

## Supporting Information

### *The Role of $\sigma/\pi$ , $\sigma$ and $\pi$ Donors on the Basicity of Silylene Superbases: A Density Functional Theory Study*

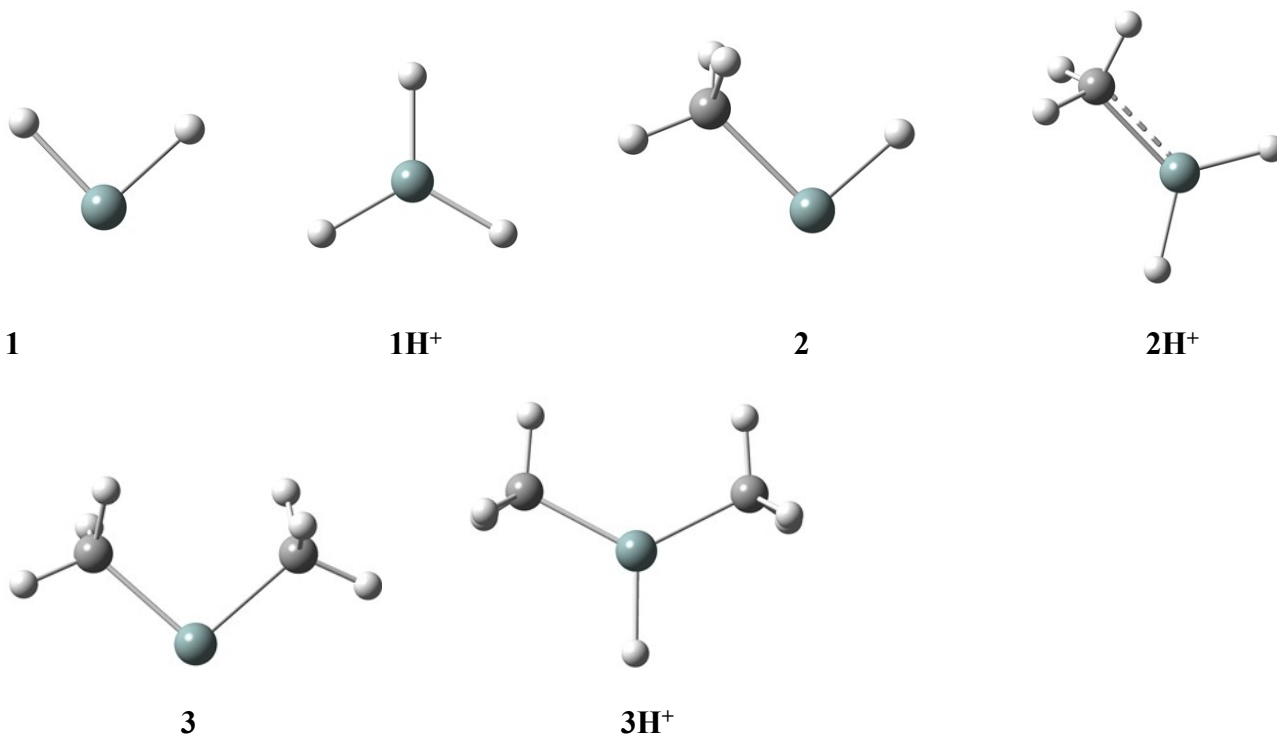
Abul Kalam Biswas,<sup>†</sup> Mrinal Kanti Si, Bishwajit Ganguly\*

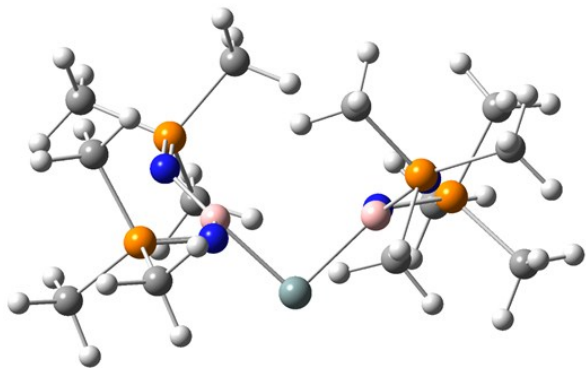
Analytical Discipline and Centralized Instrument Facility, Academy of Scientific and Innovative Research, CSIR–Central Salt & Marine Chemicals Research Institute, Bhavnagar, Gujarat, India-364 002.

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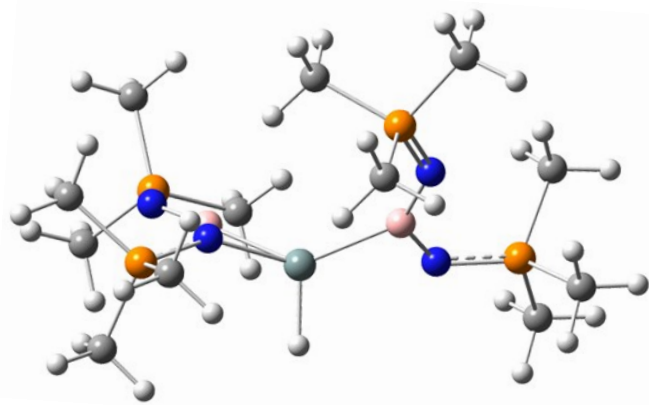
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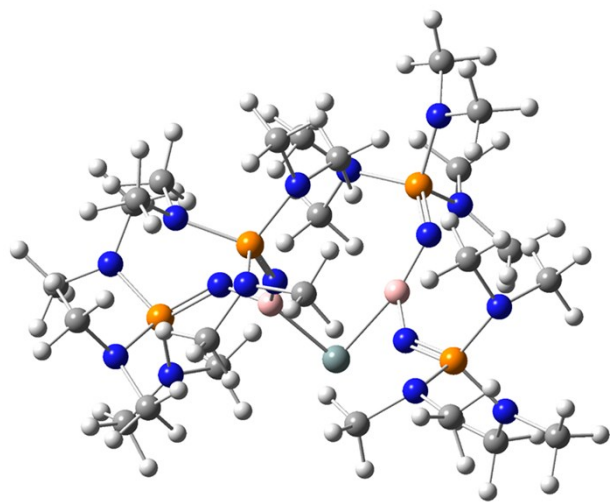




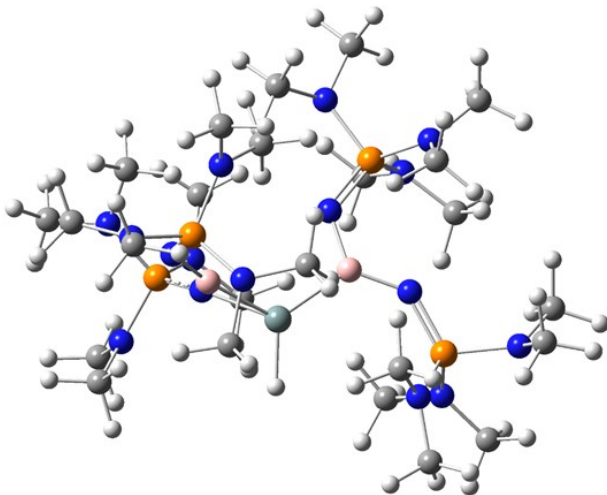
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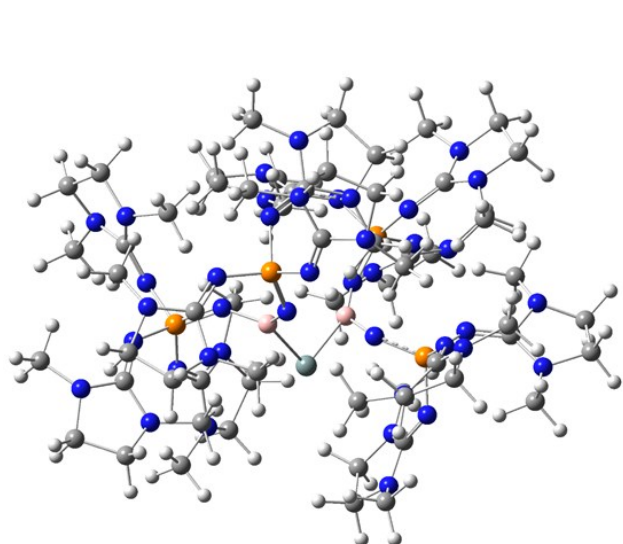
4H<sup>+</sup>



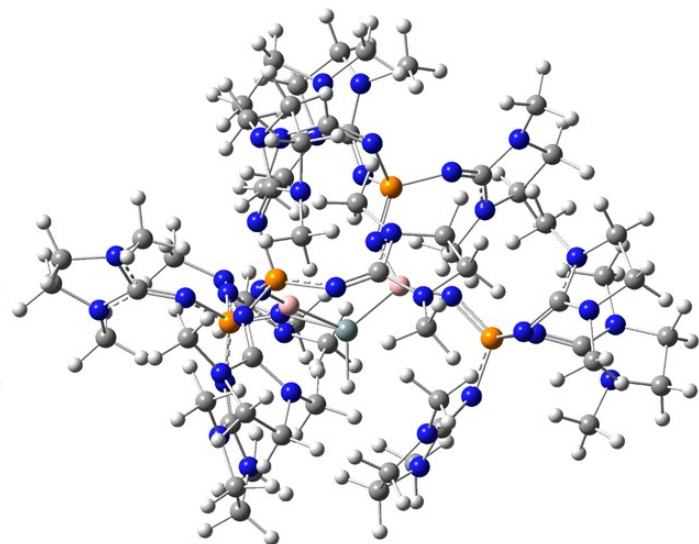
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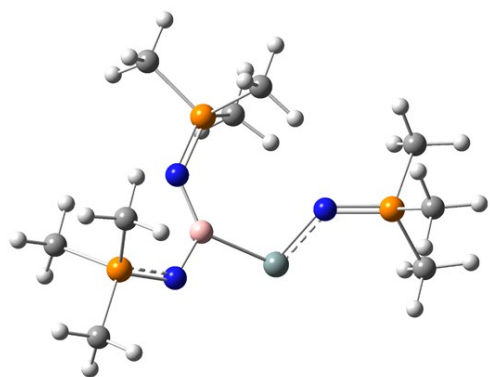
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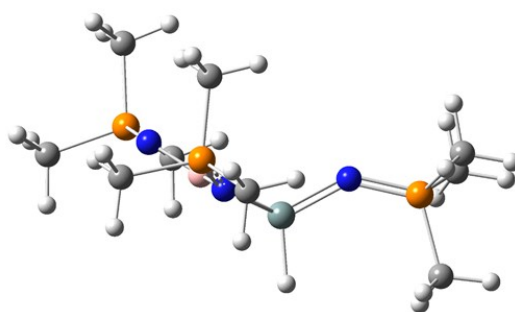
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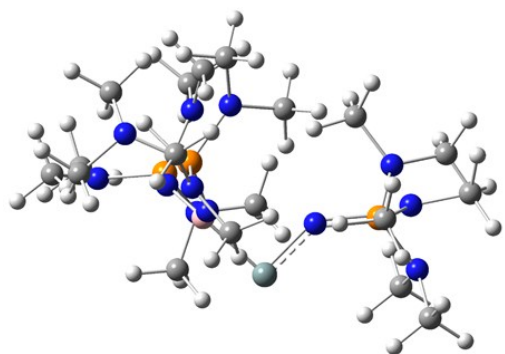
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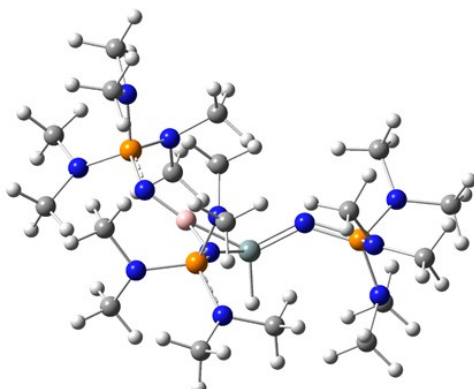
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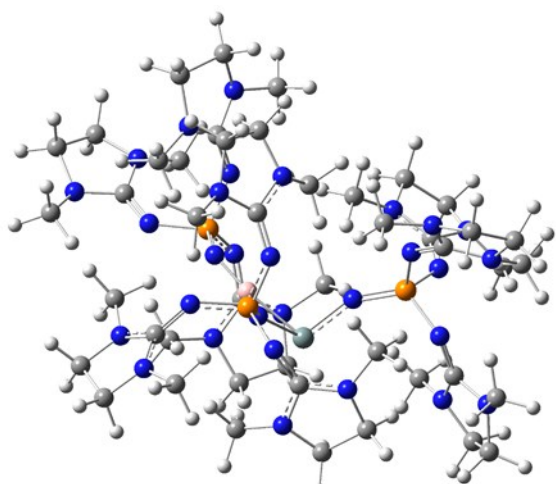
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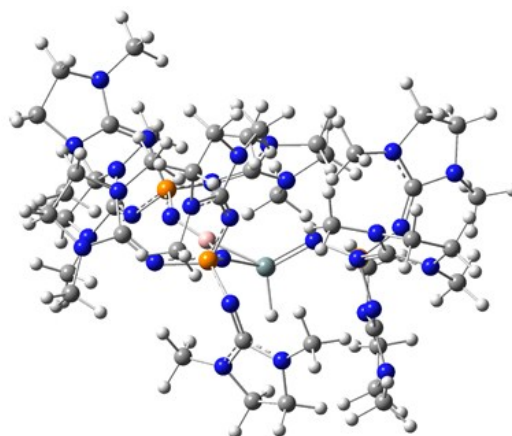
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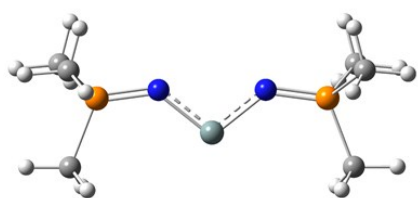
8H<sup>+</sup>



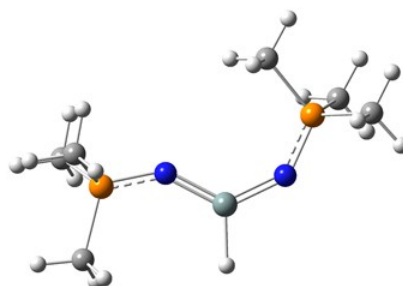
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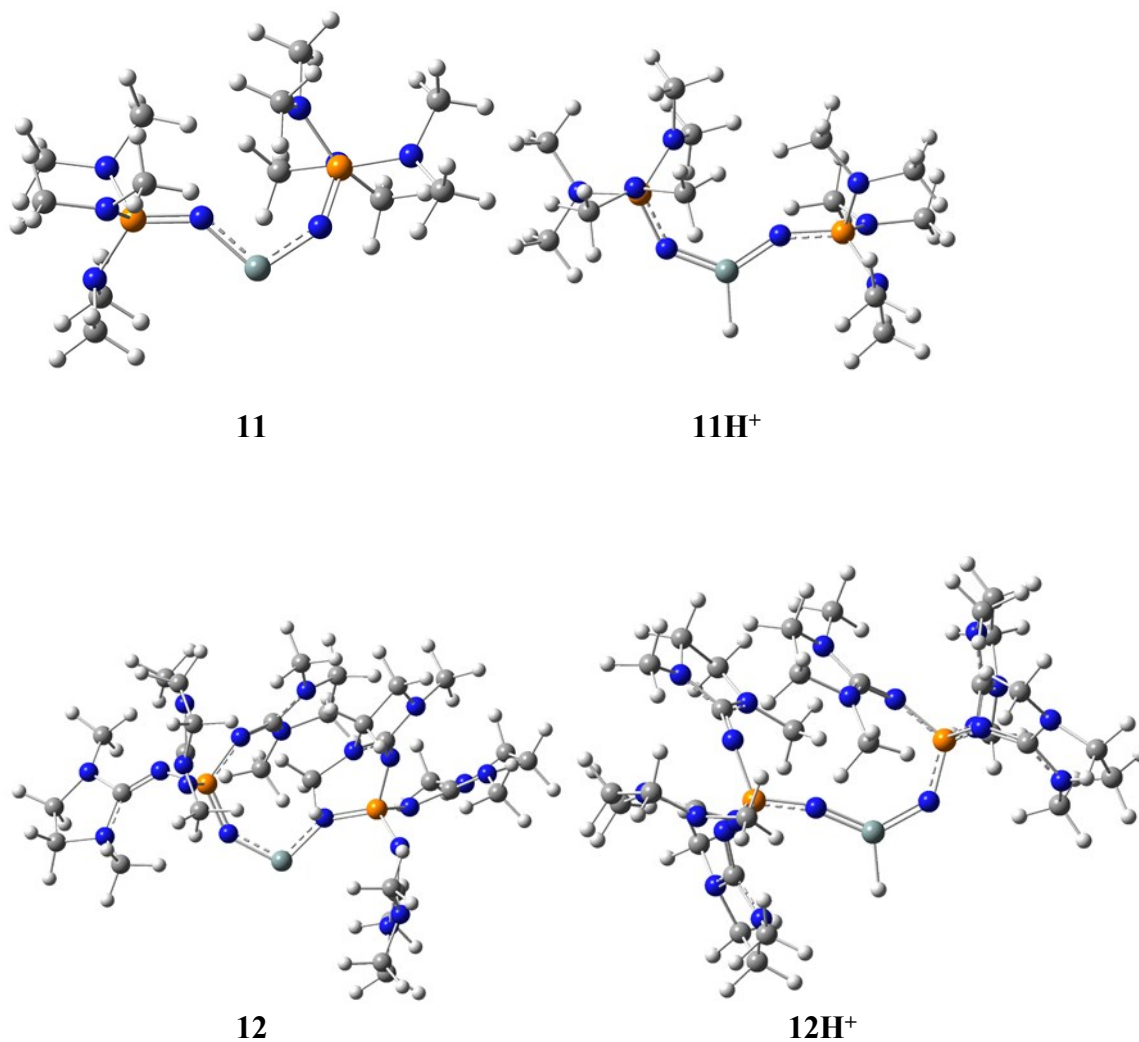
9H<sup>+</sup>



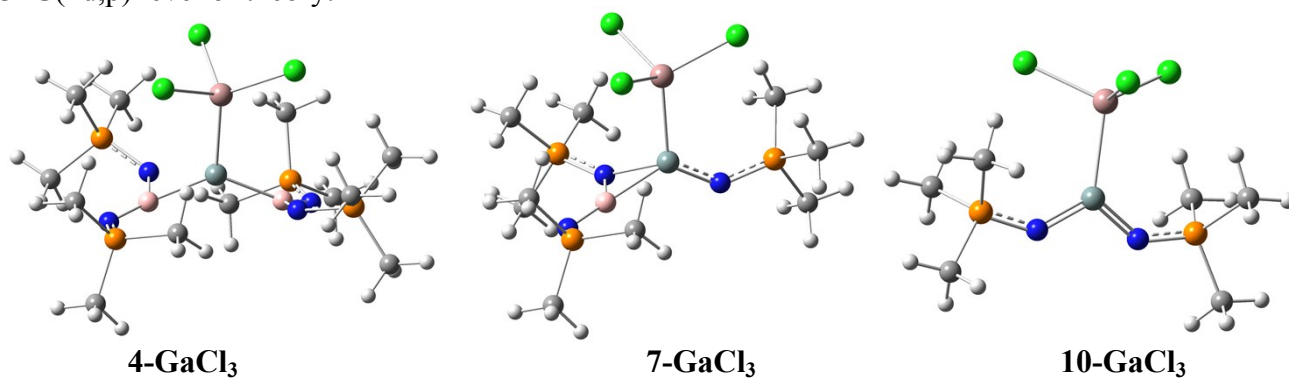
10



10H<sup>+</sup>



**Figure S1:** Optimized geometries of neutral and protonated compounds 1-12 at B3LYP-D3/6-31G(2d,p) level of theory.



**Figure S2:** Optimized structure of complexes 4, 7 and 10 with GaCl<sub>3</sub> at BP86/def2-SVP level of theory in gas phase. (green = Cl; blue = N; white = H; light gray = C; grey = Si; Creamy (small sphere) = B, Creamy = Ga; Orange = P)

**Table TS1:** The complexation energies of 4, 7 and 10 with GaCl<sub>3</sub> calculated at BP86/def2-SVP level of theory in gas phase. (energies are given in kcal/mol.).

Complexes	Complexation energies ( $\Delta E$ )
4-GaCl <sub>3</sub>	-72.5
7-GaCl <sub>3</sub>	-73.3
10-GaCl <sub>3</sub>	-53.8

Energies are calculated using the equation  $\Delta E = E_{\text{complex}} - (E_{\text{indiv}} + E_{\text{GaCl}_3})$ , Where,  $E_{\text{complex}}$  is energy of complex,  $E_{\text{indiv}}$  and  $E_{\text{GaCl}_3}$  are energies of individual silylene (4, 7, and 10) and GaCl<sub>3</sub> respectively.

**B3LYP–D3/6–31G(2d,p) optimized Cartesian coordinates of all the neutral and protonated silylene molecules and the electronic energies at B3LYP–D3/6–311+G(2d,p) level of theory**

**1**

**E= -290.64253111 a.u.**

Si	0.00000000	0.00000000	0.13312300
H	0.00000000	1.09023100	-0.93185900
H	0.00000000	-1.09023100	-0.93185900

**1H<sup>+</sup>**

**E= -290.96424020 a.u.**

Si	0.00000000	0.00000000	0.00000000
H	0.00000000	1.46768400	0.00000000
H	1.27105200	-0.73384200	0.00000000
H	-1.27105200	-0.73384200	0.00000000

**2**

**E= -329.98536465 a.u.**

Si	0.75456700	-0.11449100	-0.00000800
H	0.96121300	1.40099600	0.00001100
C	-1.14998100	0.00297400	-0.00002500
H	-1.48782100	0.57678400	-0.87518700
H	-1.64988600	-0.96881300	-0.00029300
H	-1.48755700	0.57606800	0.87573100

**2H<sup>+</sup>**

**E= -330.33206061 a.u.**

Si	-0.00736900	-0.63843600	0.00000000
H	0.01578300	-1.40852900	1.25178600
C	-0.00736900	1.18048800	0.00000000
H	1.05256500	1.49634900	0.00000000

H	-0.46837200	1.58794200	-0.90539800
H	-0.46837200	1.58794200	0.90539800
H	0.01578300	-1.40852900	-1.25178600

**3**

**E= -369.32879216 a.u.**

Si	0.00000000	0.00000000	0.76126800
C	0.00000000	1.43616100	-0.50113100
H	0.25331500	2.40634600	-0.06485000
H	0.63665100	1.25010100	-1.37505600
H	-1.03259400	1.51004500	-0.88218700
C	0.00000000	-1.43616100	-0.50113100
H	1.03259400	-1.51004500	-0.88218700
H	-0.25331500	-2.40634600	-0.06485000
H	-0.63665100	-1.25010100	-1.37505600

**3H<sup>+</sup>**

**E= -369.69600439 a.u.**

Si	0.00000000	0.00000000	0.43662200
C	0.00000000	1.62369800	-0.39884700
H	0.87773500	2.19686200	-0.06473000
H	0.00018700	1.54529700	-1.48802400
H	-0.87795600	2.19670500	-0.06503800
C	0.00000000	-1.62369800	-0.39884700
H	0.87795600	-2.19670500	-0.06503800
H	-0.87773500	-2.19686200	-0.06473000
H	-0.00018700	-1.54529700	-1.48802400
H	0.00000000	0.00000000	1.90904100

**4**

**E= -2403.16241283 a.u.**

B	1.34426600	-0.59324400	-0.42663200
B	-1.34706400	0.59832800	-0.41914600
N	1.71319200	-1.70736600	0.37756900
N	2.16194300	0.60794500	-0.54248300
N	-2.15896200	-0.60788800	-0.52978000
N	-1.71554600	1.71199900	0.38486300
P	0.81441800	-2.95560200	0.69963800
P	3.73260700	0.59830900	-0.46475300
P	-3.73019400	-0.60386700	-0.46278000
P	-0.81505900	2.96158000	0.69800000
C	1.85579200	-4.32911600	1.29813900
H	1.25055800	-5.19528200	1.58025700
C	-0.18850600	-3.67616800	-0.65049600
H	-0.93201100	-2.93023000	-0.94564300
C	-0.40861800	-2.67762400	2.03061900
H	-1.11681900	-1.93016100	1.66057900
C	4.41710600	2.23370600	-0.89134500
H	4.02697400	2.97916000	-0.19403100
C	4.55364600	-0.57029100	-1.61079400
H	5.64428500	-0.52049700	-1.54368700

C	4.45687000	0.18476500	1.16885500
H	5.55006300	0.13527700	1.14051800
C	-4.46479800	-0.17862600	1.16293300
H	-4.04576300	0.78942500	1.44776500
C	-4.40626800	-2.24508300	-0.88020000
H	-5.49925400	-2.24871600	-0.84098900
C	-4.54731900	0.55237100	-1.62396100
H	-5.63820400	0.49918600	-1.56401800
C	0.18706500	3.67248000	-0.65760900
H	0.93016100	2.92423000	-0.94826500
C	-1.85410500	4.33930300	1.29070800
H	-2.42769800	4.00599200	2.15890400
C	0.40962700	2.68913800	2.02854300
H	1.11658800	1.93915600	1.66128500
H	-1.24765800	5.20645200	1.56711100
H	-2.55334500	4.62442800	0.50059300
H	-0.45609400	3.88752300	-1.51416300
H	0.68797300	4.59057900	-0.33407300
H	-4.21139600	1.56163200	-1.37385000
H	-4.22142500	0.31913700	-2.64068000
H	-4.07685800	-2.51640200	-1.88603500
H	-4.01747700	-2.98359900	-0.17479900
H	-5.55780700	-0.12999200	1.12738500
H	-4.15790200	-0.92340200	1.90212000
H	2.43053700	-3.99067200	2.16358100
H	2.55394100	-4.61792500	0.50840000
H	0.45425000	-3.89665400	-1.50597300
H	-0.68886200	-4.59231900	-0.32062500
H	-0.94244900	-3.59656600	2.29267800
H	0.10138900	-2.28660100	2.91440000
H	4.03563300	-0.78091800	1.45829200
H	4.14594200	0.93520500	1.90061700
H	4.23589400	-0.34423500	-2.63169800
H	4.21208800	-1.57609000	-1.35455500
H	5.50986500	2.23380000	-0.84599600
H	4.09426400	2.49833600	-1.90108500
H	0.94485900	3.60881500	2.28504500
H	-0.09928900	2.30302700	2.91509700
Si	-0.00820500	-0.00105600	-1.80790700

**4H<sup>+</sup>**

**E= -2403.64737320a.u.**

B	1.87687400	-0.29315100	-0.09896700
B	-1.82480500	-0.06428600	-0.27844200
N	3.03546100	-0.81851600	0.42281600
N	1.56486200	1.07737800	-0.52216400
N	-2.19791300	-1.29233900	-0.86649600
N	-2.60043500	0.77899800	0.53516000
P	3.33991100	-2.31456400	0.85878800
P	2.58731900	2.20188700	-1.05710600
P	-3.61796800	-1.99741800	-0.78736300

P	-2.35660700	2.15905800	1.23848200
C	3.70244000	-2.41545200	2.63755800
H	3.99460300	-3.42954800	2.92288000
C	4.82837500	-2.93789200	0.02296900
H	4.64885500	-2.97222100	-1.05446300
C	2.03940500	-3.55258900	0.54673300
H	1.82899200	-3.59697200	-0.52428200
C	1.71000800	3.73164900	-1.47550000
H	1.21259900	4.12175400	-0.58463100
C	3.47770400	1.68608000	-2.55413800
H	4.15306000	2.47265900	-2.90089600
C	3.84034300	2.57655200	0.19692800
H	4.59702100	3.26277500	-0.19232800
C	-4.17692000	-2.42605400	0.89716800
H	-4.22242200	-1.50378900	1.48045200
C	-3.57872100	-3.56221900	-1.70764900
H	-4.54789500	-4.06672100	-1.67321400
C	-4.98619000	-1.03068900	-1.50980700
H	-5.93537900	-1.57047500	-1.45089700
C	-2.36481400	3.60229300	0.11412500
H	-1.53578900	3.50685200	-0.59193700
C	-3.68401500	2.49643000	2.43316700
H	-3.69286900	1.70688100	3.18846600
C	-0.80807800	2.32962400	2.19965300
H	0.04362600	2.14747100	1.53890700
H	-3.54302200	3.46396100	2.92250300
H	-4.64397200	2.49074900	1.91162600
H	-3.29961300	3.60528900	-0.45175900
H	-2.27098200	4.54477400	0.66115000
H	-5.05986900	-0.08893900	-0.96151900
H	-4.75617500	-0.81364200	-2.55578000
H	-3.31218100	-3.35633000	-2.74698600
H	-2.81540100	-4.21304000	-1.27463900
H	-5.15792600	-2.90924800	0.88573200
H	-3.44819100	-3.09867600	1.35633900
H	2.81344900	-2.12303100	3.20180100
H	4.51297000	-1.72340500	2.87769100
H	5.66075100	-2.25829900	0.22024400
H	5.08726400	-3.93901500	0.37747200
H	2.35741000	-4.53821500	0.89733000
H	1.12453700	-3.25729800	1.06530400
H	4.29961800	1.62869800	0.48968800
H	3.35838200	3.01935500	1.07159900
H	2.75494000	1.45218400	-3.33980900
H	4.05222400	0.78615300	-2.32201900
H	2.40748100	4.48172900	-1.85734400
H	0.96012000	3.51774100	-2.24142600
H	-0.72438100	3.32295100	2.65015200
H	-0.79860200	1.57577200	2.99114800
Si	0.10896400	-0.10735500	-0.94721300
H	0.21005800	-0.29820800	-2.42300300



5

E = -3539.52911587 a.u.

N	-0.76231600	-1.13745600	0.45895200
N	-2.26107200	0.67134500	-0.43514900
N	2.23619200	1.41657400	0.29016400
N	1.85256700	-0.56619700	-1.27711700
P	-1.08989600	-1.95058500	1.71157300
P	-3.61321600	0.64797700	-1.16911400
P	1.87533400	2.85799600	0.77819700
P	3.01834300	-1.59458500	-1.30571700
N	2.39281000	-3.15721900	-1.26840400
N	4.12114900	-1.61091200	-0.04289100
N	3.99882900	-1.35282000	-2.64095500
N	-3.58851600	1.17516500	-2.77431200
N	-4.73669100	1.55579000	-0.29195300
N	-4.41180400	-0.83384700	-1.37357500
N	-2.67185500	-1.81952100	2.33197800
N	-0.97247100	-3.63514500	1.56700700
N	0.00628800	-1.62922200	2.95707800
N	0.30141600	3.40980200	0.93645100
N	2.42817100	3.00127700	2.36281800
N	2.53956500	4.01999900	-0.23456300
B	-1.06979700	-0.15438500	-0.52362900
B	1.54713800	0.73821500	-0.73131000
Si	0.16417700	0.32555300	-2.09544000
C	-0.54764400	2.86336300	1.99608700
H	-1.02389400	1.92683000	1.68259300
H	0.03760900	2.68407400	2.89673000
H	-1.33488500	3.59113900	2.22932600
C	3.59074200	3.68167400	-1.18273500
H	4.56329100	4.08834700	-0.86541900
H	3.67077900	2.60017400	-1.27425100
H	3.35392700	4.10056700	-2.16986800
C	2.34231500	5.44984400	-0.06344800
H	3.22710800	5.93805300	0.37209600
H	2.14696200	5.91919000	-1.03714700
H	1.48423500	5.64324300	0.57922900
C	3.60632500	-1.98919500	1.27627400
H	4.43377900	-2.36089000	1.89215800
H	3.14206900	-1.13583400	1.78247100
H	2.85824500	-2.77352900	1.17682300
C	5.06396100	-0.48894000	0.04138900
H	5.87426000	-0.76271400	0.72653800
H	5.49700000	-0.28245400	-0.93729300
H	4.56889300	0.42074300	0.40396500
C	3.59033800	-0.49449400	-3.74580100
H	2.67302400	0.03974700	-3.49876000
H	4.38078900	0.23769000	-3.96392900
H	3.41492100	-1.08341900	-4.65720300
C	3.28942900	-4.30248200	-1.37182600
H	2.79441900	-5.18214400	-0.94382600
H	3.56353400	-4.54209900	-2.41072100
H	4.20127300	-4.11874700	-0.80126700

C	1.09826700	-3.36436400	-1.92612700
H	0.73047000	-4.35919800	-1.65277100
H	0.38292500	-2.61908100	-1.57961600
H	1.16969100	-3.32115900	-3.02305800
C	0.73251800	-0.36981800	2.96865200
H	0.18697600	0.41778200	3.51081100
H	1.69657300	-0.50746600	3.47531700
H	0.91940100	-0.03102500	1.95123700
C	-0.25158100	-2.17065000	4.28139000
H	-0.71783900	-3.15479300	4.20882100
H	0.69644900	-2.28686500	4.82223000
H	-0.90252600	-1.52024800	4.88752900
C	-1.83430300	-4.22687000	0.54438200
H	-2.82459400	-3.77020500	0.57277200
H	-1.42795400	-4.09674700	-0.46874000
H	-1.94513100	-5.30051900	0.73804700
C	0.35527400	-4.24587200	1.59104200
H	0.24259600	-5.32698400	1.73638600
H	0.91810500	-4.07468100	0.66461200
H	0.93851000	-3.84372100	2.41853800
C	-4.63184400	0.92475900	-3.75682900
H	-5.25519300	0.08765100	-3.44625700
H	-5.27586700	1.80563700	-3.90544700
H	-4.17670900	0.67975000	-4.72626400
C	-2.73685500	2.29949600	-3.13219100
H	-1.94413900	2.42181500	-2.39730000
H	-2.25762600	2.11580200	-4.10088300
H	-3.31149500	3.23786800	-3.20029200
C	-6.01295600	1.87342800	-0.91295000
H	-5.96736600	2.77675200	-1.54252600
H	-6.35190900	1.03900000	-1.52894300
H	-6.76699300	2.04602300	-0.13496500
C	-4.28290200	2.56037400	0.65594400
H	-4.99869700	2.63922600	1.48498100
H	-3.30945300	2.27619400	1.04955600
H	-4.19248900	3.55718300	0.19407900
C	-5.06953300	-1.43508000	-0.21500000
H	-5.63811700	-0.67944400	0.32697800
H	-5.76346600	-2.20953600	-0.56420800
H	-4.35029000	-1.89323200	0.47810000
C	-3.64601600	-1.82454300	-2.13811700
H	-2.87347600	-2.30493500	-1.52198400
H	-4.32707700	-2.59633600	-2.51608900
H	-3.14886100	-1.34955600	-2.98470800
C	2.38085600	4.28474600	3.04634600
H	2.30499100	4.12008700	4.12824900
H	3.27968100	4.89418100	2.86286300
H	1.50403800	4.85169600	2.73171000
C	3.46734200	2.11487100	2.86587300
H	3.40827800	1.16053400	2.34795200
H	4.47719600	2.53337900	2.72704700
H	3.31664500	1.95117600	3.94089800
C	-3.12732700	-0.45207500	2.55778300

H	-2.72534000	0.19742400	1.78017800
H	-4.22091200	-0.40994200	2.49030100
H	-2.83590400	-0.07932600	3.55396300
C	-3.29921800	-2.77854100	3.23038200
H	-4.37410100	-2.83697600	3.00950500
H	-2.86239100	-3.76753300	3.09760500
H	-3.19422900	-2.49143200	4.28811800
C	5.20541300	-2.12191900	-2.90057800
H	5.06125500	-2.85244100	-3.70972800
H	6.01994300	-1.44858700	-3.20235500
H	5.52509300	-2.65086900	-2.00274100
C	-0.47762000	3.73374900	-0.26383100
H	-1.08552400	4.62893300	-0.07339800
H	0.18055600	3.92502400	-1.11018100
H	-1.14042600	2.90075700	-0.51676300

**5H<sup>+</sup>**

**E = -3540.02809742 a.u.**

N	0.95243200	0.82369600	0.95404500
N	2.57682900	-0.75079900	-0.16232700
N	-3.34010300	-0.65042000	-0.20700300
N	-1.54948900	0.86363000	-1.28730900
P	1.89670200	1.36005900	2.09254800
P	3.35106100	-1.61309100	-1.19887300
P	-3.70937200	-1.94391900	0.61005500
P	-1.85562100	2.41584500	-1.56805400
N	-0.57578700	3.41994400	-1.27126700
N	-3.14904300	2.87370300	-0.65689900
N	-2.15966100	2.62556900	-3.17413900
N	4.09785400	-0.69481300	-2.37300300
N	2.39689900	-2.76651700	-1.95762200
N	4.65594400	-2.44467900	-0.54377900
N	2.51715400	0.15087600	3.06433100
N	3.25338200	2.27815100	1.70988900
N	1.00269500	2.47583700	2.99042500
N	-2.99868500	-3.39777500	0.17835400
N	-3.37139400	-1.69710500	2.22454000
N	-5.32479100	-2.24778600	0.41732600
B	1.33247100	-0.09218400	-0.06125200
B	-2.13028200	-0.35296400	-0.76916900
Si	-0.23821700	-0.44058300	-1.32776500
C	-1.80316800	-3.88263000	0.85908400
H	-0.89072800	-3.39608500	0.49191800
H	-1.87725900	-3.72005500	1.93393300
H	-1.71096500	-4.96128600	0.68998300
C	-6.26741900	-1.14231600	0.26792300
H	-6.86736700	-1.00664300	1.17812700
H	-5.72459700	-0.22351200	0.05010400
H	-6.95126000	-1.35035200	-0.56376200
C	-5.95654200	-3.54886500	0.59800700
H	-6.64580600	-3.53987800	1.45365400
H	-6.53846000	-3.81085100	-0.29460700
H	-5.20250400	-4.31772100	0.76055900

C	-3.32674100	2.43953700	0.72803600
H	-3.19425900	3.28181500	1.41968400
H	-4.33032600	2.02400800	0.85933800
H	-2.61299800	1.65905000	0.97583900
C	-4.02382100	3.96934100	-1.05956600
H	-3.80013500	4.89232500	-0.50744500
H	-3.92743300	4.16998700	-2.12618900
H	-5.06492100	3.69416300	-0.85802400
C	-2.95843600	1.63882000	-3.90044500
H	-3.07922000	0.73390100	-3.30580100
H	-3.95188900	2.03934500	-4.13904200
H	-2.45675400	1.37506300	-4.83809400
C	-0.45512400	4.14189200	-0.00348600
H	0.03301900	3.53230500	0.76339700
H	0.14409200	5.04307000	-0.17304200
H	-1.43559000	4.45727500	0.35236400
C	0.71642900	3.11612000	-1.89300300
H	1.33896300	2.52524500	-1.21325600
H	0.56987600	2.55637400	-2.81878700
H	1.23356400	4.05153300	-2.13554300
C	-0.41008300	2.17879300	3.20880400
H	-0.56759600	1.51745500	4.07565200
H	-0.95294800	3.11266800	3.39641700
H	-0.81506900	1.69984300	2.32093300
C	1.61545000	3.12699700	4.14731900
H	2.64730800	3.40417700	3.93134100
H	1.05841300	4.04103100	4.38051700
H	1.60194400	2.48741400	5.04255000
C	4.42948400	1.59602600	1.17206700
H	4.49043800	0.58433300	1.56228600
H	4.38735500	1.52017200	0.07743400
H	5.33144900	2.15060500	1.45682300
C	3.09276800	3.61686100	1.14792000
H	3.96952600	4.22350700	1.40298000
H	3.00897200	3.59214100	0.05158100
H	2.20560000	4.10037500	1.55311100
C	5.30866300	-1.06830900	-3.09473000
H	5.72788200	-1.98339900	-2.67991900
H	5.10261200	-1.22593400	-4.16280000
H	6.05751200	-0.26945500	-3.01556000
C	3.41464800	0.46188900	-2.93261100
H	2.58060400	0.75305000	-2.29544900
H	4.10899100	1.30917800	-3.00121200
H	3.02817100	0.25537500	-3.94058800
C	2.77320300	-3.40080500	-3.21263000
H	1.87276700	-3.58987500	-3.80867600
H	3.42599100	-2.74990300	-3.79251600
H	3.28561300	-4.36237100	-3.05883900
C	1.37048600	-3.48792300	-1.21709300
H	1.64194100	-4.54249800	-1.06318200
H	1.22462600	-3.02593700	-0.24043900
H	0.41789500	-3.46473900	-1.76265400
C	4.47979200	-3.79617400	-0.02472900

H	3.88715500	-4.40102900	-0.71018900
H	5.46261600	-4.26987200	0.07029400
H	4.00149500	-3.81239200	0.96709300
C	5.62815000	-1.66627700	0.21926200
H	5.34053000	-1.57229100	1.27653600
H	6.60824400	-2.15434500	0.17161700
H	5.72118600	-0.66476400	-0.20259200
C	-4.04603200	-2.44170900	3.27892600
H	-3.44689700	-3.29108100	3.63908000
H	-4.23401900	-1.77870800	4.13156000
H	-5.00654800	-2.82019100	2.93154900
C	-2.16234300	-1.01005100	2.66417400
H	-1.65586500	-0.52870100	1.82826400
H	-2.41609600	-0.24291500	3.40629600
H	-1.45029500	-1.70575300	3.13123700
C	2.04052100	-1.22245700	2.99242600
H	1.16556000	-1.28571900	2.34841800
H	2.81432100	-1.88589400	2.58466900
H	1.76570600	-1.57647200	3.99484100
C	3.53863300	0.36753300	4.08034300
H	4.38556600	-0.31433900	3.92032200
H	3.91724300	1.38758900	4.03449500
H	3.14380100	0.18221900	5.08812500
C	-1.91414500	3.86096200	-3.91310800
H	-1.31894200	3.64720100	-4.80868300
H	-2.85733100	4.32061500	-4.23629300
H	-1.37164300	4.57079000	-3.29056900
C	-3.06654500	-3.77632600	-1.23378100
H	-3.07366200	-4.86865200	-1.32142400
H	-3.98557600	-3.39031900	-1.67898500
H	-2.21461400	-3.37899900	-1.80177100
H	0.00696500	-0.75793600	-2.76692300

**6**

**E = -6255.31991863 a.u.**

N	-1.69385900	1.52822000	0.05800600
N	-2.52249700	-0.83516200	0.19014600
N	2.04459100	-1.54103100	0.08698200
N	1.48472700	0.73452600	1.25884700
P	-2.41822500	2.04849300	-1.22859000
P	-3.44416600	-1.95565300	0.71399100
P	3.02001000	-1.84963800	-1.06852000
P	2.55240900	1.74219000	1.84344100
N	2.38637700	3.29067900	1.29269600
N	4.08354500	1.35777000	1.33466000
N	2.49532400	1.82839500	3.48999100
N	-3.07518200	-2.66179800	2.16152200
N	-3.64840300	-3.23726800	-0.33491100
N	-5.04389600	-1.51065100	0.94644200
N	-2.02135200	1.35582400	-2.68688300
N	-4.07518400	1.89552400	-1.26222800
N	-2.03099400	3.67080700	-1.41282400
N	2.48849500	-3.08603100	-2.03632200

N	3.39113400	-0.52135100	-1.99628700
N	4.52215700	-2.40293600	-0.61323000
B	-1.63456200	0.21014200	0.61008100
B	1.31446900	-0.63770800	0.84698000
C	-1.97337900	4.38887900	-2.47240300
C	-2.25127000	5.39135100	-4.56816100
C	-1.00782400	5.97153100	-3.89549200
H	-2.06853700	5.07157800	-5.59939800
H	-3.08027200	6.11772900	-4.57917800
H	-0.08649100	5.54158400	-4.32509900
H	-0.94441900	7.06125500	-3.97959300
N	-2.57372100	4.26097400	-3.71493700
N	-1.17976900	5.54215900	-2.52086100
C	-4.98700700	2.21026800	-0.42054900
C	-6.28981600	3.20300400	1.23469900
C	-7.13027900	2.14878500	0.51252200
H	-6.37553700	3.14893800	2.32511300
H	-6.56715900	4.22364900	0.92221800
H	-7.24462200	1.23867000	1.11678800
H	-8.12460600	2.51708900	0.23860700
C	-0.91727700	1.43052700	-3.34532700
C	0.47226600	0.90587700	-5.15985200
C	1.27698500	1.69111700	-4.11546000
H	0.73217000	-0.16590200	-5.14098700
H	0.62234500	1.27322100	-6.18069000
H	2.19583600	1.17991800	-3.81843300
H	1.54202900	2.69712400	-4.47754500
N	-4.94176400	2.87259400	0.80081300
N	-6.31922300	1.89336300	-0.66742500
N	0.35818800	1.77491700	-2.99180600
N	-0.88911900	1.12626700	-4.71324700
C	1.30776100	-3.52146700	-2.31238800
C	-0.31379600	-5.15712900	-2.70985200
C	-0.95200000	-3.76904300	-2.82130000
H	-0.57983700	-5.81720700	-3.54162900
H	-0.61095400	-5.65227800	-1.77239400
H	-1.19862100	-3.51292400	-3.86464200
H	-1.85507300	-3.67115600	-2.22127500
C	4.94098300	-3.48857800	-0.09111900
C	5.22374000	-5.49470800	1.06669900
C	6.51032100	-5.17589900	0.30326600
H	5.34276800	-5.31354300	2.14728500
H	4.89115100	-6.52878500	0.93169100
H	7.41144500	-5.31744200	0.90841700
H	6.60411900	-5.80255000	-0.60017500
C	4.41641800	-0.20691800	-2.69922100
C	6.19543600	-0.17643000	-4.21159200
C	6.06285400	1.20712300	-3.57250000
H	7.22479600	-0.54889400	-4.21799900
H	5.83011900	-0.17338600	-5.25144700
H	6.86256800	1.39116800	-2.83665500
H	6.09095400	2.01795200	-4.30780500
C	5.22759100	1.90991400	1.50437500

C	7.04844800	3.28203400	2.00891200
C	7.55967200	2.01083200	1.33257100
H	7.08028200	4.14451700	1.32302500
H	7.60990600	3.54453400	2.91105400
H	8.30675100	2.20618100	0.55695700
H	8.00120900	1.31721500	2.06852900
C	2.20365300	0.88736400	4.33477700
C	1.80333100	-1.17529100	5.34401600
C	1.04576600	-0.07650700	6.11757600
H	1.10077900	-1.85228600	4.84125500
H	2.48013300	-1.76032300	5.97988000
H	-0.03771400	-0.17247300	5.95593300
H	1.24452400	-0.09679700	7.19569800
C	1.58735900	4.26289200	1.54158700
C	-0.18741600	5.64627300	2.11892200
C	0.96008700	6.51300600	1.59678000
H	-0.99276100	5.55515100	1.37490700
H	-0.61936700	6.02428500	3.05023100
H	0.62883200	7.27204100	0.88182300
H	1.49071100	7.02261000	2.41908400
C	-5.64791600	-1.00820400	1.94965500
C	-7.48622000	-0.64988200	3.34539600
C	-6.29671200	0.16534900	3.85247500
H	-8.42344200	-0.08385400	3.34225800
H	-7.63370200	-1.55919700	3.95266300
H	-6.41965100	1.23411600	3.61232600
H	-6.14556900	0.07626700	4.93248900
C	-2.04110000	-3.23477800	2.65790300
C	-0.73962600	-4.15171100	4.37479000
C	0.04992700	-4.16607100	3.05976400
H	-0.16078800	-3.74199500	5.21006100
H	-1.07820100	-5.16349800	4.65908800
H	0.80094900	-3.36378000	3.03109500
H	0.54326100	-5.12490700	2.86910300
C	-4.18556400	-3.40474500	-1.47951200
C	-5.30285900	-4.63148300	-3.12194900
C	-4.98066400	-3.23729700	-3.65928100
H	-5.08702800	-5.42878100	-3.84032300
H	-6.36340700	-4.71277000	-2.82798100
H	-4.14044700	-3.27165300	-4.37298400
H	-5.82925000	-2.75912200	-4.15788500
N	0.46184300	4.35661900	2.33039700
N	1.80362500	5.51704400	0.96890400
N	-5.18266200	-0.41148800	3.11347800
N	-7.05339900	-0.98183900	2.00116700
N	-1.85196800	-3.29661700	4.03142600
N	-0.99014000	-3.91038600	2.07526600
N	1.52979400	1.15355000	5.51353500
N	2.55328600	-0.43061000	4.35170200
N	6.33713100	1.47279000	0.77213500
N	5.67846300	2.92240800	2.33465600
N	4.27416000	-4.55356800	0.49332900
N	1.10865600	-4.84841100	-2.70108800

N	0.09942600	-2.89474100	-2.32878900
N	-4.59492700	-2.51148200	-2.45661800
N	-4.43277800	-4.69805900	-1.96381300
N	6.30929300	-3.78358400	-0.05108200
N	5.33536300	-1.00175600	-3.37537000
N	4.77609300	1.11842800	-2.91044900
Si	-0.21040100	-0.26040600	2.04533100
C	-3.82276500	3.58030500	-3.98523000
H	-3.74705700	3.04243300	-4.93670400
H	-4.05940800	2.86590600	-3.19999000
H	-4.64427100	4.30989000	-4.06518600
C	-0.05372700	5.66736300	-1.62544600
H	-0.24098900	5.05211000	-0.74938300
H	0.87941300	5.31788900	-2.09335600
H	0.08284400	6.71291300	-1.32932000
C	-3.86100000	3.74191100	1.22097100
H	-3.97451900	3.92855000	2.29390700
H	-2.90684000	3.24491300	1.05730600
H	-3.86746700	4.70346000	0.68826300
C	-6.63212800	0.74648100	-1.49890700
H	-6.31418600	-0.19512300	-1.03102000
H	-7.71187500	0.72627600	-1.67543500
H	-6.11877800	0.85048100	-2.45474700
C	-3.91293000	0.30908300	3.15822400
H	-3.80509400	0.73731400	4.15845000
H	-3.07676600	-0.36438200	2.99049400
H	-3.88034700	1.11114900	2.41275300
C	-7.81176900	-1.95074900	1.24279300
H	-8.79699700	-1.54209400	0.99449400
H	-7.26301900	-2.17172400	0.32685400
H	-7.95198300	-2.88945500	1.80256400
C	-0.60635500	-3.80637300	0.68002900
H	0.00561000	-2.92195300	0.48212600
H	-0.02954600	-4.70222500	0.42052100
H	-1.50196900	-3.78361000	0.06453200
C	-2.89767900	-3.00221400	4.97219900
H	-3.35474000	-3.92009200	5.37707600
H	-2.50200600	-2.41648700	5.81109600
H	-3.66591900	-2.42336900	4.45597200
C	-4.57797400	-5.79738600	-1.03670000
H	-5.61771100	-5.90535600	-0.68803300
H	-4.27444700	-6.73361200	-1.51717700
H	-3.94142200	-5.60019600	-0.17360000
C	-3.92379200	-1.23634300	-2.66580600
H	-3.01138200	-1.37323100	-3.26033300
H	-4.58832900	-0.56155200	-3.20784800
H	-3.64446300	-0.78060400	-1.71878700
C	2.03638700	-5.87250600	-2.27941200
H	1.70920300	-6.35161800	-1.34176100
H	2.12343700	-6.64903200	-3.04744800
H	3.00867800	-5.40879300	-2.11021500
C	-0.13299400	-1.46622800	-2.36521200
H	-0.54479500	-1.19749700	-3.34603100



H	-0.85038900	-1.17677000	-1.59382100
H	0.79393400	-0.92313500	-2.20950900
C	7.20712600	-3.17673500	-1.00794500
H	7.36266300	-3.82962800	-1.88252400
H	6.76587400	-2.23962700	-1.34847700
H	8.18199700	-2.98285200	-0.54757900
C	2.97540600	-4.45702000	1.13068600
H	3.08896100	-4.36036200	2.22133000
H	2.42822200	-3.58572800	0.76838400
H	2.39575600	-5.36367600	0.92585900
C	4.89295700	3.87069300	3.09589800
H	3.97775200	3.40672400	3.45988500
H	5.48987800	4.18709900	3.95950100
H	4.63877800	4.75892500	2.50468500
C	6.35313400	0.14882900	0.19492500
H	6.72689600	-0.60556100	0.90450600
H	5.34481200	-0.13380900	-0.09164200
H	6.99830600	0.13818700	-0.69014200
C	5.02714000	-2.32578200	-3.88039100
H	4.25452500	-2.80266200	-3.27964700
H	4.67891800	-2.27115400	-4.92424800
H	5.93105200	-2.94387100	-3.85288100
C	4.39572100	2.16803200	-1.98178800
H	3.91103100	2.99833700	-2.50672200
H	3.71269200	1.76130500	-1.24005500
H	5.28093100	2.54316500	-1.45331200
C	-1.97570100	0.43241600	-5.35191000
H	-2.06982100	0.75868800	-6.39450600
H	-1.83296800	-0.66116100	-5.34782500
H	-2.89299200	0.66206700	-4.80975800
C	0.89976200	2.05530400	-1.67381800
H	0.12559300	2.01869400	-0.91082500
H	1.64674100	1.30032000	-1.42439600
H	1.37469200	3.04292000	-1.65937400
C	-0.41949600	3.21548000	2.56623200
H	-0.87411400	2.85304000	1.63678300
H	0.13136700	2.39722000	3.01502900
H	-1.19532700	3.52974200	3.27048800
C	3.07561100	5.88917700	0.40622300
H	3.60081900	4.97482700	0.12655700
H	2.92808300	6.51303700	-0.48268700
H	3.69419000	6.45416500	1.12225800
C	3.32452900	-1.15404500	3.37089400
H	2.67746600	-1.73085100	2.70075000
H	3.91104700	-0.46734600	2.76334900
H	4.00713000	-1.83806200	3.89281300
C	0.77868800	2.36857700	5.70805200
H	1.19442600	3.14258100	5.06216700
H	-0.28272400	2.22886100	5.45558300
H	0.85043400	2.68828300	6.75449900

**6H<sup>+</sup>**

**E = -6255.85706663 a.u.**

N	1.16670900	1.32566800	0.18772100
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N	2.63114900	-0.58222600	-0.51121400
N	-3.22055100	-0.69180500	0.51551200
N	-1.75534800	0.58250200	-1.22368300
P	1.88938700	2.26689700	1.20738400
P	3.35683400	-1.79951200	-1.15513300
P	-3.47026500	-1.81230900	1.60131900
P	-2.58650600	1.67885000	-2.09443300
N	-1.93093400	3.16679400	-2.21275900
N	-3.95257600	1.86863300	-1.26248100
N	-2.71953300	1.15700800	-3.64155500
N	2.74448600	-2.32842200	-2.57150800
N	3.50161700	-3.11560300	-0.12570800
N	4.91506500	-1.35527400	-1.49420900
N	1.10664600	2.31163100	2.67186600
N	3.43090700	1.93072900	1.70690200
N	1.88155700	3.81737600	0.59657400
N	-2.26209700	-2.88825300	1.89048000
N	-3.90009000	-1.03745900	2.98967000
N	-4.79046500	-2.71672900	1.20478100
B	1.40577100	0.09562800	-0.45322400
B	-2.13762400	-0.43146200	-0.26855400
C	1.92464000	4.97194000	1.15387400
C	2.28823700	6.83483300	2.50792300
C	1.43072300	7.24861700	1.31451000
H	1.90531100	7.20528300	3.46298400
H	3.32568400	7.18616900	2.39261500
H	0.37075500	7.35495400	1.60015400
H	1.75827800	8.18601200	0.85563500
N	2.22919500	5.37694600	2.44857100
N	1.61463700	6.11793400	0.42434000
C	4.56381400	2.29545400	1.22330000
C	6.28081800	3.15379100	-0.09727700
C	6.85951500	2.76816500	1.27290800
H	6.88224000	2.78251000	-0.93101000
H	6.18466400	4.24547500	-0.19907400
H	7.46489300	1.85004800	1.21464000
H	7.48117400	3.55675000	1.70697700
C	0.01000800	2.87361100	3.02889100
C	-1.36887900	3.92350500	4.58796800
C	-2.03140200	3.98630000	3.21107100
H	-2.06384700	3.64853200	5.38640200
H	-0.90246500	4.88727100	4.85224800
H	-2.89605700	3.30949700	3.14352200
H	-2.37110000	4.99299200	2.94700100
N	4.97800200	2.51022400	-0.06706200
N	5.65287900	2.55790100	2.04877600
N	-0.96875100	3.53929200	2.32194800
N	-0.35824100	2.89969900	4.38138100
C	-0.99697100	-2.79793900	2.14548600
C	1.13500300	-3.65731400	2.56894900
C	1.18717400	-2.12659300	2.57489700
H	1.17932600	-4.07057500	3.59075800
H	1.93654800	-4.10369300	1.97804900

H	1.71336700	-1.71695900	3.44203400
H	1.65496100	-1.73139500	1.66481000
C	-4.96615700	-3.86030300	0.66038000
C	-4.82701400	-5.84943100	-0.55407900
C	-6.06521600	-5.89443100	0.34209600
H	-5.10637700	-5.68711900	-1.60751100
H	-4.22209200	-6.75909100	-0.49846100
H	-6.95557300	-6.25901800	-0.17824800
H	-5.89953700	-6.53164800	1.22620400
C	-3.80539000	-1.33561600	4.23378500
C	-3.76735000	-2.35842500	6.32388700
C	-3.42661000	-0.87612700	6.48662400
H	-4.79542600	-2.56831700	6.65783200
H	-3.08661700	-3.01857000	6.86842000
H	-3.95973100	-0.40300100	7.31618700
H	-2.34505700	-0.72814500	6.63978600
C	-5.05931100	2.51765000	-1.26309800
C	-6.85420400	3.91806700	-1.74135400
C	-7.14596900	3.14925000	-0.44458700
H	-6.59878000	4.96971900	-1.53974700
H	-7.68956000	3.89885400	-2.44706500
H	-7.49701200	3.79786500	0.36300900
H	-7.89869500	2.36113000	-0.60199800
C	-2.99351800	0.01638400	-4.18619100
C	-3.75247200	-2.11593400	-4.72059600
C	-3.11482500	-1.48705600	-5.96673900
H	-3.11295500	-2.89992700	-4.28904200
H	-4.73836600	-2.54707100	-4.91593300
H	-2.42244300	-2.16190200	-6.47726500
H	-3.87711500	-1.15974700	-6.69113300
C	-1.04720900	3.71445900	-2.97443200
C	0.86110800	4.23032000	-4.19153900
C	-0.05964400	5.45299000	-4.17736500
H	1.70854200	4.36249400	-3.50279900
H	1.25321300	3.99901400	-5.18482200
H	0.46613100	6.37891200	-3.92771800
H	-0.56709100	5.59261000	-5.14472600
C	6.00030400	-2.02377500	-1.60989900
C	8.29466900	-2.38942900	-1.37863300
C	7.66185700	-3.59150500	-2.07622700
H	9.22083300	-2.05571000	-1.85526200
H	8.51136000	-2.60946500	-0.31951700
H	7.88193200	-3.58469800	-3.15506100
H	7.99018500	-4.55024500	-1.66508700
C	1.70305200	-2.85375000	-3.09927900
C	0.02576900	-3.07392300	-4.71767400
C	-0.30034000	-3.99222700	-3.52322500
H	-0.65595700	-2.21239800	-4.75291300
H	-0.02797200	-3.59870600	-5.67823900
H	-1.26235600	-3.73204500	-3.06632900
H	-0.33099000	-5.05399000	-3.80260600
C	4.30004800	-3.31855200	0.86058600
C	5.67965900	-4.62219100	2.21041600

C	5.75158700	-3.16939000	2.67719000
H	5.58691500	-5.33587900	3.03349800
H	6.56670800	-4.89312800	1.61416000
H	5.20320200	-3.02232000	3.62080100
H	6.77663600	-2.81488400	2.82145500
N	-0.02111400	3.16591600	-3.71241700
N	-1.00828200	5.08337500	-3.14349500
N	6.23669100	-3.37648400	-1.83922900
N	7.23935000	-1.40029000	-1.49283000
N	1.37857100	-2.62979000	-4.43165500
N	0.78510900	-3.73553300	-2.59670400
N	-2.41861700	-0.34917200	-5.39134300
N	-3.85160100	-0.97938400	-3.81730600
N	-5.84994200	2.56949500	-0.14039200
N	-5.70191300	3.20105200	-2.27039500
N	-4.09835000	-4.69539400	-0.03712600
N	-0.16978200	-3.90144200	1.97418700
N	-0.23195400	-1.77773700	2.62450900
N	5.09279300	-2.45594200	1.59126000
N	4.48864100	-4.60370400	1.37580200
N	-6.19756700	-4.50040800	0.72350900
N	-3.64425400	-2.54890800	4.88163200
N	-3.84659000	-0.34304100	5.20285700
Si	-0.38282000	-0.62505100	-1.16477000
C	3.14960800	4.67175000	3.32557600
H	3.06888300	5.11304400	4.32379100
H	2.88786600	3.61974400	3.38772900
H	4.19050300	4.76464400	2.98301800
C	0.79408200	6.01714000	-0.75827800
H	0.94503800	5.03332500	-1.19644400
H	-0.27479700	6.12507900	-0.52214800
H	1.07082200	6.79507800	-1.47783400
C	4.14326300	2.41948000	-1.24725500
H	4.79234500	2.23118400	-2.10739300
H	3.47273000	1.56634600	-1.14129100
H	3.56120700	3.33374500	-1.41346600
C	5.71556600	2.09478100	3.41182600
H	6.30390600	1.16884000	3.50004100
H	6.17220200	2.85529200	4.05459000
H	4.69685700	1.89516500	3.74638900
C	5.33162400	-4.21622400	-2.60707600
H	4.32007800	-4.14245900	-2.22012700
H	5.32909200	-3.94483700	-3.67193400
H	5.66763300	-5.25325200	-2.51160000
C	7.35996700	-0.16212100	-0.76115500
H	8.13129700	0.47294000	-1.20990900
H	6.39602400	0.34691900	-0.78226900
H	7.63557800	-0.34799400	0.28927400
C	0.69084500	-4.19109100	-1.23250500
H	-0.10125500	-3.66587000	-0.68711100
H	0.46664900	-5.26594200	-1.21876200
H	1.63660300	-4.02111600	-0.71992400
C	1.89851000	-1.48116100	-5.13419800

H	2.87459700	-1.23427700	-4.71552500
H	2.00491100	-1.71074900	-6.19990500
H	1.23459400	-0.60884800	-5.02748900
C	4.22655200	-5.76324100	0.55023300
H	5.06055900	-5.97207600	-0.13725000
H	4.07509500	-6.63716200	1.19058900
H	3.32756900	-5.58878500	-0.03930400
C	4.80501200	-1.04807700	1.81103200
H	4.31334100	-0.90379200	2.78320200
H	5.74058400	-0.48087900	1.81168300
H	4.14908000	-0.64912500	1.03831400
C	-0.70005800	-5.24206700	1.93238900
H	-1.72102800	-5.20227600	1.55084000
H	-0.08549700	-5.86559800	1.27413000
H	-0.71449500	-5.70649900	2.93153800
C	-0.60475200	-0.38330600	2.73276900
H	-0.11877100	0.04097000	3.61582300
H	-0.27262300	0.18514300	1.86163700
H	-1.68085900	-0.28259600	2.83861300
C	-7.17021400	-4.13054500	1.72752900
H	-7.01829300	-4.68569900	2.66641100
H	-7.06903300	-3.06439300	1.92971800
H	-8.17878500	-4.34281100	1.35987700
C	-3.01144800	-4.21275900	-0.86477700
H	-2.59092700	-3.29282200	-0.46761200
H	-2.21544600	-4.96274100	-0.89270800
H	-3.35445400	-4.04098400	-1.89764600
C	-5.09373000	3.64383400	-3.50376300
H	-4.66647200	4.65095300	-3.41083100
H	-4.30803200	2.95267500	-3.80744000
H	-5.85891300	3.66566000	-4.28712000
C	-5.68640400	1.64948400	0.97010700
H	-6.48845100	0.89877200	0.97120100
H	-4.73418700	1.12216700	0.87580200
H	-5.72434700	2.19370200	1.92037900
C	-4.10884800	-3.81369100	4.34169500
H	-3.75682400	-3.94061800	3.32098600
H	-3.68816800	-4.61917700	4.95122100
H	-5.20534100	-3.89047700	4.36965100
C	-3.52430600	1.02491000	4.85760700
H	-2.43865400	1.20524700	4.84802800
H	-3.91419600	1.22597700	3.85932700
H	-3.99267500	1.70317100	5.57785400
C	0.64770700	2.71424600	5.40390600
H	0.16973600	2.37721400	6.32880300
H	1.35671400	1.96065200	5.06137700
H	1.19860000	3.64469300	5.61399800
C	-1.34564700	3.27638200	0.94086300
H	-0.56992600	2.71847500	0.42178500
H	-2.26718200	2.68093300	0.90690500
H	-1.52637300	4.21768600	0.41445600
C	0.60711400	1.90552600	-3.33266900
H	0.98506400	1.94009200	-2.30499500

H	-0.10145700	1.08554000	-3.43206300
H	1.43604300	1.71745900	-4.01854500
C	-2.12301800	5.93958700	-2.82381700
H	-2.72337600	5.44621400	-2.05888700
H	-1.75826600	6.89715800	-2.43865600
H	-2.75095500	6.13811500	-3.70518100
C	-4.53046800	-1.12563200	-2.54587400
H	-3.98566100	-1.77975700	-1.86206400
H	-4.63355700	-0.16212200	-2.05337000
H	-5.52703400	-1.54340500	-2.72406100
C	-1.73351700	0.60129100	-6.23646700
H	-2.40469100	1.02097100	-7.00051600
H	-1.35862600	1.41350800	-5.61229800
H	-0.89515200	0.11035100	-6.74113800
H	-0.46552700	-1.34488000	-2.47911500

7

**E = -1862.29995458 a.u.**

Si	0.82062600	-1.30453100	-1.08441100
N	-1.95742100	-1.41785100	-0.40792400
N	1.97450000	-0.50695700	-0.04922800
P	-3.42598300	-1.13939500	0.09354300
P	3.49695500	-0.84612100	0.16408100
C	-3.58623600	-0.47826800	1.79293500
H	-4.63241800	-0.33510900	2.07951400
H	-3.10589400	-1.16965000	2.48981800
H	-3.05166800	0.47373100	1.81038000
C	-4.39929800	-2.67749800	0.10672200
H	-4.42640300	-3.08699800	-0.90581400
H	-3.90708400	-3.40100700	0.76099300
H	-5.41894900	-2.49689800	0.45892100
C	-4.40710900	0.02872100	-0.91649500
H	-5.41503500	0.17180800	-0.51531500
H	-3.85717100	0.97212700	-0.92070300
H	-4.46881000	-0.35231800	-1.93887000
C	4.30179700	-2.04971600	-0.95704600
H	3.76929900	-3.00129000	-0.89656300
H	4.22552200	-1.68657300	-1.98443600
H	5.35239400	-2.18740200	-0.68611700
C	4.53644400	0.64951200	0.03718600
H	4.17112200	1.39456700	0.74791200
H	5.58695500	0.42740300	0.24523900
H	4.44438500	1.05511800	-0.97371100
C	3.83914800	-1.50001200	1.83304600
H	4.91102300	-1.64550200	1.99517600
H	3.44518100	-0.80135600	2.57476100
H	3.31969800	-2.45550900	1.94241400
B	-0.96743000	-0.39269200	-0.51110700
N	-1.27078500	0.98426200	-0.22507100
P	-0.32091600	2.21430900	-0.04532100
C	0.66627800	2.22035800	1.49205700
H	1.28008500	3.12243000	1.57865300

H	-0.00554400	2.14983700	2.35111300
H	1.29845700	1.32902900	1.44359400
C	-1.30416100	3.74841900	0.02675600
H	-1.85187600	3.86368600	-0.91187300
H	-2.02468600	3.66962800	0.84427500
H	-0.66511700	4.62188600	0.18563600
C	0.92061400	2.54881800	-1.35051800
H	0.41734200	2.59336100	-2.31950700
H	1.44580400	3.49124800	-1.16703700
H	1.63202700	1.72056500	-1.34802300

7H<sup>+</sup>

E = -1862.78348515 a.u.

Si	-0.81581000	-0.28425900	-0.93159700
N	0.23389500	1.17505400	-0.55792900
N	-2.03176100	-0.61482200	0.14822400
P	0.54183700	2.64351400	0.04808900
P	-3.55736400	-0.97407800	0.13967500
C	0.78450100	2.56150900	1.83921500
H	1.04357600	3.54023100	2.25090400
H	-0.13101900	2.19028500	2.30558800
H	1.59410000	1.85037100	2.02298600
C	-0.82337400	3.77520800	-0.29605600
H	-0.96308100	3.84963800	-1.37710600
H	-1.73481500	3.37842900	0.15791900
H	-0.61270800	4.76586500	0.11476700
C	2.06613100	3.30071800	-0.66599600
H	2.34364700	4.24920700	-0.19914200
H	2.84337600	2.55066900	-0.49622600
H	1.93044800	3.44067300	-1.74074200
C	-4.42859000	-0.82262100	-1.45502700
H	-4.35053600	0.20558600	-1.81677500
H	-3.96605400	-1.48834800	-2.18780200
H	-5.48364500	-1.08686200	-1.34428100
C	-3.87071800	-2.67930400	0.68759600
H	-3.41215000	-2.82483100	1.66849700
H	-4.94311300	-2.88215100	0.75191900
H	-3.41233300	-3.37271900	-0.02189300
C	-4.49965500	0.06904300	1.29386400
H	-5.54777500	-0.23904900	1.33390600
H	-4.05780700	-0.01569500	2.28949500
H	-4.44163100	1.11036100	0.96735100
B	1.06133800	-0.03846800	-0.46230600
N	2.36184000	-0.17420700	-0.04454300
P	3.20951700	-1.51281800	0.07077700
C	3.73015800	-1.80913500	1.78401600
H	4.37324300	-2.69061500	1.84922200
H	4.27481100	-0.93432700	2.14696500
H	2.84386500	-1.95851100	2.40559300
C	4.74144600	-1.39300100	-0.89297500
H	4.49148100	-1.28674800	-1.95134400
H	5.29569400	-0.50887400	-0.56955500

H	5.36014500	-2.28305700	-0.75212400
C	2.39104400	-3.04401100	-0.47222600
H	2.10953300	-2.94930900	-1.52340300
H	3.06034100	-3.89913000	-0.34732200
H	1.48590800	-3.19583000	0.12006900
H	-1.28216000	-0.14516200	-2.33643800

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**E = -2714.57635554 a.u.**

Si	0.96962600	0.03511100	-2.04947700
N	-1.63074900	1.08402100	-0.53412100
N	1.79988900	-0.19346700	-0.55372200
P	-1.28827000	2.53888100	-0.13290200
P	3.22090900	-0.49113200	-0.01882200
N	3.38488400	-2.12627400	0.31776400
N	3.49321400	0.41001500	1.37295700
N	4.60361700	-0.09820800	-0.91840000
N	-0.99454300	2.61653600	1.52703800
N	-2.56320900	3.53839600	-0.60328900
N	0.02060400	3.41620100	-0.72960800
B	-0.88700500	0.03846800	-1.14998700
N	-1.26844000	-1.33691600	-1.10058900
P	-2.25042100	-2.11672000	-0.18383600
N	-3.84513300	-1.61516400	0.09216300
N	-1.67573200	-2.25462800	1.39704000
N	-2.52296600	-3.62186900	-0.89059800
C	4.57712700	-2.67152600	0.94227800
H	4.30935700	-3.30366000	1.79995700
H	5.15374500	-3.29165600	0.23860700
H	5.23464000	-1.87871900	1.29408100
C	2.51373200	-3.13360300	-0.26978100
H	1.59910200	-2.67358700	-0.63972200
H	3.00770300	-3.66364300	-1.09908300
H	2.24614400	-3.87813400	0.49171800
C	4.78849400	0.56854600	2.01494600
H	4.91483300	-0.11540000	2.86885600
H	5.59082000	0.39107400	1.29905300
H	4.88868400	1.59303900	2.39769400
C	2.36824500	0.64138100	2.27042400
H	1.43839500	0.61082700	1.70546700
H	2.32465800	-0.10705300	3.07708900
H	2.46847700	1.63092400	2.73529700
C	4.93566400	-0.97994900	-2.03920700
H	4.80854500	-2.02481800	-1.75457700
H	4.30930300	-0.78229800	-2.92042500
H	5.98609100	-0.82783800	-2.31551900
C	4.76812600	1.31334800	-1.27504400
H	4.15993800	1.58855700	-2.14836400
H	4.47701200	1.94876000	-0.43752700
H	5.82170400	1.50882900	-1.50965200
C	-1.49316700	-4.21455700	-1.73431100
H	-0.84972700	-4.91022800	-1.17133300



H	-1.96619900	-4.78113500	-2.54696500
H	-0.87881200	-3.42346200	-2.16065900
C	-3.44898000	-4.59460200	-0.33459200
H	-4.24506600	-4.08955700	0.21229900
H	-3.90773900	-5.17113200	-1.14858400
H	-2.95394700	-5.31113400	0.33973900
C	0.02968900	3.78617000	-2.14315200
H	0.59299000	3.06078200	-2.74782100
H	-0.98982700	3.83899600	-2.52502300
H	0.50095300	4.77037500	-2.26503100
C	1.36589200	3.30065500	-0.17457600
H	1.85365700	4.28491700	-0.19303100
H	1.32540900	2.94490400	0.85236700
H	1.98171000	2.59661300	-0.74574800
C	-0.82846900	3.87585100	2.23248300
H	-1.76678200	4.22607800	2.68958500
H	-0.09075200	3.75608400	3.03740500
H	-0.46091700	4.64962400	1.55865200
C	-1.34374800	1.50298200	2.39592400
H	-1.43539400	0.59179400	1.80891300
H	-0.55939000	1.36458800	3.15292000
H	-2.29344700	1.67730700	2.92618200
C	-3.87806500	2.97330500	-0.86838200
H	-4.36582400	3.54382500	-1.66957600
H	-3.76766400	1.93824500	-1.18654800
H	-4.53439400	3.00779600	0.01592800
C	-2.58393900	4.96424400	-0.32313000
H	-1.56812100	5.35842100	-0.28385900
H	-3.11619100	5.48857100	-1.12717100
H	-3.09258400	5.20385400	0.62365000
C	-4.10793300	-0.55041000	1.06215600
H	-3.80556800	0.43166000	0.67980900
H	-5.18132700	-0.53996600	1.28622500
H	-3.56507800	-0.73283700	1.98842600
C	-4.66000600	-1.45736800	-1.11451000
H	-5.72151200	-1.50684000	-0.84444800
H	-4.47199300	-0.49537700	-1.61262300
H	-4.44161500	-2.25903800	-1.82061800
C	-0.26795100	-2.03177300	1.69700100
H	-0.17572700	-1.51057300	2.65963600
H	0.28567100	-2.98001100	1.77731500
H	0.20133800	-1.42291200	0.92583100
C	-2.34793600	-3.09044500	2.38005700
H	-1.92967800	-4.10838200	2.41690400
H	-2.23518600	-2.64912100	3.37928200
H	-3.41411600	-3.16124200	2.16308000

**8H<sup>+</sup>**

**E = -2715.07016575 a.u.**

Si	-0.64232500	-0.48188400	-1.13168000
N	2.46495000	0.06071100	-0.21153200
N	-1.73996800	-1.18098800	-0.09942300

P	3.34599600	-1.24545000	-0.06038600
P	-3.29372500	-1.28435300	-0.01175400
N	-3.90377700	0.01421200	0.87570100
N	-3.68596600	-2.76562100	0.64239100
N	-4.24590000	-1.22603100	-1.38736200
N	3.90011300	-1.30415900	1.51667400
N	4.56250100	-1.21790000	-1.19732000
N	2.66968800	-2.75663900	-0.25117200
B	1.15367600	0.05665000	-0.61880100
N	0.12624900	1.10097400	-0.59181500
P	0.13608800	2.62166700	-0.05058900
N	1.51969800	3.42720800	-0.46525400
N	-0.05198800	2.61117400	1.59026900
N	-1.08681000	3.48112100	-0.73489800
C	-5.33449100	0.12631100	1.16028000
H	-5.61946500	-0.41102800	2.07579300
H	-5.59314000	1.18267500	1.29682800
H	-5.92374800	-0.26218700	0.33005500
C	-3.07720600	0.56591100	1.94700700
H	-2.02530500	0.48949400	1.67966800
H	-3.32932400	1.62374400	2.08944100
H	-3.24083000	0.04781600	2.90401400
C	-5.06989200	-3.17147800	0.86430300
H	-5.37706900	-3.02475500	1.90882600
H	-5.74291300	-2.60957300	0.21743900
H	-5.18264600	-4.23597600	0.62672800
C	-2.71353400	-3.55789400	1.38767400
H	-1.70621300	-3.21681100	1.15629500
H	-2.87794300	-3.47957100	2.47173700
H	-2.80713200	-4.61415500	1.10699400
C	-4.47673900	0.04118400	-2.08251400
H	-4.51438900	0.86615400	-1.37325800
H	-3.69104900	0.24757500	-2.82262900
H	-5.43634800	-0.00752200	-2.60930400
C	-4.20644900	-2.36249400	-2.31140000
H	-3.43203400	-2.23136600	-3.07974700
H	-4.00610300	-3.28571400	-1.76914600
H	-5.17533500	-2.45457600	-2.81434400
C	-2.42303700	2.89377900	-0.81277600
H	-3.12796100	3.46087100	-0.19137800
H	-2.78421800	2.90706600	-1.84726100
H	-2.42193900	1.86339400	-0.46128100
C	-1.02174400	4.89343000	-1.10095200
H	-0.01663100	5.27985100	-0.94093900
H	-1.28925600	5.02104700	-2.15635100
H	-1.72601500	5.48134100	-0.49802800
C	2.41663800	-3.29847200	-1.58702300
H	1.39351800	-3.07675600	-1.91700400
H	3.11288900	-2.87427000	-2.30887200
H	2.54781300	-4.38641800	-1.56755200
C	1.71310000	-3.24900100	0.74388800
H	1.80506900	-4.33788000	0.82809100
H	1.91716800	-2.80597500	1.71808500

H	0.68190100	-3.00497900	0.45687300
C	4.71919000	-2.41314400	2.00218900
H	5.79374900	-2.20685000	1.90351200
H	4.50413400	-2.58250300	3.06337000
H	4.48514500	-3.32887900	1.46013800
C	4.09337600	-0.07321300	2.27801100
H	3.41806800	0.69619800	1.90987300
H	3.87354600	-0.26346100	3.33530400
H	5.12758600	0.29442500	2.20937000
C	4.91295100	-0.00192000	-1.92337500
H	5.14323700	-0.25143700	-2.96593900
H	4.07574100	0.69286600	-1.90333900
H	5.79442300	0.48963400	-1.48795700
C	5.61713000	-2.22849900	-1.19776800
H	5.26477600	-3.15262900	-0.73960800
H	5.90598100	-2.45432400	-2.23053600
H	6.51260400	-1.88592900	-0.66142500
C	2.65921300	3.48592100	0.45400600
H	3.27714600	2.58347200	0.37610500
H	3.26567100	4.36207000	0.20433500
H	2.31571200	3.59819900	1.48246300
C	1.91369500	3.38251000	-1.87848300
H	2.47933000	4.28616000	-2.12558400
H	2.53411200	2.50234600	-2.08690600
H	1.02988300	3.34283600	-2.51743900
C	0.51130500	1.57248700	2.45141800
H	1.39091300	1.94129900	2.99484000
H	-0.24032400	1.26362500	3.18628100
H	0.80790700	0.70335400	1.86756500
C	-0.48315400	3.80996600	2.30550400
H	-1.21000200	3.52989100	3.07598800
H	0.35825700	4.31680100	2.79616600
H	-0.96228000	4.51378400	1.62490400
H	-1.16152800	-0.25803500	-2.50654700

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**E = -4751.40666185 a.u.**

Si	-0.97544600	0.45170600	-1.61407500
N	2.18995200	0.20439800	-0.43810900
N	-1.77729300	-0.63168100	-0.48677100
P	2.92799700	-1.13845800	-0.79589400
P	-3.06023700	-1.09432400	0.22209500
N	-3.02666400	-0.73740200	1.84777100
N	-3.37453800	-2.73493000	0.08584800
N	-4.53343900	-0.43112000	-0.22641700
N	4.51472200	-0.75953100	-1.18402600
N	2.26380700	-2.06584000	-1.96771000
N	3.02939700	-2.21085500	0.47485100
B	0.89854700	0.55961000	-0.85199000
N	0.11210600	1.70274500	-0.54928200
P	0.14573500	2.88546600	0.55190200
N	1.56008800	3.70325300	0.45441000
N	0.06069400	2.29714000	2.06123400

N	-1.15419000	3.83075200	0.33471500
C	0.88362200	1.84053000	2.93236900
C	1.85754700	0.33539600	4.42173400
C	2.33226500	1.75864000	4.75026900
H	1.49302900	-0.20100000	5.30461700
H	2.65043300	-0.26535400	3.95759300
H	1.83403700	2.14904100	5.65296000
H	3.41404400	1.82320600	4.90749800
C	-2.66159500	-3.79735000	0.07980500
C	-1.02536600	-5.44622800	0.28353900
C	-2.23793000	-6.03800600	-0.43678800
H	-0.07886600	-5.66365700	-0.22118600
H	-0.95294400	-5.81243400	1.32103800
H	-2.05361600	-6.11409200	-1.52271700
H	-2.51719200	-7.02998100	-0.06775900
C	-3.94347800	-0.49323500	2.70711700
C	-4.91206500	0.60424700	4.53285800
C	-5.88737500	-0.45270200	4.01006500
H	-4.80626400	0.57859800	5.62266300
H	-5.23089700	1.62126300	4.24884300
H	-5.94653200	-1.31659800	4.69240600
H	-6.90215700	-0.06421100	3.87331300
C	-5.23421500	-0.41009100	-1.28925700
C	-6.18224300	-0.71324600	-3.40111200
C	-6.99310400	0.34024500	-2.63845200
H	-5.93583700	-0.40569600	-4.42226900
H	-6.72329200	-1.67269200	-3.45237600
H	-6.75569300	1.35849500	-2.99237700
H	-8.07424300	0.19191600	-2.72396900
C	1.60729300	-1.69434800	-3.02532200
C	0.73616600	-0.50628400	-4.83923900
C	-0.14993500	-1.73728800	-4.56660600
H	0.18994400	0.42138200	-4.62635800
H	1.11562400	-0.47315100	-5.86837800
H	-1.13374500	-1.42326700	-4.19585100
H	-0.28917900	-2.36577700	-5.45439300
C	5.60615300	-1.42340700	-1.12685600
C	7.90601600	-1.64132000	-0.79436200
C	7.29127500	-3.03448300	-0.94433400
H	8.83099800	-1.51970600	-1.36661300
H	8.12619500	-1.41147300	0.26270700
C	2.08728300	4.50345800	-0.39939100
C	3.70331300	5.38127600	-1.83276800
C	2.54124600	6.38258400	-1.71167300
H	4.59059000	5.72405900	-1.27581100
H	4.00195200	5.20030500	-2.86957200
H	2.87847300	7.40402500	-1.50852800
H	1.92591200	6.39993800	-2.62517500
C	-2.08281500	3.67031500	-0.56714400
C	-4.15835000	3.10576200	-1.47804100
C	-3.17134600	3.45091800	-2.61575500
H	-4.47363100	2.05946200	-1.53731400
H	-5.05192300	3.74472700	-1.48009800

H	-2.88602100	2.54440500	-3.16785500
H	-3.56463100	4.20260900	-3.30971600
N	-4.98630500	-0.82283200	-2.58593900
N	-6.52889800	0.12743000	-1.28301400
N	-3.26047800	-5.04939700	-0.14778000
N	-1.31389800	-4.02491400	0.25336100
N	-5.28900700	-0.84445800	2.74442000
N	-3.68148900	0.24664100	3.85709200
N	1.83531200	-0.66666500	-3.89987900
N	0.57290400	-2.45687300	-3.52599400
N	5.86318200	-2.76345000	-0.88036800
N	6.84369500	-0.79461600	-1.29971900
N	3.13682500	4.18976600	-1.22951300
N	1.79240700	5.83836100	-0.59491400
N	0.79451000	0.57758700	3.46449600
N	1.91713200	2.50799000	3.57330300
N	-2.00650500	3.96215500	-1.90507700
N	-3.36667600	3.31853300	-0.28122500
H	7.60386600	-3.72553000	-0.15475000
H	7.55581500	-3.48441400	-1.91432700
C	3.65774500	-2.16373200	1.58633700
C	4.31279000	-2.98258200	3.67761400
C	5.01390900	-1.64816200	3.41160000
H	3.47317800	-2.85345700	4.38229900
H	4.98305900	-3.74933400	4.07771500
H	4.97194100	-0.96495500	4.26578600
H	6.07137600	-1.79510600	3.13833700
N	4.24745500	-1.12947300	2.29273000
N	3.84291300	-3.32456700	2.34911700
C	4.46890600	0.22722500	1.83590300
H	5.44525200	0.34047300	1.34868700
H	3.68005900	0.51854300	1.13753800
H	4.42743200	0.89547600	2.70291000
C	2.95590000	-4.45227700	2.17950400
H	2.70209900	-4.53507800	1.12268700
H	3.45714700	-5.36787900	2.51015000
H	2.02232200	-4.33592800	2.75250800
C	-0.36714100	-3.11460100	0.86221700
H	0.62853100	-3.29078900	0.44771900
H	-0.64700700	-2.08904300	0.61846100
H	-0.32820300	-3.25705600	1.95239400
C	-4.51166100	-5.12587300	-0.86414500
H	-5.10494200	-4.24475700	-0.61898200
H	-4.36005200	-5.15323000	-1.95665900
H	-5.05657300	-6.02957400	-0.57096400
C	-5.84983200	-2.00382500	2.07931400
H	-6.74225200	-1.72502600	1.50799200
H	-5.12532600	-2.43995600	1.39376000
H	-6.13419700	-2.76184500	2.82513100
C	-2.54869100	1.14666300	3.93178300
H	-1.96263700	1.07439300	3.01750000
H	-2.89279900	2.18414800	4.04011600
H	-1.90286100	0.90845900	4.78432500

C	-3.93319300	-1.72839200	-2.98522700
H	-3.69530700	-1.54450200	-4.03819200
H	-3.04037800	-1.53221200	-2.39282300
H	-4.22699900	-2.78052800	-2.86510800
C	-6.96337400	0.99985100	-0.21907400
H	-6.43978900	0.71103200	0.69404100
H	-6.74238900	2.05787100	-0.43067200
H	-8.04457600	0.89780400	-0.07334000
C	-3.78785200	2.82497100	1.00691300
H	-2.96571900	2.97645900	1.70605600
H	-4.67408000	3.37198000	1.35677300
H	-4.02536800	1.75848500	0.94846900
C	-0.76397000	4.07287700	-2.63042500
H	0.00403200	4.47710700	-1.97460600
H	-0.43939000	3.08846700	-2.99341200
H	-0.90224000	4.75532400	-3.47747300
C	0.61718700	6.50326700	-0.08723800
H	-0.14907100	6.62410500	-0.86511600
H	0.18240700	5.90053700	0.70897200
H	0.88871400	7.49543000	0.29325400
C	3.90517200	2.97217200	-1.10283800
H	4.77908200	3.11559100	-0.44805200
H	3.27807800	2.16959600	-0.70682300
C	0.27555400	-0.52834500	2.68066700
H	-0.40461800	-0.14996900	1.91854100
H	1.09391100	-1.05923300	2.17965100
H	-0.27788500	-1.21656000	3.32481400
C	1.96048100	3.95343100	3.63147800
H	1.30149400	4.34817500	4.42106700
H	2.98608100	4.27183200	3.84554500
H	1.66584600	4.35828800	2.66504100
C	-0.17743900	-3.32513300	-2.64309400
H	-0.68989100	-4.09214200	-3.23450800
H	0.51692400	-3.80531500	-1.95487600
H	-0.91109400	-2.76004700	-2.05605500
C	2.73765600	0.44084700	-3.70412300
H	3.60209500	0.13078100	-3.11774900
H	3.08287300	0.78727100	-4.68593700
H	2.24271900	1.27028300	-3.18140700
C	4.96725100	-3.85848100	-1.20911600
H	4.00023200	-3.48783500	-1.54505700
H	5.40958500	-4.46257900	-2.01454500
H	4.81237700	-4.49881700	-0.33476600
C	6.96886100	0.63760800	-1.17057200
H	6.02524900	1.09264800	-1.46829000
H	7.19388300	0.94259100	-0.13598700
H	7.77499400	1.00037200	-1.81724800
H	4.26172500	2.66828900	-2.09245500

**9H<sup>+</sup>**

**E = -4751.95078014 a.u.**

Si	0.64936200	-0.73027500	1.16765600
N	-2.52988000	-0.23336900	0.52292800

N	1.79688800	-1.07231400	-0.00223300
P	-3.32401900	-1.49681500	-0.01981200
P	3.36677300	-0.97301200	0.06840000
N	3.86636200	0.57403500	-0.16305100
N	4.08126500	-1.93702100	-1.07330100
N	4.04834000	-1.46115700	1.49523300
N	-4.36432000	-2.03008000	1.12834500
N	-2.42115000	-2.78910800	-0.44794100
N	-4.20467600	-1.07240200	-1.36724300
B	-1.20523400	-0.20949500	0.86171000
N	-0.23496000	0.85165800	1.07973600
P	-0.08259500	2.46956400	1.00259600
N	-1.46587100	3.21239900	1.43772200
N	0.36444100	2.87421200	-0.51954400
N	1.11956000	2.94108400	1.97667400
C	0.24605900	3.94615200	-1.21920700
C	-0.02274500	5.14923900	-3.19833300
C	-0.03612300	6.12150700	-2.01322700
H	0.61712200	5.48720000	-4.01811600
H	-1.03617000	4.98819900	-3.59999700
H	0.88856800	6.71552300	-1.96985100
H	-0.88316500	6.81270500	-2.04078300
C	4.12441800	-1.95026700	-2.35327800
C	3.98338300	-1.51051900	-4.63777900
C	4.63537100	-2.87957100	-4.43313600
H	3.19386800	-1.52033900	-5.39454500
H	4.72613100	-0.74920900	-4.92318500
H	3.92157200	-3.69471300	-4.63783300
H	5.51981800	-3.03241300	-5.05718800
C	4.91417400	1.11802100	-0.67037300
C	6.16185200	2.85682100	-1.61340700
C	7.03032300	1.59551300	-1.52508200
H	6.22007100	3.34638500	-2.58957200
H	6.43908200	3.59328800	-0.84215600
H	7.16519300	1.12809500	-2.51280100
H	8.01912300	1.78568800	-1.09868700
C	3.88608300	-2.52668800	2.20110700
C	3.42815900	-4.65289800	3.04200200
C	4.03104700	-3.79970500	4.15676100
H	2.52949100	-5.19262700	3.35247300
H	4.15684800	-5.38400400	2.65897000
H	3.25960200	-3.46263300	4.86822300
H	4.81378700	-4.31750800	4.71819100
C	-1.36066700	-2.97332500	-1.15558300
C	0.33962500	-4.27511500	-2.08938500
C	0.49388100	-2.82549500	-2.55436700
H	1.28368100	-4.70877400	-1.74626800
H	-0.07260800	-4.92244900	-2.88107600
H	1.29926700	-2.32113300	-2.01371400
H	0.66006000	-2.73507900	-3.63207400
C	-5.26901400	-2.93848500	1.20223300
C	-7.08271400	-4.02044100	2.20108400
C	-6.69998300	-4.75316900	0.91381800

H	-7.24256300	-4.69529900	3.04662300
H	-7.99486600	-3.41642400	2.06470400
C	-2.56798000	3.57754800	0.87940400
C	-4.36032100	4.01261700	-0.53850200
C	-4.66806600	4.59728000	0.84392500
H	-4.12112700	4.80223600	-1.26742300
H	-5.17299800	3.40295200	-0.94069400
H	-5.05035900	5.62070700	0.80115100
H	-5.39770000	3.98037100	1.39124900
C	1.62724900	2.34297800	3.01730700
C	3.29019200	1.74841800	4.54075000
C	1.97636400	1.03771200	4.90730400
H	4.13452200	1.06026400	4.46960600
H	3.54836800	2.53890600	5.26108800
H	2.00811900	-0.03033400	4.64814500
H	1.71870400	1.13694100	5.96516900
N	3.11270900	-3.65883700	2.02130800
N	4.56514800	-2.68138000	3.40210400
N	4.97837800	-2.82554200	-3.02220900
N	3.43709600	-1.23740100	-3.31604500
N	6.23786400	0.74352100	-0.65093500
N	4.83879700	2.31495600	-1.36685400
N	-0.60232900	-4.12247300	-0.99619900
N	-0.79402000	-2.24663000	-2.17640800
N	-5.81638400	-3.79191400	0.26235600
N	-5.92033500	-3.17693400	2.40294300
N	-3.19389000	3.18522900	-0.27297000
N	-3.36270400	4.54400400	1.47923400
N	0.48456400	3.93408100	-2.58474500
N	-0.11481700	5.22530300	-0.86445600
N	1.00730700	1.72980100	4.06815600
N	2.97041200	2.31114600	3.24364100
H	-7.55999100	-4.98665100	0.28017400
H	-6.16530600	-5.69067100	1.13121900
C	-5.19540900	-0.28174100	-1.56655800
C	-6.77892400	0.84203000	-2.86704200
C	-7.04117700	1.12295100	-1.38723800
H	-6.29943700	1.70524500	-3.35930200
H	-7.68493800	0.58900100	-3.42430300
H	-7.23774100	2.17829200	-1.17734800
H	-7.89107100	0.53267500	-1.01169000
N	-5.79030900	0.68938600	-0.77515500
N	-5.87142200	-0.28621400	-2.78104100
C	-5.64816100	0.80141400	0.66587900
H	-6.23285300	0.04310900	1.19990100
H	-4.59802100	0.70997300	0.94494700
H	-6.00880900	1.79210000	0.95847300
C	-5.26010900	-0.81392400	-3.97874100
H	-4.58883300	-1.62523600	-3.69764800
H	-6.03302800	-1.19432600	-4.65326700
H	-4.67915600	-0.04544800	-4.51283200
C	2.71542300	-0.00095200	-3.10325100
H	1.96113200	0.09326300	-3.89093300



H	2.21082300	-0.01919000	-2.13801000
H	3.37914700	0.87322200	-3.14274600
C	5.45926200	-4.02055100	-2.36437200
H	5.64523200	-3.78863500	-1.31570000
H	4.72663400	-4.84150800	-2.41964500
H	6.38812300	-4.35202300	-2.83727500
C	6.75656500	-0.54140100	-0.23347500
H	7.76957600	-0.39615000	0.15654700
H	6.12767100	-0.95522200	0.55394200
H	6.79338500	-1.25702000	-1.06467300
C	3.67966900	3.17431800	-1.31100800
H	2.83198300	2.60052700	-0.93616500
H	3.84920600	4.03232800	-0.64401800
H	3.44038200	3.56235900	-2.30694200
C	2.62546800	-4.16172000	0.74972700
H	1.84408600	-4.89847900	0.95879700
H	2.18468800	-3.35617800	0.16840400
H	3.42345900	-4.64501000	0.16967900
C	5.13094200	-1.55757800	4.10557900
H	5.35375000	-0.77431100	3.38077200
H	4.43272900	-1.16309500	4.86075500
H	6.05143400	-1.85777800	4.61654100
C	3.96551600	2.89181500	2.38107400
H	3.45344200	3.30364700	1.51322800
H	4.51301900	3.69169700	2.89750200
H	4.67121700	2.12569600	2.04397200
C	-0.40707500	1.46795100	4.20787600
H	-0.97643100	2.17761700	3.60803200
H	-0.66562500	0.45342200	3.88576200
H	-0.68518300	1.59158200	5.26042700
C	-3.23544500	4.85425200	2.88639300
H	-3.82116000	4.16384800	3.51168900
H	-2.18522300	4.77700100	3.16709800
H	-3.58753300	5.87380000	3.06805900
C	-2.64871700	2.38864600	-1.34696200
H	-2.16945600	3.01964500	-2.10792300
H	-1.94011700	1.66481100	-0.96134700
C	0.49494300	2.69752200	-3.33243900
H	0.73335800	1.88751900	-2.64475500
H	-0.48213300	2.49367200	-3.79553000
H	1.25089900	2.74222600	-4.12262400
C	0.02553200	5.79122100	0.46870100
H	0.61825200	6.71152900	0.40532300
H	-0.95203600	6.02797500	0.89964700
H	0.54244300	5.09547800	1.12928900
C	-1.00727700	-0.83842800	-2.43397100
H	-0.78197700	-0.64575600	-3.48932800
H	-2.04789800	-0.57699400	-2.25245300
H	-0.35565800	-0.21075800	-1.81454400
C	-1.12201800	-5.27783000	-0.30803000
H	-1.78967200	-4.93593000	0.48304600
H	-1.68022600	-5.94593900	-0.98311800
H	-0.29620900	-5.84671200	0.13123400

C	-5.19200200	-4.19235200	-0.98422100
H	-4.77154300	-3.32873100	-1.49470200
H	-4.39610900	-4.93116100	-0.82690300
H	-5.96552600	-4.63364000	-1.62066300
C	-5.90010500	-2.21062100	3.47572600
H	-4.95074100	-1.67613800	3.44028500
H	-6.72155800	-1.48210000	3.38694300
H	-5.99828100	-2.72489100	4.43671900
H	-3.46661300	1.83085900	-1.80724800
H	1.19203600	-0.85487400	2.55564600

## 10

**E = -1321.46307165 a.u.**

Si	0.00000100	0.74487300	-0.00028300
N	1.33963700	-0.31754700	-0.00182500
N	-1.33963800	-0.31754400	-0.00242600
P	2.88357300	-0.11029600	-0.00018400
P	-2.88357400	-0.11029500	-0.00023300
C	3.70256600	-0.87745800	-1.44116000
H	4.79067200	-0.78034100	-1.38121900
H	3.42832400	-1.93409400	-1.48112900
H	3.34255900	-0.38881700	-2.35000800
C	3.70024000	-0.88421200	1.43851200
H	3.33867200	-0.39987300	2.34904000
H	3.42596900	-1.94103300	1.47304200
H	4.78844700	-0.78677100	1.38088200
C	3.54418600	1.60184600	0.00442100
H	4.63819000	1.60079800	0.00550800
H	3.17809200	2.12819300	-0.88025200
H	3.17634400	2.12403900	0.89082800
C	-3.54418600	1.60184100	0.00604900
H	-3.17623700	2.12319700	0.89290300
H	-3.17820200	2.12902400	-0.87817200
H	-4.63819000	1.60079000	0.00727200
C	-3.70290000	-0.87618100	-1.44169700
H	-3.42861200	-1.93276500	-1.48272100
H	-4.79099500	-0.77917700	-1.38138000
H	-3.34315900	-0.38667600	-2.35018400
C	-3.69990500	-0.88548800	1.43796900
H	-4.78812300	-0.78794900	1.38070700
H	-3.42567000	-1.94235100	1.47145000
H	-3.33808200	-0.40200600	2.34885000

## 10H<sup>+</sup>

**E = -1321.90663232 a.u.**

N	1.09841900	-0.05876100	0.01499300
P	2.67414000	0.15244300	0.00141400
Si	-0.01653800	-1.23628900	-0.00307000
N	-1.62093400	-1.05396000	-0.00569400
P	-2.71807800	0.10116200	-0.00100900
C	3.16045400	1.20221800	-1.39129200
H	4.23684500	1.39135900	-1.36763800
H	2.90043900	0.70351200	-2.32811500

H	2.62122100	2.15019800	-1.32970900
C	3.21912900	0.99942900	1.50602200
H	3.00207100	0.37177700	2.37366600
H	4.29297800	1.19921900	1.46230700
H	2.67595800	1.94226400	1.60218200
C	3.67401800	-1.35881400	-0.12589500
H	3.42557500	-1.88639700	-1.05019000
H	4.73786400	-1.10637900	-0.13262000
H	3.46623100	-2.01057900	0.72645000
C	-2.08394900	1.77210400	-0.32001800
H	-1.31561000	2.00952700	0.41928100
H	-1.63527000	1.80127300	-1.31586500
H	-2.89231700	2.50594900	-0.26320800
C	-3.97284900	-0.23188100	-1.26076500
H	-4.40850300	-1.21653900	-1.07631100
H	-4.75663400	0.52940300	-1.22890700
H	-3.50273700	-0.23018500	-2.24703300
C	-3.57674700	0.16210800	1.59172300
H	-4.38111900	0.90178400	1.56217400
H	-3.99322700	-0.82433300	1.80787700
H	-2.86542300	0.42906300	2.37695300
H	0.41952700	-2.63886300	-0.01814400

## 11

**E = -1889.64953755 a.u.**

N	-0.93211300	0.01791200	-0.60741700
P	-2.39867100	-0.00134400	-0.11405900
N	-3.23351100	-1.31133500	-0.76338600
N	-3.46606300	1.26929700	-0.43399700
N	-2.42993700	-0.01708900	1.57218800
Si	0.00786900	0.96224900	-1.69359300
N	1.62910400	0.51076900	-1.39300100
P	2.53590000	0.08648800	-0.20917700
N	2.88139600	1.26424400	0.96023800
N	4.05491000	-0.32154400	-0.78981900
N	1.93303900	-1.15293900	0.76694700
C	5.04194100	-0.92549500	0.08782700
H	6.04895600	-0.60768100	-0.21122800
H	4.88600700	-0.60166800	1.11796900
H	5.01503200	-2.02583500	0.05740500
C	4.30529800	-0.50359600	-2.21106200
H	5.27009000	-0.05352500	-2.48146400
H	4.34121300	-1.56925000	-2.48414100
H	3.51174700	-0.02054300	-2.77988000
C	3.77053600	2.34948400	0.54201400
H	4.12233400	2.88274100	1.43229000
H	4.63218600	1.94529000	0.01168800
H	3.26319300	3.07125000	-0.11560800
C	1.71649500	1.78358100	1.68124700
H	1.11258900	2.45948000	1.05605500
H	1.07491900	0.96902100	2.01349500
H	2.05879600	2.34015600	2.56084000

C	2.45046200	-1.49411000	2.08403800
H	1.62214300	-1.81621000	2.72980400
H	3.18115300	-2.31662200	2.04475200
H	2.92700200	-0.62761500	2.54146600
C	1.30638900	-2.28003000	0.08681800
H	0.91121300	-1.95714300	-0.87417700
H	2.01631300	-3.10835200	-0.06544100
H	0.46687200	-2.65393500	0.68504600
C	-1.31551000	-0.61716800	2.29145100
H	-1.53023100	-1.65570200	2.59142700
H	-0.42773000	-0.60618200	1.66000500
H	-1.11325200	-0.04407300	3.20657400
C	-3.66067400	0.03762400	2.34669500
H	-4.03514900	-0.96328200	2.61099000
H	-3.48105700	0.58201000	3.28310400
H	-4.43602000	0.56592600	1.79225600
C	-3.14434800	2.56779600	0.16310200
H	-2.75752300	2.43432600	1.17341900
H	-2.39465000	3.11327000	-0.42815500
H	-4.05443400	3.17748400	0.21405000
C	-3.94833100	1.41718300	-1.80969000
H	-4.87080700	2.01005900	-1.80342700
H	-3.21179400	1.92502700	-2.44854900
H	-4.16326100	0.43962400	-2.24013800
C	-2.50664300	-2.44049700	-1.32397600
H	-2.39473800	-3.26190700	-0.59824400
H	-3.04846200	-2.83344800	-2.19413500
H	-1.51693300	-2.11594700	-1.64002800
C	-4.58322200	-1.63812900	-0.33120200
H	-5.13720400	-2.09087800	-1.16339000
H	-4.59442100	-2.35366600	0.50566300
H	-5.11481500	-0.73590900	-0.02729800

**11H<sup>+</sup>**

**E = -1890.09616761 a.u.**

N	1.07068400	-0.03115000	-0.60781100
P	2.56450500	-0.01022200	-0.10591500
N	3.34418900	1.26814000	-0.82430000
N	3.55844200	-1.30187400	-0.42685200
N	2.52729300	0.03357000	1.55757300
Si	-0.07506000	-0.80495400	-1.43792900
N	-1.67102900	-0.61476600	-1.26346200
P	-2.66039800	-0.04562400	-0.15890100
N	-3.06283200	-1.17606500	1.00042200
N	-4.02435600	0.44970300	-0.93863200
N	-2.03647800	1.20601800	0.73341700
C	-5.02718000	1.25851100	-0.25102200
H	-5.89910200	0.65901800	0.04239200
H	-4.61049600	1.71736000	0.64538500
H	-5.37157300	2.05787500	-0.91585400
C	-4.48290100	-0.13490700	-2.19961400
H	-5.34831200	-0.79148700	-2.04012700

H	-4.78210700	0.66702700	-2.88314800
H	-3.67947600	-0.70740900	-2.65951400
C	-4.17535000	-2.09422400	0.74172100
H	-4.52691600	-2.49772800	1.69609500
H	-5.00575600	-1.56837200	0.27201600
H	-3.87931800	-2.93504000	0.09935000
C	-1.95867700	-1.80902600	1.72537500
H	-1.53792700	-2.65764800	1.16603700
H	-1.16248800	-1.08746500	1.91464200
H	-2.32147400	-2.17890500	2.68945700
C	-2.38486100	1.51074300	2.11990700
H	-1.47233600	1.66598700	2.70773200
H	-2.98338900	2.42915400	2.18229700
H	-2.95308300	0.69223200	2.55771300
C	-1.41173200	2.32191500	0.02361400
H	-1.24889800	2.06729300	-1.02359200
H	-2.04763500	3.21506600	0.06618400
H	-0.44144300	2.55818900	0.47321200
C	1.38066300	0.58990900	2.27232000
H	1.56333800	1.62889400	2.58141700
H	0.49481900	0.56064400	1.63986700
H	1.19382400	-0.00120000	3.17678300
C	3.76141900	0.04320800	2.34479500
H	4.06947800	1.06442700	2.60519300
H	3.60156500	-0.51159600	3.27582600
H	4.57051800	-0.44009000	1.79808900
C	3.34090500	-2.57139300	0.27380800
H	2.93545500	-2.39547300	1.26895100
H	2.64856800	-3.22081600	-0.28040600
H	4.29534500	-3.09859500	0.37051600
C	4.08013200	-1.49682800	-1.78437500
H	5.05584600	-1.98983600	-1.72761600
H	3.41109200	-2.13062300	-2.38246900
H	4.19930500	-0.54026400	-2.29035400
C	2.60820300	2.43308800	-1.31412300
H	3.09772100	2.81523300	-2.21649800
H	1.58547600	2.15661500	-1.56317800
H	2.58760500	3.24119600	-0.56974200
C	4.74523100	1.55825200	-0.51117700
H	5.23536900	1.96791500	-1.40071200
H	4.83839900	2.29323900	0.29917300
H	5.27218300	0.64827800	-0.22495300
H	0.30856400	-1.73656200	-2.50677000

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**E = -3247.53032238 a.u.**

N	0.76574700	-0.98191900	0.59959400
P	2.20309500	-0.42954800	0.38855000
N	3.19386000	-1.65517500	-0.17019400
N	2.87878400	0.33737800	1.70367800
N	2.41361100	0.70795300	-0.80594100
C	2.87475900	0.02564900	2.95307000
C	2.82762500	-1.04811200	5.02704300

C	2.60189700	0.45721800	5.22737100
H	2.04000800	-1.65311100	5.48698200
H	3.79621100	-1.37865900	5.43211500
H	1.54142400	0.67082700	5.43425200
H	3.20169100	0.87270300	6.04332000
C	4.31189800	-1.66692200	-0.79304300
C	5.84867200	-2.52693500	-2.32628200
C	6.41840400	-1.24841800	-1.71130000
H	6.58065700	-3.33882300	-2.37827700
H	5.46415300	-2.34626900	-3.34459500
H	7.21916000	-1.47753700	-0.98990600
H	6.82058700	-0.55469800	-2.45615100
C	2.18007600	1.96539200	-0.85844800
C	1.41405300	4.15623200	-0.56161600
C	2.30836300	4.10581500	-1.81399800
H	0.43978100	4.61605700	-0.76209700
H	1.89016000	4.71775600	0.25545100
H	1.71189200	4.18064600	-2.73894900
H	3.05540700	4.90589900	-1.83187900
N	1.25902000	2.75500700	-0.22103500
N	2.92975100	2.80317900	-1.68742700
N	2.99215800	1.00911800	3.93871100
N	2.81103200	-1.18177100	3.58262300
N	5.26347800	-0.68010900	-1.02740000
N	4.76916900	-2.83250100	-1.40867600
C	2.91882700	-2.49322900	2.98919000
H	1.96654600	-3.02917700	3.07645600
H	3.17501400	-2.41597900	1.93357400
H	3.70616200	-3.06044000	3.50445600
C	2.61621600	2.37133000	3.63573800
H	2.84704400	2.56709200	2.58821900
H	1.53959200	2.54323900	3.79683200
H	3.17616000	3.06369000	4.27331300
C	5.53936000	0.42047900	-0.12135300
H	5.83520800	1.30266400	-0.69901100
H	4.66473400	0.66824800	0.47448100
H	6.36629200	0.15922800	0.55756700
C	3.85199300	-3.90089700	-1.73349600
H	3.06731300	-3.92417700	-0.97732700
H	3.38525700	-3.75526000	-2.72056000
H	4.38682300	-4.85618900	-1.74125700
C	0.15525000	2.29667400	0.59017600
H	-0.76063600	2.80201800	0.26776300
H	0.01668800	1.22719800	0.44840900
H	0.31615700	2.49709200	1.65618900
C	3.73793300	2.27137200	-2.75503300
H	4.03707100	1.25795100	-2.48213700
H	3.18530500	2.23308600	-3.70825100
H	4.62872400	2.89278500	-2.90184900
Si	-0.33842900	-1.31862000	1.87705400
N	-1.90897500	-1.10095600	1.27283900
P	-2.66021400	-0.39303900	0.09120800
N	-3.27612900	1.05418600	0.64111100

N	-3.95087500	-1.27626700	-0.48038100
N	-1.81790300	0.02498400	-1.25170900
C	-4.95493300	-1.83415900	0.09103600
C	-6.68072100	-2.50520800	1.49849900
C	-6.76742500	-3.30104200	0.19508300
H	-6.77399800	-3.13185900	2.39038000
H	-7.45735200	-1.72440500	1.54256400
H	-6.38139900	-4.32598900	0.32836800
H	-7.78517900	-3.36655900	-0.20181900
C	-3.45947000	2.18656200	0.08270400
C	-3.42244100	4.51941000	-0.01832600
C	-3.88617400	3.96812700	-1.36962300
H	-4.03260700	5.35856900	0.33072400
H	-2.37228700	4.85892600	-0.06288400
H	-4.96521000	4.13458700	-1.51842900
H	-3.35624000	4.41662000	-2.21629700
C	-0.89903400	-0.53503000	-1.95398700
C	0.71348400	-1.94917000	-2.84410900
C	0.83481300	-0.58274400	-3.53540200
H	1.51379100	-2.09509900	-2.10905200
H	0.71877300	-2.78498200	-3.55234500
H	1.85522600	-0.18961600	-3.48666600
H	0.51633000	-0.62236600	-4.59058400
N	-0.57438700	-1.85165800	-2.17021300
N	-0.06336400	0.22701400	-2.74557500
N	-5.90362400	-2.52223300	-0.67185900
N	-5.35277700	-1.91833500	1.40835600
N	-3.59969700	2.54668700	-1.25048000
N	-3.55460600	3.35892600	0.83891500
C	-4.90192000	-1.04747200	2.47951700
H	-5.18007300	-1.51341900	3.43003600
H	-3.81628600	-0.94570300	2.43990300
H	-5.36506600	-0.05348200	2.42009100
C	-5.55048300	-3.04566800	-1.97090100
H	-4.84433900	-2.35937100	-2.43857500
H	-5.07875900	-4.03923300	-1.90032700
H	-6.44793200	-3.13171300	-2.59236000
C	-4.14709200	1.66845000	-2.26787700
H	-3.50293500	1.65549600	-3.15254500
H	-4.22729700	0.65042600	-1.89228800
H	-5.14738600	2.02039100	-2.56228300
C	-3.01683400	3.40733400	2.18010800
H	-3.03103200	2.39558200	2.58670700
H	-1.97897800	3.77487400	2.18945500
H	-3.62476500	4.06933200	2.80592900
C	-1.00962200	-2.97350400	-1.37047100
H	-0.32678600	-3.14856000	-0.53237000
H	-2.01065100	-2.79267900	-0.98389500
H	-1.03819500	-3.86289300	-2.01220500
C	-0.33500700	1.59436000	-3.07912700
H	-1.00661700	2.00549700	-2.32324900
H	0.59717800	2.16831600	-3.09388400
H	-0.81043600	1.69102000	-4.06977800

12H<sup>+</sup>

E = -3248.02447318 a.u.

N	-0.93988100	0.34543600	1.12298700
P	-2.39248700	0.19411800	0.51848500
N	-3.07274400	1.68599300	0.57766200
N	-3.25249200	-0.98372600	1.28669900
N	-2.46737600	-0.21210600	-1.06152600
C	-3.30379100	-1.32611600	2.53196200
C	-3.32272300	-1.40646100	4.85969800
C	-3.43594600	-2.83018900	4.30745900
H	-2.55850000	-1.30589600	5.63447400
H	-4.28085300	-1.05887600	5.27292900
H	-2.48820300	-3.38118800	4.40928000
H	-4.22436200	-3.41348000	4.79055400
C	-4.04112500	2.22380400	-0.08766400
C	-5.12063500	3.95360100	-1.21367900
C	-6.01050800	2.70891400	-1.23175900
H	-5.66253400	4.86318700	-0.94210300
H	-4.63595700	4.11813900	-2.18879400
H	-6.85595500	2.81110100	-0.53547000
H	-6.40855900	2.47802900	-2.22328600
C	-2.43554000	-1.35330400	-1.66809800
C	-2.09495200	-3.57516800	-2.28884600
C	-2.83143400	-2.84500200	-3.42619000
H	-1.21856200	-4.12692600	-2.64041800
H	-2.75590200	-4.27950600	-1.76436900
H	-2.17600900	-2.66928000	-4.29372900
H	-3.71366400	-3.38912100	-3.77456500
N	-1.70085900	-2.47648400	-1.41938700
N	-3.19918700	-1.59504700	-2.78746500
N	-3.73402500	-2.58155200	2.90613200
N	-2.97673800	-0.62592000	3.67224300
N	-5.10068900	1.66116600	-0.77010500
N	-4.13601800	3.59365000	-0.20625500
C	-3.05618400	0.81920100	3.80179300
H	-2.26948300	1.16628300	4.47778600
H	-2.92967500	1.30933400	2.83921200
H	-4.02957300	1.11322400	4.22054800
C	-3.77136200	-3.68506100	1.97334800
H	-3.91648100	-3.28459200	0.96999900
H	-2.83667300	-4.26581500	1.99564000
H	-4.59917200	-4.35503900	2.22397300
C	-5.70009900	0.37939900	-0.44337000
H	-6.10407000	-0.07031900	-1.35550200
H	-4.96682200	-0.29885600	-0.01503600
H	-6.52465400	0.50909600	0.27276400
C	-2.99076200	4.44947600	0.01459000
H	-2.38840000	4.02842100	0.81866700
H	-2.36655300	4.53423800	-0.88780500
H	-3.33314400	5.44856100	0.29797100
C	-0.74090200	-2.64839100	-0.35204600
H	0.01536800	-3.36779000	-0.67917200



H	-0.24202900	-1.70197100	-0.15268000
H	-1.20682200	-3.01511900	0.56945900
C	-3.95195700	-0.57937600	-3.47899300
H	-4.03653500	0.28967700	-2.82472800
H	-3.45903600	-0.27906100	-4.41532100
H	-4.95268300	-0.94958100	-3.72888100
Si	0.29101400	0.35079800	2.14933900
N	1.87392000	0.29420200	1.81471200
P	2.69272400	0.12969100	0.44044000
N	3.63397300	-1.19416900	0.61813400
N	3.59701900	1.46266100	0.13564500
N	1.78879100	-0.14826100	-0.88420600
C	4.57403400	2.06177000	0.73443600
C	6.35616600	2.68836200	2.08689300
C	6.09866600	3.79493100	1.06011800
H	6.46496800	3.06687500	3.10638200
H	7.25448900	2.10524700	1.83532600
H	5.59122600	4.65876100	1.51766300
H	7.01146300	4.14908800	0.57402100
C	4.15005400	-2.02015700	-0.22483600
C	4.86027200	-4.11644300	-0.95505500
C	5.09875400	-3.09072800	-2.06574000
H	5.72096200	-4.76877500	-0.78467100
H	3.98608800	-4.75129500	-1.17162500
H	6.16804000	-2.85323500	-2.16963600
H	4.72714200	-3.41904200	-3.04047700
C	0.98256300	0.48980900	-1.65989000
C	-0.51367100	1.96618700	-2.66132900
C	-0.31484400	0.76150400	-3.58767500
H	-1.48965700	1.92218900	-2.16337200
H	-0.41031000	2.92386300	-3.18016100
H	-1.26316700	0.33676600	-3.92730000
H	0.28710900	1.01821300	-4.47355700
N	0.55579600	1.79139300	-1.68219000
N	0.39850300	-0.16459900	-2.72982800
N	5.22275200	3.11622900	0.11900000
N	5.15592100	1.86768700	1.96023500
N	4.36678900	-1.92173600	-1.58492800
N	4.60032000	-3.25913300	0.18856800
C	5.02340600	0.68554700	2.79225500
H	5.35201900	0.94791400	3.80183100
H	3.98265100	0.36953500	2.83707200
H	5.63439500	-0.14735300	2.42347300
C	4.61664800	3.85504800	-0.96536800
H	3.97306700	3.18138400	-1.53110200
H	4.01093700	4.69637900	-0.59557000
H	5.39671400	4.25221100	-1.62165900
C	4.57795600	-0.67962300	-2.30561700
H	4.05209400	-0.71281400	-3.26528700
H	4.20898900	0.17029700	-1.73805400
H	5.64998200	-0.53332100	-2.50208400
C	4.14842000	-3.84636000	1.43100500
H	3.94061100	-3.04454300	2.13887900

H	3.23254600	-4.43999600	1.28793700
H	4.92710100	-4.50086800	1.83341500
C	0.63145300	2.74358700	-0.59339600
H	-0.27020700	2.69998100	0.02785700
H	1.51330000	2.55043900	0.01270600
H	0.72838600	3.74896500	-1.01824500
C	0.94761800	-1.38081400	-3.27480600
H	1.56120100	-1.85649600	-2.50915500
H	0.14102900	-2.05928000	-3.57200400
H	1.57303400	-1.18090400	-4.15877900
H	0.01765700	0.46715700	3.59206300