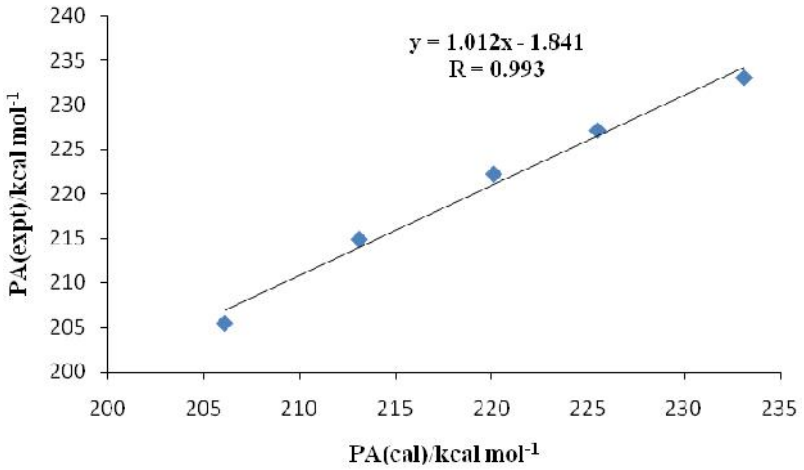


Fig. S1 Correlation between experimental and calculated proton affinities of amine and imine bases.

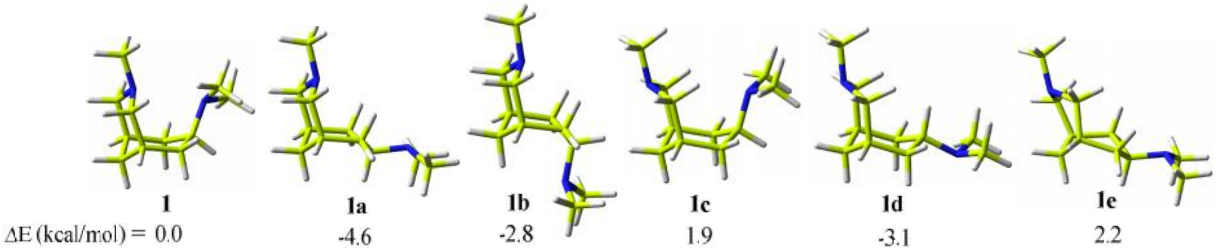


Fig. S2 B3LYP/6-31+G* optimized geometry of different conformations of **1** and their corresponding relative energies. [Green-yellow = carbon; blue = nitrogen; and white = hydrogen].

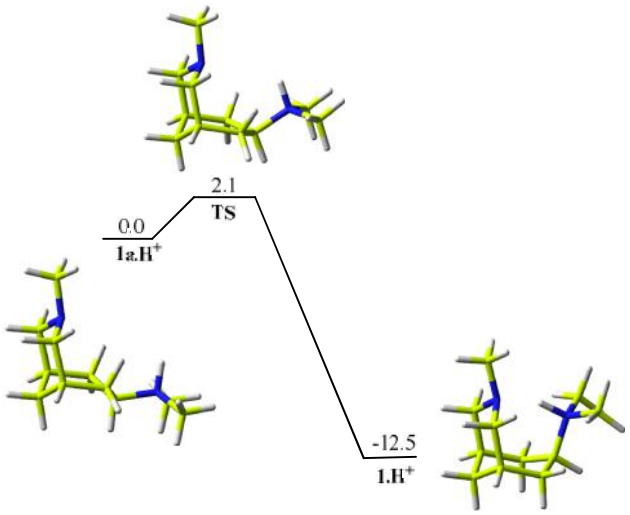


Fig. S3 B3LYP/6-31+G* calculated relative energy (kcal/mol) profile diagram for the flipping of chair-boat conformation (**1a.H**$^+$) to chair-chair conformation (**1.H**$^+$) [Green-yellow = carbon; blue = nitrogen; and white = hydrogen]

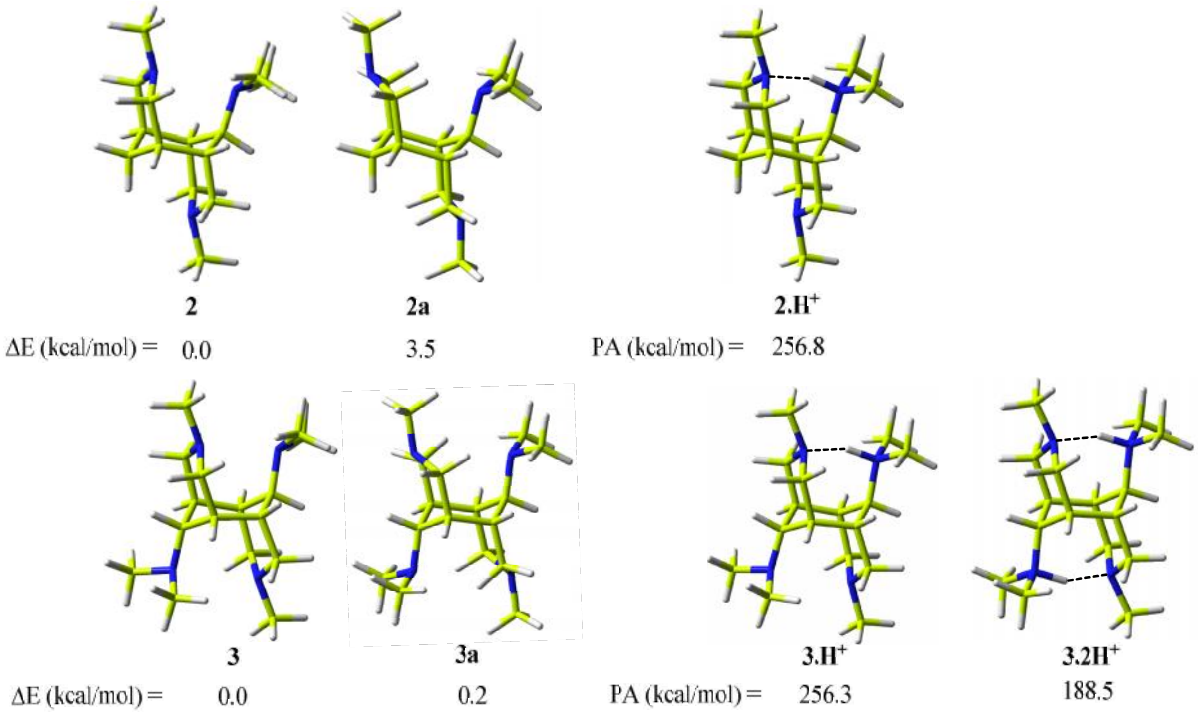


Fig. S4 B3LYP/6-31+G* calculated geometries for different conformations of **2** and **3**, relative energies (kcal/mol), and protonated forms of their most stable conformer. Proton affinity values (PA) were calculated at B3LYP/6-311+G**//B3LYP/6-31+G* level of theory with zero point vibrational energy correction. [Green-yellow = carbon; blue = nitrogen; and white = hydrogen].

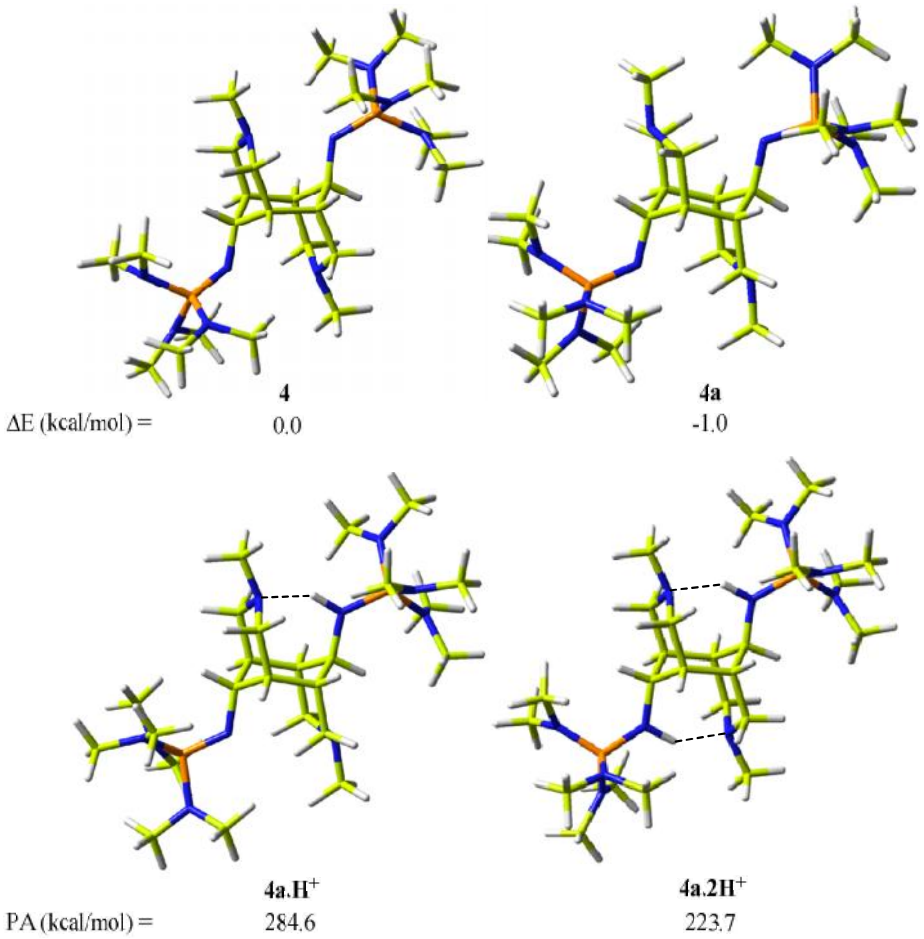


Fig. S5 B3LYP/6-31+G* calculated geometries for different conformations of **4**, relative energies (kcal/mol), and protonated forms of their most stable conformer **4a**. Proton affinity values (PA) were calculated at B3LYP/6-311+G**//B3LYP/6-31+G* level of theory with zero point vibrational energy correction. [Green-yellow = carbon; blue = nitrogen; orange = phosphorus; and white = hydrogen]

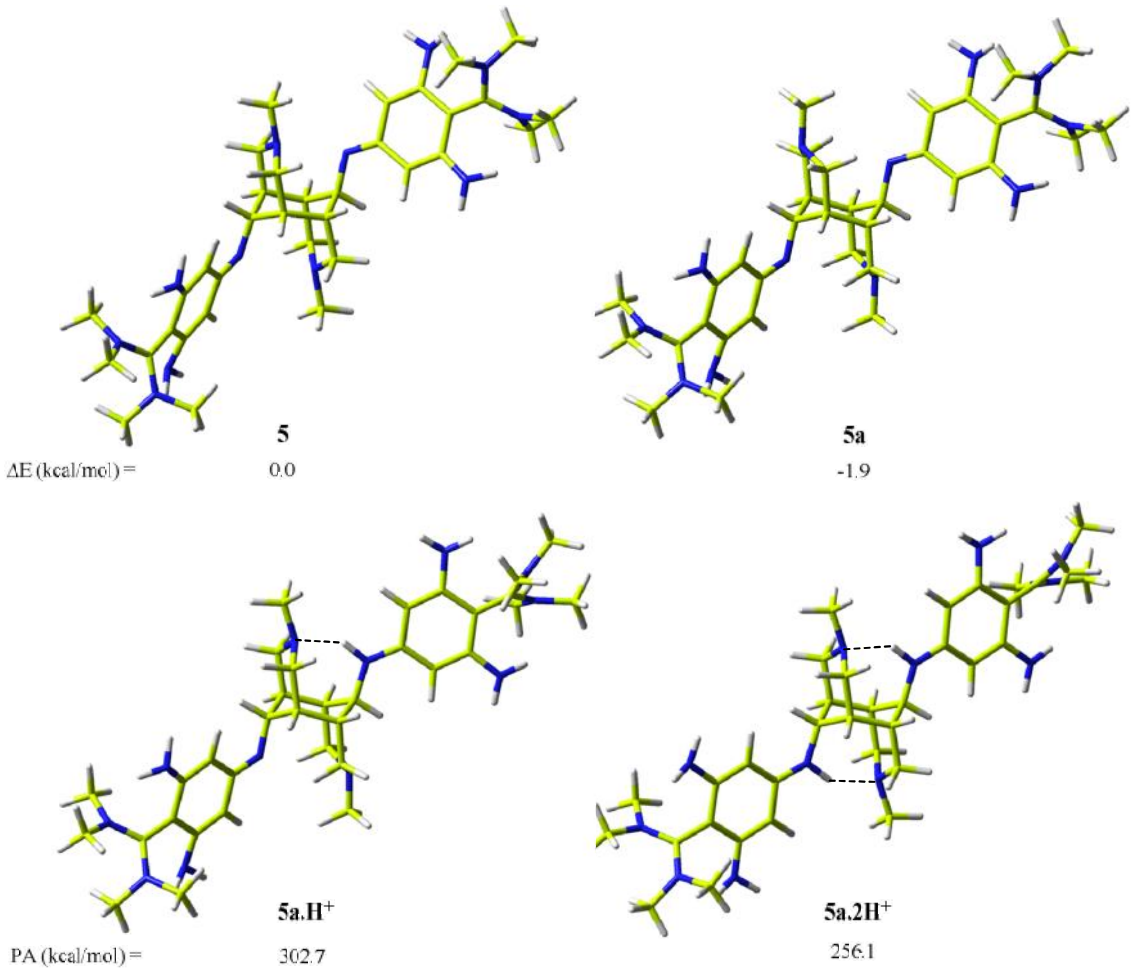


Fig. S6 B3LYP/6-31+G* calculated geometries for different conformations of **5**, relative energies (kcal/mol), and protonated forms of their most stable conformer **5a**. Proton affinity values (PA) were calculated at B3LYP/6-311+G**//B3LYP/6-31+G* level of theory with zero point vibrational energy correction. [Green-yellow = carbon; blue = nitrogen; and white = hydrogen].

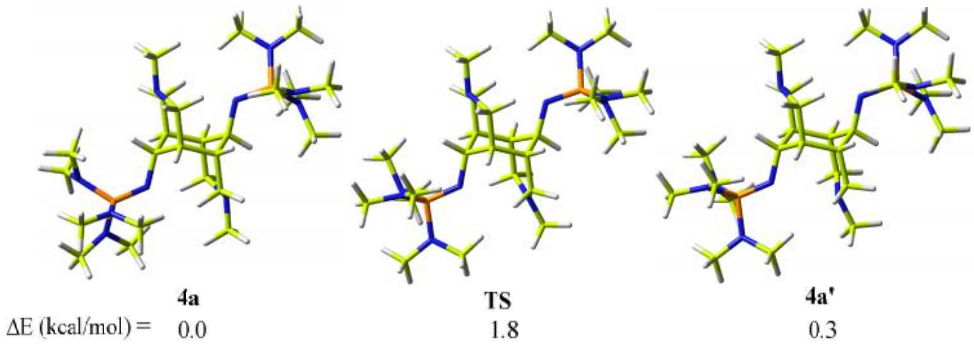


Fig. S7 B3LYP/6-31+G* calculated relative energies (kcal/mol) for the flipping of piperidine ring from boat form (**4a**) to chair form (**4a′**) [Green-yellow = carbon; blue = nitrogen; orange = phosphorus; and white = hydrogen]

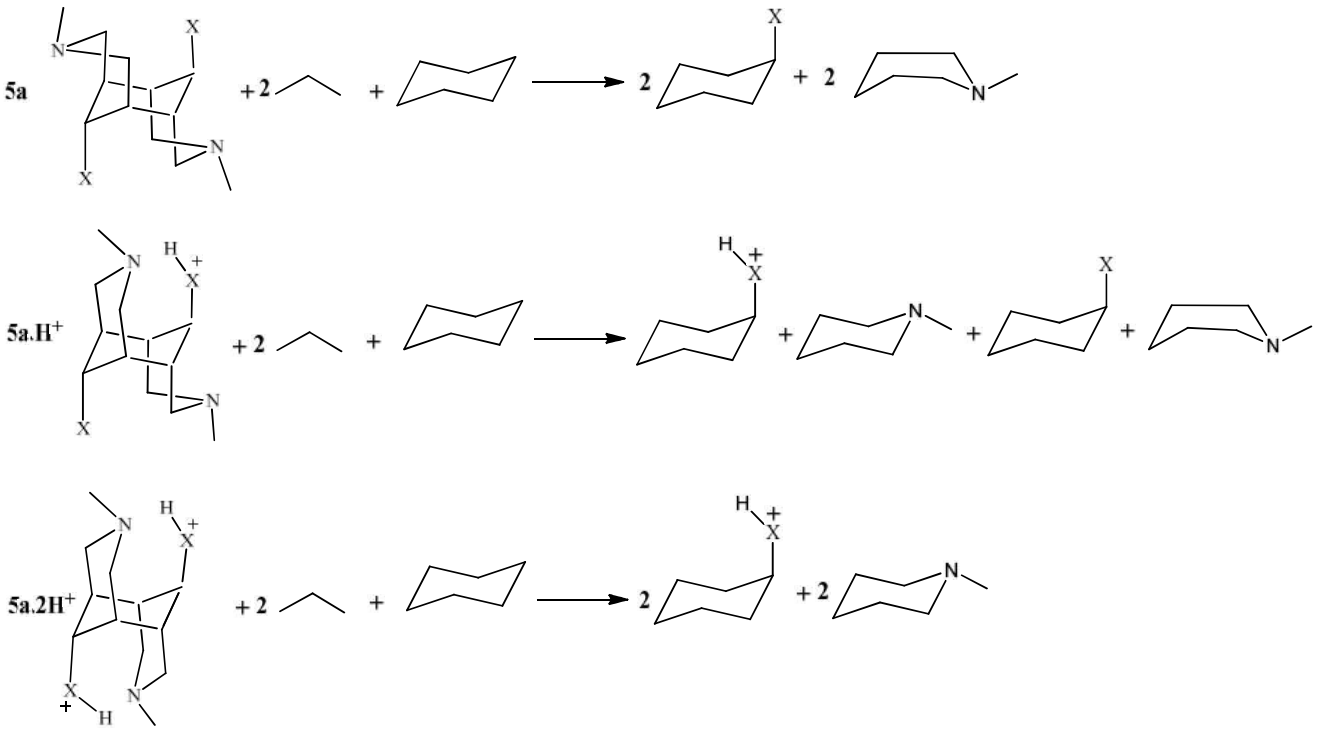


Fig. S8 Isodesmic reactions used to obtain strain energy of unprotonated bases and the sum of the cation strain and the H-bond energies $(SE+HB)^+$ for their corresponding protonated cations.

Table S3 Strain energies (SE) for the unprotonated bases **5a** and Hydrogen bond + Strain Energies $(HB+SE)^+$ and Hydrogen bond energies (HB) for their monoprotonated and bis-protonated cations (all in kcal/mol).

Compounds	SE	$(HB+SE)^+$		HB	
		monoprotonated	bis-protonated	monoprotonated	bis-protonated
5a	16.9	3.0	36.9	-5.8	-5.1

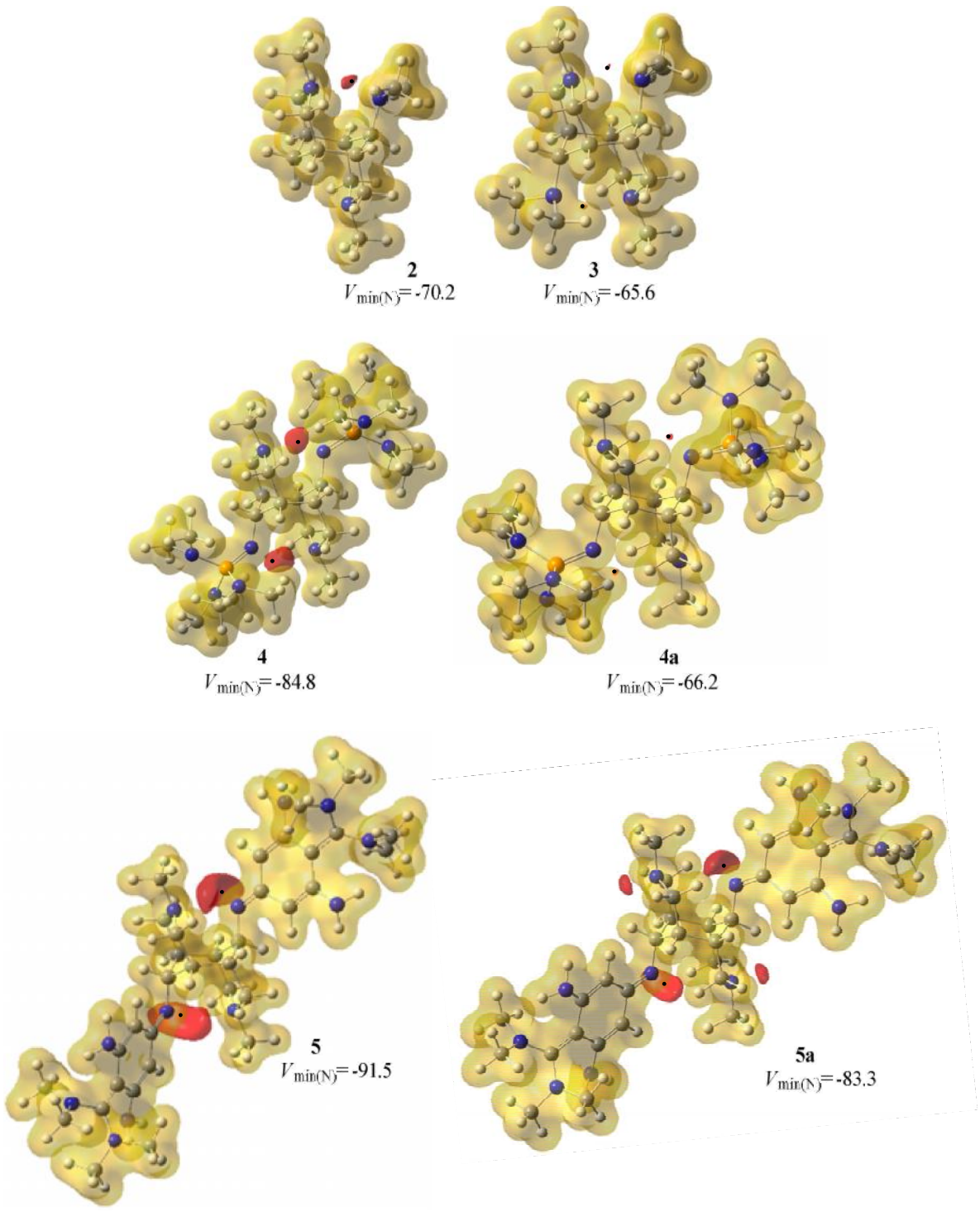


Fig. S9 Molecular electrostatic isopotential surfaces of compounds **2-5** and **4a-5a** at isosurface value of -0.104 au. The black dot represents the location of the V_{min} point in each case and is given in kcal/mol.

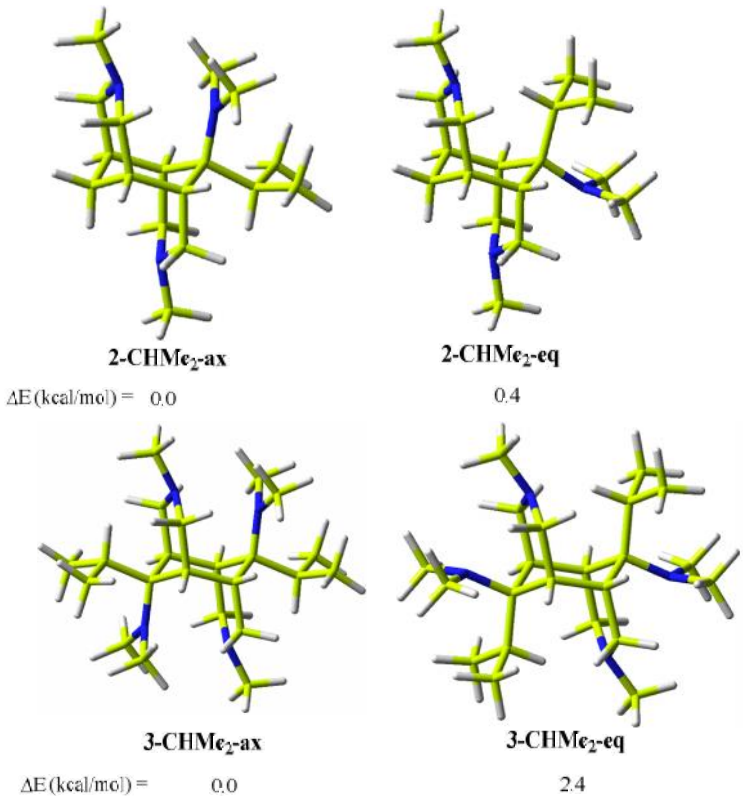


Fig. S10 B3LYP/6-31+G* optimized geometries of **2** and **3** with isopropyl substitution and their corresponding relative energies. [Green-yellow = carbon; blue = nitrogen; and white = hydrogen].

Table S4 B3LYP/6-311+G**//B3LYP/6-31+G* calculated p*K*a(MeCN) and gas phase proton affinities (kcal/mol) of amino and imino bases. Experimental [a] p*K*a(MeCN) values are given in parenthesis.

Compounds	p*K*a	Gas phase Proton affinity (PA)[b]
I	22.1 (21.6)	243.3
II	19.2 (20.0)	238.5
III	25.9 (25.4)	254.8
IV	24.3 (24.3)	251.0
V	26.6 (26.0)	253.1
VI	22.2 (23.3)	247.0

[a] ref. 19, [b] Zero point vibrational energy corrected.

19 *(a)* I. Kaljurand, A. Kütt, L.Sooväli, T. Rodima, V. Mäemets, I. Leito and I. A. Koppel, *J. Org. Chem.,* 2005, 70, 1019; *(b)* E. Rõõm, A. Kütt, I. Kaljurand, I. Koppel, I. Leito, I. A. Koppel, M. Mishima, K. Goto and Y. Miyahara, *Chem. Eur. J*., 2007, 13, 7631.

Thermodynamics of the capture of CO_2

The thermodynamics of binding are critical for designing a system that can efficiently capture CO_2. We have calculated the thermodynamic data for CO_2 capture with the designed superbase **4a** using propylcarbonic acid as reported (Fig. S11, ESI†).[20] The calculations have been performed with B3LYP/6-31+G* level of theory. The reliability of the method employed in this study has been examined with variety of simple amidine or guanidine base and propylcarbonic acid, because their experimental results are known. The computed free energy (ΔG) value for these system are found to be in good agreement with the experimental data available (Table S5, ESI†). The binding of propylcarbonic acid with the designed superbase (**4a**) containing two capturing sites was examined. The sequential free energy of binding of acid with **4a** is given in Table S5, ESI†. The thermodynamic data suggest that the compound **4a** binds much strongly at both ends to stablize the propylcarbonate anions compare to the reported DBU, TMG and Barton's base. The extra stabilization comes from the delocalization of the superbase in protonated form due to cation resonance effect.

20 *(a)* D. J. Heldebrant, C. R. Yonker, P. G. Jessop and L. Phan, *Energy Environ. Sci*., 2008, **1**, 487; (*b*) Z. Yang, L. He, Y. Zhao, B. Li and B. Yu, *Energy Environ. Sci*., 2011, **4**, 3971.

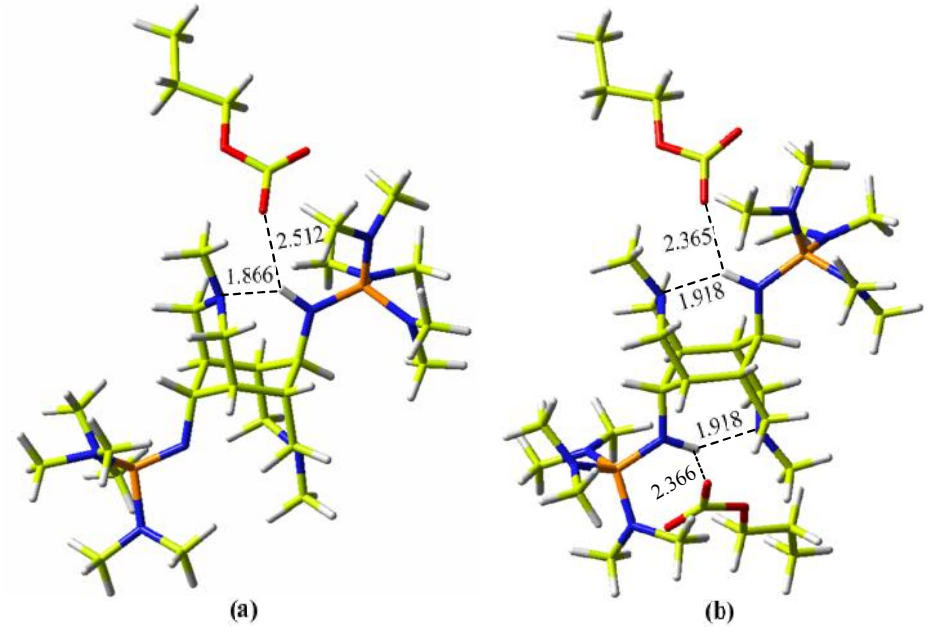


Fig. S11 B3LYP/6-31+G* optimized geometry of propylcarbonate salt made from superbase **4a** (a) 1st site, (b) 2nd site [distances are given in Å]. [Green-yellow = carbon; blue = nitrogen; orange = phosphorus; red = oxygen; and white = hydrogen].

Table S5 Thermodynamics of the capture of CO_2 by different organic bases in acetonitrile solvent.

Base/alcohol pair	ΔG/kcal mol^{-1}	
	Experimental[a]	Calculated
DBU/PrOH	-1.9	-6.7
TMG/PrOH	0.6	-3.5
Barton's/PrOH	-2.2	-6.5
4a/PrOH	-	-10.3 (-11.5)*

[a] Ref 20a.

*The 1st and 2nd free energies of binding of propylcarbonic acid with **4a** are given, where the 2nd value is given in ( ).

B3LYP/6-31+G* SCF energies in gas phase (E), B3LYP/6-31+G* zero point vibrational energies (ZPVE), and Cartesian coordinates for 1-5, 1a-5a and protonated forms. B3LYP/6-311+G//B3LYP/6-31+G* SCF energies in gas phase are given in ( ). (All energies are given in Hartee).**

1

E = -541.90549 (-542.03627)

ZPVE = 0.325450

C	1.50055882	1.59024510	-0.97614706
C	0.11455882	1.19424510	-1.50414706
C	-0.95644118	1.56024510	-0.45314706
C	-0.74844118	0.97024510	0.96885294
C	0.76355882	0.94824510	1.34285294
C	1.80055882	0.68124510	0.22385294
C	0.14955882	-0.28475490	-1.93714706
N	-1.51144118	-0.29775490	1.10885294
C	1.87855882	-0.76775490	-0.27814706
N	0.63255882	-1.18975490	-0.89814706
C	0.67355882	-2.56575490	-1.35514706
C	-0.99844118	-1.26475490	2.06585294
C	-2.91344118	-0.01375490	1.38985294
H	-0.11544118	1.77324510	-2.41014706
H	-1.94744118	1.27224510	-0.82314706
H	-1.19644118	1.68724510	1.68585294
H	0.94355882	0.28524510	2.19585294
H	2.78855882	0.92824510	0.63885294
H	2.26555882	1.46024510	-1.75514706
H	-0.85644118	-0.61575490	-2.22714706
H	0.78855882	-0.35575490	-2.84714706
H	2.73855882	-0.84675490	-0.98314706
H	2.09455882	-1.45275490	0.55385294
H	0.95855882	-3.22575490	-0.52714706
H	-0.31844118	-2.86975490	-1.70714706
H	-1.67544118	-2.12675490	2.08585294
H	-0.01644118	-1.62675490	1.75685294
H	-3.49444118	-0.94275490	1.35285294
H	-3.32944118	0.66824510	0.64285294
H	1.51455882	2.64824510	-0.68114706
H	-0.96244118	2.65724510	-0.37414706
H	0.98455882	1.95924510	1.71485294
H	1.39655882	-2.72475490	-2.18314706
H	-0.92744118	-0.87475490	3.10285294
H	-3.06644118	0.44924510	2.38885294

1.H$^+$

E = -542.32251 (-542.45550)

ZPVE = 0.341256

C	1.61238835	1.54300971	-0.93633010
C	0.20538835	1.25200971	-1.48033010
C	-0.84761165	1.68100971	-0.42733010
C	-0.69061165	1.05100971	0.97766990
C	0.79938835	1.06700971	1.39666990
C	1.81238835	0.65200971	0.29966990
C	0.14338835	-0.22499029	-1.91733010
N	-1.29661165	-0.36199029	1.04866990
C	1.74638835	-0.82199029	-0.14233010
N	0.46638835	-1.16499029	-0.81333010
C	0.47438835	-2.55799029	-1.29033010
C	-1.14961165	-1.00299029	2.39366990
C	-2.73661165	-0.41099029	0.63966990
H	0.01938835	1.85100971	-2.37933010
H	-1.86261165	1.56000971	-0.81533010
H	-1.27461165	1.63100971	1.70066990
H	0.96738835	0.50500971	2.31966990
H	2.81438835	0.80900971	0.71666990
H	2.37238835	1.32400971	-1.69633010
H	-0.85261165	-0.48599029	-2.29633010
H	0.85138835	-0.37199029	-2.75033010
H	2.58938835	-1.01999029	-0.82533010
H	1.86438835	-1.49999029	0.71266990
H	0.66038835	-3.23499029	-0.45033010
H	-0.49561165	-2.80399029	-1.73133010
H	-1.67061165	-1.96199029	2.38166990

H	-0.10061165	-1.17699029	2.61966990
H	-3.10661165	-1.42599029	0.78766990
H	-2.84361165	-0.14799029	-0.41033010
H	1.71738835	2.60300971	-0.67433010
H	-0.72961165	2.76200971	-0.27533010
H	1.01538835	2.11100971	1.65766990
H	1.25438835	-2.72299029	-2.04933010
H	-1.59161165	-0.35799029	3.15766990
H	-3.31561165	0.28200971	1.25666990
H	-0.68661165	-0.90099029	0.31566990

1a

E = -541.91283 (-542.04320)

ZPVE= 0.32595

C	0.91664400	0.00087000	1.87629500
C	0.83875500	1.23678600	0.96654700
C	-0.50720300	1.27309800	0.18034100
C	-1.37108300	0.00022100	0.33822700
C	-0.50730900	-1.27286800	0.18167800
C	0.83876000	-1.23583400	0.96771800
C	2.05059500	1.21215700	0.01647000
C	2.05064100	-1.21204700	0.01772200
N	2.06517800	-0.00036400	-0.79829800
C	3.14990400	-0.00083700	-1.76611600
H	0.92648000	2.14617800	1.57505200
H	0.92654300	-2.14471600	1.57698000
H	1.86393100	0.00112000	2.43375500
H	2.01637900	2.07631300	-0.65982600
H	2.98316500	1.30413400	0.61581900
H	2.98318300	-1.30333100	0.61723700
H	2.01651000	-2.07690700	-0.65767100
H	3.07792800	-0.88874200	-2.40462200
H	3.07747200	0.88603500	-2.40601200
H	0.11081700	0.00118900	2.62042600
H	4.15231800	-0.00021800	-1.28993400
H	-0.30736700	1.40402500	-0.89031200
H	-1.08067000	2.14429300	0.51267400
H	-0.30756800	-1.40522900	-0.88882800
H	-1.08079600	-2.14363000	0.51514900
H	-1.79794400	0.00073500	1.36437600
N	-2.49149700	-0.00016600	-0.62877500
C	-3.33020600	1.19233300	-0.52302700
H	-2.76962000	2.09192700	-0.78615700
H	-4.16305100	1.10641400	-1.22843200
H	-3.75625200	1.33090700	0.49279100
C	-3.32960100	-1.19305800	-0.52282900
H	-4.16234600	-1.10772800	-1.22841700
H	-2.76848700	-2.09241600	-0.78562400
H	-3.75578400	-1.33158500	0.49294900

1a.H$^+$

E = -542.30259 (-542.43540)

ZPVE = 0.34228

C	1.02723400	0.00056900	1.90987800
C	0.92000000	1.24049400	1.00833800
C	-0.46674600	1.29537400	0.29458300
C	-1.28804600	0.00019600	0.45167800
C	-0.46679300	-1.29509400	0.29531600
C	0.91994400	-1.23987500	1.00906000
C	2.06268000	1.20583300	-0.02340300
C	2.06263300	-1.20586700	-0.02269000
N	1.97832700	-0.00025900	-0.84874700
C	2.97259500	-0.00059400	-1.92178900
H	1.03768700	2.14845100	1.60962200
H	1.03757900	-2.14749200	1.61086700
H	1.99383600	0.00069700	2.42728200
H	2.00429400	2.08145900	-0.68167000
H	3.03144100	1.26649700	0.51114900
H	3.03138600	-1.26625400	0.51190800
H	2.00421800	-2.08187800	-0.68044100
H	2.83792700	-0.88795900	-2.54885600
H	2.83796200	0.88641000	-2.54937300
H	0.25671400	0.00081300	2.69228300
H	4.01009000	-0.00050300	-1.54105100
H	-0.30177800	1.48434600	-0.77526300
H	-1.04128300	2.13679300	0.69388700
H	-0.30182000	-1.48466700	-0.77442200
H	-1.04138000	-2.13626900	0.69506800
H	-1.80738000	0.00046700	1.41626500
N	-2.44432700	-0.00014600	-0.58146700
C	-3.30852800	1.23163400	-0.51203200
H	-2.71030900	2.11397700	-0.72927300
H	-4.10808300	1.13778500	-1.24843300
H	-3.73253700	1.29925400	0.49158600
C	-3.30827500	-1.23206000	-0.51137400
H	-4.10783000	-1.13878900	-1.24784900
H	-2.70985400	-2.11439400	-0.72810600
H	-3.73229200	-1.29921000	0.49227100
H	-1.98678200	-0.00035700	-1.50133800

2

E = -713.96485 (-714.13469)

ZPVE = 0.40666

C	1.29163636	0.72291667	-1.45230303
C	-0.20336364	0.44691667	-1.65730303
C	-1.03236364	0.87491667	-0.40730303
C	-0.70636364	0.06491667	0.86669697
C	0.83963636	0.18191667	1.01969697
C	1.71363636	-0.12808333	-0.24230303
C	-0.33536364	-1.03708333	-2.07330303
C	-0.82536364	2.35691667	-0.01430303
N	-1.38036364	-1.24808333	0.92669697
C	1.04963636	1.64691667	1.48469697
C	1.69163636	-1.58808333	-0.72530303
N	0.49963636	2.63891667	0.55469697
C	0.59363636	3.98891667	1.07769697
N	0.38163636	-1.97808333	-1.21530303
C	0.33663636	-3.32908333	-1.72330303

C	-0.75936364	-2.19908333	1.83569697
C	-2.78436364	-1.07708333	1.28369697
H	-0.58036364	1.03891667	-2.50430303
H	-2.09436364	0.76891667	-0.65930303
H	-1.10536364	0.64291667	1.72769697
H	1.19263636	-0.44908333	1.84469697
H	2.75263636	0.09991667	0.03269697
H	-0.95136364	3.01091667	-0.88930303
H	2.12263636	1.85991667	1.59069697
H	1.62763636	4.20591667	1.36869697
H	0.29963636	4.70991667	0.30569697
H	-0.05436364	4.15491667	1.96469697
H	1.85563636	0.40191667	-2.34030303
H	-1.63036364	2.62691667	0.70169697
H	0.60463636	1.75091667	2.49669697
H	-1.38936364	-1.34508333	-2.08430303
H	0.03263636	-1.10608333	-3.12130303
H	2.48163636	-1.68908333	-1.50430303
H	1.97163636	-2.28108333	0.08269697
H	-0.70436364	-3.62808333	-1.90030303
H	0.89363636	-3.45508333	-2.67830303
H	0.76863636	-4.02208333	-0.99030303
H	-1.35436364	-3.11908333	1.84769697
H	0.24363636	-2.46008333	1.49469697
H	-0.69336364	-1.82908333	2.88069697
H	-3.29236364	-2.04708333	1.24269697
H	-2.92336364	-0.65808333	2.30369697
H	-3.28936364	-0.40908333	0.57969697
H	1.48963636	1.78191667	-1.29230303

2.H$^+$

E = -714.38692 (-714.55941)

ZPVE = 0.422193

C	1.42712030	0.68464662	-1.33644361
C	-0.06587970	0.50364662	-1.65044361
C	-0.96387970	0.92164662	-0.43844361
C	-0.69987970	0.12464662	0.86155639
C	0.82312030	0.22864662	1.11455639
C	1.71312030	-0.18735338	-0.10344361
C	-0.24387970	-0.95135338	-2.13544361
C	-0.76487970	2.40264662	-0.01544361
N	-1.27087970	-1.29235338	0.88455639
C	1.03012030	1.70664662	1.54455639
C	1.57212030	-1.65635338	-0.55744361
N	0.55412030	2.66964662	0.55355639
C	0.69212030	4.04764662	1.01055639
N	0.24012030	-1.96135338	-1.15144361
C	0.21112030	-3.31735338	-1.72444361
C	-0.97687970	-2.01235338	2.16155639
C	-2.74287970	-1.32735338	0.62855639
H	-0.35687970	1.14464662	-2.49144361
H	-2.01387970	0.84564662	-0.74144361
H	-1.22387970	0.62364662	1.68655639
H	1.12012030	-0.36935338	1.98255639
H	2.75612030	-0.06335338	0.21355639
H	-0.89387970	3.05564662	-0.88744361
H	2.09812030	1.89564662	1.71155639
H	1.72812030	4.23664662	1.30955639
H	0.44412030	4.73464662	0.19455639
H	0.03512030	4.27964662	1.87055639
H	2.03112030	0.33864662	-2.18544361
H	-1.57987970	2.65964662	0.69455639
H	0.52812030	1.84264662	2.52555639
H	-1.29387970	-1.18835338	-2.35144361
H	0.30812030	-1.06135338	-3.08244361
H	2.36312030	-1.85935338	-1.29544361
H	1.72412030	-2.36035338	0.27155639
H	-0.79887970	-3.54735338	-2.07844361
H	0.90812030	-3.41435338	-2.57044361
H	0.49012030	-4.04835338	-0.95944361
H	-1.44687970	-2.99635338	2.12355639
H	0.09612030	-2.13835338	2.28755639
H	-1.38287970	-1.44735338	3.00555639
H	-3.08487970	-2.36135338	0.69755639
H	-3.26187970	-0.72135338	1.37755639
H	-2.96287970	-0.94735338	-0.36644361
H	1.67212030	1.72864662	-1.15244361
H	-0.72987970	-1.78135338	0.04455639

2a

E= -713.95930

C	-0.01916500	-2.01504800	0.00003600
C	0.27712200	-1.14322300	1.22654700
C	-0.64575500	0.11359700	1.22809900
C	-0.45735300	1.04457000	-0.00005700
C	-0.64578900	0.11334600	-1.22819500
C	0.27716900	-1.14342400	-1.22662000
N	0.77932400	1.86334600	-0.00016900
N	-2.85163900	-0.00519500	0.00008900
C	-4.22001900	-0.48017500	0.00008800
N	2.46509500	-1.23723300	0.00000900
C	3.87690500	-0.90832400	-0.00001900
C	0.85748300	2.71725300	-1.18553900
C	0.85839900	2.71673900	1.18551600
H	0.03146800	-1.70099500	2.14082100
H	-0.45269000	0.66446300	2.15376900
H	-1.30973500	1.74964300	-0.00000200
H	-0.45294200	0.66418400	-2.15393400
H	0.03167600	-1.70144000	-2.14080300
H	-4.74486300	-0.10570400	-0.88705000
H	-4.29621400	-1.58797800	-0.00081700
H	-4.74430700	-0.10718800	0.88817500
H	0.61212900	-2.90903500	0.00004200
H	4.06920000	0.18428100	-0.00064300
H	4.35832900	-1.33626700	0.88804600
H	4.35867900	-1.33739500	-0.88734700
H	1.73871400	3.36187500	-1.10520200
H	0.96900900	2.12625600	-2.09768200

H	-0.03453100	3.36657900	-1.30231800
H	1.73972300	3.36121600	1.10497200
H	-0.03338700	3.36624000	1.30318800
H	0.97040100	2.12544300	2.09738600
H	-1.05849700	-2.35740900	0.00007800
C	1.80422500	-0.83156000	1.24719200
H	1.98347400	0.23095000	1.47401200
H	2.28152800	-1.41292200	2.04796400
C	1.80428700	-0.83173000	-1.24726900
H	2.28167100	-1.41311400	-2.04799300
H	1.98367500	0.23070600	-1.47410500
C	-2.15110100	-0.30597800	-1.25152800
H	-2.67692500	0.25048100	-2.03889700
H	-2.23488800	-1.37583400	-1.52698000
C	-2.15113200	-0.30580200	1.25169500
H	-2.23477300	-1.37562000	1.52718800
H	-2.67704500	0.25070700	2.03894900

3

E = -847.90783 (-848.11073)

ZPVE = 0.479660

C	0.92717308	0.35280769	-1.26544872
C	-0.59182692	0.10680769	-1.33044872
C	-1.34982692	0.55280769	-0.04244872
C	-1.03382692	-0.31619231	1.18855128
C	0.51917308	-0.21919231	1.31855128
C	1.37117308	-0.42319231	0.01255128
N	1.32417308	1.75880769	-1.49444872
C	-0.74582692	-1.38919231	-1.70644872
C	-1.08482692	2.01180769	0.41155128
N	-1.73282692	-1.61919231	1.20655128
C	0.73217308	1.17980769	1.93155128
C	1.36817308	-1.89519231	-0.45144872
N	0.20317308	2.22380769	1.07255128
C	2.65617308	2.08680769	-1.00844872
C	1.23417308	2.07580769	-2.91644872
C	0.32817308	3.55180769	1.62655128
N	0.04917308	-2.31019231	-0.89244872
C	0.00117308	-3.66619231	-1.38744872
C	-1.12782692	-2.60519231	2.08955128
C	-3.13182692	-1.42919231	1.57655128
H	-1.02982692	0.67180769	-2.16244872
H	-2.41982692	0.50180769	-0.27544872
H	-1.41282692	0.23080769	2.07655128
H	0.89217308	-0.93919231	2.05655128
H	2.40917308	-0.18419231	0.27155128
H	-1.12382692	2.69480769	-0.44744872
H	1.80617308	1.37480769	2.07755128
H	3.45217308	1.44380769	-1.44044872
H	2.88717308	3.12380769	-1.27744872
H	2.69717308	2.01180769	0.07955128
H	1.45417308	3.13880769	-3.06744872
H	1.94217308	1.48580769	-3.53744872
H	0.22517308	1.88980769	-3.29544872
H	1.35417308	3.71880769	1.97655128
H	0.10717308	4.30080769	0.85655128
H	-0.35582692	3.73280769	2.48455128
H	1.38317308	-0.21919231	-2.09944872
H	-1.92182692	2.28980769	1.08755128
H	0.27817308	1.18580769	2.94655128
H	-1.79382692	-1.70219231	-1.61744872
H	-0.46882692	-1.47619231	-2.77844872
H	2.14217308	-2.01019231	-1.24244872
H	1.67317308	-2.55819231	0.37255128
H	-1.04082692	-3.98519231	-1.50644872
H	0.51017308	-3.79119231	-2.36844872
H	0.48317308	-4.34519231	-0.67244872
H	-1.74482692	-3.51119231	2.08755128
H	-0.13482692	-2.88319231	1.73255128
H	-1.04482692	-2.25919231	3.14155128
H	-3.65982692	-2.38619231	1.51055128
H	-3.25582692	-1.03719231	2.60955128
H	-3.62582692	-0.73019231	0.89455128

3.H$^+$

E = -848.32879 (-848.53435)

ZPVE = 0.494869

C	0.98652866	0.27068153	-1.21631210
C	-0.53747134	0.07468153	-1.35131210
C	-1.36947134	0.49468153	-0.09431210
C	-1.04847134	-0.33231847	1.17268790
C	0.49852866	-0.20131847	1.31768790
C	1.37952866	-0.51731847	0.05668790
N	1.48852866	1.71368153	-1.28331210
C	-0.67947134	-1.42131847	-1.75831210
C	-1.21247134	1.97068153	0.33668790
N	-1.71547134	-1.63831847	1.22368790
C	0.70052866	1.25368153	1.81468790
C	1.34052866	-1.98731847	-0.41531210
N	0.13652866	2.27868153	0.88968790
C	2.97552866	1.81068153	-1.17731210
C	1.04052866	2.42468153	-2.51931210
C	0.17152866	3.61868153	1.49768790
N	0.02752866	-2.35331847	-0.89431210
C	-0.07947134	-3.72931847	-1.34131210
C	-1.11147134	-2.57831847	2.16168790
C	-3.13247134	-1.46631847	1.54968790
H	-0.93147134	0.63668153	-2.20631210
H	-2.42247134	0.37268153	-0.36931210
H	-1.44447134	0.24468153	2.03568790
H	0.86552866	-0.84131847	2.12668790
H	2.42052866	-0.32431847	0.33968790
H	-1.38347134	2.66268153	-0.49831210
H	1.76652866	1.48568153	1.93468790
H	3.44152866	1.24568153	-1.98931210
H	3.26352866	2.86068153	-1.25331210
H	3.31452866	1.42068153	-0.21931210
H	1.45752866	3.43268153	-2.51331210

H	1.39952866	1.88768153	-3.40231210
H	-0.04547134	2.48968153	-2.54731210
H	1.19352866	3.85868153	1.80768790
H	-0.15747134	4.36568153	0.76768790
H	-0.48447134	3.68168153	2.37868790
H	1.47352866	-0.20131847	-2.07931210
H	-1.98547134	2.18868153	1.08868790
H	0.24052866	1.35168153	2.80868790
H	-1.73947134	-1.70031847	-1.75231210
H	-0.33247134	-1.49631847	-2.81131210
H	2.13952866	-2.11131847	-1.18131210
H	1.60952866	-2.65731847	0.41068790
H	-1.13347134	-3.99231847	-1.47831210
H	0.44952866	-3.91531847	-2.29731210
H	0.34152866	-4.40031847	-0.58531210
H	-1.70847134	-3.49431847	2.17768790
H	-0.10347134	-2.85131847	1.84368790
H	-1.06447134	-2.19031847	3.19968790
H	-3.63047134	-2.44031847	1.51868790
H	-3.29147134	-1.03031847	2.55768790
H	-3.63247134	-0.82131847	0.82168790
H	1.01952866	2.16768153	-0.38831210

3.2H$^+$

E = -848.64230 (-848.85030)

ZPVE = 0.510503

C	0.96915823	0.30049367	-1.22911392
C	-0.56884177	0.14449367	-1.33311392
C	-1.36084177	0.51649367	-0.02811392
C	-0.96884177	-0.30050633	1.22888608
C	0.56815823	-0.14450633	1.33188608
C	1.36115823	-0.51650633	0.02688608
N	1.51015823	1.72349367	-1.30611392
C	-0.76284177	-1.31950633	-1.81011392
C	-1.20384177	1.99249367	0.42388608
N	-1.51084177	-1.72250633	1.30588608
C	0.76315823	1.31849367	1.80988608
C	1.20315823	-1.99250633	-0.42411392
N	0.16415823	2.32049367	0.89388608
C	3.00715823	1.78049367	-1.19811392
C	1.08315823	2.43949367	-2.55511392
C	0.22015823	3.67849367	1.47488608
N	-0.16484177	-2.32050633	-0.89311392
C	-0.22184177	-3.67950633	-1.47311392
C	-1.07984177	-2.43950633	2.55288608
C	-3.00684177	-1.77950633	1.20088608
H	-0.97884177	0.76149367	-2.13811392
H	-2.42484177	0.40349367	-0.26111392
H	-1.41984177	0.18349367	2.10188608
H	0.97815823	-0.76250633	2.13688608
H	2.42415823	-0.40350633	0.25988608
H	-1.44584177	2.67549367	-0.39911392
H	1.82915823	1.55349367	1.90888608
H	3.45615823	1.19449367	-2.00511392
H	3.31915823	2.82149367	-1.29011392
H	3.33515823	1.39849367	-0.23311392
H	1.53215823	3.43449367	-2.55211392
H	1.42915823	1.88749367	-3.43211392
H	-0.00084177	2.54249367	-2.58311392
H	1.25415823	3.92749367	1.72888608
H	-0.14484177	4.40649367	0.74388608
H	-0.39384177	3.75649367	2.38388608
H	1.41915823	-0.18250633	-2.10311392
H	-1.94284177	2.18849367	1.21688608
H	0.33015823	1.40949367	2.81888608
H	-1.82884177	-1.55350633	-1.91011392
H	-0.32884177	-1.41050633	-2.81811392
H	1.94115823	-2.18850633	-1.21811392
H	1.44515823	-2.67550633	0.39788608
H	-1.25584177	-3.92750633	-1.72811392
H	0.39215823	-3.75850633	-2.38211392
H	0.14215823	-4.40650633	-0.74211392
H	-1.53084177	-3.43350633	2.55288608
H	0.00315823	-2.54550633	2.57688608
H	-1.42084177	-1.88650633	3.43188608
H	-3.31984177	-2.82150633	1.28988608
H	-3.45484177	-1.19650633	2.01088608
H	-3.33784177	-1.39350633	0.23888608
H	1.06115823	2.20249367	-0.43611392
H	-1.06184177	-2.20150633	0.43388608

3a

E=-847.90760

C	0.69827500	1.43002600	0.00007400
C	-0.00981300	0.78098500	1.21526200
C	0.00959800	-0.78096800	1.21533200
C	-0.69842900	-1.43013300	0.00016100
C	0.00945700	-0.78104100	-1.21522400
C	-0.00960900	0.78094300	-1.21526500
N	2.18176800	1.37872700	0.00016200
N	-2.18196400	-1.37906400	0.00009300
N	1.84379100	-2.02088800	-0.00007700
C	2.73457300	2.03948200	-1.18325600
C	2.73455200	2.03955700	1.18349400
C	3.22635800	-2.45055100	-0.00009500
N	-1.84364900	2.02108100	-0.00012000
C	-3.22581500	2.45156600	-0.00016700
C	-2.73444200	-2.04030400	-1.18320200
C	-2.73469800	-2.03990600	1.18346700
H	0.47801500	1.08605800	2.14655600
H	-0.47821900	-1.08596200	2.14665800
H	-0.41823600	-2.49951200	0.00018100
H	-0.47883400	-1.08609500	-2.14628100
H	0.47861100	1.08597800	-2.14637700
H	2.38310500	3.08655400	-1.28720700
H	3.82687300	2.05310400	-1.10956200
H	2.47591200	1.50359700	-2.09938700
H	3.82685200	2.05314600	1.10983400

H	2.38311700	3.08665800	1.28739500
H	2.47582600	1.50377900	2.09966800
H	3.42504400	-3.06455900	-0.88753600
H	3.94444600	-1.60543500	0.00018800
H	3.42497600	-3.06508900	0.88700700
H	0.41813900	2.49946900	-0.00005500
H	-3.94451500	1.60691500	-0.00093100
H	-3.42431600	3.06530000	0.88750600
H	-3.42400400	3.06659300	-0.88703800
H	-3.82674400	-2.05416500	-1.10962100
H	-2.47583800	-1.50461900	-2.09946300
H	-2.38268800	-3.08731000	-1.28679400
H	-3.82699500	-2.05368400	1.10976400
H	-2.38311100	-3.08695200	1.28743100
H	-2.47609600	-1.50402000	2.09960100
C	1.45494400	-1.37207300	-1.25579900
H	1.49936600	-2.15468800	-2.02712200
H	2.17298500	-0.59401900	-1.55443500
C	1.45512800	-1.37189800	1.25555100
H	2.17324200	-0.59382000	1.55408800
H	1.49965300	-2.15443000	2.02699500
C	-1.45497100	1.37231000	-1.25579100
H	-1.49923800	2.15488100	-2.02718700
H	-2.17309700	0.59435600	-1.55471000
C	-1.45523900	1.37206800	1.25536200
H	-2.17345700	0.59407800	1.55407600
H	-1.49960700	2.15452300	2.02692400

4

E = -2178.42715

C	-1.47770400	0.64275000	-0.26441100
C	-0.48219700	0.61050800	-1.44518600
C	0.48223300	-0.61054200	-1.44522400
C	1.47777900	-0.64277400	-0.26450500
C	0.55364100	-0.55579600	0.99615100
C	-0.55350400	0.55574400	0.99619800
C	0.21947500	1.99085300	-1.40805000
C	-0.21938600	-1.99092000	-1.40807200
C	-0.03268600	-1.97692800	1.10887000
C	0.03280200	1.97686100	1.10894200
N	-0.73571300	-2.38537300	-0.09723500
C	-1.17927500	-3.75674500	-0.06778900
N	0.73575400	2.38538900	-0.09718100
C	1.17908400	3.75683400	-0.06776300
N	-2.61469100	-0.24665800	-0.40702000
P	-4.09089300	0.07637000	-0.03371800
N	-4.72437000	1.66744500	-0.02505800
N	-4.51532300	-0.40182500	1.55842700
N	-5.08744100	-0.69350300	-1.17948800
C	-5.79494800	-0.13221100	2.20611600
C	-3.84120400	-1.57546800	2.10926300
C	-6.51526600	-0.85260500	-0.93487900
C	-4.53889700	-1.68228500	-2.10282700
C	-4.95440700	2.34802800	-1.29922800
C	-4.38270500	2.60094900	1.04975900
N	2.61477800	0.24665400	-0.40731300
P	4.09096800	-0.07640300	-0.03391300
N	4.72448300	-1.66744200	-0.02528400
N	4.51546000	0.40186900	1.55820400
N	5.08753400	0.69331500	-1.17989900
C	5.79480600	0.13202500	2.20624000
C	3.84063400	1.57477300	2.10970900
C	6.51528000	0.85261700	-0.93478000
C	4.53889300	1.68338800	-2.10185200
C	4.95444500	-2.34807800	-1.29945400
C	4.38279400	-2.60089700	1.04956300
H	-1.05430900	0.57602500	-2.38245100
H	1.05430200	-0.57602700	-2.38251300
H	1.86235700	-1.67687900	-0.24674400
H	1.17196700	-0.39403900	1.89014500
H	-1.17179000	0.39393900	1.89020700
H	-1.06231300	-2.01778800	-2.11292900
H	-0.73901700	-2.04285600	1.95048300
H	-1.70344600	-3.96642500	0.87331200
H	-1.87852800	-3.94464600	-0.89236500
H	-0.34513900	-4.48889600	-0.15826000
H	-1.86225100	1.67687200	-0.24661700
H	0.52414800	-2.73403500	-1.77204100
H	0.80420300	-2.66864500	1.35697500
H	1.06245000	2.01766100	-2.11284400
H	-0.52400000	2.73399900	-1.77206800
H	-0.80409600	2.66855700	1.35710800
H	0.73915200	2.04278600	1.95054000
H	1.87819200	3.94486200	-0.89242500
H	0.34481000	4.48884800	-0.15809800
H	1.70334500	3.96658400	0.87327800
H	-6.27228100	0.74783600	1.77251700
H	-6.48965500	-0.98454400	2.12500700
H	-5.63019200	0.05916800	3.27678600
H	-3.60614200	-1.40843600	3.17052400
H	-4.47448900	-2.47672100	2.04181700
H	-2.91645000	-1.75380800	1.55951800
H	-6.91121900	0.00283100	-0.38288800
H	-7.04206200	-0.90225300	-1.89731900
H	-6.75137000	-1.77395700	-0.37570200
H	-5.03489200	-1.58629400	-3.07963700
H	-3.46918100	-1.51059100	-2.21547400
H	-4.69554300	-2.71215100	-1.74016500
H	-4.06605100	2.90567600	-1.63686800
H	-5.22488400	1.62342200	-2.06917200
H	-5.78038800	3.06401000	-1.18442800
H	-5.24735500	3.24406600	1.27126900
H	-4.11041600	2.05996800	1.95730200
H	-3.54018900	3.25224800	0.77090500
H	6.27244300	-0.74770800	1.77233700
H	6.48946700	0.98447000	2.12591700
H	5.62968200	-0.05999700	3.27675200
H	3.60459000	1.40661600	3.17058400

H	4.47387700	2.47616900	2.04380800
H	2.91637300	1.75357600	1.55928500
H	6.91140300	-0.00345700	-0.38388600
H	7.04217300	0.90372900	-1.89707100
H	6.75101800	1.77327500	-0.37431400
H	5.03555500	1.58926800	-3.07848600
H	3.46935000	1.51122800	-2.21540800
H	4.69465300	2.71277400	-1.73742400
H	4.06608300	-2.90579100	-1.63696600
H	5.22480400	-1.62348200	-2.06943800
H	5.78047100	-3.06401400	-1.18467800
H	5.24739900	-3.24408200	1.27105100
H	4.11060600	-2.05988400	1.95711800
H	3.54022000	-3.25214800	0.77076500

4a

E= -2178.42872 (-2178.85111)

ZPVE= 0.82811

C	1.46705900	-0.60465600	-0.16068800
C	0.51290600	-0.58592300	-1.38537800
C	-0.51307900	0.58606500	-1.38533600
C	-1.46712200	0.60471600	-0.16062600
C	-0.50711000	0.59197600	1.06003400
C	0.50711000	-0.59191300	1.06001400
N	2.53137400	0.40807400	-0.18125900
P	4.03598600	0.00622300	0.01382500
N	4.66710500	-1.45197900	-0.62443700
N	4.52793100	-0.18322400	1.64744700
N	4.98371100	1.18017100	-0.76213500
C	5.82381500	-0.69987900	2.08167100
C	3.90935800	0.66873500	2.65993500
C	6.41348700	1.27055600	-0.49574800
C	4.40280900	2.40681400	-1.29605200
C	4.80006400	-1.56582000	-2.07733600
C	4.37757700	-2.74462000	0.00405900
N	-2.53132900	-0.40819200	-0.18122600
P	-4.03595200	-0.00626400	0.01382800
N	-4.66700100	1.45194100	-0.62441500
N	-4.52788000	0.18312400	1.64747900
N	-4.98365500	-1.18020300	-0.76208200
C	-5.82372000	0.69976300	2.08181000
C	-3.90925200	-0.66886400	2.65991800
C	-6.41339400	-1.27072000	-0.49557500
C	-4.40269200	-2.40659300	-1.29648100
C	-4.80016300	1.56578000	-2.07728900
C	-4.37769500	2.74460800	0.00409900
H	1.11992100	-0.47576300	-2.29418200
H	-1.12014600	0.47593000	-2.29411100
H	-1.91206300	1.60496900	-0.16501400
H	-1.10371800	0.50119300	1.97721900
H	1.10376400	-0.50110200	1.97717000
H	1.91188600	-1.60495700	-0.16515000
H	6.28240400	-1.30782200	1.30124300
H	6.52072900	0.11107100	2.34946900
H	5.68843900	-1.32866600	2.97406500
H	3.75552900	0.09433600	3.58452000
H	4.54128200	1.53962700	2.90386200
H	2.94250800	1.02737000	2.30720800
H	6.83627600	0.28150500	-0.30608800
H	6.91783000	1.68447600	-1.37903000
H	6.64548200	1.92532700	0.36110400
H	4.90381700	2.66805300	-2.23953100
H	3.34147500	2.25217700	-1.47913100
H	4.52064700	3.25437600	-0.60074000
H	3.87227100	-1.92335900	-2.55186800
H	5.06200200	-0.59772000	-2.50829100
H	5.59968100	-2.28214700	-2.31041800
H	5.24563200	-3.41038400	-0.11139800
H	4.17497300	-2.61866500	1.06843400
H	3.50653900	-3.23595400	-0.45419900
H	-6.28246600	1.30760400	1.30139300
H	-6.52055900	-0.11120600	2.34976700
H	-5.68828800	1.32864500	2.97412900
H	-3.75521600	-0.09444600	3.58446000
H	-4.54125900	-1.53965800	2.90397000
H	-2.94250000	-1.02762800	2.30705800
H	-6.83611800	-0.28178600	-0.30518200
H	-6.91790600	-1.68403200	-1.37905300
H	-6.64526900	-1.92604300	0.36088600
H	-4.90433200	-2.66793600	-2.23959200
H	-3.34154600	-2.25155700	-1.48034900
H	-4.51965700	-3.25426800	-0.60115900
H	-3.87235100	1.92305900	-2.55198500
H	-5.06244200	0.59774400	-2.50818000
H	-5.59962000	2.28232000	-2.31024900
H	-5.24604900	3.41008300	-0.11082200
H	-4.17448100	2.61861800	1.06835200
H	-3.50706600	3.23630400	-0.45455000
N	-0.02650600	-2.73083200	-0.17278300
C	-0.73760500	-3.99106100	-0.17121500
H	-0.47827000	-4.56544800	-1.07012100
H	-0.44255100	-4.58292000	0.70549900
H	-1.83961700	-3.87685600	-0.14586300
C	-0.20086600	-1.98528300	1.08269000
H	0.24818600	-2.60993200	1.86929200
H	-1.26546400	-1.86274300	1.33019000
C	-0.18740600	-1.98119100	-1.42875900
H	-1.24590600	-1.85412900	-1.69996900
H	0.27692300	-2.60035100	-2.21088400
N	0.02634100	2.73095900	-0.17278600
C	0.20088000	1.98534000	1.08264500
H	-0.24805700	2.60999500	1.86930800
H	1.26550800	1.86279400	1.33001000
C	0.73758300	3.99111200	-0.17124900
H	0.47823900	4.56555200	-1.07011600
H	0.44265200	4.58297800	0.70550400
H	1.83958700	3.87678500	-0.14597800
C	0.18726500	1.98131900	-1.42874400

H	1.24576700	1.85425800	-1.69987800
H	-0.27703500	2.60050700	-2.21085000

4a.H$^+$

E = -2178.89550 (-2179.32012)

ZPVE = 0.84361

C	1.38041500	0.60100200	0.02663000
C	0.34478400	0.47145000	1.16751300
C	-0.63237800	-0.73640600	1.02090800
C	-1.49150300	-0.70724700	-0.27823400
C	-0.43127600	-0.61636800	-1.41212500
C	0.55199700	0.59047700	-1.27885300
N	2.51100400	-0.34536400	0.10105600
P	4.09336200	0.04809300	0.05740400
N	4.44318400	1.56825100	0.64622300
N	4.71664500	0.09502800	-1.48961900
N	4.82308500	-1.15518800	0.95309400
C	5.97888500	0.75419900	-1.85503200
C	4.23691800	-0.84565400	-2.50897900
C	6.24258500	-1.48620300	0.77603500
C	4.25405100	-1.70316100	2.19341000
C	4.59240800	1.79512300	2.08964600
C	4.15250000	2.80095900	-0.10781900
N	-2.54993000	0.28110100	-0.35395400
P	-4.05736400	-0.02193500	-0.00607900
N	-4.57532100	-0.31970200	1.59729300
N	-4.64985300	-1.43103800	-0.77023800
N	-4.93634200	1.37157400	-0.38316800
C	-5.96908300	-2.01002100	-0.49244300
C	-4.22820400	-1.69539100	-2.14871500
C	-6.39362200	1.37389300	-0.23792200
C	-4.46983500	2.28839700	-1.42358800
C	-4.54263200	0.78980900	2.55636700
C	-4.23177400	-1.59085800	2.24106000
H	0.87687900	0.34985500	2.12079100
H	-1.29853400	-0.70683100	1.89259200
H	-1.91960200	-1.72176700	-0.36288400
H	-0.94943600	-0.49340800	-2.37230600
H	1.23287800	0.55425400	-2.13978500
H	1.81344600	1.59624300	0.11697300
H	6.35961500	1.34994600	-1.02524700
H	6.73910700	0.01267200	-2.13539200
H	5.81352600	1.41313500	-2.71620500
H	4.18111400	-0.33053100	-3.47478500
H	4.91297200	-1.70590100	-2.61164600
H	3.23871200	-1.20499800	-2.25659200
H	6.58613300	-1.21575300	-0.22227800
H	6.87334000	-0.97780600	1.51848800
H	6.37163600	-2.56755000	0.89633700
H	4.84097100	-1.38892100	3.06755600
H	3.22394300	-1.37129600	2.32082400
H	4.27018800	-2.79872300	2.14754100
H	3.64590200	2.10568900	2.55295400
H	4.95414600	0.89535800	2.58907700
H	5.33159200	2.58857400	2.24589500
H	5.00840700	3.48200000	-0.02778300
H	3.98167300	2.57661500	-1.16136300
H	3.26314300	3.30573400	0.28973200
H	-6.29728500	-1.76646800	0.51760400
H	-6.72732900	-1.64672200	-1.20297700
H	-5.91528500	-3.10289200	-0.58829400
H	-4.14457100	-2.77887700	-2.30601000
H	-4.95515700	-1.30322400	-2.87788100
H	-3.26086800	-1.23450600	-2.34989200
H	-6.70228100	0.72461700	0.58279700
H	-6.72992400	2.39392800	-0.01321700
H	-6.90172100	1.04681800	-1.15882600
H	-4.79790600	3.30628400	-1.17654000
H	-3.38328300	2.26578500	-1.47221200
H	-4.87967400	2.02903700	-2.41322600
H	-3.54689200	0.90806300	3.01391600
H	-4.81182800	1.72721500	2.06901200
H	-5.26327700	0.58905100	3.35887300
H	-4.99401200	-1.83516700	2.99209400
H	-4.19204800	-2.40072600	1.51166500
H	-3.25952300	-1.53796800	2.75771100
N	-0.12800000	2.65294300	-0.00110200
C	-0.85465500	3.91221300	0.00312000
H	-0.64056500	4.45870600	0.92949900
H	-0.52558400	4.53138400	-0.83977500
H	-1.94981900	3.78347600	-0.07141600
C	-0.20350300	1.96370500	-1.30170500
H	0.27699300	2.63215700	-2.02883200
H	-1.23880900	1.80375700	-1.62808400
C	-0.41978700	1.83982800	1.19191400
H	-1.49620000	1.66125200	1.31113200
H	-0.08064300	2.43105700	2.05349600
N	0.83786400	-2.42628300	-0.16788700
C	0.24158700	-2.00502900	-1.45737800
H	-0.51847900	-2.73791300	-1.78047300
H	1.04227900	-2.03495300	-2.20990200
C	1.24379100	-3.83110200	-0.20325100
H	1.77138400	-4.09030900	0.72121300
H	0.38057500	-4.51110400	-0.30886100
H	1.91964000	-4.00373700	-1.04809800
C	0.03902900	-2.12628300	1.04315700
H	0.71084500	-2.22916600	1.90709500
H	-0.75557800	-2.88275300	1.16949500
H	2.18455800	-1.33829700	0.01237000

4a.2H$^+$

E = -2179.26355 (-2179.69092)

ZPVE = 0.858002

C	1.45549100	-0.64117300	-0.12219700
C	0.50880200	-0.59464200	-1.34851200
C	-0.50867200	0.59449100	-1.34853400
C	-1.45539900	0.64104600	-0.12227600
C	-0.51179100	0.59328500	1.10803000

C	0.51176400	-0.59348700	1.10804100
C	-0.14846100	-1.99582900	-1.37801900
C	0.14856900	1.99568900	-1.37800300
C	0.13971600	1.99743800	1.13784800
C	-0.13973300	-1.99767400	1.13773100
N	0.82918800	2.36163100	-0.11757000
C	1.23053900	3.77218900	-0.11698300
N	-0.82915900	-2.36176100	-0.11768400
C	-1.23070300	-3.77225100	-0.11719200
N	2.58125300	0.30196000	-0.15216200
P	4.17855100	-0.05433800	0.04355500
N	4.58764000	-1.58083400	-0.47134400
N	4.63682200	-0.04214100	1.64234400
N	4.93779700	1.14319600	-0.82268000
C	5.87921400	-0.66051000	2.14434700
C	4.07879800	0.95259400	2.56980400
C	6.32833000	1.52702300	-0.52169900
C	4.48013300	1.63058900	-2.13512000
C	5.01352300	-1.84311800	-1.85473800
C	4.31978400	-2.80399000	0.30278800
N	-2.58121600	-0.30202800	-0.15240600
P	-4.17851700	0.05440900	0.04352200
N	-4.58728900	1.58101400	-0.47126500
N	-4.63672200	0.04202800	1.64230600
N	-4.93795100	-1.14299400	-0.82268200
C	-5.87888500	0.66076100	2.14446500
C	-4.07893500	-0.95300000	2.56961800
C	-6.32826800	-1.52725900	-0.52131000
C	-4.48063400	-1.62998700	-2.13540600
C	-5.01427500	1.84343800	-1.85428800
C	-4.31911800	2.80406700	0.30290700
H	1.10463400	-0.51238100	-2.26638600
H	-1.10449900	0.51224400	-2.26641100
H	-1.91689600	1.63261100	-0.12713300
H	-1.10558100	0.51008000	2.02713000
H	1.10549000	-0.51035700	2.02718600
H	0.89119500	2.06180600	-2.18312100
H	0.87400400	2.07118700	1.94989600
H	1.83172700	3.98766200	0.77208600
H	1.83542500	3.98627600	-1.00373300
H	0.36181700	4.45201200	-0.11956800
H	1.91703400	-1.63271800	-0.12701400
H	-0.64019000	2.73063000	-1.61977000
H	-0.65393900	2.72987000	1.37129800
H	-0.89100100	-2.06193400	-2.18322300
H	0.64032400	-2.73077000	-1.61976200
H	0.65395400	-2.73008400	1.37117400
H	-0.87400900	-2.07146000	1.94979100
H	-1.83554400	-3.98621800	-1.00400400
H	-0.36207800	-4.45220400	-0.11973400
H	-1.83199500	-3.98769300	0.77181400
H	6.35026200	-1.27326100	1.37578400
H	6.59187100	0.11013300	2.46345700
H	5.64826400	-1.29220400	3.00961200
H	3.95124900	0.49014800	3.55465000
H	4.74452400	1.81926900	2.67638500
H	3.10374100	1.29579000	2.22159600
H	6.58165400	1.30244400	0.51420800
H	7.03901100	1.01279100	-1.18161600
H	6.43489000	2.60641900	-0.67040300
H	5.16736300	1.31519400	-2.93085500
H	3.48290400	1.25234700	-2.35956800
H	4.45230000	2.72626600	-2.12367000
H	4.20207800	-2.28545600	-2.44750900
H	5.34672600	-0.92589300	-2.34038700
H	5.85482800	-2.54457500	-1.84136500
H	5.23960800	-3.39415600	0.39130200
H	3.96662100	-2.56009400	1.30577600
H	3.56575300	-3.42272200	-0.20092900
H	-6.34986200	1.27360600	1.37593600
H	-6.59170200	-0.10971600	2.46361500
H	-5.64766200	1.29237800	3.00970900
H	-3.95075500	-0.49061000	3.55440700
H	-4.74513900	-1.81927000	2.67643600
H	-3.10422000	-1.29680100	2.22105000
H	-6.58137800	-1.30260800	0.51463400
H	-7.03926600	-1.01334600	-1.18113200
H	-6.43448500	-2.60671400	-0.66985600
H	-5.16812400	-1.31438600	-2.93083700
H	-3.48348400	-1.25165100	-2.36003400
H	-4.45277000	-2.72566900	-2.12430100
H	-4.20331400	2.28589600	-2.44763100
H	-5.34776500	0.92624900	-2.33979700
H	-5.85561500	2.54483900	-1.84018400
H	-5.23898200	3.39404800	0.39226400
H	-3.96510200	2.56007000	1.30557500
H	-3.56560200	3.42303300	-0.20129100
H	-2.25046100	-1.28936500	-0.13384400
H	2.25038900	1.28930500	-0.13364700

5

E = -1986.22965

C	1.45835700	0.69788000	1.50662900
C	0.47742400	0.70133700	2.69560800
C	-0.47777400	-0.52821100	2.73477200
C	-1.46633600	-0.59421100	1.55409600
C	-0.54789500	-0.55035400	0.28768200
C	0.53102000	0.57998200	0.25113700
C	-0.24626900	2.06633300	2.62659800
C	0.24632800	-1.89474800	2.74028500
C	0.07804400	-1.95692500	0.22826000
C	-0.09581300	1.98092400	0.11407200
N	0.79298900	-2.28248400	1.44508000
C	1.40645400	-3.58308200	1.44483100
N	-0.80202900	2.37793300	1.31484200
C	-1.41519400	3.67672200	1.24289800
N	2.57338400	-0.21562500	1.69432400
C	3.65491800	-0.07341800	0.97715400

C	4.76534500	-0.96811600	1.26267000
C	3.90160400	0.89994000	-0.07808900
C	5.95900400	-0.91765000	0.60835400
C	5.08632600	0.96518900	-0.76195200
C	6.19625500	0.05466800	-0.46589500
C	7.40992300	0.10540900	-1.16222700
N	8.08325500	-1.04568600	-1.54983600
N	8.01406300	1.30963200	-1.50605200
C	9.53484800	-1.15799100	-1.51056300
C	7.38077400	-2.17175600	-2.15430900
C	8.73149600	1.49693500	-2.75967600
C	8.12639300	2.40454700	-0.54825400
N	-2.58028000	0.32900200	1.69160700
C	-3.65890200	0.14230600	0.98056200
C	-4.77482200	1.04696000	1.20813000
C	-3.89456800	-0.89104500	-0.01833300
C	-5.96490500	0.95213200	0.55194100
C	-5.07659800	-1.00464300	-0.70029000
C	-6.19287200	-0.08524000	-0.46194600
C	-7.40389100	-0.18565100	-1.15717500
N	-8.08374500	0.93546700	-1.61440700
N	-7.99908400	-1.41249700	-1.42860200
C	-9.53624600	1.03874100	-1.58740900
C	-7.38689100	2.02911200	-2.28164800
C	-8.71020000	-1.68208400	-2.67077800
C	-8.10767900	-2.44709500	-0.40555500
N	-5.14994100	-1.90025100	-1.78328900
N	-7.06404800	1.72420300	0.99401400
N	7.05262000	-1.66456300	1.10384700
N	5.16881000	1.79454300	-1.89590100
H	1.06084400	0.69445100	3.62610500
H	-1.05507900	-0.46725200	3.66711100
H	-1.88925100	-1.61506100	1.57240400
H	-1.16089700	-0.42533400	-0.61449300
H	1.13703700	0.40207400	-0.64676700
H	1.08336900	-1.88326800	3.45140400
H	0.79190600	-2.02821500	-0.60720300
H	1.96411100	-3.73647600	0.51208200
H	2.11574800	-3.66139700	2.27846900
H	0.67318200	-4.41614400	1.54344800
H	1.88143600	1.71789200	1.46238900
H	-0.48420700	-2.65096600	3.10520900
H	-0.73661600	-2.68720500	0.00691700
H	-1.07811200	2.09711400	3.34314700
H	0.48718900	2.84195100	2.94158000
H	0.71700900	2.69682300	-0.15548600
H	-0.81584800	2.00321700	-0.71877100
H	-2.11822000	3.80405000	2.07582300
H	-0.68108400	4.51366900	1.28718400
H	-1.97968900	3.77556700	0.30690700
H	4.62675600	-1.65088500	2.09819300
H	3.10176400	1.56665100	-0.38446400
H	9.95566300	-0.33020800	-0.93718700
H	9.82442900	-2.09688800	-1.01716400
H	9.97982100	-1.16034300	-2.51727800
H	7.50289100	-3.09419800	-1.56790500
H	7.77454700	-2.36307400	-3.16454000
H	6.31699100	-1.94148200	-2.22165700
H	8.50031200	0.67914100	-3.44460900
H	8.41908900	2.43928200	-3.23211500
H	9.82153900	1.54439800	-2.61385000
H	7.65604900	3.32470900	-0.92435000
H	7.63928500	2.12130300	0.38535600
H	9.18648100	2.62691100	-0.34995000
H	-4.64307100	1.77905200	2.00191700
H	-3.08861200	-1.56872000	-0.28267000
H	-9.95312500	0.24313300	-0.96752700
H	-9.83521700	2.00295100	-1.15175100
H	-9.97682900	0.97773900	-2.59424200
H	-7.52000200	2.98387800	-1.75216100
H	-7.77617900	2.15642200	-3.30366600
H	-6.32086600	1.80430600	-2.32932900
H	-8.48150400	-0.90708300	-3.40451700
H	-8.38972600	-2.64981400	-3.08261600
H	-9.80052100	-1.72787300	-2.52629500
H	-7.62811400	-3.38478400	-0.72190900
H	-7.62777600	-2.10274100	0.51116100
H	-9.16702200	-2.66546600	-0.19888000
H	-6.05940600	-2.30006700	-1.96661700
H	-4.42083600	-2.60406000	-1.77580200
H	-7.68504900	2.05196000	0.26624400
H	-6.78233900	2.48725400	1.60013200
H	7.67845800	-2.03659200	0.40208800
H	6.76450300	-2.38885900	1.75291800
H	6.08168500	2.17631400	-2.09953500
H	4.44520200	2.50315600	-1.93175100

5a

E= -1986.23265 (-1986.71340)

ZPVE= 0.89728

C	1.44494300	0.62857600	1.38032500
C	0.49928700	0.59848200	2.60366200
C	-0.49955000	-0.59797400	2.60355200
C	-1.44486900	-0.62809300	1.37999100
C	-0.48993200	-0.60500400	0.15274800
C	0.49031500	0.60535400	0.15283000
N	2.45961200	-0.41223600	1.41594400
C	3.59760600	-0.21597600	0.80278000
C	4.61456100	-1.24755000	0.92513100
C	3.97278000	0.93168600	-0.00953500
C	5.84974900	-1.15607900	0.35531000
C	5.19357800	1.03456800	-0.62068400
C	6.22132600	0.00143600	-0.46671800
C	7.48176200	0.11152000	-1.06677500
N	8.11320600	-0.97420100	-1.65742000
N	8.17616900	1.31370100	-1.10362500
C	9.55004000	-1.19404100	-1.56383400
C	7.39036700	-1.89616100	-2.52653000

C	8.98601700	1.71970700	-2.24443500
C	8.25362200	2.18624400	0.06340300
N	-2.45945400	0.41284000	1.41521300
C	-3.59742200	0.21646800	0.80204100
C	-4.61434000	1.24813000	0.92402400
C	-3.97261800	-0.93140400	-0.01000700
C	-5.84957900	1.15647900	0.35432800
C	-5.19344500	-1.03443700	-0.62104500
C	-6.22124900	-0.00135400	-0.46719000
C	-7.48191100	-0.11193600	-1.06667800
N	-8.11378300	0.97336900	-1.65761600
N	-8.17602800	-1.31431000	-1.10264700
C	-9.55055700	1.19326500	-1.56321700
C	-7.39145100	1.89496700	-2.52753000
C	-8.98635800	-1.72107700	-2.24284900
C	-8.25263800	-2.18636000	0.06480600
N	-5.39148900	-2.05542300	-1.56821100
N	-6.85193600	2.07996500	0.72603600
N	6.85215200	-2.07939800	0.72725800
N	5.39155000	2.05536700	-1.56802700
H	1.11230700	0.49470500	3.50884800
H	-1.11279800	-0.49418300	3.50858300
H	-1.92659000	-1.61499600	1.38985700
H	-1.09111800	-0.51756700	-0.76250800
H	1.09171900	0.51784700	-0.76227600
H	1.92655100	1.61554600	1.39022400
H	4.37623000	-2.08154200	1.58145500
H	3.23239100	1.69692300	-0.22077700
H	9.97767500	-0.53423700	-0.80706700
H	9.75001700	-2.23270200	-1.26400300
H	10.06130600	-1.02018200	-2.52273100
H	7.43939800	-2.93035300	-2.15595100
H	7.82657300	-1.88225200	-3.53727300
H	6.34337300	-1.59678500	-2.58334600
H	8.77042400	1.07756100	-3.10012900
H	8.74547000	2.75570400	-2.52322300
H	10.06379500	1.67655200	-2.02638000
H	7.82950000	3.17996000	-0.14049200
H	7.70332300	1.73689500	0.89058700
H	9.30460500	2.32391700	0.35987100
H	-4.37594000	2.08237100	1.58000700
H	-3.23221000	-1.69663900	-0.22117700
H	-9.97768300	0.53395000	-0.80573600
H	-9.75032500	2.23211200	-1.26390200
H	-10.06246500	1.01880300	-2.52166000
H	-7.43999000	2.92929200	-2.15724200
H	-7.82845200	1.88083900	-3.53792300
H	-6.34455800	1.59537100	-2.58506700
H	-8.77108200	-1.07955100	-3.09908900
H	-8.74594500	-2.75728000	-2.52097000
H	-10.06405200	-1.67774200	-2.02441300
H	-7.82812200	-3.17996100	-0.13880500
H	-7.70223600	-1.73638300	0.89158100
H	-9.30344500	-2.32437000	0.36172800
H	-6.33786000	-2.39370600	-1.66871900
H	-4.72359700	-2.81375300	-1.49210000
H	-7.49708900	2.34514400	-0.00571700
H	-6.47410700	2.89763400	1.19217200
H	7.49741300	-2.34462600	-0.00437900
H	6.47441900	-2.89699300	1.19359400
H	6.33788100	2.39367600	-1.66871000
H	4.72356300	2.81362900	-1.49215000
N	-0.12333900	2.72327600	1.38468200
C	-0.21640400	1.98120600	2.65627700
H	-1.26104300	1.84989100	2.97218500
H	0.28156700	2.61566900	3.40560300
C	-0.24879500	1.97722200	0.12337400
H	0.20628300	2.61650100	-0.64984300
H	-1.30136900	1.82884500	-0.16401700
C	-0.92773200	3.92507800	1.39319300
H	-0.68302700	4.52985000	2.27659400
H	-0.70993300	4.52681000	0.50026400
H	-2.01763000	3.72034300	1.41004900
N	0.12320300	-2.72295400	1.38483800
C	0.21619500	-1.98069000	2.65639100
H	1.26082600	-1.84930200	2.97225300
H	-0.28177000	-2.61508500	3.40575600
C	0.92771900	-3.92471200	1.39363800
H	2.01758100	-3.71985900	1.41077400
H	0.68280700	-4.52943500	2.27700800
H	0.71019100	-4.52649900	0.50068500
C	0.24925500	-1.97684300	0.12359200
H	-0.20538500	-2.61612700	-0.64986400
H	1.30197000	-1.82841400	-0.16322400

5a.H$^+$

E = -1986.72845 (-1987.21208)

ZPVE = 0.91345

C	-1.55438200	0.61845300	-0.90229100
C	-0.45384200	0.53547700	-1.98870700
C	0.59456900	-0.59524400	-1.74650700
C	1.36497100	-0.48604700	-0.40608300
C	0.27350800	-0.34544800	0.68429200
C	-0.76262700	0.79277000	0.42611400
N	-2.49579300	-0.47600300	-0.96156600
C	-3.73180500	-0.28326600	-0.55472600
C	-4.66291000	-1.38193600	-0.71153000
C	-4.28034700	0.91827200	0.04478100
C	-5.98608100	-1.29835400	-0.37814600
C	-5.60092000	1.02124200	0.41215500
C	-6.53951100	-0.07503500	0.20319800
C	-7.90754600	0.04490200	0.52153700
N	-8.59956500	-0.96351900	1.15950100
N	-8.62842000	1.17748900	0.20084300
C	-9.98934300	-1.28945300	0.85036800
C	-8.00489400	-1.72692700	2.25478800
C	-9.69833400	1.70597200	1.04318400
C	-8.41760300	1.88905300	-1.05862000

N	2.42547100	0.51271000	-0.36758500
C	3.73693100	0.30398300	-0.15282600
C	4.61101100	1.43145100	-0.17781200
C	4.30336400	-0.97455000	0.09817900
C	5.97040400	1.30481400	0.02357600
C	5.66375500	-1.12820300	0.31274300
C	6.55857500	0.00666100	0.27983400
C	7.96707300	-0.14742300	0.48494900
N	8.63848200	0.63635000	1.37877900
N	8.67992100	-1.08188900	-0.20881800
C	10.03044500	1.05957200	1.19675000
C	8.00441700	1.11835100	2.61126900
C	9.84269200	-1.78550400	0.34193100
C	8.32020000	-1.46674700	-1.57856700
N	6.13005000	-2.37338500	0.70827300
N	6.78720000	2.41296700	-0.18169200
N	-6.86193800	-2.32099800	-0.78374200
N	-6.00638300	2.13285900	1.16252600
H	-0.93274400	0.31946900	-2.95273600
H	1.31448800	-0.55680700	-2.57487300
H	1.83949900	-1.45121800	-0.24645900
H	0.75829400	-0.13620800	1.64728600
H	-1.46515800	0.77278700	1.26996100
H	-2.07940800	1.57418600	-1.08011600
H	-4.28281500	-2.27188000	-1.20743000
H	-3.62019900	1.74183000	0.30079000
H	-10.28696400	-0.80316400	-0.07974900
H	-10.08876400	-2.37493200	0.71763700
H	-10.67560900	-0.98661600	1.65338400
H	-7.92069500	-2.79465500	2.00931700
H	-8.63404500	-1.63655500	3.15137900
H	-7.00995100	-1.33788100	2.47205700
H	-9.66658500	1.23607600	2.02743400
H	-9.56052600	2.78801600	1.17238800
H	-10.69128400	1.54733000	0.60032000
H	-8.02677500	2.90245600	-0.89288100
H	-7.70844500	1.33656100	-1.67530000
H	-9.37287700	1.97703200	-1.59406600
H	4.19639900	2.40709400	-0.41903300
H	3.66857800	-1.84859400	0.18254500
H	10.34533900	0.88461300	0.16762000
H	10.10000700	2.13421300	1.40336500
H	10.71282100	0.54144300	1.88123600
H	7.86938300	2.20699200	2.59188200
H	8.64699300	0.86726100	3.46350300
H	7.03301700	0.64184600	2.73833600
H	9.88656900	-1.65231900	1.42338300
H	9.73791800	-2.85581200	0.12772800
H	10.78316400	-1.44405100	-0.10685900
H	7.93794200	-2.49426900	-1.61745000
H	7.55923300	-0.78945600	-1.96451300
H	9.21452800	-1.40691300	-2.20978200
H	7.10346200	-2.59975700	0.57602300
H	5.50451000	-3.15607000	0.56950500
H	7.67671200	2.44824000	0.29270100
H	6.31660500	3.30847600	-0.20857000
H	-7.64289800	-2.51565700	-0.17369200
H	-6.38801600	-3.17130800	-1.06565900
H	-6.98161300	2.38878200	1.11059400
H	-5.39253500	2.93522800	1.09509400
N	0.63365100	2.50163700	-0.82078100
C	0.13163300	1.95784100	-2.10180300
H	0.96884600	1.98531900	-2.81400000
H	-0.65785300	2.61408100	-2.51167500
C	-0.18060400	2.22153600	0.38093300
H	-1.02830500	2.92971700	0.44016300
H	0.45590300	2.41700900	1.25630800
C	0.95771300	3.91926900	-0.92957700
H	1.65173400	4.08056900	-1.76266400
H	0.06221900	4.54357000	-1.10552200
H	1.43649900	4.26531000	-0.00593200
N	-0.06381600	-2.61149300	-0.37673600
C	-0.06532100	-2.01320500	-1.72692500
H	-1.07601500	-1.95723500	-2.14919400
H	0.52932600	-2.69321500	-2.35392100
C	-0.78196500	-3.87290800	-0.34402200
H	-1.86901700	-3.75484400	-0.51161500
H	-0.38778600	-4.54301300	-1.11819400
H	-0.63694300	-4.35739000	0.62975600
C	-0.41607100	-1.74777600	0.76478600
H	-0.05671700	-2.27377400	1.66090200
H	-1.50224100	-1.62292600	0.86919600
H	2.07785600	1.47438500	-0.52627700

5a.2H$^+$

E = -1987.14859 (-1987.63473)

ZPVE = 0.92807

C	-1.48486300	-0.53818100	-0.35657300
C	-0.71124700	-0.64428800	0.98548800
C	0.37213200	0.46377400	1.19938200
C	1.47492300	0.53128200	0.10922900
C	0.70148300	0.63772500	-1.23264800
C	-0.38324000	-0.46908500	-1.44673200
N	-2.52862700	0.46850100	-0.43980400
C	-3.86749600	0.27173300	-0.27716100
C	-4.70458700	1.41754400	-0.27483200
C	-4.46745700	-0.99994100	-0.12965000
C	-6.08087200	1.31489000	-0.14158100
C	-5.84942300	-1.13286300	-0.00172900
C	-6.70470400	0.02273100	-0.00313500
C	-8.13943900	-0.10551800	0.12499200
N	-8.96723500	0.46381600	-0.78895500
N	-8.68115600	-0.79679100	1.16149400
C	-10.31045900	0.96806200	-0.47066700
C	-8.56274900	0.65152100	-2.18995700
C	-9.95074500	-1.53231000	1.07776100
C	-8.01045800	-0.88670800	2.46631100
N	2.51540300	-0.47830700	0.19167300

C	3.86088500	-0.28262300	0.11908200
C	4.69776500	-1.42485300	0.18137900
C	4.47010700	0.98901400	-0.01601100
C	6.08179600	-1.32218900	0.14923900
C	5.85456000	1.11865200	-0.04971700
C	6.71131000	-0.02970000	0.03848500
C	8.15289200	0.10953800	0.08257200
N	8.94385700	-0.61500300	-0.75774400
N	8.73831700	0.94087800	0.97364400
C	10.29697600	-1.06915500	-0.40881500
C	8.49731100	-1.01116600	-2.09991500
C	9.99036500	1.66358200	0.71064400
C	8.08291900	1.31727700	2.23379000
N	6.40320700	2.39394100	-0.16999800
N	6.83832500	-2.45901600	0.36288300
N	-6.82878900	2.47348100	-0.00884900
N	-6.38756800	-2.40514900	0.00221800
H	-1.41935200	-0.57133100	1.82122800
H	0.84023400	0.27960200	2.17476400
H	1.98383100	1.48563600	0.25987000
H	1.40931100	0.56376600	-2.06855900
H	-0.85167200	-0.28345000	-2.42164800
H	-1.99102600	-1.49400400	-0.50677000
H	-4.25078300	2.40231300	-0.35174900
H	-3.87141200	-1.90479200	-0.15821300
H	-10.43358600	1.06180100	0.60834800
H	-10.42077000	1.96068800	-0.92160300
H	-11.09877800	0.32475800	-0.87683000
H	-8.41107900	1.71302300	-2.41837500
H	-9.35816400	0.26808600	-2.83821500
H	-7.64094100	0.10653500	-2.38830200
H	-10.24380100	-1.66428500	0.03613500
H	-9.80535900	-2.52109600	1.52728000
H	-10.75532400	-1.02911300	1.62528100
H	-7.63213500	-1.89982000	2.64685800
H	-7.18214100	-0.18079600	2.50858100
H	-8.73580000	-0.64246300	3.24999000
H	4.24377900	-2.40270600	0.32064200
H	3.87030500	1.88414700	-0.13462200
H	10.45404300	-0.99340100	0.66743300
H	10.39385400	-2.12038700	-0.70282000
H	11.07297000	-0.50104500	-0.93398500
H	8.40256200	-2.10075800	-2.17704300
H	9.23889500	-0.67798700	-2.83498500
H	7.53458300	-0.55335500	-2.32350400
H	10.26265400	1.58865000	-0.34231000
H	9.83067400	2.71942700	0.95586200
H	10.81440500	1.29071900	1.32853600
H	7.63896500	2.31494100	2.15228200
H	7.30476300	0.59518300	2.47844800
H	8.83814500	1.31678500	3.02610100
H	7.28546600	2.47511600	-0.65903400
H	5.75291900	3.11656200	-0.45496000
H	7.80906400	-2.47752000	0.09337700
H	6.36965300	-3.35262400	0.30555100
H	-7.81771500	2.45085800	-0.20537700
H	-6.38107200	3.34183900	-0.27015600
H	-7.32812400	-2.55867200	0.33007700
H	-5.75986200	-3.18457100	0.14204300
N	0.64453700	-2.42228900	-0.19181100
C	0.18418800	-1.90905800	-1.49836200
H	-0.60577800	-2.56081900	-1.91521000
H	1.03595500	-1.96730000	-2.18887300
C	0.95037500	-3.84980200	-0.25323800
H	1.41083700	-4.17254200	0.68690200
H	0.04921600	-4.46599900	-0.42348500
H	1.65457600	-4.04476500	-1.06924200
N	-0.65627700	2.41507300	-0.05774100
C	-0.19575500	1.90358500	1.24928200
H	-1.04741100	1.96228500	1.93986600
H	0.59408000	2.55613600	1.66523000
C	-0.96425700	3.84222900	0.00246400
H	-1.42483600	4.16335500	-0.93814600
H	-1.66903000	4.03686800	0.81803800
H	-0.06407800	4.45988900	0.17261100
C	0.15360200	2.08281800	-1.24452600
H	1.01926500	2.76654500	-1.33174100
H	-0.47333800	2.25796600	-2.12896600
C	-0.16308200	-2.08930600	0.99669900
H	0.46568000	-2.26458300	1.87986100
H	-1.02868900	-2.77266500	1.08562200
H	2.15038400	-1.43757200	0.12145900
H	-2.16347900	1.42772300	-0.37192000

B3LYP/6-31+G* SCF energies in gas phase (E), and Cartesian coordinates for 1b-1e (All energies are given in Hartee).

1b

E= -541.90997

C	-0.20906500	0.20578300	1.52308600
C	-0.51512000	-1.14205300	0.84960500
C	0.38880700	-1.36829500	-0.40419200
C	1.27175900	-0.15412300	-0.78550800
C	0.37842400	1.10637000	-0.79340700
C	-0.49345800	1.30386400	0.48515400
C	-2.01210600	-1.16030600	0.48589400
N	2.47362200	-0.06575200	0.08594900
C	-1.99434900	1.25006000	0.13967000
N	-2.36381900	-0.05595500	-0.40789900
C	-3.75690600	-0.10551800	-0.81980800
C	3.45518600	-1.09071700	-0.25819700
C	3.12505200	1.23999900	0.10283800
H	-0.34763800	-1.95490200	1.56768000
H	1.61905900	-0.29802700	-1.82947000
H	-0.29153300	2.29015600	0.92377100
H	-0.85948300	0.34213400	2.39913400

H	-2.27013700	-2.09965200	-0.02129800
H	-2.61009200	-1.12161500	1.42262500
H	-2.58590900	1.48633500	1.05071300
H	-2.24132400	2.01265200	-0.61121500
H	-3.95761100	0.68841800	-1.54841800
H	-3.96881600	-1.06887600	-1.29780600
H	4.28603900	-1.05796800	0.45486400
H	3.01516600	-2.08947800	-0.20712200
H	4.02311000	1.17629100	0.72670600
H	2.47401000	1.99947600	0.54444300
H	0.82847800	0.24068700	1.86392200
H	-4.46191000	0.01969100	0.02781400
H	3.87043500	-0.95453200	-1.27870000
H	3.43840100	1.58936300	-0.90257600
H	-0.24952000	-1.58247100	-1.27035500
H	1.01154800	-2.25565800	-0.25536600
H	-0.29095300	0.97783600	-1.65171500
H	0.97071700	2.00170600	-1.00479200

1c

E= -541.90247

C	1.41261500	-1.79106900	0.00011700
C	0.83734200	-1.08055500	1.23435400
C	-0.69651500	-1.27431900	1.25806500
C	-1.46194800	-0.78508300	0.00003000
C	-0.69639500	-1.27440200	-1.25791500
N	-1.74222000	0.67450400	-0.00009300
C	-2.48230400	1.09835700	-1.18831600
C	-2.48214200	1.09865400	1.18813600
H	1.22858000	-1.55760600	2.14268000
H	-1.11944700	-0.84314800	2.17059100
H	-2.44445100	-1.30659700	-0.00000500
H	-1.11935800	-0.84328200	-2.17045300
H	2.50634700	-1.75013900	0.00023200
H	-2.74674000	2.15548100	-1.08712200
H	-1.87765900	1.00291300	-2.09282000
H	-2.74672800	2.15571100	1.08663600
H	-1.87731000	1.00359200	2.09255700
H	1.11720600	-2.84972700	0.00018000
H	-0.88682800	-2.35476200	1.33293200
H	-0.88670300	-2.35485000	-1.33276100
H	-3.42002600	0.52347600	-1.33629500
H	-3.41977300	0.52372400	1.33649200
N	2.01937800	0.75302300	0.00006800
C	2.46036500	2.13581800	-0.00007600
H	3.07431400	2.32974000	-0.88789400
H	1.61936500	2.85970000	-0.00025700
H	3.07418800	2.33000200	0.88776200
C	1.29568800	0.41040700	-1.22927000
H	1.98922900	0.58728400	-2.06158300
H	0.43102000	1.07947100	-1.38203200
C	0.83746900	-1.08067900	-1.23422500
H	1.22861200	-1.55791000	-2.14251100
C	1.29533200	0.41067200	1.22919900
H	0.43048600	1.07959700	1.38151900
H	1.98853500	0.58783500	2.06173100

1d

E= -541.91048 Ha

C	1.16879200	0.00162400	1.81635400
C	0.84252900	1.23511900	0.96354900
C	-0.67071400	1.27062300	0.65969900
C	-0.67052600	-1.26959700	0.66195500
H	1.07862900	2.14499400	1.52989800
H	-0.87969700	2.15468300	0.04566700
H	-0.87938900	-2.15478800	0.04951800
H	2.22171500	0.00198400	2.11631800
H	0.55927200	0.00238600	2.73030300
H	-1.22082600	1.39922900	1.60294800
H	-1.22069700	-1.39653700	1.60539000
N	2.51758300	-0.00026800	-0.43624900
C	3.35333400	-0.00125600	-1.62323300
H	3.99639300	-0.88909900	-1.62434300
H	2.76651700	-0.00210000	-2.56555300
H	3.99632000	0.88663200	-1.62587200
C	1.71916900	-1.22208200	-0.32565700
H	2.42190800	-2.06423500	-0.31108900
H	1.08134900	-1.36536800	-1.22348800
C	0.84270600	-1.23342600	0.96577200
H	1.07888500	-2.14228400	1.53372200
C	1.71893400	1.22158200	-0.32786700
H	1.08106300	1.36306600	-1.22596700
H	2.42149600	2.06391600	-0.31490900
C	-1.20268300	-0.00012700	-0.03914600
H	-0.82154100	-0.00099200	-1.08145200
N	-2.68459200	-0.00037700	-0.08188600
C	-3.23115500	1.19167900	-0.72847400
H	-4.32222200	1.10878100	-0.76460300
H	-2.99035900	2.09279400	-0.16046900
H	-2.86422200	1.32523500	-1.76747400
C	-3.23056300	-1.19293300	-0.72805300
H	-2.98930200	-2.09373700	-0.15975300
H	-4.32167400	-1.11063600	-0.76424400
H	-2.86350400	-1.32663600	-1.76699200

1e

E= -541.90200

C	0.91704700	-0.37057600	1.67247000
C	0.82545800	1.01761200	1.01768100
H	0.78739300	1.79387100	1.79105100
H	1.89144800	-0.49545200	2.15557200
H	0.14850700	-0.50796200	2.44314400
N	2.69481100	-0.05402600	-0.23548900
C	3.75308700	0.12227600	-1.21201000
H	4.22716400	-0.84220900	-1.42771300
H	3.39302600	0.55272400	-2.16974300
H	4.51858300	0.79575800	-0.80815900
C	1.67769300	-1.01750800	-0.64983500

H	2.19719100	-1.91688700	-1.00138400
H	1.09287400	-0.64414900	-1.51507300
C	0.72478500	-1.38550100	0.53440600
H	0.98949500	-2.38980400	0.88636200
C	2.12490000	1.22682300	0.19726100
H	1.91772900	1.88960900	-0.66784400
H	2.88437300	1.73293200	0.80937700
C	-0.45849300	1.14112900	0.12868200
H	-0.94063300	2.09619700	0.35662600
H	-0.18633100	1.18458300	-0.93350100
C	-1.46448400	-0.01384700	0.31298300
H	-1.83777200	0.03363400	1.35852900
C	-0.76570900	-1.38831000	0.11370700
H	-0.85675500	-1.67579300	-0.94216600
H	-1.29614900	-2.14996300	0.69753500
N	-2.62270500	0.11233400	-0.59958900
C	-3.30226900	1.40272500	-0.49892500
H	-2.65686200	2.21563100	-0.83891300
H	-4.18380200	1.39108200	-1.14813200
H	-3.64218400	1.63240200	0.53240400
C	-3.59394100	-0.96176000	-0.39599000
H	-4.42912900	-0.82888600	-1.09140300
H	-3.14657200	-1.93729200	-0.59871900
H	-4.00478600	-0.97656200	0.63511300

B3LYP/6-31+G* SCF energies in gas phase (E), and Cartesian coordinates for 2-CHMe$_2$-ax, 2-CHMe$_2$-eq, 3-CHMe$_2$-ax and 3-CHMe$_2$-eq (All energies are given in Hartee).

2-CHMe$_2$-ax

E= -831.87414

C	-0.58124300	-2.32214200	0.00002300
C	-0.70347800	-1.39353800	-1.21451500
C	0.43934900	-0.31331600	-1.21538500
C	0.44966100	0.68900600	-0.00004100
C	0.43941400	-0.31324800	1.21532300
C	-0.70338500	-1.39349600	1.21453700
C	-2.17765400	-0.93689100	-1.25422200
C	1.81369700	-1.02707500	-1.26702200
N	-0.71288400	1.58586400	-0.00002600
C	1.81381600	-1.02695000	1.26688000
C	-2.17755500	-0.93680300	1.25435500
N	2.21969500	-1.64533100	-0.00005500
C	3.59964600	-2.08054000	-0.00010000
N	-2.69460600	-0.38718600	0.00007500
C	-4.14110600	-0.30894500	0.00011500
C	-1.26370900	2.19390800	1.18646300
C	-1.26365700	2.19379800	-1.18658800
H	-0.55388400	-1.96642100	-2.14098200
H	0.36312600	0.23486900	-2.16021100
H	0.36322200	0.23498100	2.16013000
H	-0.55372600	-1.96635700	2.14100500
H	1.76744000	-1.82774700	-2.02140500
H	1.76768900	-1.82752400	2.02137500
H	3.79920400	-2.69432500	0.88680900
H	3.79914600	-2.69437400	-0.88699000
H	4.32312700	-1.23756800	-0.00014600
H	-1.40681700	-3.04839000	0.00007400
H	2.57594900	-0.31723600	-1.63415300
H	2.57607400	-0.31702300	1.63383100
H	-2.34709700	-0.19340400	-2.04520800
H	-2.75760900	-1.83765700	-1.55005200
H	-2.75752000	-1.83750900	1.55034100
H	-2.34684100	-0.19323300	2.04529700
H	-4.48861200	0.23433400	-0.88703600
H	-4.63062200	-1.30792500	0.00021600
H	-4.48856400	0.23448300	0.88719700
H	-2.35326300	2.02266400	1.22756200
H	-0.82699800	1.79574700	2.10184000
H	-1.10895500	3.28966300	1.20146400
H	-2.35322900	2.02263000	-1.22766400
H	-1.10883100	3.28954500	-1.20181700
H	-0.82704200	1.79546300	-2.10193700
H	0.35475200	-2.87879600	0.00000400
C	1.78089400	1.56688200	-0.00009800
H	2.65212700	0.90731500	-0.00042000
C	1.92392200	2.45717200	1.24939900
H	2.90465500	2.94972300	1.23826000
H	1.16411700	3.24395400	1.27481800
H	1.85757000	1.89333100	2.18665100
C	1.92335500	2.45782700	-1.24915600
H	1.16373600	3.24481300	-1.27356100
H	2.90423500	2.95008900	-1.23836300
H	1.85620000	1.89456400	-2.18670100

2-CHMe$_2$-eq

E= -831.87347

C	-0.81601800	-2.26830800	-0.00057000
C	-0.86427900	-1.33256700	-1.21433100
C	0.34664600	-0.32353800	-1.21333500
C	0.34665600	-0.32401600	1.21318800
C	-0.86406600	-1.33338900	1.21387800
C	-2.31055500	-0.79463200	-1.27226400
C	1.66797600	-1.13662500	-1.25695900
C	1.66798700	-1.13713400	1.25660000
C	-2.31051100	-0.79596200	1.27269400
N	1.98968100	-1.82325400	-0.00031700
C	3.33313500	-2.36383000	-0.00042000
N	-2.83699300	-0.29545700	0.00054500
C	-4.27430100	-0.13596100	0.00041200
H	-0.73826500	-1.91181900	-2.13953300
H	0.28865500	0.22391800	-2.16139900
H	0.28851200	0.22310000	2.16144000
H	-0.73754500	-1.91322000	2.13864300
H	1.57813900	-1.91130800	-2.03503000
H	1.57808000	-1.91213800	2.03434600
H	3.48423500	-2.99145500	0.88653800

H	3.48419500	-2.99122400	-0.88755000
H	4.11681000	-1.57734300	-0.00034000
H	-1.69595000	-2.92852400	-0.00069200
H	2.49430200	-0.48037500	-1.56783000
H	2.49433600	-0.48110700	1.56780400
H	-2.41044100	0.01071000	-2.01683700
H	-2.93099700	-1.63696700	-1.63935200
H	-2.93054600	-1.63898600	1.63892100
H	-2.41053700	0.00847200	2.01825700
H	-4.59007800	0.42830200	-0.88566300
H	-4.81732500	-1.10468200	-0.00141700
H	-4.59053700	0.42520300	0.88827500
H	0.07580200	-2.89084300	-0.00086100
C	0.42866900	0.68547400	0.00005500
N	1.79615900	1.30724800	0.00003900
C	2.31266200	1.97284900	-1.18581600
H	2.15441300	3.06624700	-1.17320100
H	3.40050700	1.80933800	-1.25150800
H	1.86611600	1.58906200	-2.10350400
C	2.31335600	1.97133700	1.18651100
H	3.40084800	1.80572600	1.25298100
H	2.15715200	3.06501900	1.17402000
H	1.86532600	1.58832000	2.10377800
C	-0.70298100	1.77795500	0.00024400
H	-1.65072100	1.24400300	0.00122100
C	-0.73909800	2.68469800	1.24891500
H	-1.68894900	3.23535300	1.26100600
H	-0.68461400	2.12634400	2.18978400
H	0.06102600	3.43185500	1.25480400
C	-0.74099200	2.68360800	-1.24915200
H	-1.69129700	3.23348000	-1.26086200
H	0.05851900	3.43139700	-1.25634700
H	-0.68680700	2.12461900	-2.18966600

3-CHMe$_2$-ax

E= -1083.71871

C	-1.66766900	0.14712500	0.00005100
C	-0.73859900	-0.29274300	1.19185300
C	0.73861200	0.29274000	1.19184600
C	1.66764400	-0.14712100	0.00002500
C	0.73859100	0.29268800	-1.19183100
C	-0.73863600	-0.29268400	-1.19181500
N	-1.97055200	1.58737200	0.00009800
C	-0.79494100	-1.83828200	1.27074100
C	0.79501600	1.83827400	1.27072200
N	1.97046100	-1.58737300	0.00004800
C	0.79499700	1.83821200	-1.27084100
C	-0.79503800	-1.83821400	-1.27080800
N	0.62006300	2.54273800	-0.00007300
C	-2.35646700	2.32127900	-1.18305700
C	-2.35641800	2.32118300	1.18333300
C	1.15182200	3.88568300	-0.00009900
N	-0.62006400	-2.54274400	-0.00005500
C	-1.15177200	-3.88570500	-0.00004900
C	2.35638800	-2.32120400	-1.18316300
C	2.35657900	-2.32114400	1.18323100
H	-1.15645800	0.04718400	2.14652300
H	1.15649900	-0.04721000	2.14649500
H	1.15645200	-0.04736900	-2.14645200
H	-1.15652500	0.04735800	-2.14642800
H	0.03562200	2.19144300	1.98062400
H	0.03554500	2.19130500	-1.98072800
H	-3.42626300	2.60327000	-1.16982800
H	-1.78070200	3.26073900	-1.24599000
H	-2.18494100	1.75785700	-2.09991200
H	-1.78067700	3.26066200	1.24628800
H	-3.42621400	2.60314800	1.17021500
H	-2.18476900	1.75771300	2.10014300
H	0.80138400	4.43018500	-0.88555600
H	0.80110600	4.43035800	0.88514500
H	2.26470600	3.92558800	0.00008300
H	1.76267600	2.11002900	1.72637700
H	1.76261600	2.10997100	-1.72657300
H	-0.03547200	-2.19141500	1.98058200
H	-1.76255000	-2.11006100	1.72648500
H	-1.76267600	-2.10998200	-1.72650200
H	-0.03561000	-2.19129500	-1.98072700
H	-0.80097400	-4.43037900	0.88516500
H	-2.26465700	-3.92566000	0.00021300
H	-0.80138100	-4.43019300	-0.88553200
H	1.78075900	-3.26074900	-1.24604300
H	2.18465600	-1.75779700	-2.09999300
H	3.42622800	-2.60302000	-1.17005900
H	1.78092900	-3.26067100	1.24626400
H	3.42640100	-2.60300900	1.16995300
H	2.18501600	-1.75769000	2.10007000
C	-3.04629200	-0.66063600	-0.00002800
H	-2.84392800	-1.73168600	-0.00012500
C	-3.91287300	-0.40009000	-1.24851500
H	-4.75048900	-1.10940800	-1.26389400
H	-4.34143600	0.60615100	-1.24729100
H	-3.36370600	-0.53075900	-2.18749900
C	-3.91296300	-0.40034200	1.24845000
H	-4.34141700	0.60594000	1.24747100
H	-4.75065300	-1.10957900	1.26352400
H	-3.36391400	-0.53133700	2.18745400
C	3.04626500	0.66061000	0.00000000
H	2.84390800	1.73166200	-0.00000400
C	3.91292500	0.40022700	1.24846800
H	4.34145000	-0.60602200	1.24739800
H	4.75056600	1.10952000	1.26364900
H	3.36383400	0.53109100	2.18746600
C	3.91285100	0.40013600	-1.24850100
H	4.75049000	1.10942800	-1.26381000
H	4.34138100	-0.60611900	-1.24736500
H	3.36369700	0.53090400	-2.18747800

3-CHMe$_2$-eq

E= -1083.71493

C	1.65945200	-0.31470900	-0.00008400
C	0.76744700	0.21606300	1.19102800
C	-0.76740700	-0.21617600	1.19104100
C	-1.65944400	0.31468600	-0.00001600
C	-0.76748300	-0.21608200	-1.19113100
C	0.76738000	0.21613000	-1.19115500
C	0.96432800	1.75221100	1.27509100
C	-0.96420500	-1.75235000	1.27501900
C	-0.96437500	-1.75224800	-1.27519000
C	0.96430700	1.75227800	-1.27513900
N	-0.91424100	-2.47141200	-0.00011300
C	-1.65707000	-3.71099800	-0.00007600
N	0.91406700	2.47142100	-0.00000900
C	1.65700500	3.71098400	0.00000900
H	1.13616400	-0.17752800	2.14629000
H	-1.13605100	0.17736800	2.14634500
H	-1.13617300	0.17753200	-2.14638900
H	1.13605900	-0.17741000	-2.14644600
H	-0.19040500	-2.16706400	1.94301700
H	-0.19070000	-2.16692800	-1.94334400
H	-1.39732100	-4.30562600	-0.88481800
H	-1.39685300	-4.30587400	0.88436800
H	-2.75561700	-3.55839900	0.00024000
H	-1.92283300	-1.95443400	1.76838300
H	-1.92310000	-1.95423500	-1.76840600
H	0.19066900	2.16689800	1.94325800
H	1.92306200	1.95423200	1.76824100
H	1.92305400	1.95428700	-1.76828200
H	0.19065400	2.16702700	-1.94326900
H	1.39709700	4.30564400	0.88467800
H	2.75552100	3.55829500	-0.00010900
H	1.39693100	4.30577000	-0.88452900
N	2.95831700	0.44376800	0.00002100
N	-2.95834500	-0.44387200	-0.00001100
C	-3.80027700	-0.47497000	-1.18683500
H	-4.26777700	-1.46836700	-1.28303000
H	-4.62238300	0.26190500	-1.15041000
H	-3.23462500	-0.28516200	-2.09938600
C	-3.79998600	-0.47534700	1.18698200
H	-4.62211000	0.26154800	1.15097300
H	-4.26746700	-1.46877300	1.28300600
H	-3.23415800	-0.28577800	2.09947300
C	3.80003800	0.47511700	1.18696600
H	4.62234300	-0.26154900	1.15064500
H	4.26724000	1.46864700	1.28327900
H	3.23429200	0.28507700	2.09941100
C	3.80014400	0.47528500	-1.18685100
H	4.26754000	1.46875600	-1.28280100
H	4.62231400	-0.26153800	-1.15070900
H	3.23444300	0.28567400	-2.09940700
C	-1.93643500	1.86406700	0.00010000
H	-0.97387200	2.36684600	0.00019900
C	-2.67182100	2.40183500	-1.24772000
H	-2.56630600	3.49433200	-1.27500200
H	-2.26361700	2.02125100	-2.19033700
H	-3.74528700	2.18736500	-1.23600100
C	-2.67208400	2.40157300	1.24785400
H	-2.56696000	3.49411300	1.27518300
H	-3.74547900	2.18674800	1.23607900
H	-2.26380500	2.02113200	2.19049400
C	1.93649000	-1.86409800	-0.00003200
H	0.97398500	-2.36690100	-0.00001900
C	2.67203800	-2.40146800	1.24782200
H	2.56711900	-3.49402300	1.27513900
H	3.74539300	-2.18642600	1.23619700
H	2.26353300	-2.02107900	2.19039300
C	2.67207700	-2.40177600	-1.24775100
H	2.56672200	-3.49428900	-1.27503700
H	2.26393500	-2.02127200	-2.19042900
H	3.74552200	-2.18717600	-1.23593800