

Supplementary data

Superbasicity of Silylene derivatives achieved via non-covalent intramolecular cation... π interactions and exploiting as molecular container for CO₂

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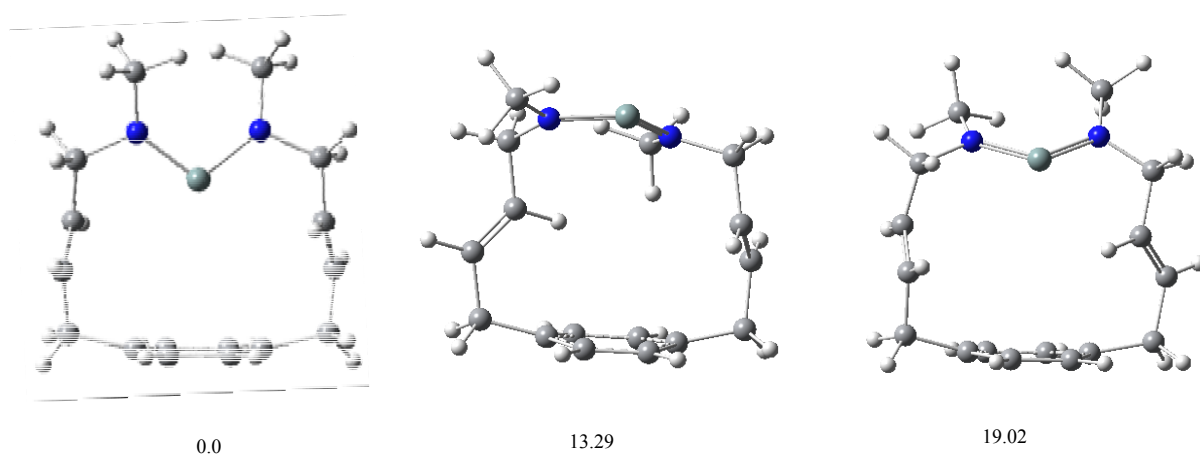
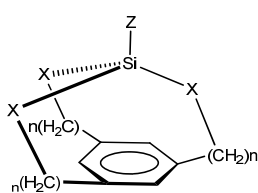
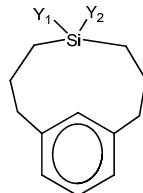


Figure S1. Different conformers of compound **1** are obtained by conformational search using semi-empirical AM1 method. The relative energies (kcal/mol) with respect to the lowest energy conformer are given at B3LYP/6-31+G* level of theory. [Blue-grey = silicon; blue = nitrogen; grey = carbon; and white = hydrogen]



- I. X = C, Z = CH₃, n = 1
- II. X = O, Z = *t*-Bu, n = 2
- III. X = O, Z = *t*-Bu, n = 3
- IV. X = O, Z = *t*-Bu, n = 9



- V. Y₁ = CH₃, Y₂ = CH₃
- VI. Y₁ = CH₃, Y₂ = (CH₂)₃Ph
- VII. Y₁ = CH₃, Y₂ = CH₂CH=CH₂

Scheme S1: Reported synthesized Si (IV) compounds.

Table S1: Comparison of experimental and calculated proton affinities of simplest silylene molecules in gas phase.

Systems	Proton affinity (kcal/mol)		
	Experimental	Calculated	
		B3LYP/6-311+G**// B3LYP/6-31+G* (using electronic energy)	B3LYP/6-311+G**// B3LYP/6-31+G* (using enthalpy energy)
:SiH ₂	201±3	201.5	193.3
:SiHMe	215±3	216.5	209.6
:SiMe ₂	231	228.8	221.7

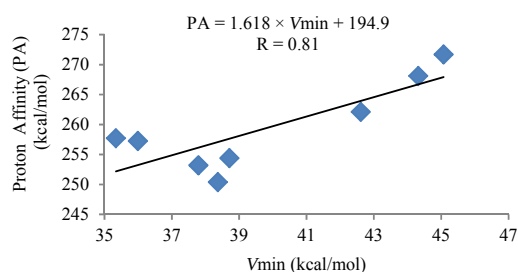
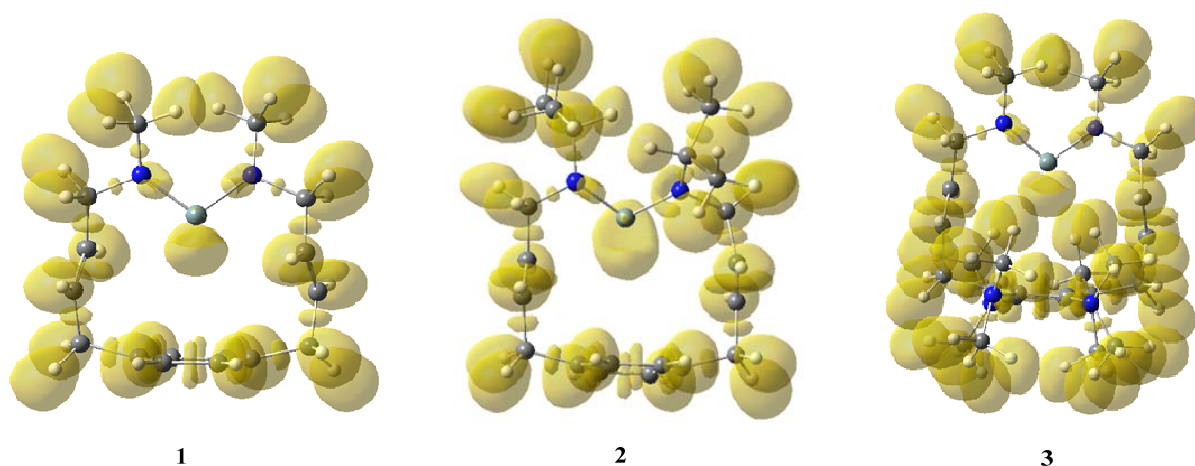


Fig. S2 Relationship between the $V_{\min}$ and the gas phase proton affinities for **1–8**.



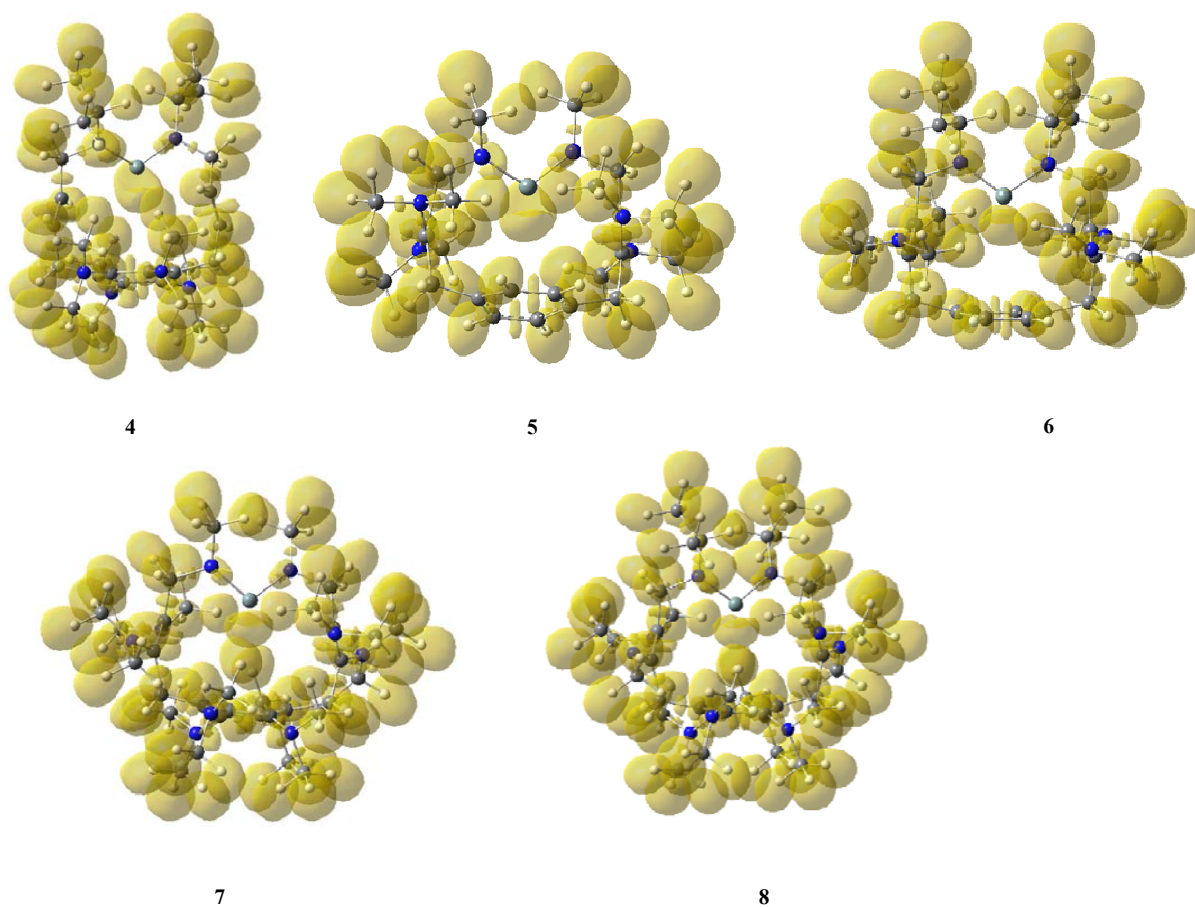


Fig. S3 Three-dimensional representations of ELF isosurfaces with ELF = 0.85 for the silylene systems (1-8).

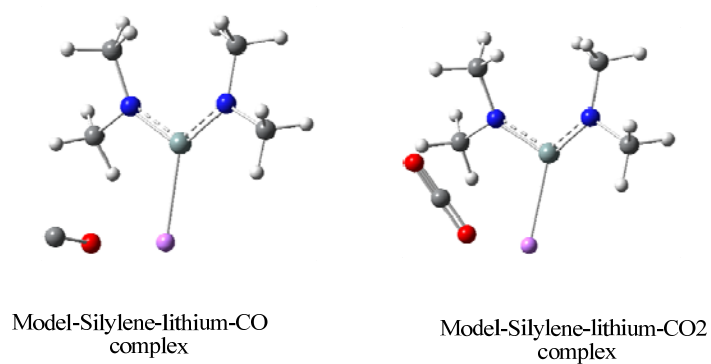


Fig. S4 Model systems of Silylene-lithium-CO and Silylene-lithium-CO₂ for interaction energy calculation in GAMESS. [Blue-grey = silicon; blue = nitrogen; red = oxygen; grey = carbon; pink = lithium and white = hydrogen]

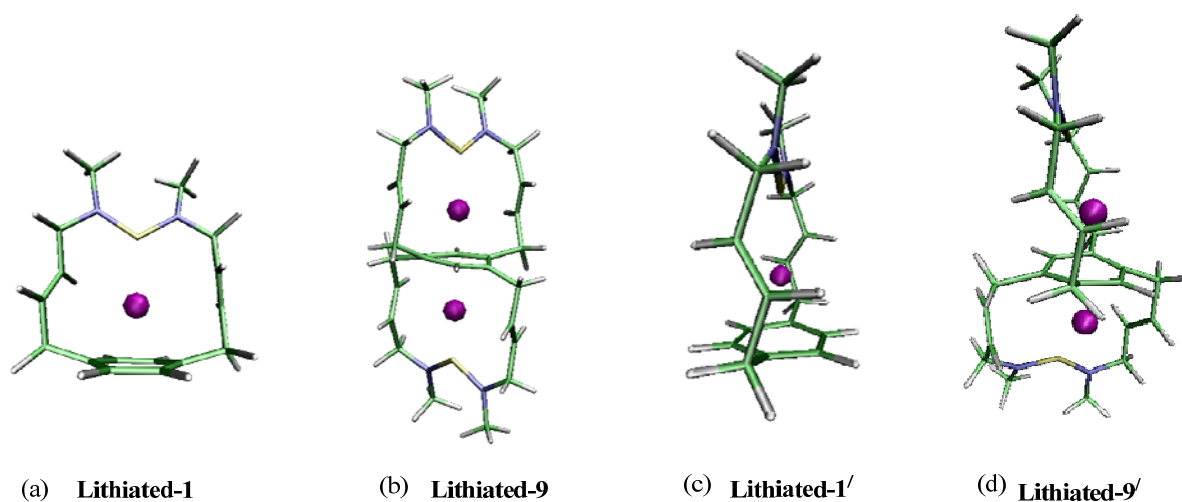


Fig. S5 (a-b) Front view and (c-d) side view of lithiated silylenes (**1** and **9**) at M06-2X/6-31+G* level of theory. [Yellow = silicon; blue = nitrogen; green = carbon; pink = lithium and white = hydrogen]

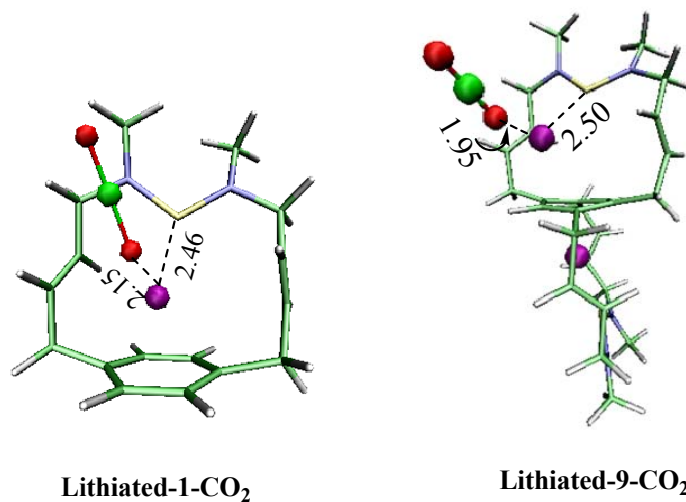


Fig. S6 Geometries of carbon dioxide trapped lithiated silylenes (**1** and **9**) at M06-2X/6-31+G* level of theory. [Yellow = silicon; blue = nitrogen; red = oxygen; green = carbon; pink = lithium and white = hydrogen]

Table S2. The calculated NBO charge on lithium ion at M06-2X/6-311+G** level of theory.

Compound	NBO charge
Lithiated system-1	0.314
Lithiated system-9	0.415

Table S3: Binding of CO₂ with reported organic systems.

Systems	Binding energy
N-doped molecular models of coal surface	-3.6 kcal/mol at BLYP-D3/6-311++G** level of theory
Benzoic acid	-3.9 kcal/mol at PW91/DNP level of theory

imidazopyridamine

-6.4 kcal/mol at CCSD(T)/CBS level of theory and (-6.9 kcal/mol M06-2X/6-311+G**//M06-2X/6-31+G* level of theory)

B3LYP/6-31+G* optimized Cartesian coordinates of all the neutral and protonated silylene molecules and the electronic energies at B3LYP/6-311+G level of theory.**

1.

E = -1022.11142 a.u

C	2.62488200	0.59040700	1.25548400
C	2.63391800	-0.80039300	1.13457500
C	2.56302400	-1.41339200	-0.12357000
C	2.62493100	-0.59035500	-1.25546100
C	2.63393600	0.80044500	-1.13455100
C	2.56299100	1.41344300	0.12359100
H	2.60756600	1.03926600	2.24696500
H	2.60765300	-1.03921500	-2.24694200
C	-0.30909200	-2.74920300	-0.52794100
C	-0.30915700	2.74919000	0.52792100
C	-1.72197300	-2.74900900	-0.00087500
H	-1.74704600	-3.26967400	0.97056000
H	-2.36657500	-3.32895800	-0.68367000
C	-1.72203500	2.74897300	0.00084800
H	-1.74711300	3.26962700	-0.97059300
H	-2.36664500	3.32892200	0.68363600
N	-2.31741400	1.40087500	-0.15505000
N	-2.31736800	-1.40092000	0.15504700
H	2.62392400	1.41285900	-2.03457500
H	2.62389400	-1.41280700	2.03459900
Si	-1.25020600	-0.00001200	-0.00005000
C	2.20823200	2.88969100	0.25193300
C	2.20829700	-2.88964700	-0.25192100
H	2.32813200	3.20747300	1.29466800

H	2.87520000	3.51356300	-0.35596600
H	2.87527000	-3.51350800	0.35598500
H	2.32821600	-3.20742400	-1.29465500
C	-3.69808700	1.49857700	-0.61995200
H	-4.05183300	0.53436600	-0.98855700
H	-4.38265400	1.84655300	0.17116900
H	-3.76812200	2.21680900	-1.45195100
C	-3.69801900	-1.49864400	0.62001000
H	-3.76800800	-2.21688700	1.45200300
H	-4.05175800	-0.53444100	0.98864300
H	-4.38262000	-1.84661900	-0.17108300
C	0.76706200	3.07193700	-0.20207700
C	0.76712500	-3.07192200	0.20207100
H	-0.17785100	2.44270300	1.56697500
H	0.62412700	3.34643000	-1.24870100
H	0.62418400	-3.34641000	1.24869600
H	-0.17778300	-2.44272500	-1.56699700

1 H+

E= -1022.51050 a.u

C	-2.64668000	-0.59016900	1.25934000
C	-2.65635800	0.80128500	1.13669500
C	-2.58521300	1.41035700	-0.12469900
C	-2.64672100	0.59007100	-1.25932200
C	-2.65633800	-0.80138300	-1.13667700
C	-2.58515100	-1.41045200	0.12471600
H	-2.65179400	-1.03911900	2.25030400
H	-2.65186600	1.03902100	-2.25028600
C	0.27593700	2.77002000	-0.54608100
C	0.27606000	-2.77000000	0.54606300

C	1.67615500	2.80111300	-0.00615400
H	1.69988100	3.31400900	0.96300000
H	2.34372800	3.34649500	-0.68693700
C	1.67627500	-2.80105200	0.00612600
H	1.70001300	-3.31393900	-0.96303200
H	2.34386400	-3.34642100	0.68690300
N	2.30084400	-1.44938300	-0.19540800
N	2.30076400	1.44946500	0.19540000
H	-2.67275800	-1.41506700	-2.03519100
H	-2.67279300	1.41496900	2.03521000
Si	1.47661500	0.00002300	-0.00003900
C	-2.24304000	-2.88818800	0.25223000
C	-2.24316400	2.88810800	-0.25221700
H	-2.36257300	-3.21347600	1.29130800
H	-2.90196900	-3.50846700	-0.36496700
H	-2.90211000	3.50836000	0.36498700
H	-2.36272100	3.21339000	-1.29129400
C	3.71108000	-1.56227700	-0.61786300
H	4.09398100	-0.60963900	-0.98555100
H	4.33956800	-1.91271700	0.20922700
H	3.77661300	-2.28826400	-1.43562800
C	3.71097400	1.56241100	0.61792800
H	3.77643900	2.28840200	1.43569500
H	4.09388900	0.60978700	0.98564000
H	4.33949300	1.91287100	-0.20913000
C	-0.80212600	-3.05102500	-0.19883400
C	-0.80225100	3.05099900	0.19882900
H	0.15821800	-2.50519000	1.59900000
H	-0.65409800	-3.32383000	-1.24516100
H	-0.65422200	3.32380100	1.24515700

H	0.15809200	2.50521500	-1.59901900
H	0.02265100	0.00000100	-0.00012700

2.

E = -1179.40777 a.u

C	3.26861500	0.45717200	1.24505300
C	3.03544600	-0.90251000	1.45156200
C	3.04041500	-1.80322200	0.37662300
C	3.43053100	-1.32311800	-0.87924600
C	3.67976100	0.03553900	-1.08284000
C	3.52902500	0.95670800	-0.03878600
H	3.18468200	1.14742200	2.08251900
H	3.47891500	-2.00693700	-1.72440500
C	0.04847000	-2.84022700	-0.23570900
C	0.88695500	2.81865500	-0.25382100
C	-1.42147300	-2.60760000	0.01749400
H	-1.62671900	-2.84068400	1.07285700
H	-1.99531000	-3.32995600	-0.58174700
C	-0.49845400	2.70191100	-0.85044900
H	-0.41054300	2.59046700	-1.93722100
H	-1.07259700	3.62102700	-0.68701000
N	-1.27546500	1.55495700	-0.28920100
N	-1.89096900	-1.23424100	-0.28486200
H	3.91642400	0.38949000	-2.08462400
H	2.77974600	-1.25447300	2.44958400
Si	-0.68442000	-0.03610300	-0.80065300
C	3.39430200	2.44476800	-0.33035600
C	2.44488700	-3.19572400	0.52719500
H	3.48946300	3.02196200	0.59691400
H	4.17619600	2.79036100	-1.01815700
H	2.89341700	-3.72939500	1.37466200

H	2.65530200	-3.78420800	-0.37374500
C	2.01777000	2.63733800	-0.94544900
C	0.94368400	-3.06493200	0.73609900
H	0.93650300	2.95562900	0.82685700
H	1.94947300	2.44394100	-2.01716800
H	0.60234200	-3.04418400	1.77301800
H	0.37568900	-2.83181000	-1.27562100
C	-3.36397000	-1.09444600	-0.30790500
C	-4.04075900	-1.51238700	1.01067900
C	-4.00798900	-1.82358800	-1.50609400
H	-3.56216400	-0.03133400	-0.46258300
H	-3.57526200	-1.01960500	1.87207300
H	-5.10324300	-1.23982100	0.99329200
H	-3.98462200	-2.59557800	1.17085100
H	-3.53975700	-1.51005600	-2.44548700
H	-3.92265100	-2.91348100	-1.42741900
H	-5.07793900	-1.58522300	-1.55871400
C	-2.27717900	1.91021400	0.73852200
C	-3.47506400	2.68920800	0.16133400
C	-1.67332100	2.65762900	1.94286200
H	-2.65069500	0.96018800	1.12763700
H	-3.91761300	2.16094800	-0.69022500
H	-4.25105500	2.82075200	0.92628800
H	-3.18356500	3.68920800	-0.18185200
H	-0.85266900	2.08312700	2.38571700
H	-1.29303000	3.64882400	1.66857200
H	-2.44171400	2.80549100	2.71210900

2H+

E= -1179.81317 a.u

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C	3.65231800	0.16156200	-1.14130000
C	3.50728300	1.09064200	-0.10221200
H	3.25522900	1.30316300	2.03111200
H	3.54472600	-1.90351500	-1.73825500
C	0.26303800	-2.83026800	-0.23005900
C	0.80922800	2.82377500	-0.21197400
C	-1.21973500	-2.73367400	-0.01126900
H	-1.46128100	-3.01283200	1.02003600
H	-1.73806700	-3.43203400	-0.67628200
C	-0.58611500	2.71255900	-0.76253600
H	-0.56400300	2.60826000	-1.85218300
H	-1.16876500	3.61200100	-0.55091700
N	-1.36140500	1.56028400	-0.16206400
N	-1.79528200	-1.37334300	-0.27284100
H	3.86064900	0.50770800	-2.15183400
H	2.97029000	-1.10929500	2.44984500
Si	-0.82334700	-0.00977200	-0.42337200
C	3.32221000	2.57000900	-0.40653600
C	2.65409300	-3.09676700	0.57609900
H	3.44120500	3.16615400	0.50446700
H	4.05513900	2.92753600	-1.13800000
H	3.11636500	-3.56082400	1.45387300
H	2.91278600	-3.71377900	-0.29171100
C	1.91367800	2.69946900	-0.95756100
C	1.14419900	-3.05036100	0.75656300
H	0.88864900	2.96045200	0.86705700
H	1.80819000	2.54669500	-2.03336900

H	0.77260200	-3.14259700	1.77862500
H	0.61353200	-2.74682100	-1.26004600
C	-3.29690100	-1.31721800	-0.34586900
C	-3.95730000	-1.81639400	0.94492300
C	-3.82142900	-2.05101100	-1.58993800
H	-3.54997700	-0.26146100	-0.47367400
H	-3.55331000	-1.31057200	1.82925700
H	-5.03365900	-1.61877400	0.90325600
H	-3.83132200	-2.89569200	1.07911900
H	-3.32004300	-1.70315100	-2.49934200
H	-3.70206500	-3.13655500	-1.51850400
H	-4.89324800	-1.85153000	-1.69664200
C	-2.52530900	1.92451200	0.71232800
C	-3.65134600	2.59586700	-0.08523100
C	-2.07688600	2.76857100	1.91423300
H	-2.90535600	0.97992900	1.11299000
H	-3.96693600	1.98190300	-0.93588800
H	-4.51969000	2.75056200	0.56426400
H	-3.35434600	3.57739400	-0.46934900
H	-1.29493200	2.25949500	2.48742400
H	-1.70350500	3.75384700	1.61612400
H	-2.93240300	2.93344100	2.57794200
H	0.52437100	-0.13158900	-0.96914000

3.

E= -1558.06784 a.u

C	-1.50964700	0.66889600	1.24700300
C	-1.49419300	1.40595200	0.04094600
C	-1.39383900	0.73789600	-1.19914000
C	-1.51049300	-0.66823800	-1.24664500

C	-1.49511100	-1.40532000	-0.04061500
C	-1.39385800	-0.73730800	1.19944400
C	1.51099200	1.35270200	-2.46319800
C	1.51116900	-1.35340200	2.46298400
C	2.89601500	1.80395300	-2.07606500
H	2.87426300	2.87516900	-1.81632200
H	3.57309200	1.70427900	-2.94179700
C	2.89581600	-1.80538600	2.07527900
H	2.87337400	-2.87655200	1.81539500
H	3.57320900	-1.70620500	2.94080800
N	3.48441100	-1.04022600	0.94955800
N	3.48440500	1.03872400	-0.95032000
Si	2.41550600	-0.00103600	-0.00070600
C	-1.02158200	-1.55013100	2.44133700
C	-1.02155400	1.55053400	-2.44114800
H	-1.07983300	-0.92434200	3.33171400
H	-1.70506300	-2.39237200	2.58292800
H	-1.70481800	2.39297400	-2.58265500
H	-1.08026900	0.92475200	-3.33150400
C	4.85617700	-1.46795500	0.69178900
H	5.20028400	-1.10208700	-0.27718700
H	5.55590800	-1.11892400	1.46901900
H	4.91323300	-2.56769700	0.67046900
C	4.85616100	1.46632600	-0.69234400
H	4.91329900	2.56606200	-0.67090600
H	5.20006400	1.10031500	0.27663600
H	5.55597000	1.11732300	-1.46951900
C	0.39648900	-2.06726500	2.25293200
C	0.39675200	2.06727900	-2.25326900
H	1.44165400	-0.36199000	2.90939300

H	0.48113500	-3.04439400	1.77991300
H	0.48190700	3.04467800	-1.78089200
H	1.44071000	0.36110200	-2.90905500
N	-1.59736700	2.83886500	-0.01805400
N	-1.69963000	1.39221700	2.47931500
N	-1.59961400	-2.83818200	0.01865100
N	-1.70120500	-1.39142200	-2.47893600
C	-0.69703400	-3.66184900	-0.77212600
H	-0.60043900	-4.64432200	-0.28683500
H	-1.03604300	-3.82529600	-1.80682400
H	0.29465400	-3.20155800	-0.79732700
C	-2.96738500	-3.34204100	0.02564300
H	-3.44942800	-3.29399400	-0.96818300
H	-2.96661700	-4.39051700	0.35237300
H	-3.57488900	-2.76528600	0.73096100
C	-2.93616200	-1.11856800	-3.19918600
H	-2.90822600	-0.19958900	-3.81507900
H	-3.15302100	-1.95988100	-3.87199100
H	-3.76534200	-1.02742100	-2.49142200
C	-0.56655500	-1.66278700	-3.34916900
H	0.33665900	-1.80520500	-2.75196900
H	-0.75111200	-2.58684400	-3.91593900
H	-0.36669200	-0.86412500	-4.08692300
C	-2.96446400	3.34438900	-0.02454000
H	-3.44598600	3.29759500	0.96961400
H	-2.96263600	4.39265900	-0.35195600
H	-3.57309600	2.76790100	-0.72909600
C	-0.69332400	3.66141000	0.77215600
H	-1.03176900	3.82565500	1.80691600
H	0.29767100	3.19960600	0.79718100

H	-0.59536500	4.64362000	0.28657500
C	-0.56480500	1.66255800	3.34962800
H	-0.74854400	2.58679200	3.91636500
H	-0.36562500	0.86373600	4.08738000
H	0.33853700	1.80423100	2.75244800
C	-2.93488600	1.12033200	3.19941000
H	-3.76420700	1.03071900	2.49160500
H	-2.90804800	0.20084200	3.81460000
H	-3.15070500	1.96141300	3.87282800

3H+

E = -1558.47134 a.u

C	-1.50971600	-0.53107300	-1.31853800
C	-1.49556200	-1.40022400	-0.19990100
C	-1.38982000	-0.86055500	1.10445300
C	-1.50842100	0.53129400	1.31942800
C	-1.49509200	1.40043200	0.20077700
C	-1.39060200	0.86075700	-1.10367000
C	1.51550000	-1.62893700	2.31538400
C	1.51393300	1.62866900	-2.31670400
C	2.88121300	-2.07145100	1.87796600
H	2.84915500	-3.09926500	1.49586200
H	3.58798500	-2.05145300	2.71878400
C	2.87993600	2.07087600	-1.87989500
H	2.84821100	3.09870300	-1.49781100
H	3.58639200	2.05070400	-2.72097500
N	3.48930100	1.21345500	-0.80708100
N	3.49025200	-1.21394800	0.80507800
Si	2.65399500	-0.00076700	-0.00130600
C	-1.02076900	1.80093300	-2.25092300
C	-1.01927300	-1.80082400	2.25138900

H	-1.06614200	1.27466400	-3.20320800
H	-1.69472100	2.65910100	-2.30933600
H	-1.69329600	-2.65890100	2.31023100
H	-1.06391100	-1.27462200	3.20374500
C	4.88698700	1.59329500	-0.52727700
H	5.25608100	1.11242500	0.37966300
H	5.53877400	1.32919900	-1.36853500
H	4.93541400	2.67776900	-0.37820200
C	4.88823900	-1.59290300	0.52559800
H	4.93736300	-2.67733400	0.37640300
H	5.25730100	-1.11170700	-0.38118100
H	5.53963600	-1.32850300	1.36706300
C	0.39116800	2.27970000	-1.97789000
C	0.39240300	-2.27981700	1.97735900
H	1.46521600	0.73004800	-2.93350600
H	0.46972700	3.17877100	-1.36809500
H	0.47040800	-3.17896900	1.36761000
H	1.46731400	-0.73024400	2.93213000
N	-1.61702200	-2.82484000	-0.28149200
N	-1.72393700	-1.09742300	-2.62150300
N	-1.61624300	2.82508100	0.28245800
N	-1.72117300	1.09769600	2.62260400
H	1.19948500	-0.00187200	-0.00244800
C	-2.99482300	-3.31286100	-0.18927600
H	-3.56002500	-3.15730900	-1.12406600
H	-2.98468800	-4.38708900	0.03051000
H	-3.52288900	-2.80173100	0.62138500
C	-0.82231200	-3.58282400	-1.23949100
H	-1.24793200	-3.61013400	-2.25221600
H	0.18830200	-3.16597200	-1.29862500

H	-0.73625000	-4.61625000	-0.87699400
C	-2.97648100	-0.74126200	-3.28161900
H	-2.95202600	0.23621800	-3.79671500
H	-3.21390800	-1.50588700	-4.03212000
H	-3.78834300	-0.72238300	-2.54950300
C	-0.61176500	-1.28812900	-3.54046100
H	-0.40080700	-0.41230500	-4.18129800
H	0.29818700	-1.53036400	-2.98510500
H	-0.82909200	-2.13010600	-4.21108600
C	-0.82056500	3.58292600	1.23977600
H	-0.73485300	4.61638900	0.87731300
H	-1.24515500	3.61011700	2.25293100
H	0.19010600	3.16603800	1.29783100
C	-2.99410500	3.31323500	0.19157900
H	-3.55852700	3.15746600	1.12680200
H	-2.98403800	4.38751600	-0.02791300
H	-3.52289600	2.80237300	-0.61877700
C	-2.97313600	0.74188100	3.28400100
H	-2.94844000	-0.23559700	3.79908800
H	-3.20959800	1.50658400	4.03472700
H	-3.78574200	0.72321200	2.55270400
C	-0.60800300	1.28824300	3.54036000
H	-0.39628500	0.41231600	4.18081700
H	0.30132900	1.53059800	2.98403800
H	-0.82460100	2.13009500	4.21137700

4.

E = -1715.36205 a.u

C	-2.31542400	-0.45573800	-1.17119400
C	-2.19708800	-1.36952900	-0.10058500

C	-1.90022800	-0.90272200	1.19839900
C	-1.93967500	0.48190200	1.47391200
C	-2.04299700	1.39651000	0.40082700
C	-2.11944300	0.92064600	-0.92814100
C	1.10854600	-1.84040100	1.91524600
C	0.65695200	1.58746400	-2.47455200
C	2.40262700	-2.31862600	1.30501500
H	2.22233200	-3.26306800	0.76744000
H	3.10757900	-2.55191500	2.11410800
C	2.09973500	1.91077900	-2.16184900
H	2.15289100	2.96622500	-1.87400000
H	2.70868400	1.79978600	-3.07143000
N	2.69729000	1.09322400	-1.06384100
N	3.03502700	-1.29610300	0.43110500
Si	1.91345400	-0.43603400	-0.65623700
C	-1.83533500	1.89281500	-2.07292900
C	-1.41334900	-1.90918600	2.24060900
H	-2.03290300	1.41473000	-3.03210700
H	-2.46507700	2.78496200	-2.00891900
H	-2.12272800	-2.73382000	2.35855800
H	-1.30684200	-1.42533500	3.21128700
C	3.84172700	1.75098000	-0.39362400
H	4.19432000	1.03925000	0.35288800
C	4.49309900	-1.47248100	0.24410000
H	4.79210900	-0.74301700	-0.51500300
C	-0.37105500	2.28542900	-1.97234800
C	-0.07377200	-2.45436700	1.77055800
H	0.46617500	0.72725800	-3.11234500
H	-0.16046100	3.13095300	-1.31837600
H	-0.12365600	-3.35419900	1.16033600

H	1.17892600	-0.91802100	2.49292800
N	-2.37975900	-2.78834000	-0.23866900
N	-2.67756100	-0.97014500	-2.46656800
N	-2.09844900	2.82181300	0.56658000
N	-1.94043600	1.00578000	2.81657600
C	-1.11714800	3.50405000	1.39554300
H	-1.03410900	4.54644800	1.05427000
H	-1.36886700	3.51435200	2.46724100
H	-0.13765600	3.03394700	1.27173100
C	-3.44422500	3.35898100	0.72597000
H	-3.85672400	3.19105100	1.73816000
H	-3.42908200	4.44158100	0.54187200
H	-4.12072100	2.89796700	-0.00094300
C	-3.09015300	0.66037400	3.63954600
H	-3.03716200	-0.34838400	4.09133600
H	-3.17565500	1.38591900	4.46040500
H	-4.00389300	0.71649200	3.04043900
C	-0.69457400	1.10212700	3.56288200
H	0.13400900	1.30912500	2.88211600
H	-0.75972100	1.93122000	4.28229400
H	-0.44311500	0.19198900	4.13747700
C	-3.76522300	-3.22706700	-0.12917900
H	-4.35862100	-3.00881500	-1.03633100
H	-3.79081800	-4.31199100	0.03975500
H	-4.24701300	-2.73740100	0.72376200
C	-1.63298200	-3.51960100	-1.25243300
H	-2.11685400	-3.52287200	-2.24130800
H	-0.63214100	-3.09173200	-1.35392500
H	-1.52381000	-4.56409400	-0.92446000
C	-1.65534800	-1.15997100	-3.48597300

H	-1.93252800	-2.00305800	-4.13546500
H	-1.51398400	-0.27953300	-4.13946300
H	-0.69709800	-1.38948100	-3.01466500
C	-3.96421600	-0.54601200	-2.99586900
H	-4.70738800	-0.52586000	-2.19313200
H	-3.95114400	0.45108900	-3.47635900
H	-4.29846000	-1.27093400	-3.75113400
C	3.42926700	3.01200600	0.39310700
H	4.27124900	3.35539400	1.00732600
H	3.14296700	3.84660500	-0.25658100
H	2.58811600	2.78979300	1.05862900
C	5.00659600	2.05390100	-1.35263000
H	4.73723400	2.82258400	-2.08670900
H	5.87476500	2.42377300	-0.79292600
H	5.31097900	1.15532600	-1.90187900
C	5.31643700	-1.18418000	1.51477300
H	5.14782000	-1.93808300	2.29272400
H	6.38867300	-1.19421600	1.28135700
H	5.06681900	-0.20494500	1.93753000
C	4.84827500	-2.86026300	-0.32781700
H	5.91908100	-2.91080900	-0.56216800
H	4.63027400	-3.66488300	0.38418700
H	4.28595100	-3.05740600	-1.24768200

4H+.

E = -1715.77275 a.u

C	-2.18981100	0.26694000	1.39640700
C	-2.18264100	1.33456800	0.46700400
C	-2.06811800	1.05622900	-0.91620600
C	-2.19028900	-0.26702600	-1.39612400

C	-2.18273400	-1.33467900	-0.46669700
C	-2.06776500	-1.05633500	0.91643600
C	0.85740100	2.02444400	-1.87454800
C	0.85802700	-2.02466700	1.87447800
C	2.21387700	2.42445300	-1.37042200
H	2.12231500	3.32261100	-0.75207000
H	2.87244100	2.66414200	-2.21290900
C	2.21433500	-2.42466600	1.36988000
H	2.12255000	-3.32266300	0.75131900
H	2.87309000	-2.66464200	2.21213100
N	2.92841200	-1.37320000	0.56243000
N	2.92810400	1.37318400	-0.56282400
Si	2.13429500	-0.00013500	-0.00027600
C	-1.67831100	-2.19831900	1.85376800
C	-1.67885000	2.19825800	-1.85354800
H	-1.70218800	-1.86652700	2.89077200
H	-2.35324100	-3.05269600	1.76141100
H	-2.35382800	3.05259600	-1.76112500
H	-1.70286500	1.86648700	-2.89055500
C	4.36068100	-1.70180200	0.24662300
H	4.69428500	-0.93820300	-0.46018300
C	4.36027100	1.70209000	-0.24695900
H	4.69398900	0.93857500	0.45988500
C	-0.27325700	-2.61786400	1.46679900
C	-0.27374200	2.61790100	-1.46686000
H	0.82560700	-1.23110500	2.62322100
H	-0.21072400	-3.41032300	0.72246100
H	-0.21101400	3.41063500	-0.72283400
H	0.82469000	1.23062800	-2.62301600
N	-2.31334100	2.71628000	0.81975600

N	-2.39749700	0.56884000	2.78669500
N	-2.31360900	-2.71643400	-0.81940500
N	-2.39825400	-0.56897900	-2.78637500
C	-1.53849300	-3.28119600	-1.91597500
H	-1.45680000	-4.36558000	-1.75938200
H	-1.97740200	-3.11052700	-2.90913400
H	-0.52554700	-2.86663000	-1.90790100
C	-3.69054700	-3.21360200	-0.79445300
H	-4.27312000	-2.88895700	-1.67385000
H	-3.68001700	-4.31011700	-0.77765200
H	-4.20280400	-2.86125200	0.10578200
C	-3.63846400	-0.06937700	-3.37198300
H	-3.60108000	0.99449500	-3.66857200
H	-3.87064300	-0.65607500	-4.26982300
H	-4.45987300	-0.19735400	-2.66173000
C	-1.27654400	-0.58225200	-3.71393100
H	-0.37714700	-0.95111900	-3.21308700
H	-1.49793300	-1.26210700	-4.54749900
H	-1.04309600	0.40373700	-4.15571900
C	-3.69012000	3.21385000	0.79450700
H	-4.27265400	2.89015000	1.67429000
H	-3.67931800	4.31035400	0.77673600
H	-4.20263100	2.86080200	-0.10530000
C	-1.53827100	3.28104200	1.91633500
H	-1.97723600	3.11039100	2.90947600
H	-0.52532500	2.86649500	1.90832900
H	-1.45657700	4.36542700	1.75971900
C	-1.27565700	0.58204100	3.71407300
H	-1.49677900	1.26206600	4.54757900
H	-1.04234000	-0.40393000	4.15597100

H	-0.37626300	0.95064400	3.21302800
C	-3.63769900	0.06946800	3.37248200
H	-4.45921100	0.19769000	2.66239000
H	-3.60050400	-0.99444700	3.66895500
H	-3.86959600	0.65612500	4.27042200
C	4.48105300	-3.05215800	-0.47613700
H	5.50625400	-3.16935000	-0.84327500
H	4.27474900	-3.89880200	0.18600000
H	3.80582500	-3.10738000	-1.33715800
C	5.26016400	-1.63496200	1.48919300
H	5.04372300	-2.44057100	2.19801600
H	6.30740900	-1.74392500	1.18681800
H	5.15568200	-0.68048000	2.01681400
C	5.25984300	1.63544400	-1.48947400
H	5.04318000	2.44094400	-2.19834900
H	6.30703500	1.74475000	-1.18704300
H	5.15568600	0.68090200	-2.01705200
C	4.48035500	3.05248800	0.47578800
H	5.50548500	3.16982700	0.84307300
H	4.27403700	3.89908800	-0.18640200
H	3.80499500	3.10764200	1.33671000
H	0.67972900	-0.00027000	-0.00049300

5.

E= -1558.07572 a.u

C	-0.92224200	-2.64555400	0.62963900
C	0.46627800	-2.77252500	0.55256900
C	1.31078200	-2.02318500	1.38343000
C	0.70854400	-1.29388800	2.41808700
C	-0.67940500	-1.17312300	2.49819200

C	-1.51903800	-1.76980000	1.54635200
H	-1.54334600	-3.19041300	-0.07636100
H	1.33484300	-0.75827800	3.12471700
C	2.86763600	0.54247200	0.28425000
C	-2.86235800	-0.15352900	-0.86129600
C	2.86721500	1.60925100	-0.80295100
H	3.43516300	1.25190600	-1.67026900
H	3.38964500	2.49865800	-0.41681000
C	-2.55697400	1.13831200	-1.63725200
H	-3.37004000	1.84191800	-1.43739100
H	-2.59593500	0.92165800	-2.71123500
N	-1.28375900	1.83017700	-1.29219900
N	1.51249700	2.05037900	-1.22720000
H	-1.10948600	-0.55753200	3.28416800
H	0.89298200	-3.42173100	-0.20699700
Si	0.19316200	0.87356500	-1.31355500
C	-2.98101400	-1.36017500	1.40793200
C	2.79808700	-1.87331600	1.08569300
H	-3.57034800	-2.21505200	1.05864400
H	-3.38847500	-1.09564300	2.39117200
H	3.20905000	-2.81881800	0.71290100
H	3.33701300	-1.63706900	2.00886500
C	-1.47572200	3.23318600	-0.92283700
H	-0.57904700	3.62151800	-0.43460000
H	-1.69688600	3.87218000	-1.79368000
H	-2.31240300	3.31941400	-0.21857500
C	1.58689400	3.33718600	-1.91426300
H	2.37252900	3.31644200	-2.68696900
H	0.64438100	3.57201300	-2.41255900
H	1.82845600	4.16157100	-1.22219300

C	-3.09719700	-0.13213000	0.48298400
C	3.03365400	-0.77772600	0.02476800
N	-2.99179700	-1.32145100	-1.62507600
C	-2.14939800	-1.63444700	-2.76638200
H	-1.72652500	-2.64547000	-2.66238000
H	-2.71651000	-1.60509200	-3.71150500
H	-1.30607100	-0.94445300	-2.82287000
C	-4.06858700	-2.26315500	-1.40466200
H	-3.74648200	-3.19216800	-0.90215800
H	-4.85265900	-1.79943900	-0.80066000
H	-4.50192800	-2.55249700	-2.37388300
N	2.77442700	0.96709900	1.65613200
C	1.84963100	2.05395900	1.95439400
H	1.80517300	2.18444600	3.04250300
H	2.14234700	3.02374900	1.51100900
H	0.84871700	1.80357500	1.59845700
C	4.08716900	1.19962700	2.26200200
H	3.96660500	1.34862900	3.34202300
H	4.73357700	0.33156200	2.10424400
H	4.60148700	2.09116400	1.85314200
N	-3.42387600	1.14761600	1.07044100
N	3.46767300	-1.16215100	-1.29281500
C	4.90836500	-1.40609500	-1.36071200
H	5.20411100	-1.52261600	-2.41063300
H	5.45112500	-0.55317200	-0.94164300
H	5.22368500	-2.31927600	-0.81856400
C	2.70912100	-2.20973300	-1.96525800
H	1.64573300	-1.96431700	-1.93892200
H	3.02790400	-2.25273200	-3.01380400
H	2.85906700	-3.21772400	-1.53190500

C	-4.84373900	1.27114100	1.39864000
H	-5.06108400	2.30486600	1.69719600
H	-5.44983900	1.03050400	0.51933200
H	-5.16163900	0.60980100	2.22909700
C	-2.58376300	1.61598800	2.16442700
H	-1.53226700	1.52920800	1.88312900
H	-2.80805500	2.67282600	2.36025100
H	-2.73861300	1.06783600	3.11402900

5H+.

E= -1558.48566 a.u

C	0.74408800	-2.55708800	1.17294500
C	-0.65164700	-2.56224100	1.22187200
C	-1.41936300	-2.46408000	0.05150500
C	-0.74409900	-2.55710300	-1.17293900
C	0.65163500	-2.56225900	-1.22186700
C	1.41935100	-2.46408400	-0.05150100
H	1.31331800	-2.57307200	2.09682700
H	-1.31332900	-2.57309800	-2.09682100
C	-2.79913800	0.29366200	-0.69968300
C	2.79914400	0.29365500	0.69968600
C	-2.78544700	1.78726600	-0.41708000
H	-3.47619800	2.00464100	0.39877900
H	-3.10652800	2.35075500	-1.30261700
C	2.78545400	1.78725900	0.41708200
H	3.47620700	2.00463500	-0.39877600
H	3.10653500	2.35074800	1.30261800
N	1.46190600	2.36403100	-0.00540500
N	-1.46189800	2.36403800	0.00540400
H	1.14377500	-2.60766600	-2.18899400
H	-1.14378700	-2.60763300	2.18900000

Si	0.00000300	1.53781100	0.00000400
C	2.90106400	-2.11924900	-0.10420600
C	-2.90107500	-2.11924100	0.10420700
H	3.39537500	-2.45876200	0.81077100
H	3.38857700	-2.63698000	-0.93699700
H	-3.38859000	-2.63697000	0.93699900
H	-3.39538500	-2.45875500	-0.81077000
C	1.60951000	3.76806200	-0.43281000
H	0.70065000	4.13768000	-0.90941500
H	1.85905400	4.41474400	0.41737800
H	2.42250800	3.82872200	-1.16463300
C	-1.60949800	3.76807200	0.43279500
H	-2.42249800	3.82874200	1.16461500
H	-0.70063900	4.13769100	0.90940100
H	-1.85903600	4.41474800	-0.41739900
C	3.07502700	-0.59961500	-0.28761000
C	-3.07503400	-0.59960700	0.28761000
N	2.64089500	-0.16334600	2.04792300
C	1.66749100	0.52739900	2.88034400
H	1.61104000	0.02682200	3.85236900
H	1.90374000	1.59045500	3.07189400
H	0.66648100	0.45981300	2.43637300
C	3.91568600	-0.35854600	2.75563000
H	3.73245600	-0.90974300	3.68424500
H	4.60043200	-0.94479900	2.13854000
H	4.41185500	0.59389100	3.01473300
N	-2.64087800	-0.16334100	-2.04791900
C	-1.66746800	0.52740300	-2.88033200
H	-1.61101200	0.02682700	-3.85235900
H	-1.90371200	1.59046000	-3.07188200

H	-0.66646000	0.45981200	-2.43635600
C	-3.91566300	-0.35854200	-2.75563600
H	-3.73242600	-0.90974300	-3.68424700
H	-4.60041500	-0.94479200	-2.13854900
H	-4.41182900	0.59389400	-3.01474700
N	3.59313500	-0.08817000	-1.52816400
N	-3.59315300	-0.08816000	1.52815900
C	-5.06161300	-0.17636900	1.58430600
H	-5.41687100	0.36361800	2.46855100
H	-5.49850000	0.28885500	0.69587700
H	-5.42783700	-1.21605200	1.64971600
C	-2.98792200	-0.57854000	2.76433400
H	-1.90408800	-0.43907600	2.73532300
H	-3.38496700	0.00915700	3.59895900
H	-3.19907100	-1.64158200	2.97764200
C	5.06159500	-0.17636700	-1.58432000
H	5.41684400	0.36362100	-2.46856900
H	5.49848500	0.28886200	-0.69589500
H	5.42782700	-1.21604700	-1.64972900
C	2.98790000	-0.57855600	-2.76433400
H	1.90406500	-0.43910300	-2.73531500
H	3.38493400	0.00914400	-3.59896200
H	3.19905800	-1.64159700	-2.97764200
H	-0.00000100	0.08466800	0.00001800

6.

E= -1715.36718 a.u

C	-0.70900700	-3.05604100	-1.19620700
C	0.68666300	-3.05925700	-1.20468400
C	1.42200700	-2.95977400	-0.01522800
C	0.71067500	-3.06004600	1.18770400

C	-0.68500300	-3.06471800	1.19616900
C	-1.42043700	-2.96125400	0.00711500
H	-1.25109100	-3.05287900	-2.13683400
H	1.25274400	-3.06011600	2.12835900
C	2.75000100	-0.19207300	0.83301100
C	-2.75042900	-0.19170000	-0.83137500
C	2.70744200	1.31935900	0.60194800
H	3.50847700	1.56113700	-0.09957400
H	2.94518500	1.81678600	1.55279000
C	-2.71015000	1.31904400	-0.59602800
H	-3.51007900	1.55742000	0.10793900
H	-2.95081300	1.81859600	-1.54505100
N	-1.43349900	1.87812500	-0.06480500
N	1.43110800	1.87774800	0.06910200
H	-1.20497300	-3.08948800	2.15004700
H	1.20667600	-3.07983200	-2.15863300
Si	-0.00137600	0.83141900	0.00355800
C	-2.89916800	-2.59438100	0.01894600
C	2.90048200	-2.59188600	-0.02563000
H	-3.38272800	-2.96985400	-0.88915700
H	-3.40298600	-3.07894700	0.86421200
H	3.40460500	-3.07305000	-0.87265800
H	3.38424700	-2.97062300	0.88100600
C	-1.59142600	3.23490200	0.50851500
H	-0.59062300	3.54908700	0.81217500
C	1.58924000	3.23396600	-0.50548400
H	0.58841900	3.54827100	-0.80891900
C	-3.06495500	-1.06657100	0.15672600
C	3.06534100	-1.06349200	-0.15796000
N	-2.59024000	-0.69202700	-2.16729600

C	-1.65103700	-0.01319700	-3.04882100
H	-1.48595100	-0.63620800	-3.93633200
H	-2.00266300	0.97635100	-3.39744000
H	-0.69076200	0.11442800	-2.54382600
C	-3.85616100	-0.95809700	-2.85252700
H	-3.66383000	-1.54942500	-3.75661800
H	-4.52842500	-1.52732600	-2.20602500
H	-4.37743400	-0.03065300	-3.15997000
N	2.59078700	-0.69652000	2.16733500
C	1.65370500	-0.01988200	3.05276900
H	1.48567400	-0.64798000	3.93615000
H	2.00914800	0.96593000	3.40806800
H	0.69420400	0.11478900	2.54817400
C	3.85665400	-0.96786700	2.85053500
H	3.66402300	-1.56334000	3.75185700
H	4.52798600	-1.53470500	2.20103400
H	4.37915600	-0.04255500	3.16228500
N	-3.57163800	-0.53037300	1.39673600
N	3.57237600	-0.52276100	-1.39588800
C	5.00609000	-0.75361000	-1.56233200
H	5.36489500	-0.18151900	-2.42712600
H	5.54415000	-0.40899200	-0.67321000
H	5.26484600	-1.81714600	-1.73362700
C	2.83437500	-0.83676500	-2.61299100
H	1.76829700	-0.65986700	-2.45520000
H	3.18289600	-0.17648500	-3.41740500
H	2.97038700	-1.87955400	-2.95966800
C	-5.00499300	-0.76304000	1.56353500
H	-5.36366000	-0.19380700	2.43026700
H	-5.54402600	-0.41627400	0.67583500

H	-5.26267500	-1.82730500	1.73189800
C	-2.83227100	-0.84744400	2.61224500
H	-1.76646400	-0.66923400	2.45398700
H	-3.18058900	-0.18981500	3.41891800
H	-2.96722800	-1.89135400	2.95592500
C	-2.12327300	4.26730700	-0.50267100
H	-3.16854400	4.07114300	-0.76931200
H	-2.07814700	5.27670100	-0.07490500
H	-1.53253600	4.26099100	-1.42622400
C	-2.44054400	3.24302000	1.79688300
H	-2.41054800	4.24128000	2.25231100
H	-3.49221600	2.99912400	1.61188500
H	-2.04841800	2.52145500	2.52113600
C	2.12191800	4.26693100	0.50468200
H	3.16706900	4.07025200	0.77142300
H	2.07744200	5.27597600	0.07602600
H	1.53126500	4.26185300	1.42830600
C	2.43768900	3.24059800	-1.79427000
H	2.40893100	4.23882100	-2.24986900
H	3.48905900	2.99504200	-1.60982800
H	2.04407300	2.51948700	-2.51815200

6H+.

E= -1715.78488 a.u

C	-0.66273000	-3.07531200	-1.22085800
C	0.73280700	-3.07934800	-1.17539400
C	1.41867700	-2.98049100	0.04434100
C	0.66242400	-3.07553700	1.22017200
C	-0.73311000	-3.07943400	1.17470800
C	-1.41896800	-2.98034500	-0.04501100
H	-1.16817900	-3.09147600	-2.18120500

H	1.16787300	-3.09187200	2.18051500
C	2.72462800	-0.20665400	0.85174500
C	-2.72473500	-0.20614800	-0.85156500
C	2.74899400	1.28853900	0.56534100
H	3.52026400	1.48563500	-0.17632600
H	2.99882700	1.83345300	1.48203800
C	-2.74898900	1.28895300	-0.56470900
H	-3.52002000	1.48576600	0.17728100
H	-2.99911200	1.83414900	-1.48116800
N	-1.47514900	1.88495000	-0.02615200
N	1.47532800	1.88468200	0.02653100
H	-1.29033800	-3.12117600	2.10596100
H	1.29002900	-3.12100000	-2.10665300
Si	0.00001600	1.07642600	0.00023600
C	-2.89881600	-2.62966000	-0.09250100
C	2.89855200	-2.62993200	0.09193000
H	-3.32949100	-2.95686300	-1.04346700
H	-3.44551800	-3.15450000	0.69818900
H	3.44522800	-3.15457300	-0.69890900
H	3.32920800	-2.95742800	1.04280100
C	-1.63523600	3.27315500	0.52874600
H	-0.63326500	3.59782800	0.82160600
C	1.63567600	3.27278600	-0.52858000
H	0.63375900	3.59759300	-0.82145700
C	-3.07909000	-1.11150600	0.09782000
C	3.07887500	-1.11172200	-0.09793600
N	-2.46808900	-0.65163500	-2.19027500
C	-1.43364500	0.04103500	-2.94322400
H	-1.31376500	-0.44720000	-3.91592200
H	-1.64795300	1.10866300	-3.13644500

H	-0.46625900	-0.04311400	-2.43268000
C	-3.69002300	-0.82600000	-2.99004000
H	-3.44527500	-1.36559700	-3.91138400
H	-4.42188700	-1.41425100	-2.43191100
H	-4.15931000	0.13434500	-3.27006900
N	2.46806800	-0.65249000	2.19035800
C	1.43354300	0.03990100	2.94347000
H	1.31367700	-0.44861200	3.91602800
H	1.64777700	1.10749200	3.13699800
H	0.46619700	-0.04417300	2.43285800
C	3.69006800	-0.82681200	2.99004300
H	3.44540600	-1.36646500	3.91137500
H	4.42192300	-1.41500600	2.43183900
H	4.15932600	0.13354500	3.27008500
N	-3.69310600	-0.61660200	1.30213100
N	3.69288700	-0.61641600	-1.30207900
C	5.15868800	-0.73795700	-1.25299000
H	5.58822200	-0.21486000	-2.11430300
H	5.54224400	-0.27387400	-0.33944000
H	5.50589900	-1.78591200	-1.28361800
C	3.16668500	-1.10629400	-2.57396500
H	2.08577800	-0.95008400	-2.62006200
H	3.62998700	-0.53173300	-3.38336700
H	3.37409600	-2.17435400	-2.76513700
C	-5.15888000	-0.73846800	1.25313900
H	-5.58844500	-0.21570900	2.11464000
H	-5.54262000	-0.27420600	0.33975700
H	-5.50584600	-1.78651100	1.28350000
C	-3.16667200	-1.10664600	2.57386400
H	-2.08580300	-0.95017000	2.61987800

H	-3.63002100	-0.53236400	3.38343700
H	-3.37381500	-2.17480000	2.76480500
H	-0.00010800	-0.37784200	0.00041900
C	2.48589400	3.27241200	-1.80892300
H	2.45825800	4.27260300	-2.25550900
H	3.53522000	3.03009100	-1.61644800
H	2.09691500	2.55949600	-2.54294600
C	2.17215500	4.25917000	0.51693500
H	3.21834500	4.05690200	0.76818000
H	2.12486600	5.27745900	0.11636000
H	1.58542800	4.23083200	1.44216700
C	-2.17154300	4.25947200	-0.51691300
H	-3.21781300	4.05742400	-0.76801200
H	-2.12395300	5.27781200	-0.11651000
H	-1.58490200	4.23081200	-1.44218900
C	-2.48550000	3.27313300	1.80905800
H	-3.53484100	3.03083500	1.61662600
H	-2.09656100	2.56041200	2.54329600
H	-2.45782000	4.27344100	2.25537700

7.

E= -2093.98252 a.u

C	-0.71248700	-1.81244900	-1.20207500
C	0.69860100	-1.70665400	-1.21242900
C	1.41687000	-1.55592900	0.00118900
C	0.71198800	-1.81187500	1.20297100
C	-0.69906800	-1.70567000	1.21325600
C	-1.41727700	-1.55563600	-0.00045800
C	2.86277900	1.30813300	0.53944100
C	-2.86242100	1.30788300	-0.54023700

C	2.76651700	2.74056500	0.03662300
H	3.28563100	2.83962400	-0.92183200
H	3.27578500	3.43242900	0.73366400
C	-2.76637400	2.74065700	-0.03835800
H	-3.28594300	2.84032900	0.91979200
H	-3.27534200	3.43207700	-0.73607100
N	-1.38154500	3.24465500	0.16564400
N	1.38156500	3.24437400	-0.16721000
Si	0.00008200	2.14905600	0.00036800
C	-2.91560700	-1.22342200	-0.03204400
C	2.91524200	-1.22360500	0.03264300
H	-3.30466900	-1.47239400	-1.02134800
H	-3.47198400	-1.84315800	0.67538200
H	3.47175800	-1.84391500	-0.67422300
H	3.30412100	-1.47183000	1.02221500
C	-1.42028200	4.60384000	0.69302300
H	-0.43736100	4.90847400	1.05599600
H	-1.75910000	5.33951900	-0.05718700
H	-2.12212500	4.66311200	1.54116200
C	1.42004700	4.60311600	-0.69575000
H	2.12213300	4.66183200	-1.54371300
H	0.43712600	4.90708000	-1.05929700
H	1.75839800	5.33957000	0.05390200
C	-3.25947900	0.26023200	0.26169400
C	3.25915800	0.25989800	-0.26210600
N	-2.75547300	1.06356600	-1.96094100
C	-1.84371900	1.88752900	-2.74577800
H	-1.87783200	1.55711700	-3.79128800
H	-2.09182900	2.96468400	-2.73192300
H	-0.81842600	1.76672900	-2.38754200

C	-4.07710400	1.04511700	-2.59978600
H	-3.97964600	0.71636000	-3.64204800
H	-4.73751100	0.34500100	-2.08123100
H	-4.56365300	2.04027700	-2.60587300
N	2.75703900	1.06494400	1.96038600
C	1.84603700	1.88941000	2.74553700
H	1.88094400	1.55953200	3.79118900
H	2.09430100	2.96653000	2.73096300
H	0.82043900	1.76858300	2.38817600
C	4.07913300	1.04637500	2.59823200
H	3.98236900	0.71782500	3.64063100
H	4.73900500	0.34601400	2.07933300
H	4.56589600	2.04143800	2.60376300
N	-4.14192500	0.50551400	1.32484000
N	4.14087300	0.50477500	-1.32594600
C	5.23997300	1.44697400	-1.20988000
H	5.12414200	2.32543000	-1.86607900
H	5.33553500	1.79772500	-0.18047900
H	6.17877800	0.94811800	-1.50063800
C	4.17646900	-0.24404300	-2.56794800
H	3.35496400	-0.95701400	-2.58903600
H	4.07016300	0.43480500	-3.42983800
H	5.13773600	-0.77217900	-2.68197900
C	-5.24059100	1.44810200	1.20798400
H	-5.12446400	2.32712300	1.86338300
H	-5.33599600	1.79794900	0.17825100
H	-6.17956400	0.94985400	1.49918400
C	-4.17773100	-0.24229700	2.56746400
H	-3.35674800	-0.95586900	2.58895800
H	-4.07074500	0.43711000	3.42884000

H	-5.13934700	-0.76964100	2.68206400
N	1.46014800	-1.87116200	-2.41804200
N	-1.34896600	-2.42899500	-2.34583800
N	-1.46062900	-1.86901600	2.41906800
N	1.34831000	-2.42760900	2.34718800
C	1.86999100	-3.76060200	2.07384000
H	2.86081700	-3.75894600	1.57888800
H	1.97579000	-4.30602300	3.02232300
H	1.17248900	-4.31502600	1.43892100
C	2.14877900	-1.71690200	3.33011400
H	3.21994700	-1.66191600	3.06767400
H	1.78704800	-0.69985400	3.45172400
H	2.07842600	-2.24084100	4.29560800
C	-1.90666200	-3.23472800	2.68026300
H	-1.09511900	-3.87694900	3.06463300
H	-2.71149600	-3.22012200	3.42865600
H	-2.29971300	-3.68470400	1.76373800
C	-1.03061700	-1.18948500	3.63481200
H	-0.27561100	-1.74679700	4.20530600
H	-0.63148200	-0.20382500	3.38264400
H	-1.90350300	-1.04286000	4.28748800
C	1.90837000	-3.23665700	-2.67656000
H	2.30240100	-3.68398800	-1.75918100
H	1.09778200	-3.88101600	-3.05937300
H	2.71297500	-3.22232400	-3.42520300
C	1.02966900	-1.19436400	-3.63511500
H	0.62947500	-0.20865000	-3.38487100
H	1.90258000	-1.04803300	-4.28784000
H	0.27534200	-1.75348700	-4.20474200
C	-2.14968800	-1.71894700	-3.32903300

H	-1.78651200	-0.70268500	-3.45314300
H	-2.08120600	-2.24496900	-4.29349400
H	-3.22046300	-1.66167500	-3.06546500
C	-1.87085200	-3.76168100	-2.07115400
H	-1.97726200	-4.30782900	-3.01914500
H	-1.17314500	-4.31573100	-1.43613800
H	-2.86141300	-3.75942600	-1.57568000

7H+.

E= -2094.40979 a.u

C	0.60127600	-1.77481200	1.27290700
C	-0.80766700	-1.68587400	1.15109100
C	-1.40766600	-1.54977800	-0.12734000
C	-0.60245100	-1.77539400	-1.27164900
C	0.80664000	-1.68714800	-1.14991400
C	1.40675300	-1.55055000	0.12832000
C	-2.82940500	1.28811200	-0.57696000
C	2.83087700	1.28690100	0.57617900
C	-2.79210300	2.66982200	0.03088500
H	-3.30259400	2.69317800	0.99502700
H	-3.26960500	3.43060800	-0.60864600
C	2.79407500	2.66838000	-0.03212400
H	3.30399600	2.69121800	-0.99658500
H	3.27237600	3.42907200	0.60691800
N	1.40380000	3.17675100	-0.29978400
N	-1.40167800	3.17736200	0.29920600
Si	0.00089200	2.29740300	-0.00024400
C	2.90283700	-1.25907500	0.28365800
C	-2.90354900	-1.25785900	-0.28235000
H	3.17367200	-1.39449200	1.33168400
H	3.50805800	-1.97019600	-0.28088200

H	-3.50860300	-1.96777200	0.28392000
H	-3.17538400	-1.39497700	-1.32991800
C	1.41123100	4.53979800	-0.85142900
H	0.41047700	4.84813700	-1.15875900
H	1.79614700	5.26081200	-0.11821600
H	2.06170300	4.57000500	-1.73417200
C	-1.40855700	4.54042300	0.85082700
H	-2.05946700	4.57102800	1.73323200
H	-0.40776900	4.84814200	1.15868900
H	-1.79264900	5.26169300	0.11742800
C	3.31291500	0.17694800	-0.10962000
C	-3.31259800	0.17895200	0.10924200
N	2.62407700	1.14687000	1.99966900
C	1.62209200	1.97831100	2.64371500
H	1.60485100	1.76313700	3.71783200
H	1.78692900	3.06576500	2.53430000
H	0.61335000	1.73539200	2.27260100
C	3.88765100	1.20964400	2.75444600
H	3.70644600	0.94689600	3.80288600
H	4.60184000	0.49182900	2.34344900
H	4.35156200	2.21288200	2.73114700
N	-2.62168800	1.14731300	-2.00024900
C	-1.61962900	1.97872700	-2.64420000
H	-1.60185800	1.76309900	-3.71822300
H	-1.78473000	3.06618200	-2.53530900
H	-0.61095600	1.73619400	-2.27263000
C	-3.88485200	1.20938700	-2.75581600
H	-3.70300200	0.94602900	-3.80398000
H	-4.59917100	0.49173100	-2.34479200
H	-4.34888100	2.21258500	-2.73337100

N	4.28728500	0.32348400	-1.08107100
N	-4.28742100	0.32721000	1.08005900
C	-5.31472700	1.36289800	0.99617800
H	-5.21114100	2.12870000	1.77869300
H	-5.29157300	1.84899700	0.01921600
H	-6.29925100	0.89438200	1.12755100
C	-4.60992300	-0.67193900	2.09585900
H	-3.76577700	-1.34033500	2.23707900
H	-4.81716600	-0.16473500	3.04658500
H	-5.50946400	-1.24102500	1.81709900
C	5.31460700	1.35929600	-0.99940100
H	5.21009900	2.12443200	-1.78244500
H	5.29260000	1.84624200	-0.02281400
H	6.29896400	0.89069000	-1.13155000
C	4.60945500	-0.67768000	-2.09505200
H	3.76493800	-1.34583200	-2.23526300
H	4.81722500	-0.17225500	-3.04659200
H	5.50862300	-1.24674100	-1.81503900
H	0.00052700	0.84579900	-0.00011600
N	-1.68707400	-1.86666700	2.26972700
N	1.14309800	-2.32490700	2.48943400
N	1.68546500	-1.86826800	-2.26897000
N	-1.14449800	-2.32577700	-2.48792700
C	-1.75711000	-3.64275900	-2.33293500
H	-2.80364500	-3.60924100	-1.97751900
H	-1.75487900	-4.15246800	-3.30523000
H	-1.17570500	-4.24816400	-1.63188200
C	-1.78394800	-1.53544700	-3.52863300
H	-2.87188600	-1.42125700	-3.38561400
H	-1.34714300	-0.54078100	-3.57384200

H	-1.63450000	-2.03034200	-4.49858400
C	2.04000800	-3.26746200	-2.52433200
H	1.21122500	-3.83311500	-2.97855500
H	2.89620800	-3.30734800	-3.21029400
H	2.32777000	-3.75866700	-1.58982200
C	1.43281800	-1.13272600	-3.50358100
H	0.71574400	-1.62709900	-4.17124300
H	1.06625300	-0.12965700	-3.26760700
H	2.37867100	-1.02270600	-4.05177100
C	-2.04555800	-3.26548700	2.52158700
H	-2.33685900	-3.75285300	1.58610200
H	-1.21767300	-3.83518100	2.97241200
H	-2.90048300	-3.30473800	3.20914300
C	-1.43356800	-1.13420500	3.50590700
H	-1.06498700	-0.13135500	3.27214300
H	-2.37950900	-1.02342000	4.05381000
H	-0.71787800	-1.63127400	4.17302300
C	1.78131500	-1.53422400	3.53068000
H	1.34230000	-0.54057800	3.57724300
H	1.63321800	-2.03038200	4.50015800
H	2.86890000	-1.41740700	3.38741300
C	1.75632200	-3.64170200	2.33490100
H	1.75358600	-4.15129500	3.30725300
H	1.17547800	-4.24730500	1.63355700
H	2.80304700	-3.60797200	1.98016400

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C	0.42394900	-2.27484100	1.29152000
C	-0.96877200	-2.04849200	1.18516400

C	-1.57395500	-1.88324700	-0.08611300
C	-0.80316900	-2.23623000	-1.22043200
C	0.60817900	-2.24928600	-1.12012200
C	1.23904600	-2.12211700	0.14356300
C	-2.69347100	1.07062200	-0.78463100
C	2.84205200	0.63542000	0.71764500
C	-2.54640800	2.51419400	-0.31754000
H	-3.18121400	2.67810300	0.55240600
H	-2.91766200	3.19195400	-1.10402200
C	2.94987600	2.06351800	0.19437600
H	3.56777600	2.07098800	-0.70386200
H	3.47408300	2.68605200	0.93836800
N	1.65053400	2.71912900	-0.13298900
N	-1.16098800	2.93047000	0.05007200
Si	0.16139800	1.74521400	-0.07174200
C	2.75184300	-1.90567300	0.28616200
C	-3.03056400	-1.42788600	-0.24632300
H	3.04184500	-2.15155300	1.30960100
H	3.30942700	-2.58897200	-0.35870700
H	-3.69131400	-1.98201300	0.42453100
H	-3.35971700	-1.66739500	-1.25934400
C	1.81569000	4.04763400	-0.76394400
H	0.80456000	4.41103900	-0.95765800
C	-1.11597500	4.24536700	0.72788400
H	-0.06057500	4.43937500	0.92815700
C	3.22531200	-0.46170300	-0.02092000
C	-3.25812800	0.08591600	-0.00407200
N	2.59593200	0.43724000	2.12959900
C	1.67856300	1.34130800	2.81282200
H	1.61535900	1.05140000	3.86897800

H	1.98771100	2.40160300	2.77851300
H	0.67728800	1.26045800	2.38115600
C	3.85460000	0.35388100	2.88072700
H	3.64816600	0.06062400	3.91760900
H	4.50996400	-0.39978800	2.43644500
H	4.40274300	1.31628300	2.90803700
N	-2.49151800	0.77474300	-2.18668200
C	-1.45643100	1.50060600	-2.91274900
H	-1.43201300	1.14394800	-3.94988300
H	-1.61666700	2.59418100	-2.94346300
H	-0.47744300	1.30757800	-2.46613000
C	-3.75435800	0.84750800	-2.93239900
H	-3.60004800	0.48772800	-3.95728300
H	-4.51073800	0.21575500	-2.45919100
H	-4.15461900	1.87848400	-2.99573400
N	4.18824400	-0.29890300	-1.03299300
N	-4.18757600	0.44682100	0.98762600
C	-5.22814200	1.42714100	0.71846200
H	-5.16645900	2.30249100	1.38489200
H	-5.17061300	1.77546800	-0.31425600
H	-6.21862100	0.96838500	0.87687200
C	-4.46672000	-0.33481400	2.17829900
H	-3.66700000	-1.05374900	2.34132200
H	-4.53080900	0.32660700	3.05578400
H	-5.43292000	-0.86365600	2.09582000
C	5.39220400	0.48494700	-0.79993400
H	5.49084000	1.32324300	-1.50786400
H	5.40029600	0.88752600	0.21434400
H	6.28260800	-0.15404100	-0.92723700
C	4.31283100	-1.15979500	-2.19421800

H	3.39759800	-1.73289900	-2.32523300
H	4.48158900	-0.55163000	-3.09599700
H	5.17226700	-1.84714800	-2.09765100
N	-1.83359200	-2.10541100	2.32985900
N	0.91338500	-2.90668500	2.49831900
N	1.44388300	-2.50983200	-2.25721700
N	-1.40218900	-2.83330300	-2.39428700
C	-2.05955900	-4.10622300	-2.12816900
H	-3.08489000	-4.00155000	-1.72248100
H	-2.13216400	-4.67627400	-3.06532400
H	-1.47004200	-4.69329100	-1.41781800
C	-2.05725200	-2.08999100	-3.45708200
H	-3.13841900	-1.94236500	-3.28703300
H	-1.60440400	-1.10916800	-3.56829800
H	-1.95170400	-2.64449400	-4.40218200
C	1.81015800	-3.91104100	-2.44123400
H	0.98926300	-4.50716200	-2.87701800
H	2.67494600	-3.97887100	-3.11634700
H	2.08948300	-4.35664300	-1.48198400
C	1.16041700	-1.84516900	-3.52247000
H	0.41660700	-2.37112700	-4.13593800
H	0.81157100	-0.82744700	-3.33142900
H	2.09039200	-1.77822100	-4.10613100
C	-2.40304800	-3.42309800	2.59867200
H	-2.75990000	-3.87622000	1.66897100
H	-1.67411800	-4.10896200	3.06428900
H	-3.25819000	-3.31965600	3.28140000
C	-1.44201500	-1.41739000	3.55376300
H	-0.93963900	-0.48020900	3.30195400
H	-2.34633700	-1.17096700	4.12925300

H	-0.78498600	-2.01473800	4.20021200
C	1.69339900	-2.23789400	3.52600200
H	1.40300500	-1.19439800	3.60507300
H	1.51195300	-2.73426900	4.49150600
H	2.78181700	-2.26995300	3.34298300
C	1.34114900	-4.28586900	2.29817900
H	1.31963700	-4.81134900	3.26334100
H	0.65509700	-4.79720600	1.61660300
H	2.36656700	-4.38009300	1.89063000
C	2.50613100	3.97901600	-2.14387900
H	2.42634100	4.95097500	-2.64753700
H	3.57318400	3.73993800	-2.07073400
H	2.02805400	3.22458300	-2.77857500
C	2.52129600	5.08311900	0.13415700
H	3.58449800	4.85108800	0.26715200
H	2.46000000	6.08071000	-0.31910300
H	2.06046300	5.13170700	1.12735100
C	-1.65421200	5.40739300	-0.12981500
H	-2.74083300	5.34640300	-0.26203800
H	-1.43762800	6.36820200	0.35431600
H	-1.19453000	5.41615200	-1.12476900
C	-1.80621300	4.23501900	2.10996700
H	-1.57836400	5.16569200	2.64555500
H	-2.89743100	4.16395200	2.03765100
H	-1.44718700	3.39485700	2.71451300

8H+.

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C	0.51635100	-2.23617200	1.30844800
C	-0.88113400	-2.14687000	1.09505100

C	-1.39452700	-2.00540100	-0.21989500
C	-0.51668900	-2.23632500	-1.30828700
C	0.88080600	-2.14707000	-1.09490800
C	1.39421400	-2.00547300	0.22001000
C	-2.74877300	0.84380200	-0.78394300
C	2.74898600	0.84352700	0.78384300
C	-2.78621700	2.24174600	-0.20547700
H	-3.39704400	2.26600400	0.69421200
H	-3.21678800	2.96079500	-0.91601400
C	2.78649700	2.24139100	0.20520600
H	3.39707100	2.26544200	-0.69465300
H	3.21737200	2.96043700	0.91555400
N	1.43947300	2.79007100	-0.19085100
N	-1.43920200	2.79025800	0.19080400
Si	0.00008800	1.93128900	0.00010200
C	2.87315800	-1.69975300	0.47389300
C	-2.87341000	-1.69940800	-0.47384200
H	3.07927500	-1.84999500	1.53444400
H	3.52286100	-2.39329200	-0.06254200
H	-3.52326900	-2.39282500	0.06256000
H	-3.07948200	-1.84961600	-1.53440800
C	1.47851700	4.13628200	-0.84800000
H	0.43535400	4.41775800	-1.01491300
C	-1.47816100	4.13651400	0.84786100
H	-0.43497600	4.41795000	1.01470800
C	3.28889600	-0.25334400	0.12573400
C	-3.28893500	-0.25294200	-0.12582900
N	2.43120400	0.68188300	2.18566600
C	1.38285800	1.50634900	2.76138200
H	1.27194700	1.26617700	3.82483200

H	1.56501500	2.59442300	2.69284200
H	0.40992100	1.27930600	2.29886900
C	3.63379100	0.74349000	3.03360600
H	3.37475500	0.47545200	4.06414400
H	4.37929700	0.03009400	2.67386800
H	4.09448600	1.74863100	3.05062100
N	-2.43072400	0.68200200	-2.18568400
C	-1.38189300	1.50605600	-2.76111200
H	-1.27087500	1.26593600	-3.82455900
H	-1.56357900	2.59420900	-2.69251100
H	-0.40915400	1.27853000	-2.29841700
C	-3.63313200	0.74424500	-3.03385000
H	-3.37404500	0.47620100	-4.06437200
H	-4.37902400	0.03114700	-2.67431200
H	-4.09339500	1.74958700	-3.05083800
N	4.32859200	-0.08435700	-0.77682200
N	-4.32875700	-0.08375700	0.77654700
C	-5.37024400	0.92064800	0.57364300
H	-5.35965800	1.70404500	1.34576800
H	-5.26924300	1.38843500	-0.40714100
H	-6.35161700	0.42907000	0.62286200
C	-4.71086100	-1.06095000	1.79156300
H	-3.87138000	-1.71705500	2.00420200
H	-4.98732700	-0.53395600	2.71384100
H	-5.58412700	-1.64799300	1.46817700
C	5.37006700	0.92014400	-0.57434500
H	5.35926200	1.70336300	-1.34664600
H	5.26923900	1.38815900	0.40634700
H	6.35145500	0.42860400	-0.62366100
C	4.71049800	-1.06171500	-1.79176700

H	3.87094500	-1.71781100	-2.00420200
H	4.98684600	-0.53486200	-2.71416200
H	5.58379300	-1.64873800	-1.46842700
H	0.00010000	0.47806700	0.00039000
N	-1.83207100	-2.33146000	2.15276500
N	0.97843500	-2.79858900	2.55290900
N	1.83170600	-2.33185300	-2.15261200
N	-0.97884900	-2.79893400	-2.55263900
C	-1.59985700	-4.11485300	-2.42216300
H	-2.66775300	-4.07774000	-2.13715000
H	-1.53328900	-4.63661500	-3.38582100
H	-1.06586600	-4.71031400	-1.67641100
C	-1.55566800	-2.02232700	-3.63895900
H	-2.64989500	-1.90427800	-3.55988500
H	-1.11439900	-1.02927800	-3.67440300
H	-1.35270800	-2.53224200	-4.59124900
C	2.23218200	-3.72691100	-2.35628200
H	1.44718400	-4.32015500	-2.85197000
H	3.13223200	-3.76000000	-2.98408100
H	2.46834000	-4.19467800	-1.39581900
C	1.64624500	-1.62568600	-3.41575900
H	0.98131500	-2.14582200	-4.11686300
H	1.24838700	-0.62525800	-3.22378900
H	2.62350500	-1.50922000	-3.90462100
C	-2.23263500	-3.72647600	2.35658900
H	-2.46894900	-4.19428100	1.39618200
H	-1.44765700	-4.31976400	2.85224200
H	-3.13262500	-3.75942000	2.98448000
C	-1.64652600	-1.62516300	3.41582600
H	-1.24864400	-0.62477200	3.22372600

H	-2.62375700	-1.50860300	3.90472200
H	-0.98157200	-2.14523400	4.11695300
C	1.55524300	-2.02184800	3.63914500
H	1.11406900	-1.02874000	3.67440100
H	1.35217700	-2.53160800	4.59149400
H	2.64948200	-1.90389800	3.56011800
C	1.59939200	-4.11455700	2.42269200
H	1.53274300	-4.63615700	3.38643400
H	1.06543400	-4.71013200	1.67700800
H	2.66730600	-4.07753500	2.13774100
C	-2.14642800	4.07373400	2.23182900
H	-2.01335200	5.03342000	2.74401000
H	-3.22334900	3.88919900	2.16493100
H	-1.69881900	3.29151900	2.85436800
C	-2.12161000	5.21621700	-0.03609800
H	-3.20578100	5.08830900	-0.11823200
H	-1.94461800	6.20242600	0.40710200
H	-1.70102200	5.21958700	-1.04770700
C	2.12191200	5.21600800	0.03593700
H	3.20602300	5.08791000	0.11847600
H	1.94525800	6.20216300	-0.40752700
H	1.70098900	5.21966300	1.04740700
C	2.14688200	4.07340700	-2.23193300
H	2.01343300	5.03290200	-2.74436400
H	3.22388100	3.88933400	-2.16494600
H	1.69961700	3.29084000	-2.85428500