Electronic Supplementary Information

First Principle studies Toward the Design of a New Class of Carbene Superbases involving Intramolecular H···π Interactions

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Computational Section

Calculations were performed for compound **1-9** 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. The geometry optimization of compound **10** was performed at the Hartree-Fock method[3] using 6-31G* basis set. Single-point calculations were then carried out with the B3LYP/6-311+G** level using HF/6-31G* optimized geometries. Zero-point vibrational energies (ZPVE) computed at B3LYP/6-31+G* and HF/6-31G* level used in the proton affinity calculations are unscaled. Proton affinities calculated at B3LYP/6-311+G**//B3LYP/6-31+G* and B3LYP/6-311+G**// HF/6-31G* 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.[4]

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

In general, electron rich regions are shown by highly negative MESP whereas electron deficient regions are characterized by positive MESP.[5] The most negative valued point (V_{min}) in electron rich regions can be determined from the MESP topography calculation.[6] 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)[7-11] through single-point energy calculations at the B3LYP/6-311+G** level of theory (using the gas-phase optimized geometries). The p*K*a value of the acid BH^+ is calculated using the following relation,

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

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. All quantum chemical calculations were performed using Gaussian 03, Revision E.01 program.[16]

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.

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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.

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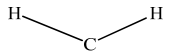
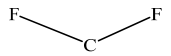
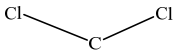
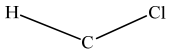
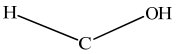
Table S1 Comparison of experimental and computed (B3LYP/6-311+G**//B3LYP/6-31+G*) Proton Affinities[a] (kcal/mol) for some carbenes.

Carbene	Proton Affinity(gas phase)
	206.9(206.3±0.8)[b]
	173.8(172.0±2.0)[b]
	207.0(205.2±1.9)[c]
	212.3(209.7±2.2)[c]
	224.9(230.9)[d]

[a] Experimental Proton Affinity value is given in parenthesis.

[b] J. R. Pliego Jr. and W. B. D. Almeida, *J. Chem. Soc., Faraday Trans.*, 1997, **93**, 1881 and references therein.

[c] Z. Tian and S. R. Kass, *Int. J. Mass Spectrom.*, 2007, **267**, 288.

[d] M. H. Matus, M. T. Nguyen and D. A. Dixon, *J. Phys. Chem. A*., 2006, **110**, 8864 and references therein.

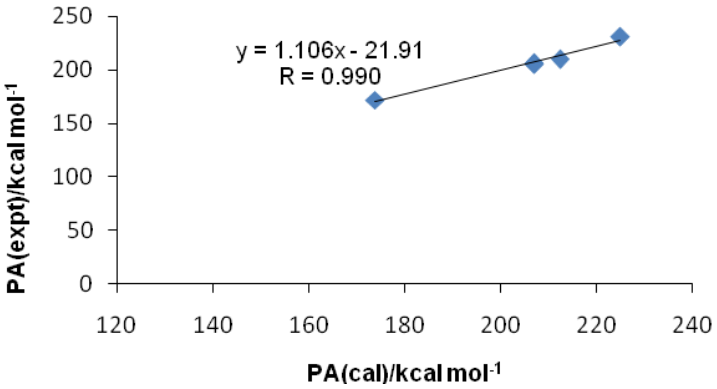


Fig. S1 Correlation between experimental and calculated proton affinities of carbene bases.

Table S2 Proton affinity values (kcal/mol) calculated at M05-2X/6-311+G**//B3LYP/6-31+G* and MP2/6-311+G**//B3LYP/6-31+G* of carbene **5** and **6**.

	M05-2X	MP2
5	280.2	281.2
6	284.5	285.8

Table S3 Calculated bond lengths (Å), bond angles (º) of the free bases **5-9** and their corresponding conjugate acids at B3LYP/6-31+G* level of theory.

	Bond length		Bond angle
	C···Ph center	H···Ph center	C-H···Ph center
5	3.214		
5H$^+$	3.225	2.200	157.0
6	3.317		
6H$^+$	3.359	2.27	180.0
7	3.420		
7H$^+$	3.387	2.298	180.0
8	3.405		

8H$^+$	3.402	2.313	180.0
9	3.410		
9H$^+$	3.360	2.269	180.0

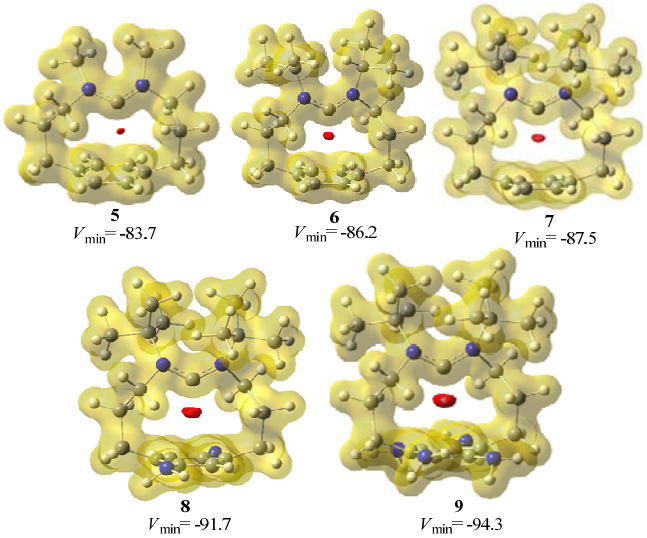


Fig. S2 Representation of the MESP isosurface at -81.6 kcal/mol. V_{min} in kcal/mol.

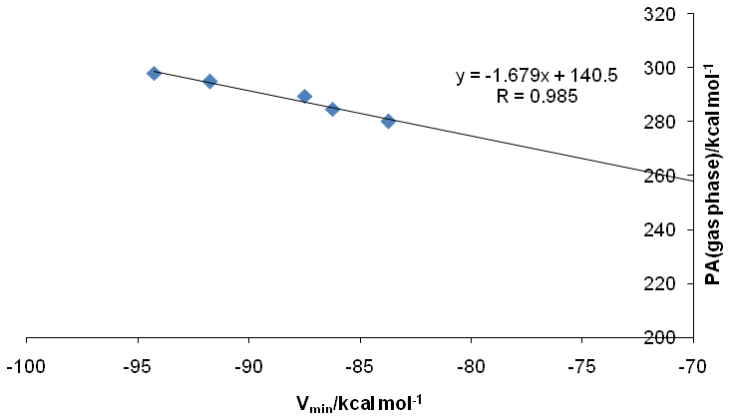
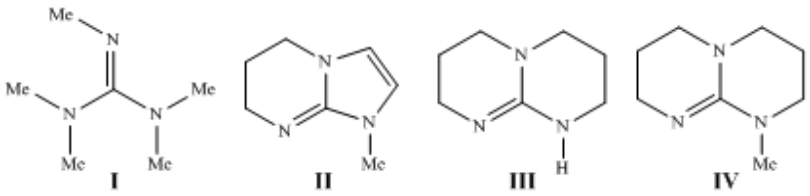


Fig. S3 Correlation between V_{min} and proton affinity in gas phase for **5-9**.



Scheme S1

Table S4 Comparison of experimental and calculated (B3LYP/6-311+G**//B3LYP/6-31+G*) p*K*a(MeCN) of some gauge molecules.

	p*K*a(MeCN)	
Compounds	Experimental[a]	Calculated
I	25.0	24.1
II	24.55	23.03
III	25.96	26.54
IV	25.43	25.86

[a] B. Kovaćević and Z. B. Maksić, *Org. Lett*., 2001, **3**, 1523.

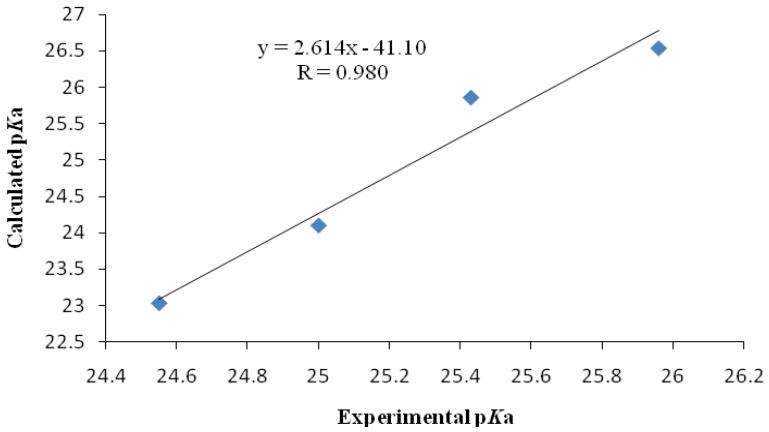


Fig. S4 Correlation between experimental and calculated p*K*a of some gauge molecules.

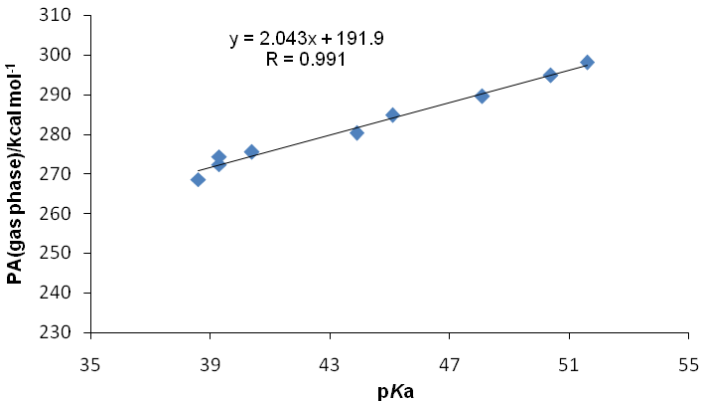


Fig. S5 Correlation between p*K*a and proton affinity in gas phase for **1**-**9**.

Table S5 Calculated parameters of carbenes **1**-**9**: HOMO energy (E_{HOMO}), HOMO-LUMO gap (HLG) and singlet-triplet energy gap ($E_{S\text{-}T}$). (E_{HOMO}, HLG in eV; $E_{S\text{-}T}$ in kcal/mol).

Carbene	E_{HOMO}	HLG	$E_{S\text{-}T}$
1	-4.98	4.90	41.9
2	-4.73	4.59	37.8
3	-4.80	4.73	41.5
4	-4.67	4.55	43.0
5	-4.72	4.45	38.1
6	-4.49	4.25	39.0
7	-4.03	3.78	17.8
8	-3.82	3.63	17.9
9	-3.72	3.44	17.5

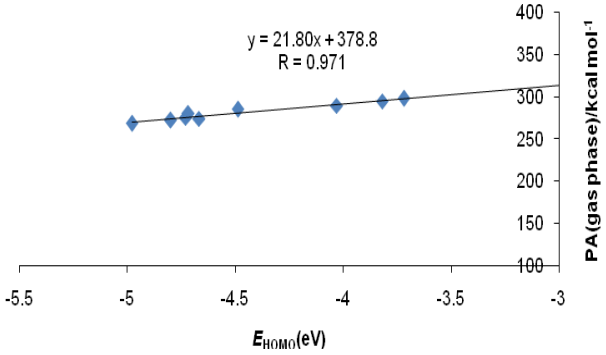


Fig. S6 Correlation between calculated PA in gas phase and E_{HOMO} of carbene bases.

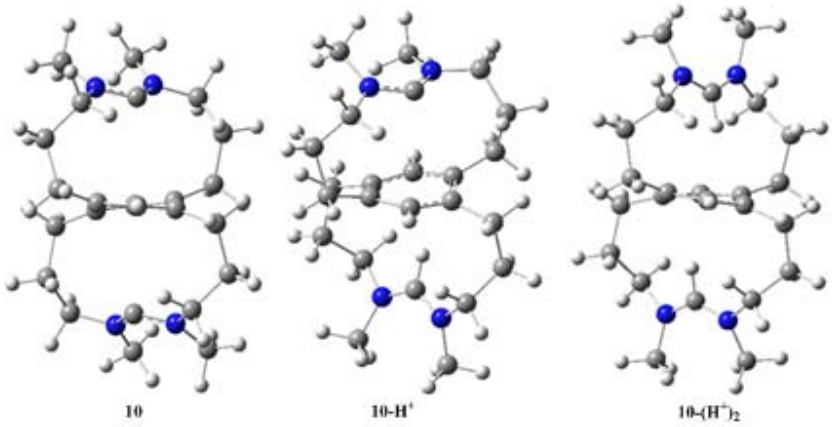


Fig. S7 HF/6-31G* optimized geometries of compound **10** and its mono- and bis-protonated form [Gray = carbon; blue = nitrogen; white = hydrogen].

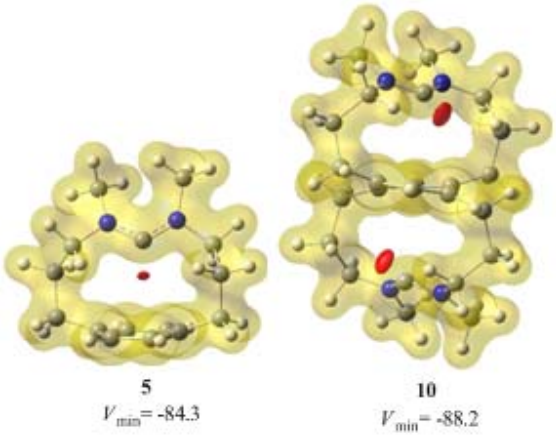


Fig. S8 Representation of the MESP isosurface of HF/6-31G* optimized **5** and **10** at -81.6 kcal/mol. V_{min} in kcal/mol.

B3LYP/6-311+G//B3LYP/6-31+G* SCF energies in gas phase (**E**), **B3LYP/6-31+G* zero point vibrational energies (**ZPVE**), and Cartesian coordinates for 1-9 and their corresponding monoprotonated cations (All energies are given in Hartee).**

1

E = -307.27343

ZPVE = 0.170815

C	0.00004700	-0.81736700	0.00001400
N	1.16886900	-0.13776100	-0.01813600
N	-1.16882500	-0.13792800	0.01767700
C	-2.38094000	-0.93629800	0.19973800
H	-2.97043500	-0.55558100	1.04567600
H	-3.01219700	-0.90322700	-0.70122200
H	-2.08649700	-1.96607100	0.40037500
C	-1.45959000	1.26431600	-0.33053000
H	-2.37062500	1.28795100	-0.94046800
H	-1.63314400	1.89551000	0.55226700
H	-0.65247700	1.69014900	-0.92605500
C	1.45946100	1.26425700	0.33062500
H	1.63315500	1.89583400	-0.55188800
H	0.65221100	1.68993900	0.92610200
H	2.37034300	1.28782700	0.94081300
C	2.38101100	-0.93621600	-0.19958400
H	2.08658900	-1.96581600	-0.40106300
H	2.97127300	-0.55509100	-1.04481900
H	3.01156100	-0.90375600	0.70192000

1H$^+$

E = -307.71688

ZPVE = 0.186217

C	-0.00000100	-0.65172700	0.00000500
N	1.20493500	-0.10220200	0.02592800
N	-1.20493700	-0.10220000	-0.02592500
C	-2.38324200	-0.97004600	0.17168000
H	-2.94165600	-0.62916400	1.04897100
H	-3.02837700	-0.91801600	-0.71009700
H	-2.07173000	-2.00293200	0.33412300
C	-1.52413200	1.31740800	-0.25735500
H	-2.46002200	1.35693500	-0.81938500
H	-1.66436800	1.85073200	0.68842900
H	-0.75053100	1.79785600	-0.85326700
C	1.52414000	1.31740500	0.25735400
H	1.66439000	1.85071900	-0.68843300
H	0.75053800	1.79786600	0.85325300
H	2.46002400	1.35692600	0.81939400
C	2.38323700	-0.97005000	-0.17168300
H	2.07172100	-2.00292700	-0.33417300
H	2.94167200	-0.62913900	-1.04894900
H	3.02835400	-0.91805600	0.71010900
H	-0.00000200	-1.73791900	-0.00000200

2

E = -464.56668

ZPVE = 0.284671

C	0.00000500	1.40849600	-0.00005500
N	1.18994000	0.76992800	0.11316900
N	-1.18992800	0.76991800	-0.11325200
C	-2.32873100	1.67260200	-0.34172500
H	-2.96903300	1.29657700	-1.14976000
H	-2.94243400	1.79245100	0.56039900
H	-1.92903900	2.64403500	-0.62651200
C	-1.57833400	-0.65550800	0.10981000
H	-0.73152700	-1.13583000	0.59601500
C	1.57835800	-0.65550600	-0.10984300
H	0.73158900	-1.13582500	-0.59611200
C	2.32871700	1.67261400	0.34176000
H	1.92898600	2.64405300	0.62647300
H	2.96892300	1.29661300	1.14988400
H	2.94252900	1.79244100	-0.56029100
C	-2.75224900	-0.78915800	1.09648600
H	-3.69944100	-0.43951700	0.67225200
H	-2.88097000	-1.84619200	1.35948800
H	-2.55912400	-0.23103000	2.01937400
C	-1.88220300	-1.38818000	-1.20780000
H	-2.09325800	-2.44862000	-1.01832400
H	-2.76019300	-0.96018300	-1.70539300
H	-1.04081100	-1.32509900	-1.90661600
C	1.88208100	-1.38816500	1.20780500
H	2.09312700	-2.44861400	1.01836500
H	2.76003500	-0.96018400	1.70547700
H	1.04062200	-1.32505300	1.90653900
C	2.75235700	-0.78920100	-1.09641500
H	3.69952200	-0.43958500	-0.67210100
H	2.88107100	-1.84624300	-1.35939100
H	2.55933300	-0.23108200	-2.01932800

2H$^+$

E = -465.02113

ZPVE = 0.300148

C	-0.00000100	1.25899600	-0.00000200
N	-1.21713200	0.73422500	-0.08825500
N	1.21713000	0.73422700	0.08825400
C	2.32729300	1.67661700	0.35430200
H	2.93711300	1.29837500	1.17774200
H	2.95196200	1.79448000	-0.53393100
H	1.92972500	2.64885400	0.64732700
C	1.60807200	-0.69942400	-0.11978600
H	0.75678200	-1.17411600	-0.60438300
C	-1.60807200	-0.69942500	0.11979400
H	-0.75678900	-1.17410900	0.60441000
C	-2.32729600	1.67661200	-0.35430900
H	-1.92972900	2.64884800	-0.64733900
H	-2.93711500	1.29836500	-1.17774700
H	-2.95196500	1.79447900	0.53392400
C	2.78720100	-0.80468600	-1.09757000
H	3.72534700	-0.44439200	-0.66487300

H	2.93059900	-1.86019000	-1.34951600
H	2.59261700	-0.26179200	-2.02860600
C	1.90137800	-1.39550200	1.21579300
H	2.10648200	-2.45584100	1.03547500
H	2.78390900	-0.97120100	1.70584500
H	1.05977500	-1.32527400	1.91327800
C	-1.90135600	-1.39551800	-1.21578100
H	-2.10646000	-2.45585600	-1.03545500
H	-2.78388100	-0.97122500	-1.70585200
H	-1.05974200	-1.32529600	-1.91325400
C	-2.78721700	-0.80467900	1.09756100
H	-3.72535500	-0.44438600	0.66484700
H	-2.93061900	-1.86018100	1.34951200
H	-2.59264600	-0.26178000	2.02859700
H	-0.00000200	2.34511700	-0.00000600

3

E = -464.57402

ZPVE = 0.283731

C	-0.00002200	-0.11974200	-0.00006500
N	-1.16292100	0.56190800	0.04865000
N	1.16288200	0.56185800	-0.04883700
C	2.40388700	-0.25215600	-0.19712200
H	3.20198200	0.47404900	-0.40110400
C	1.42373200	1.93841700	0.41611800
H	2.30714000	1.93228600	1.06491200
H	1.61625400	2.63884500	-0.40820800
H	0.58660300	2.30534900	1.01047000
C	-1.42385600	1.93837100	-0.41649100
H	-1.61695700	2.63878300	0.40771700
H	-0.58653800	2.30549100	-1.01044500
H	-2.30694300	1.93199900	-1.06573400
C	-2.40387700	-0.25215100	0.19705200
H	-3.20208600	0.47407100	0.40053700
C	2.32949600	-1.19982400	-1.39661500
H	2.08706500	-0.64883500	-2.31284700
H	3.29695200	-1.69837600	-1.53794000
H	1.55808700	-1.95901500	-1.24192000
C	2.73905900	-0.99659500	1.10277000
H	2.82252500	-0.30492100	1.95032300
H	1.94751400	-1.71909900	1.32736900
H	3.69158700	-1.53282700	1.00944600
C	-2.32970200	-1.19924700	1.39701900
H	-1.55818500	-1.95847700	1.24298500
H	-2.08754400	-0.64778000	2.31303000
H	-3.29714500	-1.69783400	1.53832200
C	-2.73868900	-0.99721900	-1.10256200
H	-3.69100800	-1.53380700	-1.00910000
H	-2.82239600	-0.30590200	-1.95037900
H	-1.94681100	-1.71948000	-1.32674900

3H$^+$

E = -465.02384

ZPVE = 0.299498

C	0.00000000	0.04724900	-0.00000800
N	1.20373500	0.59480900	-0.06215600
N	-1.20373200	0.59481400	0.06213900
C	-2.40583000	-0.29727000	0.27031600
H	-3.16195200	0.38744100	0.66708900
C	-1.52170200	2.00627500	-0.21064600
H	-2.47139500	2.03768500	-0.74911000
H	-1.63063500	2.57632800	0.71777300
H	-0.76445400	2.46275400	-0.84578000
C	1.52170100	2.00627300	0.21061600
H	1.63057200	2.57633600	-0.71780400
H	0.76448300	2.46273500	0.84580000
H	2.47142600	2.03769300	0.74902400
C	2.40582900	-0.29728100	-0.27032600
H	3.16194000	0.38741000	-0.66715300
C	-2.16949300	-1.38185600	1.32474300
H	-1.74931800	-0.96583600	2.24668700
H	-3.13090400	-1.84201600	1.57329800
H	-1.51884300	-2.18855200	0.96814400
C	-2.89153800	-0.86255700	-1.06912200
H	-3.07972600	-0.07251700	-1.80379300
H	-2.15828100	-1.55909500	-1.49272600
H	-3.82759100	-1.41099700	-0.92194700
C	2.16946000	-1.38192000	-1.32469000
H	1.51881900	-2.18859700	-0.96803200
H	1.74926000	-0.96594600	-2.24664400
H	3.13086400	-1.84209200	-1.57324800
C	2.89157100	-0.86250600	1.06912700
H	3.82761800	-1.41095700	0.92195200
H	3.07978200	-0.07243300	1.80375600
H	2.15832100	-1.55902100	1.49278300
H	-0.00000200	-1.03612600	-0.00001000

4

E = -543.21455

ZPVE = 0.339826

C	-0.00001900	-0.24573800	-0.00005200
N	-1.16007400	0.45224600	-0.03158300
N	1.16003500	0.45216100	0.03181900
C	2.43500100	-0.34913000	-0.06188600
C	-2.43500900	-0.34917400	0.06188700
C	3.55517500	0.54549500	-0.63110200
H	3.26099500	0.96671200	-1.60009700
H	3.82723700	1.37095200	0.03444500
H	4.45726900	-0.05667900	-0.78549100
C	2.82100400	-0.88713800	1.33061100
H	3.73849000	-1.48532800	1.27224800
H	3.00036000	-0.07976200	2.05070000
H	2.01630100	-1.52174300	1.71689100
C	-3.55584900	0.54574400	0.62933900
H	-3.82856400	1.36967900	-0.03782200
H	-4.45746500	-0.05684500	0.78488700
H	-3.26203300	0.96905200	1.59753100
C	-2.81975300	-0.88857800	-1.33040000
H	-3.73776100	-1.48601200	-1.27247300
H	-2.99759900	-0.08186400	-2.05161300

H	-2.01503300	-1.52418600	-1.71498400
C	-2.24684700	-1.53137600	1.02814800
H	-1.49980700	-2.23430200	0.65815100
H	-1.91845800	-1.17916400	2.01281100
H	-3.20498900	-2.05309000	1.14780100
C	2.24635900	-1.53238900	-1.02676400
H	3.20500900	-2.05279300	-1.14807400
H	1.50119100	-2.23615700	-0.65459000
H	1.91525600	-1.18150100	-2.01097100
C	1.30720700	1.79496000	0.63198100
H	2.11770800	1.78447100	1.36648700
H	1.52636900	2.58155000	-0.10043500
H	0.39292300	2.05218200	1.16776100
C	-1.30726100	1.79496100	-0.63192700
H	-2.11747000	1.78426700	-1.36676300
H	-1.52685500	2.58156400	0.10034500
H	-0.39285100	2.05233300	-1.16740200

4H$^+$

E = -543.66812

ZPVE = 0.356156

C	-0.00000500	-0.08074300	0.00000700
N	-1.20000600	0.47898900	-0.09888500
N	1.19999700	0.47898400	0.09890700
C	2.46399200	-0.37446500	-0.05427300
C	-2.46399300	-0.37447000	0.05427000
C	3.43504000	0.39964200	-0.96600300
H	2.99044100	0.58737300	-1.94973800
H	3.75026900	1.35451000	-0.53638400
H	4.33878900	-0.19909700	-1.11379300
C	3.07646900	-0.62041300	1.33715000
H	3.97072200	-1.24311400	1.23357900
H	3.38572700	0.30338700	1.83517100
H	2.37267800	-1.14757100	1.99071100
C	-3.43495500	0.39949700	0.96621000
H	-3.75021400	1.35443900	0.53677900
H	-4.33869700	-0.19925800	1.11397700
H	-2.99027200	0.58705900	1.94994000
C	-3.07658600	-0.62018000	-1.33714300
H	-3.97086400	-1.24284800	-1.23360000
H	-3.38582900	0.30371500	-1.83500100
H	-2.37287100	-1.14727500	-1.99083600
C	-2.14907000	-1.72612100	0.71735300
H	-1.58034600	-2.40304100	0.07026400
H	-1.62334900	-1.60767300	1.67170900
H	-3.09738700	-2.22826100	0.92853800
C	2.14912600	-1.72600800	-0.71760000
H	3.09746200	-2.22813000	-0.92874600
H	1.58031400	-2.40301600	-0.07068000
H	1.62352600	-1.60740800	-1.67200200
C	1.40172000	1.88066800	0.51090200
H	2.27417800	1.92652700	1.16186500
H	1.57094300	2.54343900	-0.34159100
H	0.54476100	2.22533100	1.08706500
C	-1.40173400	1.88067000	-0.51088700
H	-2.27418000	1.92651300	-1.16186700
H	-1.57098100	2.54344200	0.34159900
H	-0.54476700	2.22533800	-1.08703600
H	-0.00001000	-1.15865600	0.00000700

5

E = -694.44211

ZPVE = 0.346885

C	0.10702900	-2.42899400	-0.95101200
C	1.43274500	-2.00430600	-0.90052100
C	1.94651300	-1.39488700	0.25134000
C	1.15562700	-1.40908300	1.40787600
C	-0.17201700	-1.83361600	1.35692900
C	-0.74245100	-2.25051400	0.14697700
H	-0.29915500	-2.80686700	-1.88789900
H	2.05050900	-2.06739600	-1.79494700
H	1.55152900	-1.00067100	2.33684300
H	-0.79325700	-1.75833300	2.24781200
C	3.19747200	-0.55096900	0.18039400
H	3.86182000	-0.73765900	1.03543100
H	3.76791800	-0.80329400	-0.72337500
C	-2.23735000	-2.27281400	-0.05438300
H	-2.76017800	-2.46903500	0.89207400
H	-2.52048900	-3.07818000	-0.74537700
C	2.84811800	0.96602600	0.16472500
H	2.44173800	1.23070700	1.14857800
H	3.78556900	1.52868900	0.05434600
C	-2.73765400	-0.92642200	-0.65382100
H	-2.15372900	-0.69338300	-1.54916700
H	-3.78045100	-1.07078500	-0.96878000
C	1.82751600	1.40694400	-0.92844400
H	1.59319800	0.58047900	-1.59903400
H	2.26132300	2.21249400	-1.53714700
C	-0.49620300	1.02010700	-0.42289100
C	-2.68662800	0.28941900	0.30372500
H	-2.47214400	-0.05147300	1.32747600
H	-3.68159400	0.74665500	0.34094200
N	-1.73741300	1.38405100	-0.03105200
N	0.53477400	1.89276800	-0.39892600
C	0.65354500	3.22696600	0.23060300
H	0.43999500	4.04313600	-0.47362600
H	-0.00325100	3.31447800	1.09588400
H	1.68012000	3.35809300	0.58668200
C	-2.29329400	2.72357100	0.25142300
H	-2.30259300	2.97330400	1.32317100
H	-1.73781800	3.48658900	-0.29065800
H	-3.32839700	2.75615100	-0.10690100

5H$^+$

E = -694.90456

ZPVE = 0.362867

C	-0.43917600	-2.23087000	-1.10698300
C	0.95020700	-2.09211100	-1.05581400
C	1.59937700	-1.77089700	0.14717900

C	0.83656100	-1.78074900	1.32471300
C	-0.55224000	-1.92747100	1.27521500
C	-1.21986800	-2.05847100	0.04612900
H	-0.92373800	-2.41190800	-2.06443000
H	1.52971700	-2.18181500	-1.97254500
H	1.32237400	-1.61624500	2.28454800
H	-1.12608100	-1.88973700	2.19898000
C	3.01181400	-1.23471800	0.14197200
H	3.59905500	-1.64194600	0.97347300
H	3.52499700	-1.52861400	-0.78146000
C	-2.70256500	-1.79759400	-0.07364500
H	-3.21222000	-1.99840500	0.87662800
H	-3.15979900	-2.45311400	-0.82382200
C	3.02305000	0.31790800	0.26561200
H	2.66435700	0.59715400	1.26378500
H	4.06204700	0.66080000	0.20225800
C	-2.96637800	-0.32298400	-0.50023900
H	-2.50500800	-0.13818100	-1.47780700
H	-4.04514800	-0.19232500	-0.64298300
C	2.17284800	1.05865600	-0.80430100
H	1.80668900	0.37069900	-1.56835800
H	2.77115800	1.81210300	-1.32416200
C	-0.18061100	1.17917700	-0.18798000
C	-2.47102600	0.73691700	0.52253600
H	-2.11686400	0.25467500	1.43763000
H	-3.29573900	1.38943600	0.81350900
N	-1.38961900	1.67104800	0.06524900
N	0.99217000	1.79665200	-0.26116200
C	1.29000000	3.13842600	0.26366500
H	1.32355400	3.88361300	-0.53819600
H	0.56171000	3.43182600	1.01804400
H	2.27288300	3.09826300	0.74012900
C	-1.76618800	3.09020200	-0.03420700
H	-1.83857800	3.56309000	0.95112800
H	-1.05542000	3.63219800	-0.65613600
H	-2.74476200	3.14191700	-0.51862300
H	-0.14787200	0.11009200	-0.36330600
H	-2.48371900	3.38490800	0.75260900
H	-2.78230700	3.37817100	-0.98592400
C	-0.74115200	-2.86195300	0.46553200
H	-0.56058900	-2.29865700	1.38703500
H	-0.43947100	-3.90085700	0.65928100
C	-0.74117700	2.86191400	-0.46573600
H	-0.56086700	2.29853300	-1.38722500
H	-0.43937900	3.90076400	-0.65956900
C	0.13651300	-2.25283900	-0.66271500
H	-0.50400600	-1.82858200	-1.43670100
H	0.72475800	-3.04128900	-1.14386700
C	0.44610900	0.00005000	-0.00047400
C	0.13664000	2.25269900	0.66235100
H	-0.50376600	1.82837900	1.43640700
H	0.72495900	3.04112700	1.14350500
N	1.07330100	1.17360200	0.24586500
N	1.07314800	-1.17361000	-0.24656600
C	2.49151100	-1.59670700	-0.04497800
H	2.97115200	-0.79397800	0.51343300
C	2.49183000	1.59664400	0.04492500
H	2.97160400	0.79404900	-0.51360100
C	2.59978100	-2.84571100	0.84778800
H	2.06030000	-2.70311700	1.79009600
H	2.20764100	-3.74538600	0.36112800
H	3.65439100	-3.03458800	1.08346200
C	3.24267300	-1.79334800	-1.37213000
H	4.29869100	-2.03071100	-1.18801400
H	2.81424700	-2.61893600	-1.95277000
H	3.19635200	-0.89220600	-1.99373700
C	2.60029000	2.84591300	-0.84743800
H	2.20779100	3.74539000	-0.36070000
H	3.65494600	3.03505700	-1.08267900
H	2.06118400	2.70347800	-1.78998000
C	3.24254200	1.79291200	1.37236300
H	4.29864800	2.03020300	1.18866700
H	2.81402100	2.61840100	1.95306700
H	3.19591400	0.89161700	1.99373100

6

E = -851.73697
ZPVE = 0.460071

C	-2.87096100	0.62786300	-1.23636400
C	-2.87478700	-0.76424500	-1.15739600
C	-2.75968100	-1.41064700	0.08039600
C	-2.87030100	-0.62771100	1.23671000
C	-2.87411600	0.76438000	1.15774200
C	-2.75967600	1.41079000	-0.08012700
H	-2.85228800	1.10723300	-2.21413800
H	-2.87322100	-1.35233400	-2.07378400
H	-2.85114300	-1.10710700	2.21446100
H	-2.87204200	1.35250500	2.07411000
C	-2.27243100	-2.83804200	0.17671800
H	-2.78220600	-3.37805500	0.98606700
H	-2.48397200	-3.38473500	-0.75252500
C	-2.27240100	2.83816700	-0.17665600

6H$^+$

E = -852.20722
ZPVE = 0.476416

C	-2.81992000	0.66838800	-1.21952400
C	-2.82532400	-0.72823000	-1.18298100
C	-2.72364800	-1.41661100	0.03667100
C	-2.81991700	-0.66840300	1.21952700
C	-2.82532800	0.72821500	1.18298500
C	-2.72365500	1.41659700	-0.03666700
H	-2.82505700	1.17783500	-2.18125300
H	-2.84985100	-1.28691000	-2.11656800
H	-2.82505200	-1.17785000	2.18125700
H	-2.84986000	1.28689500	2.11657200
C	-2.28876500	-2.86279700	0.08265800
H	-2.81545700	-3.41410800	0.87043700
H	-2.51588100	-3.36741700	-0.86441900
C	-2.28878100	2.86278500	-0.08265400

H	-2.51589600	3.36740300	0.86442400
H	-2.81547900	3.41409400	-0.87043100
C	-0.76111100	-2.95201300	0.37377700
H	-0.56362200	-2.49999900	1.35228000
H	-0.47980900	-4.00793000	0.45973500
C	-0.76112900	2.95201000	-0.37377900
H	-0.56364000	2.49999500	-1.35228300
H	-0.47983300	4.00792900	-0.45974000
C	0.12846600	-2.26742400	-0.70173800
H	-0.48837400	-1.81063600	-1.47770300
H	0.75337000	-3.00450600	-1.20649600
C	0.53368900	0.00000300	-0.00000400
C	0.12845800	2.26742800	0.70173300
H	-0.48837500	1.81063900	1.47770300
H	0.75336100	3.00451500	1.20648600
N	1.06460400	1.20357000	0.20986700
N	1.06460800	-1.20356200	-0.20987500
C	2.48461700	-1.60802600	0.03302000
H	2.93957600	-0.78733900	0.58554800
C	2.48460800	1.60804300	-0.03303300
H	2.93956000	0.78737600	-0.58559700
C	2.54763800	-2.83997100	0.94790700
H	2.00674000	-2.67346700	1.88465900
H	2.14998100	-3.73983500	0.46855100
H	3.59600400	-3.03854100	1.19347000
C	3.24969400	-1.82552900	-1.27974000
H	4.30229900	-2.03220000	-1.05955000
H	2.85914000	-2.68223500	-1.83908000
H	3.20381100	-0.94823700	-1.93392000
C	2.54761300	2.84002200	-0.94787500
H	2.14995700	3.73986600	-0.46848100
H	3.59597600	3.03860700	-1.19344300
H	2.00670500	2.67355000	-1.88462700
C	3.24970500	1.82549700	1.27972300
H	4.30230600	2.03217400	1.05952500
H	2.85916100	2.68218300	1.83910000
H	3.20383000	0.94818100	1.93387200
H	-0.55155300	0.00000100	-0.00000300

7

E = -930.33599

ZPVE = 0.516624

C	3.13421500	-0.86767200	-1.08190300
C	3.13275700	0.51046000	-1.29085700
C	3.02471700	1.39504800	-0.21081400
C	3.13417900	0.86717200	1.08204100
C	3.13244400	-0.51096000	1.29099400
C	3.02443700	-1.39553000	0.21093200
H	3.11637000	-1.53818100	-1.93994600
H	3.11631000	1.53768400	1.94008100
C	2.54398500	2.81302300	-0.40524300
H	3.10576000	3.51504400	0.22625300
H	2.69244300	3.13386600	-1.44538900
C	2.54339000	-2.81340700	0.40527600
H	2.69161000	-3.13428100	1.44544700
H	3.10511900	-3.51554600	-0.22613000
C	1.03869400	2.92525500	-0.02547000
H	0.92402400	2.57027000	1.00426700
H	0.76725800	3.98881000	-0.03202100
C	1.03813800	-2.92530300	0.02525700
H	0.92366000	-2.57000600	-1.00439400
H	0.76651200	-3.98881400	0.03146500
C	0.06992900	2.12027700	-0.94164000
H	0.65511300	1.49575900	-1.61469700
H	-0.49987000	2.80216300	-1.58181100
C	-0.28729500	-0.00002300	-0.00010200
C	0.06938200	-2.12041800	0.94150400
H	0.65451800	-1.49618700	1.61487000
H	-0.50065000	-2.80241600	1.58134700
N	-0.90601300	-1.19556500	0.28144600
N	-0.90572000	1.19568800	-0.28155800
C	-2.17277500	1.84332700	0.28881000
C	-2.17320900	-1.84295800	-0.28880400
C	-1.99518300	3.37427300	0.45460500
H	-1.12975800	3.62936400	1.06820600
H	-1.92655500	3.90795700	-0.49815400
H	-2.88316900	3.75400700	0.97282400
C	-3.41367900	1.68459800	-0.61801300
H	-4.23820800	2.28957400	-0.21913400
H	-3.19249800	2.05036800	-1.62809200
H	-3.77559500	0.66336400	-0.70447200
C	-1.99569600	-3.37389800	-0.45474400
H	-1.92622300	-3.90757100	0.49795900
H	-2.88410000	-3.75368700	-0.97220600
H	-1.13075800	-3.62893800	-1.06906800
C	-3.41396500	-1.68418000	0.61822100
H	-4.23858800	-2.28912500	0.21948600
H	-3.19262800	-2.04994900	1.62826500
H	-3.77582000	-0.66292600	0.70473700
C	-2.39403500	-1.31113000	-1.72281300
H	-2.28824600	-0.23248300	-1.80350300
H	-1.65367200	-1.75741500	-2.39641500
H	-3.39171800	-1.59182300	-2.08262100
C	-2.39349700	1.31162500	1.72288200
H	-3.39110400	1.59246900	2.08278500
H	-2.28784500	0.23296600	1.80362800
H	-1.65299800	1.75785800	2.39636800
H	3.12064000	-0.89961700	2.30802000
H	3.12120000	0.89911900	-2.30788500

7H$^+$

E = -930.81394

ZPVE = 0.533174

C	-3.03159700	-0.97038500	0.99473900
C	-3.02691600	0.38335300	1.33660900
C	-2.93439200	1.37231800	0.34599300
C	-3.03161600	0.97037100	-0.99473200
C	-3.02692900	-0.38336600	-1.33660300
C	-2.93438600	-1.37233100	-0.34598700
H	-3.04018900	-1.71943000	1.78429000

H	-3.04022200	1.71941600	-1.78428300
C	-2.51581500	2.78361900	0.68303900
H	-3.13164400	3.52120900	0.15404000
H	-2.63805500	2.97958400	1.75529000
C	-2.51580500	-2.78362900	-0.68303900
H	-2.63805300	-2.97959500	-1.75528800
H	-3.13162600	-3.52122200	-0.15403400
C	-1.03806200	3.01071900	0.25897200
H	-0.96645400	2.82280400	-0.81598400
H	-0.78558200	4.06657200	0.40738100
C	-1.03804700	-3.01072400	-0.25898200
H	-0.96643600	-2.82282200	0.81597600
H	-0.78556200	-4.06657400	-0.40740400
C	-0.00383400	2.12443000	1.01413100
H	-0.51556700	1.48187500	1.73307600
H	0.67404600	2.74206300	1.60744400
C	0.36040700	0.00000100	0.00000500
C	-0.00382800	-2.12442100	-1.01413500
H	-0.51556900	-1.48185900	-1.73306700
H	0.67405100	-2.74204100	-1.60746200
N	0.88469900	-1.22063900	-0.19873200
N	0.88469300	1.22064500	0.19873200
C	2.12666300	1.84047600	-0.46893600
C	2.12667200	-1.84046900	0.46893600
C	1.84153600	3.33141800	-0.76750600
H	0.97385500	3.47065800	-1.41411400
H	1.72162400	3.93969300	0.13262500
H	2.71133400	3.72395500	-1.30241900
C	3.37112000	1.80516200	0.43823500
H	4.14786300	2.43773700	-0.00328500
H	3.14562500	2.21164400	1.43072300
H	3.79876300	0.81201900	0.56344300
C	1.84155200	-3.33141300	0.76749900
H	1.72164200	-3.93968500	-0.13263400
H	2.71135400	-3.72394700	1.30240800
H	0.97387400	-3.47066000	1.41410900
C	3.37113100	-1.80514800	-0.43823500
H	4.14787200	-2.43772900	0.00327900
H	3.14563500	-2.21161900	-1.43072700
H	3.79877500	-0.81200500	-0.56343300
C	2.34611200	-1.16690300	1.83493000
H	2.44163800	-0.08541600	1.78514800
H	1.51766600	-1.40316500	2.51174800
H	3.26484000	-1.56008600	2.28148500
C	2.34610200	1.16690700	-1.83493000
H	3.26484500	1.56007000	-2.28147300
H	2.44160100	0.08541800	-1.78515000
H	1.51766900	1.40319200	-2.51175600
H	-3.03857800	-0.67137400	-2.38596600
H	-3.03855500	0.67136100	2.38597300
H	-0.72863000	0.00000000	0.00001000

8

E = -1041.08109

ZPVE = 0.550514

C	2.85599800	0.79406500	1.11560500
C	2.85838100	-0.59372600	1.28276100
C	2.74443700	-1.40358700	0.13846400
C	2.85637600	-0.79502300	-1.11517400
C	2.85928300	0.59275300	-1.28233200
C	2.74496100	1.40264900	-0.13809200
H	2.82302100	1.42629800	2.00387500
H	2.82379100	-1.42726800	-2.00345000
C	2.26704300	-2.83859500	0.20376900
H	2.83861600	-3.46999400	-0.49075800
H	2.40324600	-3.27101600	1.20148200
C	2.26813600	2.83783200	-0.20374200
H	2.40473400	3.26991700	-1.20153700
H	2.83977400	3.46916400	0.49079100
C	0.76641800	-2.92242700	-0.19576500
H	0.66101800	-2.48426500	-1.19381600
H	0.49692800	-3.98380400	-0.27894700
C	0.76743800	2.92229200	0.19536800
H	0.66158800	2.48441800	1.19349800
H	0.49830300	3.98378400	0.27821500
C	-0.21122000	-2.19245200	0.77389900
H	0.36592900	-1.63721000	1.50984100
H	-0.79642200	-2.92382500	1.34183500
C	-0.54581600	0.00002100	-0.00041200
C	-0.21016400	2.19243500	-0.77442700
H	0.36703300	1.63685500	-1.51007500
H	-0.79495700	2.92387900	-1.34268600
N	-1.17171600	1.21305700	-0.17657400
N	-1.17230500	-1.21268200	0.17595500
C	-2.43011900	-1.80160000	-0.46995600
C	-2.42905300	1.80245900	0.46987400
C	-2.23720200	-3.30371900	-0.79984600
H	-1.37097100	-3.47996700	-1.43943600
H	-2.15580200	-3.93535700	0.08997000
H	-3.12301100	-3.63728700	-1.35248000
C	-3.67946200	-1.75036300	0.43907400
H	-4.49396300	-2.32219500	-0.02441000
H	-3.46074300	-2.21181300	1.40975200
H	-4.05519900	-0.74646500	0.62303000
C	-2.23571300	3.30464200	0.79919800
H	-2.15345100	3.93581700	-0.09086100
H	-3.12174600	3.63886100	1.35107100
H	-1.36983900	3.48084700	1.43928600
C	-3.67899400	1.75112400	-0.43830500
H	-4.49336400	2.32250500	0.02596600
H	-3.46111400	2.21301200	-1.40896500
H	-4.05449500	0.74717600	-0.62237700
C	-2.65070900	1.12131200	1.83877100
H	-2.57075000	0.03877000	1.79734300
H	-1.89542600	1.47199700	2.55143600
H	-3.63928900	1.38450800	2.23505900
C	-2.65249100	-1.12003700	-1.83856800
H	-3.64231400	-1.38096000	-2.23325100
H	-2.56993800	-0.03767900	-1.79732200
H	-1.89920900	-1.47249200	-2.55248200

N	2.80826900	1.15535200	-2.58743800
H	3.40989400	1.96506000	-2.70477600
H	3.03097100	0.47501500	-3.30717900
N	2.80647100	-1.15618600	2.58785900
H	3.40645700	-1.96710300	2.70514700
H	3.03050500	-0.47630000	3.30760500

8H$^+$

E = -1041.56785

ZPVE = 0.567519

C	2.77674900	-0.87025500	-1.06093300
C	2.78171300	0.50599200	-1.32657400
C	2.68352300	1.39319700	-0.23418000
C	2.77677100	0.87006600	1.06093300
C	2.78166200	-0.50617800	1.32657300
C	2.68345300	-1.39337900	0.23417700
H	2.76619300	-1.56315600	-1.90218400
H	2.76623500	1.56297000	1.90218200
C	2.26488000	2.83899900	-0.40045900
H	2.86875000	3.49739200	0.23605000
H	2.39983400	3.19177000	-1.42733500
C	2.26474300	-2.83916200	0.40045500
H	2.39966000	-3.19192300	1.42733800
H	2.86859900	-3.49759100	-0.23603400
C	0.77911800	3.00802900	0.01664900
H	0.69144200	2.70450400	1.06403500
H	0.51703500	4.07135700	-0.02403000
C	0.77898200	-3.00813100	-0.01667700
H	0.69134900	-2.70468000	-1.06408800
H	0.51683500	-4.07144000	0.02407600
C	-0.22541200	2.18763100	-0.84478000
H	0.31172100	1.60227400	-1.59277900
H	-0.88236200	2.85030800	-1.41242300
C	-0.62080900	-0.00001500	-0.00013700
C	-0.22551400	-2.18760400	0.84467000
H	0.31166900	-1.60218200	1.59258300
H	-0.88246900	-2.85018100	1.41242000
N	-1.14050400	-1.23275300	0.12056500
N	-1.14043700	1.23276300	-0.12074800
C	-2.39008700	1.80989400	0.56787000
C	-2.39036500	-1.80974900	-0.56781800
C	-2.12676800	3.28879000	0.93938100
H	-1.26648100	3.40988500	1.59895600
H	-2.00839500	3.93947800	0.06913000
H	-3.00627400	3.64363200	1.48476200
C	-3.62852000	1.81084900	-0.34895800
H	-4.41578100	2.40879000	0.12146300
H	-3.39881200	2.27544900	-1.31459000
H	-4.04402000	0.82269100	-0.53570600
C	-2.12737600	-3.28865500	-0.93953500
H	-2.00915300	-3.93950500	-0.06939000
H	-3.00696700	-3.64321900	-1.48496000
H	-1.26712800	-3.40985000	-1.59914200
C	-3.62860000	-1.81058400	0.34928000
H	-4.41609600	-2.40827300	-0.12106700
H	-3.39878200	-2.27539100	1.31478600
H	-4.04384000	-0.82236300	0.53628500
C	-2.60949900	-1.06971100	-1.89970500
H	-2.67575700	0.01063700	-1.80090700
H	-1.79325600	-1.29427200	-2.59484200
H	-3.54213500	-1.41963200	-2.35352600
C	-2.60901500	1.06998200	1.89986400
H	-3.54150000	1.42006200	2.35387200
H	-2.67544100	-0.01036300	1.80116100
H	-1.79258300	1.29448600	2.59479800
N	2.71815800	-0.97526600	2.65883200
H	3.28350900	-1.79880100	2.84043000
H	2.94799700	-0.26117000	3.34275700
N	2.71825900	0.97507200	-2.65883500
H	3.28359200	1.79862300	-2.84041400
H	2.94813200	0.26098100	-3.34275100
H	0.46857800	-0.00005100	-0.00019200

9

E = -1151.81958

ZPVE = 0.584241

C	-2.67863800	-0.96706200	1.00916100
C	-2.62488500	0.39887900	1.34131300
C	-2.53436500	1.37121600	0.33114400
C	-2.67930500	0.96683400	-1.00877200
C	-2.62534000	-0.39910400	-1.34099200
C	-2.53416300	-1.37136700	-0.33083500
C	-2.03274000	2.76521400	0.64564000
H	-2.62397300	3.54442300	0.14017800
H	-2.11986000	2.97240600	1.71582000
C	-2.03255500	-2.76530200	-0.64561000
H	-2.11985000	-2.97222500	-1.71581900
H	-2.62373500	-3.54453800	-0.14014700
C	-0.54445200	2.90778600	0.21268400
H	-0.45495500	2.60163900	-0.83463200
H	-0.27450500	3.97128200	0.26434900
C	-0.54419600	-2.90789500	-0.21288200
H	-0.45443700	-2.60181900	0.83444100
H	-0.27424400	-3.97138200	-0.26468400
C	0.44275400	2.06028600	1.06921000
H	-0.13071800	1.40683200	1.72223000
H	1.02345300	2.71099500	1.73231300
C	0.78512600	0.00007600	-0.00028000
C	0.44290400	-2.06030600	-1.06945400
H	-0.13066300	-1.40693800	-1.72246100
H	1.02367600	-2.71096600	-1.73253600
N	1.40880300	-1.17665200	-0.34310300
N	1.40879300	1.17676400	0.34289800
C	2.66447200	1.85199600	-0.21205500
C	2.66457600	-1.85178200	0.21189100
C	2.46951400	3.38591500	-0.32199900
H	1.59636400	3.64975200	-0.92097500
H	2.39790100	3.88400200	0.64969800
H	3.34982300	3.79530500	-0.83087800
C	3.91356800	1.67069700	0.67966900

H	4.73113200	2.29640500	0.29816800
H	3.69658800	1.99614000	1.70440400
H	4.28319500	0.64909600	0.72544700
C	2.46979500	-3.38572000	0.32181800
H	2.39831900	-3.88382100	-0.64988000
H	3.35012100	-3.79499400	0.83076200
H	1.59664900	-3.64968200	0.92074300
C	3.91364600	-1.67036100	-0.67982700
H	4.73124200	-2.29604600	-0.29835500
H	3.69668500	-1.99576300	-1.70458000
H	4.28321900	-0.64874100	-0.72554500
C	2.88350900	-1.37605800	1.66583100
H	2.80079900	-0.29915500	1.78491100
H	2.12688700	-1.82883400	2.31648100
H	3.87198000	-1.69204100	2.02234100
C	2.88348200	1.37629000	-1.66599400
H	3.87195500	1.69231000	-2.02246500
H	2.80082400	0.29938200	-1.78509400
H	2.12686800	1.82904400	-2.31666900
N	-2.50591700	-0.78506300	-2.70822600
H	-3.28318600	-1.33132600	-3.06788600
H	-2.31820100	0.00408200	-3.31759000
N	-2.50495400	0.78468800	2.70840000
H	-3.28043600	1.33379600	3.06750000
H	-2.32012000	-0.00495200	3.31798600
N	-2.69413800	-1.90915400	2.08544200
H	-3.47585000	-1.74100700	2.71662400
H	-2.76488600	-2.86691900	1.75920000
N	-2.69540500	1.90907800	-2.08470600
H	-3.47501200	1.73864600	-2.71781800
H	-2.76956900	2.86659100	-1.75848500

9H$^+$

E = -1152.31134

ZPVE = 0.600951

C	2.59849200	1.06957300	0.90903600
C	2.52669500	-0.25783800	1.38156800
C	2.45797900	-1.32948900	0.47002000
C	2.59851000	-1.06958900	-0.90902400
C	2.52669500	0.25781600	-1.38155600
C	2.45796800	1.32946700	-0.47000400
C	2.02482900	-2.70600900	0.93033800
H	2.66054600	-3.50315800	0.52106300
H	2.10051700	-2.79796400	2.01616200
C	2.02484400	2.70598600	-0.93033800
H	2.10056100	2.79791700	-2.01616100
H	2.66056200	3.50312900	-0.52105100
C	0.55931100	-2.97201800	0.49002600
H	0.49959600	-2.85199600	-0.59522000
H	0.30467500	-4.01635000	0.70543800
C	0.55931600	2.97202400	-0.49007200
H	0.49955400	2.85203400	0.59517600
H	0.30470300	4.01635400	-0.70552300
C	-0.47099900	-2.03277300	1.18039700
H	0.04570400	-1.34037400	1.84678100
H	-1.14772200	-2.60278000	1.82160500
C	-0.83287200	-0.00000400	-0.00003500
C	-0.47099300	2.03278000	-1.18044400
H	0.04570600	1.34039300	-1.84684400
H	-1.14772600	2.60279300	-1.82163600
N	-1.36045200	1.19892700	-0.29526000
N	-1.36046900	-1.19892200	0.29521800
C	-2.59536300	-1.86824400	-0.32838300
C	-2.59531300	1.86826400	0.32839900
C	-2.30742200	-3.37752200	-0.51174600
H	-1.43728400	-3.56248900	-1.14350400
H	-2.18831500	-3.91335500	0.43324800
H	-3.17520500	-3.81149200	-1.01738600
C	-3.84403900	-1.76627900	0.56783000
H	-4.62161600	-2.42585100	0.16908900
H	-3.62255200	-2.10169400	1.58747200
H	-4.26761900	-0.76506500	0.62068700
C	-2.30737400	3.37755300	0.51166800
H	-2.18807800	3.91329200	-0.43335500
H	-3.17524300	3.81159200	1.01710200
H	-1.43735100	3.56256600	1.14357100
C	-3.84405600	1.76623700	-0.56771800
H	-4.62151700	2.42602700	-0.16911400
H	-3.62257700	2.10134400	-1.58746200
H	-4.26778100	0.76506800	-0.62027700
C	-2.81194900	1.30380600	1.74401100
H	-2.91739500	0.22257900	1.77975500
H	-1.97567500	1.58303900	2.39419100
H	-3.72384700	1.73936900	2.16495700
C	-2.81211500	-1.30372700	-1.74395400
H	-3.72410500	-1.73918900	-2.16480400
H	-2.91745800	-0.22248900	-1.77965800
H	-1.97594400	-1.58302300	-2.39424100
N	2.38020200	0.50646900	-2.77138100
H	3.08865400	1.10372800	-3.18675300
H	2.25410000	-0.33009400	-3.32889700
N	2.38019000	-0.50646400	2.77138100
H	3.08843000	-1.10399300	3.18671700
H	2.25436000	0.33012000	3.32892200
N	2.62669200	2.12051100	1.86532700
H	3.31857200	1.95885200	2.59439000
H	2.82472400	3.02656600	1.45448300
N	2.62671500	-2.12054200	-1.86528100
H	3.31835500	-1.95875400	-2.59453700
H	2.82502300	-3.02655100	-1.45446600
H	0.25765700	-0.00002000	-0.00006800

B3LYP/6-311+G//HF/6-31G* SCF energies in gas phase (**E**), HF/6-31G* zero point vibrational energies (**ZPVE**) and Cartesian coordinates for 10 and their corresponding mono- and bis-protonated cations (All energies are given in Hartee).**

10

E = -1156.56536

ZPVE = 0.637618

C	-0.32438700	-1.16874900	1.22956700
C	0.00004900	-0.00002700	1.89263600
C	0.32446500	1.16870900	1.22958300
C	0.11710800	1.20696400	-0.14911800
C	-0.00003200	0.00001300	-0.81739400
C	-0.11711400	-1.20696100	-0.14914700
H	0.00008100	-0.00004300	2.97026100
H	-0.00007500	0.00003100	-1.89524900
C	0.98699500	2.28562200	2.00030400
H	0.53147900	3.25403000	1.81506200
H	0.87309200	2.09477200	3.06322800
C	0.09932400	-2.51196900	-0.87428100
H	-0.03394600	-2.37733700	-1.94482400
H	-0.63001200	-3.25515700	-0.56907300
C	2.49489600	2.38362700	1.66453500
H	2.59646100	2.84141100	0.68737300
H	2.94627800	3.07906600	2.36903700
C	1.50876600	-3.09111300	-0.59683000
H	1.74822900	-2.99829200	0.45300000
H	1.46976500	-4.15523500	-0.82512500
C	3.29574900	1.05248000	1.68235400
H	2.76045900	0.28357800	2.21332000
H	4.23326500	1.22023600	2.20881300
C	3.07902300	-0.68792700	0.04938700
C	2.66643100	-2.56124900	-1.44728600
H	2.32151200	-2.50975200	-2.47776900
H	3.45026500	-3.31745500	-1.43343000
N	3.30002700	-1.26823900	-1.13941400
N	3.60879800	0.51253000	0.35513100
C	4.53724800	1.36077500	-0.39060600
H	5.53906500	0.94491900	-0.41418200
H	4.20442700	1.54572700	-1.40111200
H	4.60844000	2.31996600	0.10107000
C	4.17096300	-0.87337500	-2.24706900
H	3.69198500	-0.15774800	-2.90900600
H	5.10766600	-0.46992600	-1.90541800
H	4.40733800	-1.75237000	-2.83277700
C	-0.98685900	-2.28569400	2.00028900
H	-0.53125800	-3.25406700	1.81508200
H	-0.87302200	-2.09481700	3.06321600
C	-2.49472900	-2.38383900	1.66442800
H	-2.59616800	-2.84163000	0.68726000
H	-2.94608800	-3.07932900	2.36889300
C	-3.29572300	-1.05277200	1.68221500
H	-2.76056600	-0.28386200	2.21330400
H	-4.23328900	-1.22064600	2.20854900
N	-3.60865400	-0.51272000	0.35500100
C	-3.07888000	0.68777900	0.04942000
C	-4.53709000	-1.36085600	-0.39087500
N	-3.30007600	1.26834400	-1.13922400
H	-5.53892700	-0.94503400	-0.41434100
H	-4.20428300	-1.54557500	-1.40142500
H	-4.60823700	-2.32015600	0.10059100
C	-2.66655500	2.56143200	-1.44692000
C	-4.17141400	0.87388800	-2.24670400
C	-1.50877700	3.09116000	-0.59653500
H	-2.32180400	2.51015200	-2.47747000
H	-3.45040100	3.31762000	-1.43278200
H	-3.69262000	0.15864000	-2.90918800
H	-5.10791500	0.47015300	-1.90484700
H	-4.40815600	1.75313400	-2.83189200
C	-0.09938500	2.51199900	-0.87418700
H	-1.74813300	2.99823600	0.45331000
H	-1.46976800	4.15530600	-0.82471900
H	0.03374400	2.37739300	-1.94475100
H	0.63000800	3.25516000	-0.56905000

10-H$^+$

E = -1157.03981

ZPVE = 0.654650

C	-0.10904900	-1.01259000	0.94159700
C	0.15448700	0.24091500	1.47736100
C	0.15878900	1.40300200	0.71923400
C	-0.30614600	1.32255500	-0.59703600
C	-0.37423300	0.06148600	-1.17291400
C	-0.19458500	-1.11191000	-0.44979700
H	0.33470400	0.31844300	2.53627800
H	-0.60906900	-0.01187000	-2.22144800
C	0.76057000	2.66717400	1.28935900
H	0.22690200	3.55326600	0.97293100
H	0.71386600	2.65154600	2.37361000
C	-0.00036800	-2.41757000	-1.18789000
H	-0.38901500	-2.33073400	-2.19762400
H	-0.53547600	-3.23568200	-0.72161600
C	2.23794800	2.80607200	0.84538200
H	2.29433300	2.82773700	-0.23790400
H	2.61229000	3.76515700	1.18672800
C	1.49785400	-2.80303400	-1.25628700
H	1.85263300	-3.03033500	-0.25669200
H	1.59007900	-3.71833200	-1.83125000
C	3.17004900	1.70103300	1.40032900
H	2.64987400	1.08493000	2.11817100
H	3.99493100	2.15368500	1.92776600
C	3.05848400	-0.01680200	-0.30250900
C	2.41033400	-1.72222400	-1.88529700
H	1.83135900	-0.92592400	-2.32459900
H	3.00830500	-2.14406600	-2.68119700
N	3.38324000	-1.10972900	-0.94497100
N	3.81052900	0.79042100	0.40841400
C	5.27103400	0.86390500	0.32890000
H	5.74631400	0.36466000	1.16357300
H	5.62157600	0.44423300	-0.59875400
H	5.54787000	1.90814200	0.34477100
C	4.60151300	-1.89290300	-0.73018300
H	5.33704800	-1.69994600	-1.50022200
H	5.02109400	-1.69278500	0.24131100
H	4.33049400	-2.93800600	-0.76698600
C	-0.41743900	-2.15909500	1.87884200
H	0.10948500	-3.06892300	1.60723400

H	-0.07360500	-1.89516300	2.87370700
C	-1.93447300	-2.47414200	1.94601100
H	-2.21831800	-3.04951100	1.07148900
H	-2.08165900	-3.13493700	2.79538600
C	-2.89393700	-1.26567500	2.07999500
H	-2.40100800	-0.42012600	2.53328000
H	-3.71067900	-1.55410300	2.73604100
N	-3.45041600	-0.81086400	0.80777000
C	-3.21311800	0.47305400	0.46014500
C	-4.47114200	-1.70522600	0.26590500
N	-3.52574800	0.87465500	-0.78405300
H	-5.21913100	-1.14532500	-0.27176600
H	-4.07518800	-2.47666600	-0.38681900
H	-4.97073900	-2.20002500	1.09030500
C	-3.45225600	2.31668600	-1.04671900
C	-3.81542300	0.06220500	-1.96130900
C	-2.15148600	3.04544300	-0.68660600
H	-3.65125500	2.46256400	-2.10195500
H	-4.25551500	2.81721600	-0.51735300
H	-3.44304100	-0.93990300	-1.83071000
H	-4.87343200	0.01885800	-2.20101400
H	-3.30437500	0.48785000	-2.81671500
C	-0.83751700	2.53607100	-1.33047200
H	-2.04430600	3.05165900	0.38937100
H	-2.29995900	4.07756900	-0.99571000
H	-1.00171000	2.29349100	-2.37608300
H	-0.11590700	3.34724300	-1.31923500
H	2.02767100	0.26215000	-0.37265600

10-$(H^+)_2$

E = -1157.42030

ZPVE = 0.670458

C	0.01625400	-1.22481800	-0.54388500
C	-0.00001500	-0.00001100	-1.20606000
C	-0.01627400	1.22480000	-0.54393600
C	0.17951100	1.21183600	0.84364700
C	0.00006900	0.00002800	1.50476100
C	-0.17944000	-1.21181800	0.84369300
H	-0.00006000	-0.00003700	-2.28297700
H	0.00012300	0.00004300	2.58188800
C	-0.38776500	2.48428500	-1.29696700
H	0.17680100	3.34311900	-0.95747200
H	-0.16887900	2.37107000	-2.35354500
C	-0.68626200	-2.41215200	1.61564200
H	-0.50205600	-2.27041700	2.67509500
H	-0.17661900	-3.32622700	1.33724400
C	-1.89695300	2.79445700	-1.11614000
H	-2.12626300	2.89181300	-0.06045400
H	-2.09513600	3.76432100	-1.55701800
C	-2.20567600	-2.61810100	1.38639000
H	-2.38236300	-2.85730500	0.34316800
H	-2.51239400	-3.48739700	1.95633000
C	-2.84731700	1.76011600	-1.77228800
H	-2.29095500	1.02149900	-2.33078600
H	-3.48429900	2.25791800	-2.48566500
C	-3.27967600	0.19910700	0.01274900
C	-3.09149700	-1.41247700	1.79190700
H	-2.51392900	-0.64205700	2.27836700
H	-3.84381300	-1.71969800	2.50358300
N	-3.83685300	-0.78234800	0.67211500
N	-3.77960600	1.03289800	-0.86593100
C	-5.21038600	1.29776200	-1.06654900
H	-5.59401600	0.77954700	-1.93535700
H	-5.77161100	1.01944000	-0.19100200
H	-5.32892300	2.36137400	-1.21182300
C	-5.12565300	-1.40931000	0.35331800
H	-5.91163500	-1.03871400	0.99745500
H	-5.38407300	-1.24959500	-0.67963700
H	-5.02038500	-2.47271700	0.51099900
C	0.38765600	-2.48430400	-1.29693400
H	-0.17689200	-3.34312900	-0.95739000
H	0.16868300	-2.37108600	-2.35349500
C	1.89684500	-2.79453100	-1.11620500
H	2.12619200	-2.89203200	-0.06053800
H	2.09494200	-3.76435500	-1.55721300
C	2.84730500	-1.76021200	-1.77225100
H	2.29103100	-1.02163300	-2.33089400
H	3.48437200	-2.25807900	-2.48550300
N	3.77952400	-1.03295100	-0.86585000
C	3.27963900	-0.19915200	0.01283700
C	5.21031200	-1.29781800	-1.06650400
N	3.83685500	0.78238600	0.67204400
H	5.59386600	-0.77972200	-1.93541600
H	5.77160000	-1.01934700	-0.19104800
H	5.32885500	-2.36145100	-1.21162000
C	3.09162900	1.41267300	1.79183900
C	5.12569800	1.40921000	0.35314300
C	2.20573000	2.61823800	1.38628500
H	2.51413000	0.64231500	2.27849100
H	3.84404500	1.72001700	2.50335100
H	5.91162900	1.03878700	0.99744400
H	5.38417300	1.24915600	-0.67974800
H	5.02046100	2.47267000	0.51047900
C	0.68632500	2.41222400	1.61551300
H	2.38244600	2.85749700	0.34308400
H	2.51240500	3.48751800	1.95627400
H	0.50216500	2.27053800	2.67497900
H	0.17661700	3.32626200	1.33709400
H	-2.24189200	0.34502700	0.22624200
H	2.24186000	-0.34500700	0.22636800