

Supporting Information

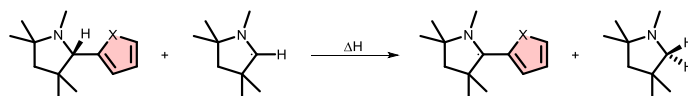
The Spin Population Determines whether Antiaromaticity can Increase or Decrease Radical Stability

Yanlin Song^a and Jun Zhu^{b*}

^aState Key Laboratory of Physical Chemistry of Solid Surfaces, Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, People's Republic of China.

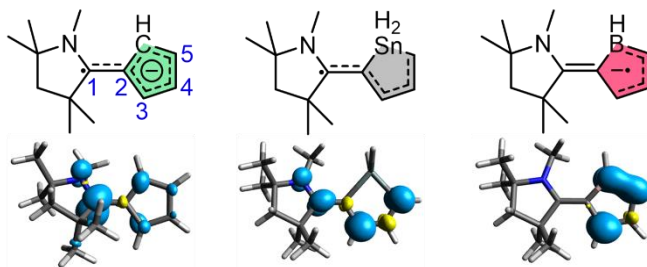
^bSchool of Science and Engineering, The Chinese University of Hong Kong, Shenzhen, 518172, People's Republic of China.

Correspondence and requests for materials should be addressed to Jun Zhu (email: jun.zhu@cuhk.edu.cn).

Table S1. NICS(1)_{zz} (Unit: ppm) and RSE Values (M06-2X/def2-TZVP Level) of CAAC Framework Bonded 5MR Radicals (Unit: kcal/mol).

X	BH (1)	PH₂⁺ (10)	AsH₂⁺ (17)	SbH₂⁺ (24)	AlH (8)	GaH (15)	InH (22)
NICS(1) _{zz} (S ₀)	37.3	1.3	2.1	3.8	14.0	15.5	11.8
NICS(1) _{zz} (D ₀)	2.2	-1.5	-1.9	-0.2	1.8	1.4	0.8
RSE	-39.6	-38.5	-36.2	-35.4	-29.3	-29.1	-26.8
X	AlH₂ (9)	NH₂⁺ (3)	SiH₂ (11)	SnH₂ (25)	GeH₂ (18)	SbH (27)	InH₂ (23)
NICS(1) _{zz} (S ₀)	2.5	-10.1	1.6	3.0	1.6	-2.7	2.6
NICS(1) _{zz} (D ₀)	1.7	-4.9	1.6	1.4	1.3	-2.4	1.8
RSE	-26.0	-25.1	-22.6	-22.2	-21.8	-19.4	-18.0
X	GaH₂ (16)	AsH (20)	PH (13)	CH₂ (4)	SnH- (26)	BH₂ (2)	GeH- (19)
NICS(1) _{zz} (S ₀)	1.8	-7.2	-12.9	-10.3	-2.8	-7.4	-11.1
NICS(1) _{zz} (D ₀)	1.1	-4.5	-7.2	-5.5	-2.4	-3.9	-6.9
RSE	-17.7	-17.6	-16.1	-15.0	-14.9	-14.2	-13.4
X	Te (28)	SiH- (12)	Se (21)	O (7)	S (14)	NH (6)	CH- (5)
NICS(1) _{zz} (S ₀)	-19.2	-19.1	-23.9	-27.2	-27.6	-31.4	-33.3
NICS(1) _{zz} (D ₀)	-25.0	-10.8	-13.7	-19.0	-18.2	-25.2	-26.8
RSE	-13.1	-12.0	-11.1	-10.7	-9.2	-6.6	-4.7

Table S2. Mülliken Spin Population and Spin Density (Isovalue: 0.01 a.u.) of Compounds **5_{rad}** (X = CH⁻), **25_{rad}** (X = SnH₂) and **1_{rad}** (X = BH) (without H atoms, Unit: e)



X	BH (1)	PH ₂ ⁺ (10)	AsH ₂ ⁺ (17)	SbH ₂ ⁺ (24)	AlH (8)	GaH (15)	InH (22)
C ₁	0.03	0.09	0.10	0.12	0.15	0.16	0.20
5MR	0.95	0.81	0.78	0.76	0.78	0.78	0.72
Other	0.02	0.10	0.12	0.12	0.07	0.06	0.08
X	AlH ₂ (9)	NH ₂ ⁺ (3)	SiH ₂ (11)	SnH ₂ (25)	GeH ₂ (18)	SbH (27)	InH ₂ (23)
C ₁	0.39	0.25	0.26	0.26	0.28	0.34	0.39
5MR	0.54	0.57	0.63	0.61	0.61	0.55	0.54
Other	0.07	0.18	0.11	0.13	0.11	0.11	0.07
X	GaH ₂ (16)	AsH (20)	PH (13)	CH ₂ (4)	SnH ⁻ (26)	BH ₂ (2)	GeH ⁻ (19)
C ₁	0.39	0.34	0.35	0.42	0.39	0.51	0.40
5MR	0.53	0.54	0.51	0.47	0.53	0.43	0.51
Other	0.08	0.12	0.14	0.11	0.08	0.06	0.09
X	Te (28)	SiH ⁻ (12)	Se (21)	O (7)	S (14)	NH (6)	CH ⁻ (5)
C ₁	0.40	0.46	0.43	0.58	0.50	0.69	0.75
5MR	0.42	0.47	0.39	0.27	0.34	0.18	0.21
Other	0.18	0.07	0.18	0.15	0.16	0.13	0.04

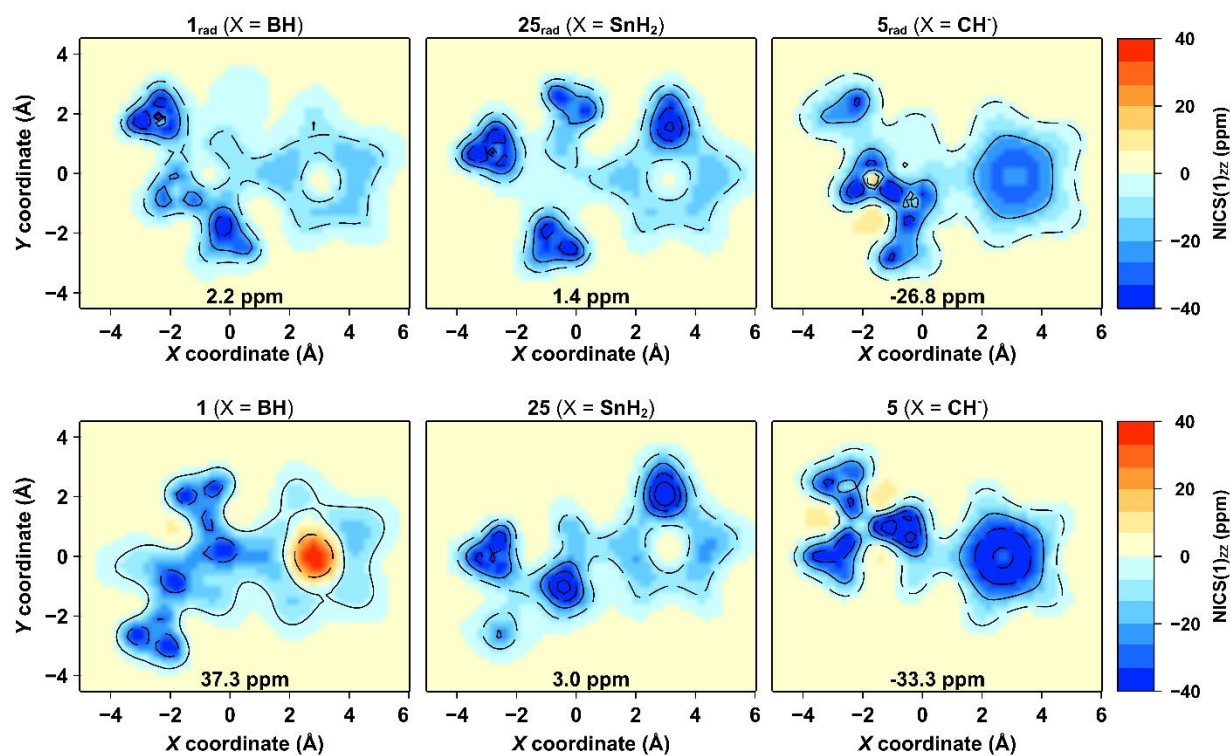


Fig. S1. NICS(1)_{zz} grid plots of compounds **1** (X = BH), **25** (X = SnH₂) and **5** (X = CH[•]) and their corresponding radicals **1_{rad}** (X = BH), **25_{rad}** (X = SnH₂) and **5_{rad}** (X = CH[•]), respectively. The numbers in each plot are the NICS(1)_{zz} of 5MR with unit in ppm.

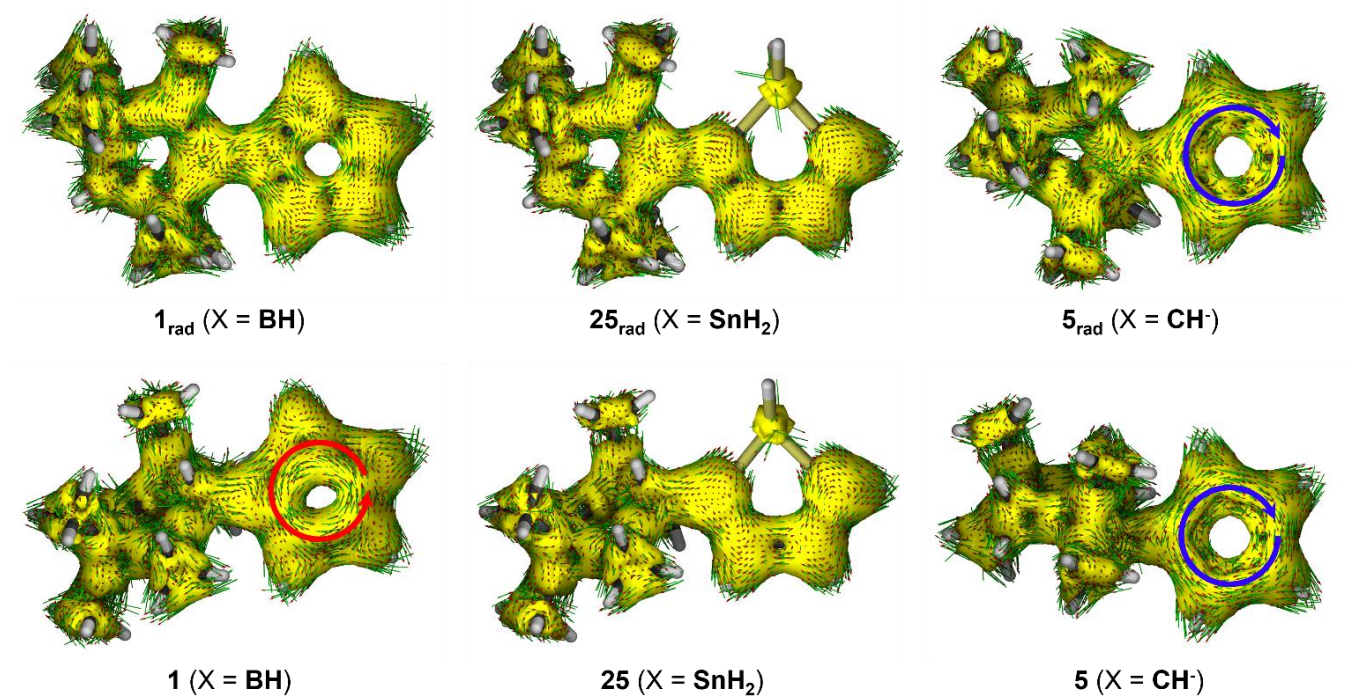


Fig. S2. AICD plots for compounds **1** ($X = \text{BH}$), **25** ($X = \text{SnH}_2$), **5** ($X = \text{CH}\cdot$) and their corresponding radicals 1_{rad} ($X = \text{BH}$), 25_{rad} ($X = \text{SnH}_2$), 5_{rad} ($X = \text{CH}\cdot$) with isovalue = 0.03 a.u., respectively.

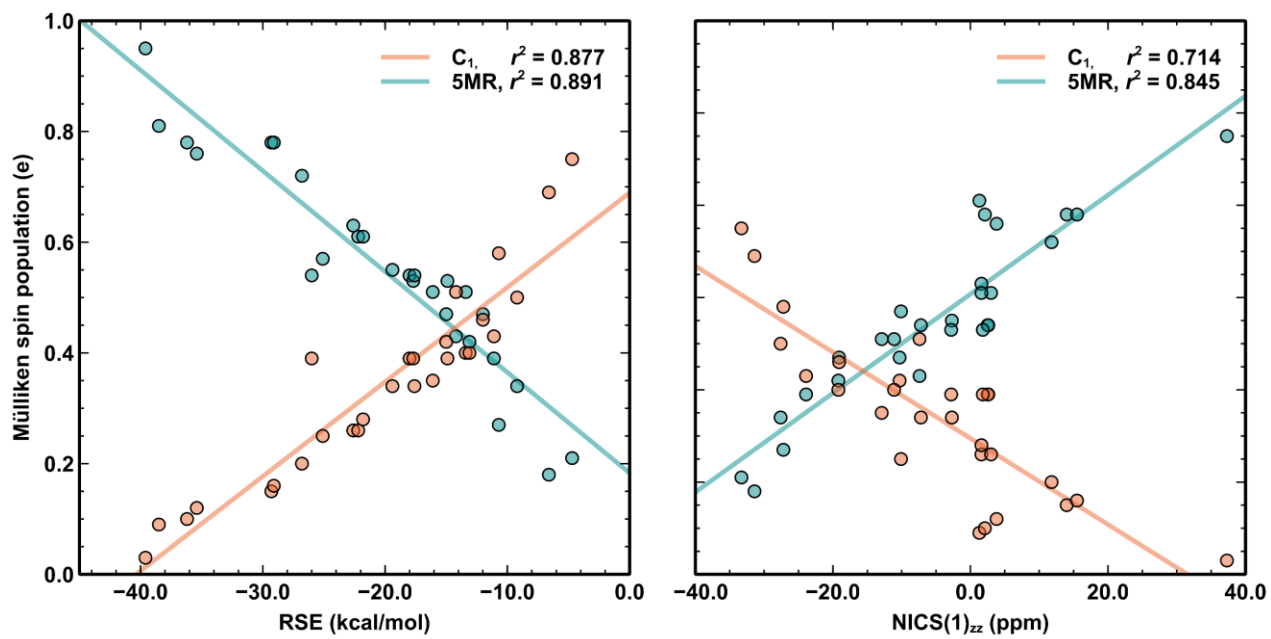


Fig. S3. Linear correlations between the Mulliken spin population and values of RSE (left) as well as NICS(1)_{zz} (right) for the 28 compounds in D₀, respectively.

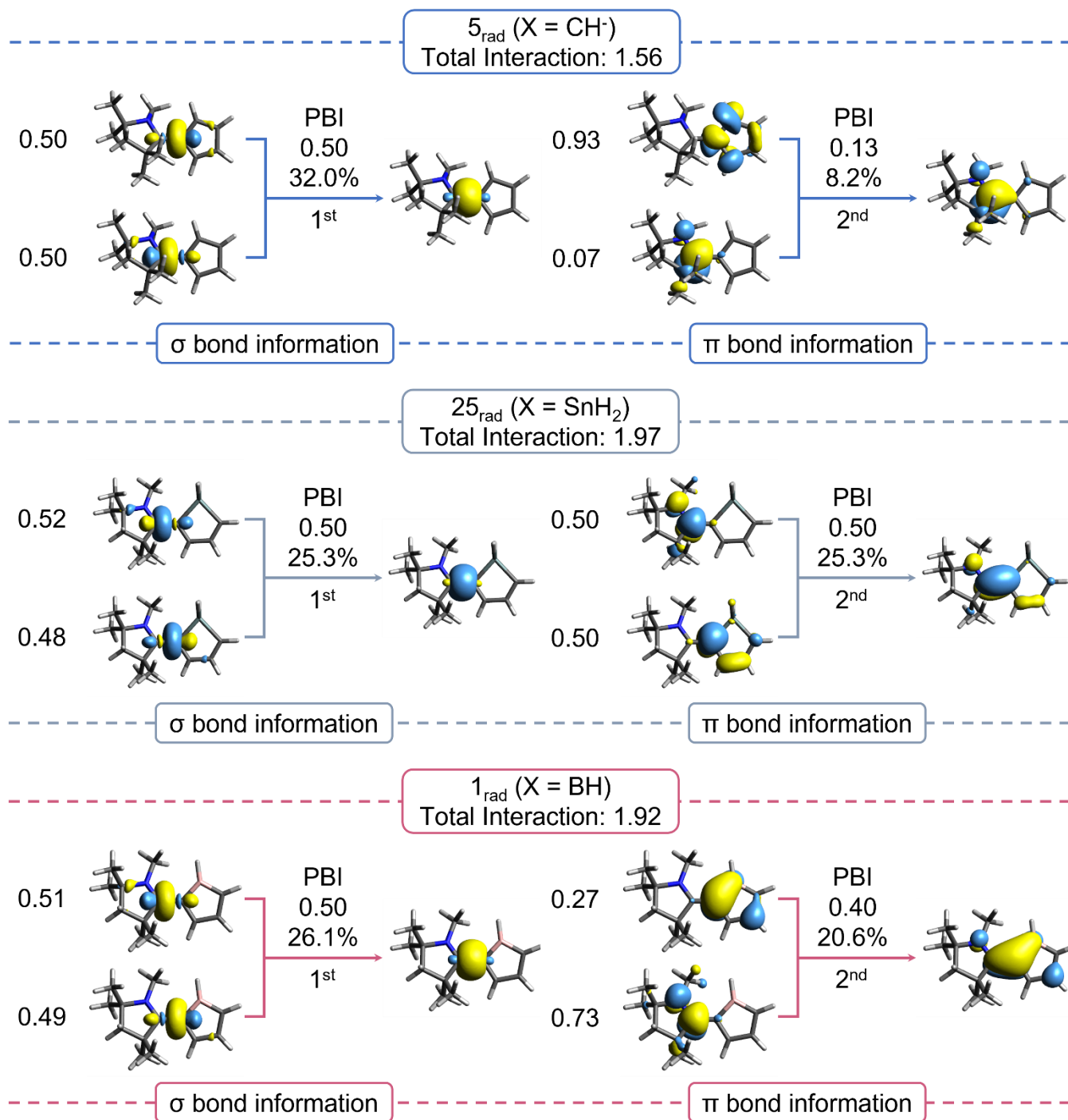


Fig. S4. PISO analysis for the α spin orbitals of compounds **5_{rad}** (X = CH⁻), **25_{rad}** (X = SnH₂) and **1_{rad}** (X = BH), including the left two PISO pairs respect to σ and π bond information, populations (Pop), PBI, and its contribution (%) of each fragment (isovalue: 0.04 a.u.).

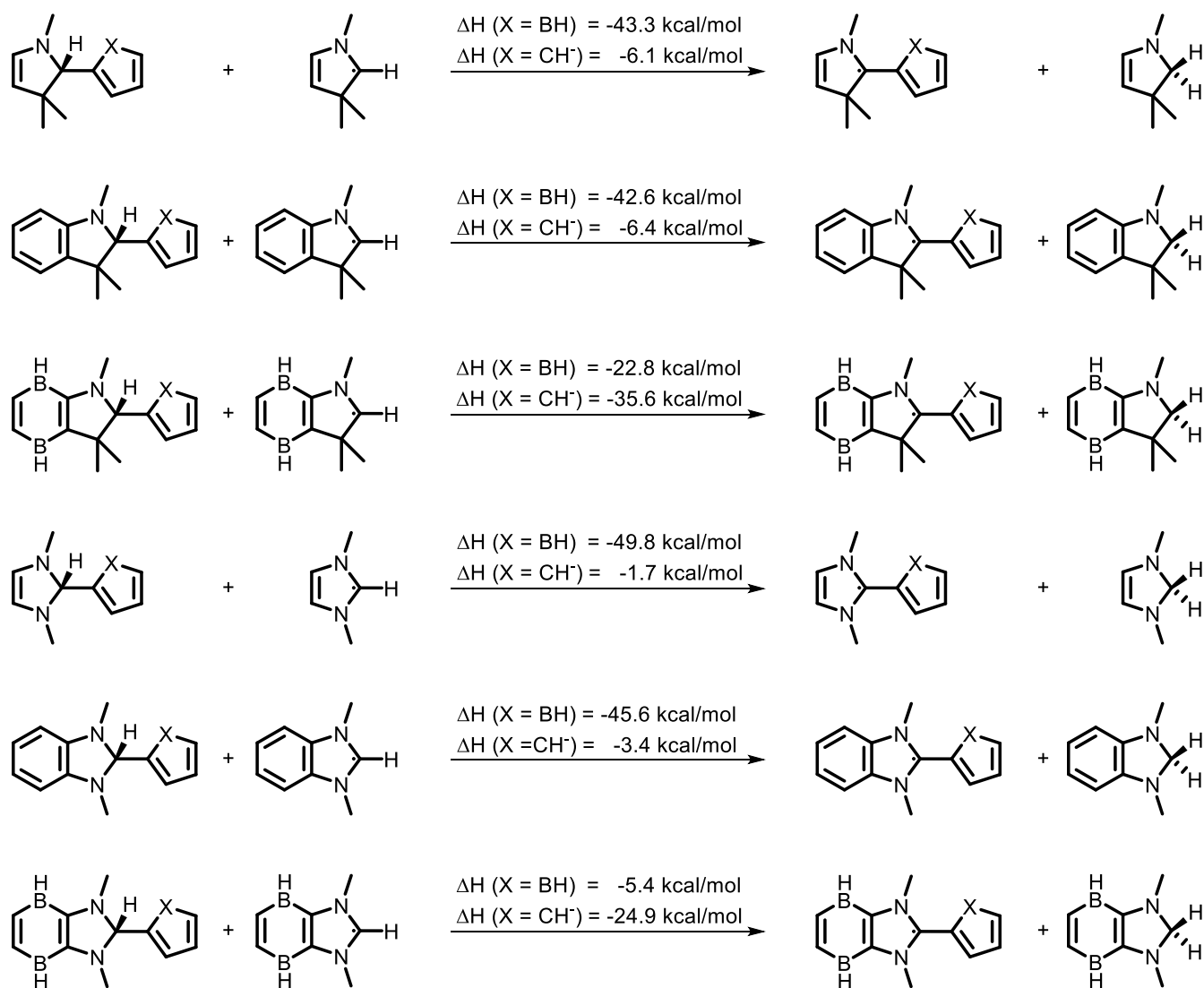


Fig. S5. The isodesmic equations in calculating RSEs for six compounds where X = CH[·] and BH, respectively.

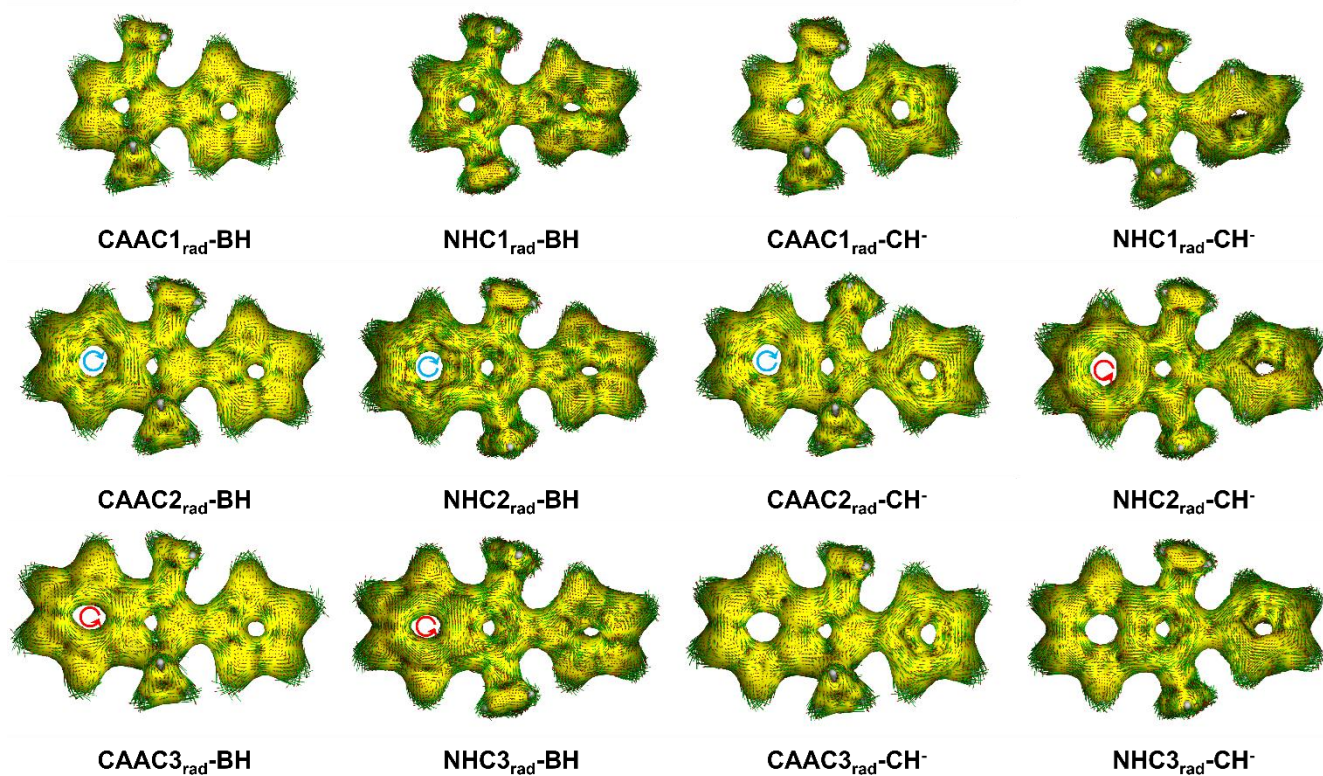


Fig. S6. The AICD plots for CAAC_n_{rad}-CH⁻ and NHC_n_{rad}-CH⁻ (n = 1 - 3) defined by 1,4-dihydro-1,4-diborinine (DHDB) plane.

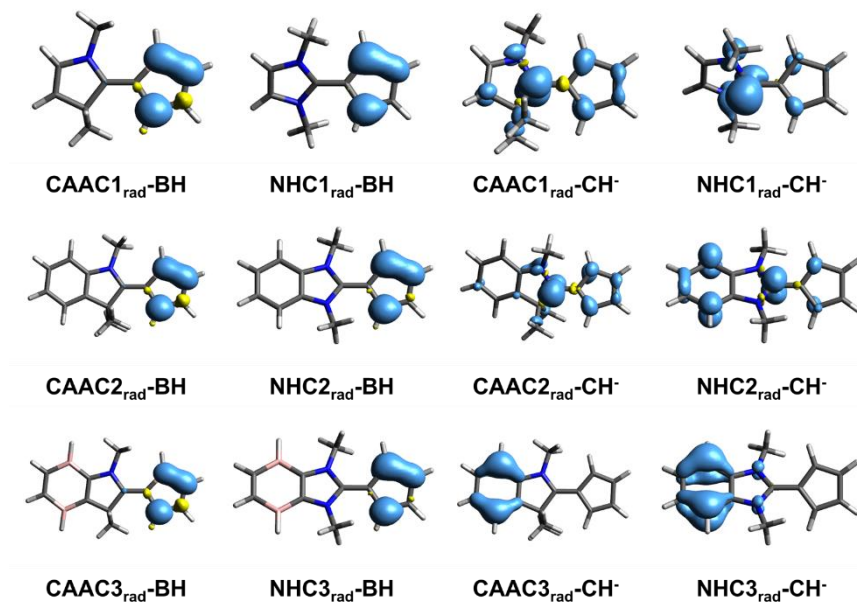


Fig. S7. The spin densities plots for CAAC_n_{rad}-CH[•] and NHC_n_{rad}-CH[•] (n = 1 - 3).

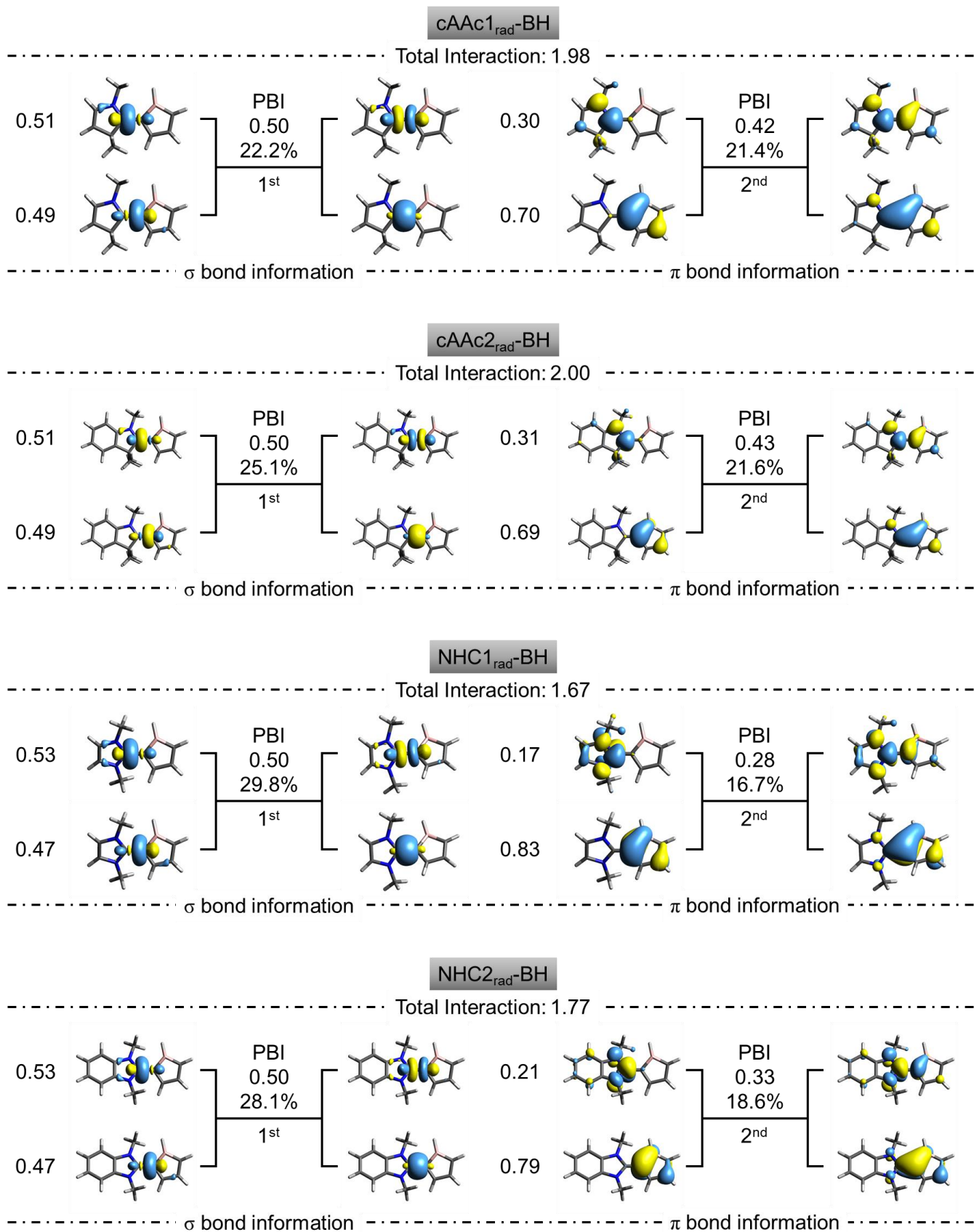


Fig. S8. The PISO analysis for **CAACn_{rad}-BH** and **NHCn_{rad}-BH** ($n = 1 - 2$).

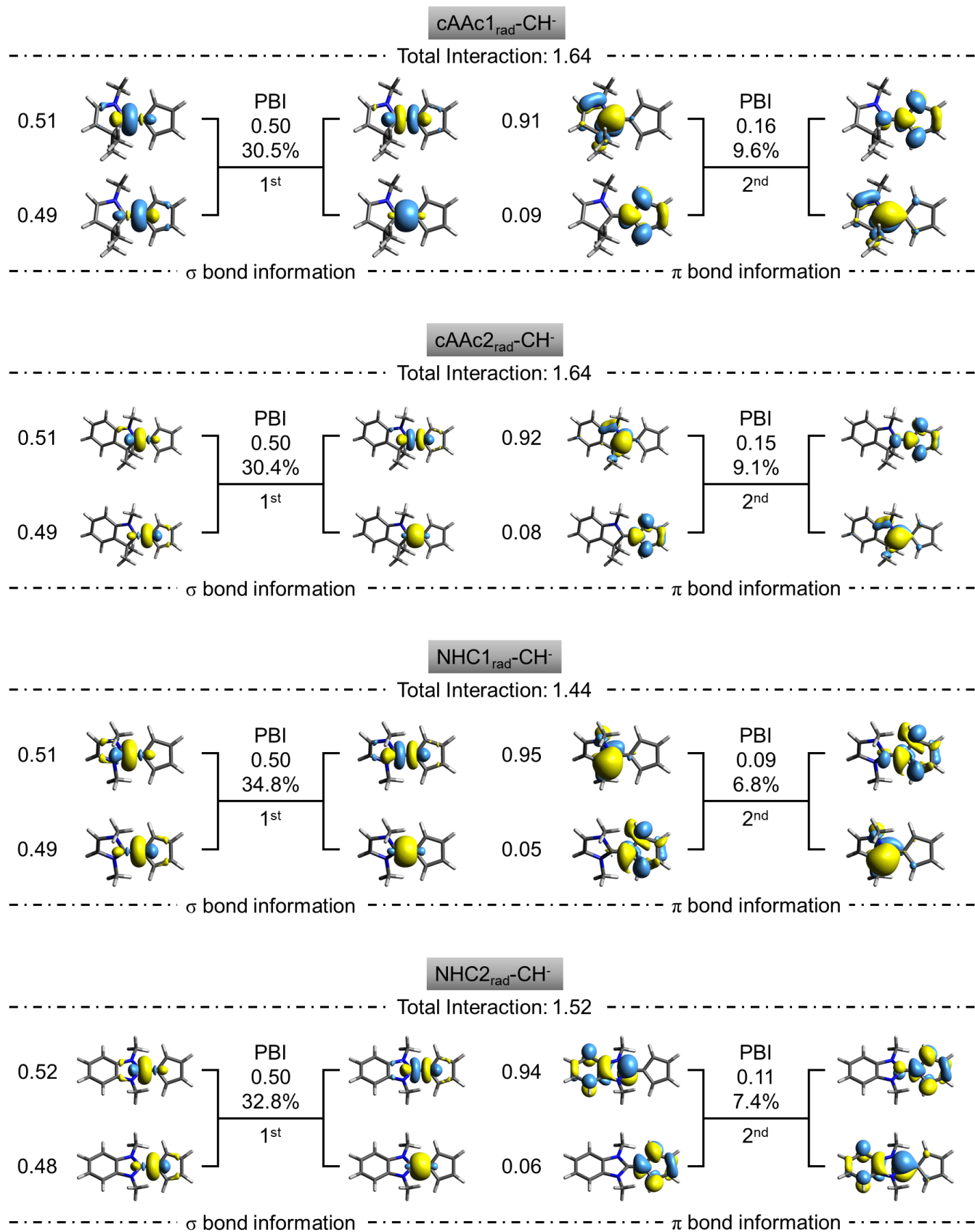


Fig. S9. The PISO analysis for **CAACn_{rad}-CH⁻** and **NHCn_{rad}-CH⁻** (n = 1 – 2).

Cartesian coordinates of all species in this study

Compounds in S_0				-805.69256343 a.u.			
AlH ₂ .anion				C	1.41044600	0.52207400	-0.62010300
-806.34584361 a.u.				Al	2.80751300	1.89018000	-0.60624800
C	0.61174600	0.31129100	-0.11009000	C	4.27483700	0.62239200	-0.63036300
Al	2.04226400	1.75222800	-0.13019100	C	3.63083900	-0.55460500	-0.65431800
C	3.42932100	0.30258300	-0.19416700	C	2.13090300	-0.60873900	-0.65260200
C	2.75966200	-0.86251000	-0.17688100	H	1.66137600	-1.59099700	-0.66348600
C	1.27382800	-0.85733000	-0.14913600	H	4.15090300	-1.51048900	-0.67450300
H	0.76148700	-1.82306900	-0.15514100	H	5.35617500	0.64329700	-0.63075200
H	3.24875900	-1.84012100	-0.18366000	H	2.73707400	3.46337400	-0.58825700
H	4.51645700	0.25225200	-0.20876400	C	-0.08478500	0.56008500	-0.54525500
H	1.95079200	2.72583600	-1.42822100	C	-2.16253500	-0.60246300	-0.45320600
H	2.08882300	2.64322300	1.23313800	N	-0.76296100	-0.66576700	-0.94258600
C	-0.88685100	0.37165400	-0.04492300	C	-0.62101100	0.79785400	0.89140100
C	-3.00808300	-0.73733600	0.02465500	C	-2.09918500	0.42925800	0.69898900
N	-1.61272700	-0.84421700	-0.44185900	H	-2.54340300	0.03979000	1.61707900
C	-1.44516200	0.63649200	1.37775400	H	-2.66105600	1.32400400	0.42001000
C	-2.92721900	0.27361100	1.19339200	H	-0.43940200	1.41032400	-1.16183800
H	-3.36444700	-0.13238700	2.10956500	C	-0.60651100	-1.01710200	-2.33684900
H	-3.49142200	1.17448300	0.93719000	H	-0.95473500	-0.22986600	-3.02307400
H	-1.22512400	1.21693400	-0.67860000	H	0.44238600	-1.20709600	-2.55740500
C	-1.44785000	-1.20219500	-1.83086000	H	-1.16406500	-1.92919700	-2.55470600
H	-1.78030500	-0.41201300	-2.52415400	C	-2.58292100	-1.98745500	0.02996800
H	-0.39567900	-1.39091200	-2.03242700	H	-3.61683900	-1.97799500	0.38177100
H	-2.01120100	-2.11175600	-2.05614000	H	-2.50901400	-2.71563500	-0.78057000
C	-3.48721800	-2.11316900	0.48602000	H	-1.93788400	-2.31764800	0.84419000
H	-4.52367000	-2.07183100	0.83259300	C	-3.15590000	-0.11143500	-1.51359000
H	-3.43102100	-2.83408600	-0.33342700	H	-3.27968400	-0.83239300	-2.32303000
H	-2.85569400	-2.47188000	1.29918600	H	-4.13184600	0.04340000	-1.05032700
C	-3.97615700	-0.20025000	-1.04072700	H	-2.83506300	0.84017600	-1.94334400
H	-4.10954100	-0.90597700	-1.86322400	C	-0.44688900	2.24173700	1.34150100
H	-4.95360600	-0.01893400	-0.58784100	H	-0.93675100	2.40413800	2.30427300
H	-3.61380200	0.74456900	-1.45177300	H	0.60920400	2.49448100	1.46865700
C	-0.78641800	-0.28406400	2.40417700	H	-0.87817500	2.93826900	0.61938300
H	0.26120900	-0.01524900	2.54207400	C	0.04057000	-0.14255200	1.89785900
H	-1.30365000	-0.19987400	3.36472100	H	1.08488400	0.12460100	2.06569700
H	-0.82164500	-1.32307900	2.07126200	H	-0.48307600	-0.08629500	2.85458800
C	-1.26653900	2.08755800	1.80344300	H	0.01317200	-1.17387700	1.54445500
H	-1.74105600	2.26133500	2.77436900	AsH ₂ .cation			
H	-0.20795100	2.33979100	1.88510300	-2799.50096976 a.u.			
H	-1.72223900	2.76495600	1.07636400	C	0.20082500	-0.17644800	-0.06655900
AlH.neutral				As	1.21516500	1.39844300	-0.47443500
				C	2.86463400	0.46409200	-0.36977300

C	2.54476800	-0.79816600	-0.07358700	N	-1.84016800	-1.41620100	-0.47580400
C	1.11311300	-1.14458600	0.07316700	C	-1.84178200	0.11126300	1.36946800
H	0.80369700	-2.16112800	0.28673200	C	-3.10296200	-0.78500200	1.37458000
H	3.30103800	-1.56311900	0.05605700	H	-2.96881900	-1.59885500	2.08953900
H	3.84705100	0.88486600	-0.50748100	H	-3.99670500	-0.23150600	1.66927000
H	1.09386500	2.52735200	0.50339600	H	-1.53722100	0.65823600	-0.70713500
H	0.91699700	1.97855100	-1.82469600	C	-1.63932100	-1.69681600	-1.88365200
C	-1.28930300	-0.25280700	0.05650700	H	-1.96351500	-0.86844400	-2.53168200
C	-3.13662300	-1.70073400	0.44786200	H	-0.58303500	-1.87621000	-2.07798300
N	-1.76060100	-1.60326600	-0.12599000	H	-2.19111500	-2.59295600	-2.16678600
C	-1.81303800	0.13834800	1.47057800	C	-3.83161400	-2.78393300	0.01482800
C	-3.21424200	-0.48816700	1.40353500	H	-4.80504900	-2.76769500	0.50893400
H	-3.56736700	-0.77347000	2.39504300	H	-3.97836700	-3.19560200	-0.98520200
H	-3.91809100	0.24636700	1.00640200	H	-3.16574100	-3.44440600	0.57080400
H	-1.73431900	0.45061300	-0.67543000	C	-4.13858900	-0.48684800	-0.91154400
C	-1.59470200	-2.14465000	-1.46131400	H	-4.23561100	-0.89332200	-1.91944100
H	-2.08705900	-1.54107700	-2.23592300	H	-5.13856700	-0.42867500	-0.47915200
H	-0.53727400	-2.22095900	-1.71460500	H	-3.75057100	0.53017600	-0.99043000
H	-2.00861500	-3.15122800	-1.49848500	C	-0.91809100	-0.30584800	2.51211200
C	-3.27441300	-3.03352900	1.17392700	H	-0.58878000	-1.33854700	2.38822900
H	-4.27984100	-3.14301500	1.58306300	H	-0.03281800	0.33031700	2.57202500
H	-3.10080100	-3.86511300	0.48858200	H	-1.45646400	-0.22794700	3.45932300
H	-2.55677300	-3.10804700	1.99064300	C	-2.18443000	1.59208700	1.51400200
C	-4.23281100	-1.57609200	-0.61383100	H	-1.28938000	2.21097900	1.41029600
H	-4.25571600	-2.43597500	-1.28356200	H	-2.90715500	1.90888800	0.75939000
H	-5.20289700	-1.51529400	-0.11935500	H	-2.61436100	1.78966800	2.49819300
H	-4.10913300	-0.67072900	-1.21272100				
C	-0.98041400	-0.50628800	2.57737300	BH ₂ .anion			
H	0.00746600	-0.04794100	2.66312700	-588.77445641 a.u.			
H	-1.48514100	-0.37582600	3.53517100	C	-1.56356700	-0.18006500	0.24506500
H	-0.84859600	-1.57461000	2.40432000	B	-2.82663100	0.32190500	1.13479200
C	-1.87591800	1.64588000	1.67629800	C	-4.02158100	-0.33056400	0.26757700
H	-0.87943200	2.08520200	1.77850700	C	-3.49630300	-0.99823100	-0.77911500
H	-2.40179100	2.14406700	0.85886700	C	-2.02674800	-0.91844800	-0.78452100
H	-2.40778300	1.87597800	2.60078400	H	-1.40732300	-1.41292100	-1.53210600
				H	-4.04993700	-1.54400500	-1.54175300
				H	-5.09798800	-0.28328400	0.42103900
				H	-2.75561500	-0.13310900	2.27525700
				H	-2.92234100	1.54398000	1.22342700
				C	-0.11067800	0.09167000	0.49379400
				C	2.18673400	-0.33487400	-0.01023300
				N	0.82609600	-0.89684500	-0.06204000
				C	0.42860100	1.41398900	-0.11276400
				C	1.94742700	1.19479900	-0.01078200
				H	2.48624000	1.68739000	-0.82501500
				H	2.31496200	1.62314500	0.92578000
				H	0.03653600	0.16445800	1.59065700
				C	0.67499300	-2.22536100	0.48179100
				H	0.80952400	-2.26389700	1.57562600
AsH.neutral							
-2799.17361461 a.u.							
C	0.27329700	-0.21808700	-0.07530300				
As	1.39257200	1.37736000	-0.04434100				
C	2.90283200	0.17023300	-0.13027900				
C	2.48755200	-1.09974600	-0.02468400				
C	1.04236000	-1.31442400	-0.00357300				
H	0.61422100	-2.30938500	0.05883100				
H	3.17193300	-1.93883900	0.03669800				
H	3.93785100	0.47798800	-0.14164100				
H	1.28454700	1.68188600	-1.53584000				
C	-1.22385900	-0.16931300	-0.04345500				
C	-3.24761100	-1.37742600	-0.03251000				

H	-0.32786300	-2.58600300	0.26207600
H	1.39900700	-2.90576700	0.02493500
C	2.96826700	-0.79314400	-1.24107200
H	3.98495700	-0.39000000	-1.23198000
H	3.03568700	-1.88348200	-1.27131200
H	2.46217500	-0.45750400	-2.14669600
C	2.96730100	-0.72673700	1.25408400
H	3.20534600	-1.79246100	1.26975900
H	3.90573700	-0.16868500	1.29476700
H	2.39229800	-0.48851300	2.15160300
C	0.00171400	1.56328200	-1.57178200
H	-1.07672800	1.70803300	-1.63926100
H	0.50818200	2.42279400	-2.02221400
H	0.25038900	0.66558300	-2.14062400
C	-0.02205300	2.63425800	0.67769900
H	0.43379700	3.54327400	0.27197600
H	-1.10714500	2.73064700	0.63756700
H	0.26595400	2.54528100	1.72836300

BH.neutral

-588.11135847 a.u.

C	0.85372200	0.39837700	-0.12004700
B	1.82486300	1.65456600	-0.01563600
C	3.27608900	1.05142400	-0.02110800
C	3.11236300	-0.27255100	-0.11836600
C	1.65607300	-0.66788800	-0.17439200
H	1.32948600	-1.70039600	-0.22922100
H	3.90411300	-1.01344300	-0.15316900
H	4.24163900	1.53287600	0.03142000
H	1.50635100	2.79865000	0.05574300
C	-0.64037700	0.39400900	-0.08431400
C	-2.62181400	-0.88568800	0.05770300
N	-1.23612900	-0.88493200	-0.44980800
C	-1.23816900	0.73135100	1.32509900
C	-2.43438200	-0.24071500	1.43566600
H	-2.20250900	-1.02348800	2.16064700
H	-3.34291700	0.26288500	1.77222900
H	-0.98199700	1.18386700	-0.77976400
C	-1.09556900	-1.19756700	-1.85763700
H	-1.49030000	-0.40349600	-2.50976300
H	-0.04425900	-1.33447500	-2.10569400
H	-1.61900500	-2.12534800	-2.08874700
C	-3.14640600	-2.31089900	0.18149300
H	-4.09909900	-2.31375200	0.71492500
H	-3.31668300	-2.76570000	-0.79588300
H	-2.43237100	-2.92343500	0.73249000
C	-3.58773600	-0.06385900	-0.80950200
H	-3.73183600	-0.52593300	-1.78744100
H	-4.56244900	-0.00622600	-0.32275200

H	-3.23114400	0.95544100	-0.96646300
C	-0.25345700	0.46044600	2.46162000
H	0.58396500	1.16340900	2.45036100
H	-0.76440300	0.56457000	3.42152500
H	0.15278200	-0.54972600	2.39342700
C	-1.67404200	2.19418000	1.38160200
H	-2.07426400	2.43601500	2.36865600
H	-0.82774600	2.85753400	1.18868700
H	-2.44712900	2.40916600	0.64183400

CH₂.neutral

-601.99672605 a.u.

C	0.82243000	0.50912200	-0.11369900
C	1.62109600	1.75685100	-0.37077600
C	3.03871200	1.27347300	-0.36699100
C	3.04735000	-0.05022100	-0.15961700
C	1.66999900	-0.52675000	-0.00821300
H	1.37781200	-1.55511900	0.15511900
H	3.92342700	-0.68157500	-0.11246000
H	3.89698500	1.91155400	-0.51502700
H	1.44248300	2.53217500	0.38219300
H	1.34662300	2.20027500	-1.33522200
C	-0.66828500	0.50068600	-0.00159300
C	-2.68724000	-0.75241000	0.01328700
N	-1.27611900	-0.74606800	-0.44107700
C	-1.22493700	0.65497900	1.43896800
C	-2.68371700	0.22898900	1.21061200
H	-3.11736100	-0.22074900	2.10589500
H	-3.28403100	1.10854300	0.96528800
H	-1.05456400	1.35766200	-0.59013100
C	-1.06062400	-1.07198200	-1.83361800
H	-1.41726100	-0.29033400	-2.52210900
H	0.00272200	-1.21941700	-2.01545500
H	-1.57485700	-2.00193500	-2.07943400
C	-3.07308700	-2.16962400	0.42635500
H	-4.11345900	-2.20582100	0.75643600
H	-2.96193100	-2.86014400	-0.41225800
H	-2.43471200	-2.51490600	1.23957000
C	-3.66670400	-0.24818200	-1.05352600
H	-3.74256300	-0.93812900	-1.89534100
H	-4.66032800	-0.14376100	-0.61437100
H	-3.36480600	0.73022400	-1.43425800
C	-0.53330100	-0.29561100	2.41430800
H	0.50373200	-0.00307800	2.58289100
H	-1.05411800	-0.27889500	3.37412500
H	-0.53825300	-1.31731400	2.03352700
C	-1.12233800	2.08338200	1.95569400
H	-1.65639500	2.18298300	2.90335000
H	-0.08224600	2.36286100	2.13525600

H	-1.55453100	2.79442200	1.24789000
CH.anion			
-601.43336715 a.u.			
C	0.88414500	0.31792500	0.32886900
C	1.68362400	1.36934200	0.82186800
C	3.03300800	1.00112900	0.68601600
C	3.07214400	-0.27690700	0.09736500
C	1.75018100	-0.70088600	-0.12199100
H	1.44061700	-1.63499100	-0.57388500
H	3.96579000	-0.83598600	-0.15066500
H	3.88906700	1.59798500	0.97351100
H	1.30544800	2.30153600	1.22660200
C	-0.60660600	0.32459200	0.31436700
C	-2.66197800	-0.31185800	-0.70609600
N	-1.21329700	-0.18881900	-0.92227400
C	-1.34761600	-0.51642800	1.38460100
C	-2.78173900	-0.49769600	0.83116400
H	-3.33551100	-1.40634200	1.08423600
H	-3.33028400	0.34606800	1.25965200
H	-0.92756500	1.37587800	0.47675500
C	-0.78957000	0.49838800	-2.11696500
H	-1.02798000	1.57565300	-2.10707200
H	0.29230600	0.39963300	-2.20183900
H	-1.25869600	0.05187100	-2.99827200
C	-3.19021200	-1.52566000	-1.46990500
H	-4.26751200	-1.64301700	-1.32109800
H	-3.00513500	-1.41769000	-2.54145600
H	-2.68491200	-2.42846800	-1.12568500
C	-3.45288400	0.93334200	-1.13610900
H	-3.43539500	1.06599100	-2.22018100
H	-4.49501600	0.83832500	-0.82123300
H	-3.03868600	1.83181200	-0.67331100
C	-0.80911200	-1.94367000	1.44611900
H	0.22763600	-1.94194600	1.78378700
H	-1.41462800	-2.54275400	2.13423900
H	-0.83338100	-2.40690900	0.45855700
C	-1.23376200	0.12851800	2.75754100
H	-1.77023700	-0.45297700	3.51366400
H	-0.18092600	0.19368800	3.04202100
H	-1.64330900	1.14234800	2.74891300

GaH ₂ .anion			
-2488.76464073 a.u.			
C	0.21390800	-0.05915700	-0.07805800
Ga	1.64002700	1.44552300	-0.09290700
C	3.03276600	-0.05296800	-0.16894700
C	2.36786400	-1.21875500	-0.16045900
C	0.88345400	-1.22110800	-0.13037600

H	0.37480900	-2.18810900	-0.14605300
H	2.86389900	-2.19213000	-0.17659600
H	4.12025600	-0.08795400	-0.18401400
H	1.53858500	2.41591700	-1.39979600
H	1.69052900	2.33225000	1.28063000
C	-1.28402500	-0.00006800	-0.01268900
C	-3.40392600	-1.11302900	0.03759800
N	-2.00744400	-1.21188900	-0.42721100
C	-1.84514100	0.24331900	1.41296500
C	-3.32658400	-0.11748000	1.21971400
H	-3.76632200	-0.53525600	2.12939400
H	-3.89015800	0.78661000	0.97361400
H	-1.62239700	0.85332700	-0.63516300
C	-1.83808500	-1.55174200	-1.82029400
H	-2.17004600	-0.75337200	-2.50439800
H	-0.78490300	-1.73562100	-2.02077000
H	-2.39903600	-2.45937400	-2.05889700
C	-4.37027100	-0.56334700	-1.02269800
H	-4.49994200	-1.25803400	-1.85510100
H	-5.34935600	-0.39029300	-0.57005900
H	-4.00893100	0.38775900	-1.41988700
C	-3.88226100	-2.49535000	0.48000100
H	-4.91930000	-2.45973400	0.82545800
H	-3.82406000	-3.20543000	-0.34870400
H	-3.25172700	-2.86408000	1.28942200
C	-1.18769900	-0.69278700	2.42596400
H	-1.22203600	-1.72630200	2.07650600
H	-0.14016600	-0.42621300	2.56872000
H	-1.70603200	-0.62388200	3.38714700
C	-1.67046600	1.68758100	1.86244600
H	-0.61319600	1.93887500	1.95871600
H	-2.11798800	2.37630200	1.14099500
H	-2.15537800	1.84644300	2.83081000

GaH.neutral			
-2488.11538095 a.u.			
C	0.18168200	-0.00937200	-0.12535200
Ga	1.53383500	1.46759200	-0.13351700
C	3.03168300	0.16664900	-0.14139100
C	2.42429700	-1.02595600	-0.14781300
C	0.92720300	-1.12014100	-0.14239800
H	0.47967200	-2.11184300	-0.13704900
H	2.97515200	-1.96390000	-0.15552300
H	4.11054400	0.23803600	-0.14380700
H	1.42143000	3.03910900	-0.13844100
C	-1.31268600	0.01363500	-0.04706000
C	-3.37395400	-1.17624600	0.06946100
N	-1.97432400	-1.22852400	-0.42113300
C	-1.85012400	0.26922700	1.38642800

C	-3.32322300	-0.12313100	1.20252300
H	-3.76088000	-0.50178200	2.12826700
H	-3.89766100	0.75865800	0.90811600
H	-1.67858200	0.84798400	-0.67864900
C	-1.81411400	-1.60360400	-1.80891000
H	-2.17457400	-0.83455500	-2.50927200
H	-0.76280400	-1.78203600	-2.02695700
H	-2.35843700	-2.52767300	-2.00898500
C	-3.77400100	-2.55813900	0.57830300
H	-4.80734800	-2.55691400	0.93194600
H	-3.69130700	-3.29946400	-0.21939800
H	-3.12304800	-2.86488600	1.39696900
C	-4.37549200	-0.71877900	-0.99797400
H	-4.48919000	-1.45564600	-1.79441900
H	-5.35322200	-0.57035400	-0.53633800
H	-4.06921900	0.22981500	-1.44466000
C	-1.69812500	1.72277500	1.81341400
H	-0.64701500	1.99011000	1.95022300
H	-2.12875100	2.40173900	1.07423000
H	-2.20238600	1.89514100	2.76700400
C	-1.17330000	-0.64434300	2.40728700
H	-1.18725900	-1.68175400	2.07150300
H	-0.13232300	-0.35990500	2.56689800
H	-1.69541600	-0.57872300	3.36429100

GeH₂.neutral

-2640.88699230 a.u.

C	0.21587500	-0.16359000	-0.07193100
Ge	1.47166200	1.35016000	-0.14442300
C	2.96876700	0.09670800	-0.14079100
C	2.44134400	-1.13221100	-0.09743200
C	0.96579000	-1.27249500	-0.06805500
H	0.51879700	-2.26200000	-0.03659100
H	3.05007800	-2.03125500	-0.08238700
H	4.03453100	0.27228900	-0.15939100
H	1.41920500	2.28619000	1.08716300
H	1.33593400	2.20627100	-1.42495200
C	-1.28030500	-0.12327600	-0.00849800
C	-3.31655500	-1.30610400	0.10914800
N	-1.92333200	-1.37882900	-0.37515900
C	-1.84934300	0.21361700	1.41099400
C	-3.12653800	-0.65579600	1.48535900
H	-2.99097300	-1.43941900	2.23301800
H	-4.00282600	-0.07267500	1.77557500
H	-1.61292700	0.67963400	-0.69224800
C	-1.77700000	-1.70678200	-1.77959900
H	-2.11107400	-0.89356500	-2.44167600
H	-0.73213000	-1.90981800	-2.00789700
H	-2.35284900	-2.60167400	-2.01511100

C	-3.91256000	-2.70292300	0.23311700
H	-4.87225700	-2.65540400	0.75160300
H	-4.08983700	-3.15590600	-0.74386100
H	-3.23796100	-3.34566600	0.79923700
C	-4.22636300	-0.44291800	-0.77832800
H	-4.35924100	-0.88861900	-1.76529800
H	-5.21155000	-0.35661600	-0.31760300
H	-3.83134500	0.56595000	-0.91064700
C	-0.89829200	-0.18890300	2.53685800
H	-0.58811800	-1.22926200	2.42752100
H	-0.00135700	0.43314300	2.55541200
H	-1.40662500	-0.07994500	3.49758700
C	-2.15536600	1.70543300	1.51641500
H	-1.25239800	2.30076900	1.35524200
H	-2.90026700	2.01177200	0.77930500
H	-2.53995000	1.94959500	2.50891600

GeH.anion

-2640.32098398 a.u.

C	0.25523500	-0.10108200	0.05596400
Ge	1.52475900	1.45337200	-0.06463200
C	2.94977200	0.06067000	-0.01515500
C	2.39999800	-1.16361100	-0.18181200
C	0.94399400	-1.24793500	-0.14834100
H	0.44969500	-2.20840500	-0.30160900
H	2.98102500	-2.06929800	-0.35847800
H	4.02859400	0.18383500	-0.05594000
H	1.55066200	1.98544000	1.44851000
C	-1.24122500	-0.05129900	0.14550100
C	-3.35973100	-1.13708700	-0.05610500
N	-1.95977800	-1.15008600	-0.51664300
C	-1.80219500	-0.12339300	1.58932700
C	-3.28453000	-0.42974800	1.31981100
H	-3.72477300	-1.04132900	2.11203400
H	-3.84918200	0.50576600	1.28163500
H	-1.57995800	0.91446300	-0.27849200
C	-1.76904600	-1.19850400	-1.94696700
H	-2.08274700	-0.27317600	-2.45731900
H	-0.71232100	-1.34770100	-2.16047700
H	-2.33123200	-2.03278700	-2.37490500
C	-3.86219200	-2.57518400	0.06475500
H	-4.90151300	-2.59967400	0.40418500
H	-3.80794500	-3.08450900	-0.90060000
H	-3.24433200	-3.12470200	0.77548300
C	-4.30375200	-0.35118300	-0.97914900
H	-4.42937200	-0.84353800	-1.94572500
H	-5.28732800	-0.26598100	-0.51134500
H	-3.92319100	0.65769100	-1.15313900
C	-1.14988800	-1.25674600	2.37877000

H	-0.09640600	-1.03906000	2.55692100
H	-1.65776500	-1.37982600	3.34026200
H	-1.20570900	-2.19591100	1.82532600
C	-1.61381800	1.19095700	2.33395100
H	-0.55084800	1.41206900	2.44685700
H	-2.07467300	2.01829500	1.78796000
H	-2.07018000	1.13977000	3.32740200

lnH₂.anion

-753.95780646 a.u.

C	-0.12576600	-0.35397600	-0.06857200
ln	1.42654500	1.29222300	-0.07503100
C	2.79437000	-0.46875900	-0.14168900
C	2.03168900	-1.57247400	-0.13746600
C	0.54663600	-1.51347600	-0.11697100
H	0.02345000	-2.47362600	-0.13128400
H	2.46215100	-2.57752600	-0.14999400
H	3.87312800	-0.61188300	-0.15067800
H	1.37779100	2.35674500	-1.51931200
H	1.49315800	2.26022100	1.44191300
C	-1.62498300	-0.31031900	0.00080000
C	-3.73728600	-1.43790000	0.06468600
N	-2.34252500	-1.52790100	-0.40794800
C	-2.18129800	-0.06963600	1.42922100
C	-3.66206700	-0.43204800	1.23803000
H	-4.10333500	-0.84099200	2.15095200
H	-4.22460700	0.47018600	0.98250500
H	-1.97532400	0.53873100	-0.62092900
C	-2.17841500	-1.86977200	-1.80101300
H	-1.12512800	-2.04656400	-2.00734300
H	-2.73354800	-2.78242600	-2.03386500
H	-2.52066400	-1.07599000	-2.48533300
C	-4.20043300	-2.82099400	0.52047500
H	-5.23621100	-2.79251600	0.87024800
H	-4.13908500	-3.53665100	-0.30315200
H	-3.56304900	-3.17799100	1.32976100
C	-4.71522700	-0.90508600	-0.99351800
H	-4.84525300	-1.60772400	-1.81913800
H	-5.69242200	-0.73614500	-0.53533600
H	-4.36452100	0.04557400	-1.40113100
C	-1.52137700	-1.00730000	2.43926500
H	-1.55656100	-2.04042200	2.08907000
H	-0.47341300	-0.74195700	2.58079000
H	-2.03746300	-0.93922400	3.40162700
C	-2.01077300	1.37363300	1.88379800
H	-0.95603100	1.62439200	2.00575600
H	-2.44231000	2.06531000	1.15546500
H	-2.51411400	1.53211900	2.84269300

lnH.neutral

-753.31171655 a.u.

C	-0.14467900	-0.31176600	-0.11861200
ln	1.32510300	1.30945900	-0.13965300
C	2.79742000	-0.27862700	-0.13969500
C	2.08573200	-1.41090900	-0.13542000
C	0.58854900	-1.42947400	-0.12733100
H	0.11229900	-2.40853800	-0.11090600
H	2.56907300	-2.38628400	-0.13516100
H	3.87854000	-0.31635000	-0.14253500
H	1.28556000	3.03299300	-0.15304600
C	-1.64012700	-0.28309100	-0.03417200
C	-3.70752700	-1.46244400	0.10448000
N	-2.31077000	-1.52644400	-0.39161800
C	-2.17170400	-0.00935700	1.39875800
C	-3.64703400	-0.39823000	1.22623200
H	-4.08115200	-0.76528400	2.15836400
H	-4.21988700	0.48262000	0.92569200
H	-2.00724300	0.54430800	-0.67410900
C	-2.15986500	-1.91607500	-1.77629100
H	-2.52112000	-1.15224100	-2.48207000
H	-1.11062400	-2.10110200	-1.99822000
H	-2.70958300	-2.83958500	-1.96409200
C	-4.11276700	-2.83696000	0.62902900
H	-5.14438400	-2.82648700	0.98760000
H	-4.03793400	-3.58675300	-0.16147700
H	-3.45953600	-3.13909500	1.44752600
C	-4.71236600	-1.01052800	-0.96268000
H	-4.83366000	-1.75454000	-1.75133500
H	-5.68706700	-0.85275800	-0.49769000
H	-4.40365100	-0.06793000	-1.42032400
C	-1.49392800	-0.91299700	2.42768900
H	-1.51608800	-1.95481800	2.10639700
H	-0.44979600	-0.63358100	2.57513200
H	-2.00913100	-0.83079000	3.38725100
C	-2.01825800	1.44828900	1.81200900
H	-0.96827400	1.71169000	1.96469200
H	-2.43418500	2.12174200	1.05927000
H	-2.53645800	1.63357900	2.75572300

NH₂.cation

-618.39866575 a.u.

C	0.79767800	0.31888200	-0.13758700
N	1.40607100	1.65218200	-0.37989800
C	2.86283700	1.43772500	-0.37456200
C	3.07817700	0.14348800	-0.16672300
C	1.79843500	-0.55119900	-0.02106700
H	1.66397800	-1.60575700	0.16254500
H	4.05060900	-0.32097500	-0.11447100

H	3.51117600	2.28218600	-0.53375200	H	-3.28919400	0.69976000	1.18982600
H	1.10588700	2.31322900	0.34933000	H	-0.96554400	1.45314600	-0.08051700
H	1.08453600	2.03491700	-1.27687600	C	-0.96427900	-0.32106200	-2.15571100
C	-0.68198100	0.23687000	-0.00507400	H	-1.27954800	0.67146800	-2.51273900
C	-2.52975300	-1.21142000	0.34017600	H	0.10656300	-0.41721200	-2.32860900
N	-1.15060300	-1.10584700	-0.22628800	H	-1.47254900	-1.07641600	-2.75619400
C	-1.19290000	0.57994500	1.42676000	C	-3.10896300	-2.12022600	-0.56461700
C	-2.59983200	-0.03146300	1.33807400	H	-4.16338800	-2.24310700	-0.30845700
H	-2.95461100	-0.34792800	2.31938600	H	-2.97487600	-2.43907700	-1.60030700
H	-3.29788600	0.72185300	0.96642100	H	-2.51395600	-2.77354600	0.07347800
H	-1.13208300	0.96789300	-0.71071700	C	-3.59358600	0.24246300	-1.21209800
C	-0.97825400	-1.61234200	-1.57502100	H	-3.63995800	-0.06786700	-2.25707900
H	-1.46969600	-0.99040100	-2.33557700	H	-4.60557000	0.20600200	-0.80524200
H	0.08083700	-1.68086600	-1.82269400	H	-3.25517600	1.28060200	-1.17472900
H	-1.39055200	-2.61805800	-1.63868000	C	-1.13337700	1.17263500	2.52761400
C	-2.68085800	-2.56714100	1.01924900	H	-1.64541300	0.91756800	3.45778400
H	-3.68832600	-2.68121200	1.42182900	H	-0.08452200	1.36254400	2.76885800
H	-2.51342600	-3.37602700	0.30597900	H	-1.57506700	2.09533000	2.14290500
H	-1.96596200	-2.67686400	1.83427500	C	-0.62104400	-1.22815100	2.08947600
C	-3.62018000	-1.04045700	-0.72068000	H	0.41480900	-1.05197800	2.38166700
H	-3.64596100	-1.87637400	-1.41993000	H	-1.17806900	-1.55290800	2.97091000
H	-4.59214400	-0.98960200	-0.22886500	H	-0.63127900	-2.03365600	1.35460900
H	-3.48770100	-0.11587300	-1.28773400				
C	-0.36015000	-0.11639500	2.50153100	O.neutral			
H	0.63632700	0.32218100	2.59450300	-637.93583880 a.u.			
H	-0.85355500	-0.01210600	3.46836300	C	0.75030400	0.54480700	-0.15809500
H	-0.24724600	-1.17892000	2.28711500	O	1.28990600	1.78501800	-0.27101400
C	-1.24003800	2.07953100	1.69446500	C	2.63585100	1.63892200	-0.31261800
H	-1.73029900	2.62524700	0.88511600	C	2.96947000	0.33225000	-0.23370800
H	-1.79787200	2.27883900	2.61069700	C	1.73411600	-0.38537800	-0.13238800
H	-0.24326500	2.50442700	1.86511400	H	1.58555800	-1.44856900	-0.04706200
				H	3.96630600	-0.07401400	-0.24936100
NH.neutral				H	3.20766700	2.54527700	-0.40473800
-618.07594721 a.u.				C	-0.73245100	0.47292700	-0.03793200
C	0.85423200	0.39739600	0.09535900	C	-2.64363400	-0.93482200	0.03513500
N	1.58648300	1.52679100	0.34425700	N	-1.25271100	-0.81261700	-0.46659100
C	2.92376900	1.24733700	0.28343900	C	-1.26668300	0.60533200	1.41051800
C	3.05438300	-0.08336200	-0.01436900	C	-2.68824500	0.05119500	1.22804200
C	1.74538900	-0.62140000	-0.13316300	H	-3.05280200	-0.42998200	2.13743800
H	1.47084800	-1.63813200	-0.36172400	H	-3.37158800	0.87211500	0.99862900
H	3.98503000	-0.61107200	-0.13873700	H	-1.15012400	1.30839800	-0.63149500
H	3.66240700	2.01274500	0.44700600	C	-1.05656500	-1.11597600	-1.86822900
H	1.18848600	2.43019500	0.53463100	H	-1.50531900	-0.36926000	-2.53999500
C	-0.63741000	0.41740500	0.15138600	H	0.00888400	-1.16694100	-2.08724500
C	-2.67691700	-0.66796900	-0.38633200	H	-1.49260000	-2.08866700	-2.09861400
N	-1.24734400	-0.53813300	-0.75398900	C	-2.89174900	-2.37758800	0.46439100
C	-1.25595500	0.03874800	1.51931500	H	-3.91421200	-2.50182300	0.82712700
C	-2.71037000	-0.22249500	1.09754100	H	-2.74726100	-3.06055900	-0.37535100
H	-3.18764100	-0.97003100	1.73382300	H	-2.20054600	-2.66127500	1.25802600

C	-3.69480700	-0.52233700	-1.00210700
H	-3.73627100	-1.21952900	-1.84027100
H	-4.67945300	-0.50326900	-0.53210000
H	-3.49126300	0.47735300	-1.39283600
C	-1.26102200	2.05117600	1.88765000
H	-1.70909800	2.12577100	2.88088300
H	-0.24133300	2.43639200	1.94718800
H	-1.82771000	2.69282100	1.20978000
C	-0.46830400	-0.26385300	2.38102100
H	-0.38461400	-1.28701600	2.01267000
H	0.54004000	0.12737000	2.52368300
H	-0.96761700	-0.28251500	3.35186400

PH₂.cation

-904.97994937 a.u.

C	0.56259100	0.18865900	-0.09356100
P	1.54118200	1.63417300	-0.47766100
C	3.13121100	0.85442800	-0.39738400
C	2.88217400	-0.42732300	-0.10053700
C	1.45759500	-0.79936500	0.05196100
H	1.14736300	-1.81519400	0.26487600
H	3.66643300	-1.16403500	0.02146400
H	4.08801300	1.32793900	-0.54690300
H	1.39558200	2.69086700	0.42389900
H	1.24260700	2.17180800	-1.73251600
C	-0.93002700	0.13410000	0.02785100
C	-2.80300500	-1.28833800	0.37896700
N	-1.42248100	-1.20395200	-0.18625500
C	-1.44766200	0.49935700	1.45102100
C	-2.86051500	-0.09873800	1.36480700
H	-3.22156900	-0.40211300	2.34803400
H	-3.54903400	0.65895500	0.98482500
H	-1.36275700	0.86273000	-0.68646700
C	-1.25918700	-1.71922300	-1.53201800
H	-1.73552600	-1.09010600	-2.29617000
H	-0.20160000	-1.81065200	-1.78096900
H	-1.69158300	-2.71681000	-1.59303300
C	-3.89118700	-1.11507700	-0.68408600
H	-3.92721800	-1.95683100	-1.37596100
H	-4.86248000	-1.04814100	-0.19282700
H	-3.74710700	-0.19714700	-1.25887700
C	-2.97033800	-2.63590700	1.07068900
H	-3.97920100	-2.73477400	1.47394700
H	-2.81158800	-3.45358400	0.36530800
H	-2.25721200	-2.74546800	1.88746400
C	-1.48031200	2.00205700	1.69439600
H	-0.47526500	2.41863700	1.80716000
H	-1.99541700	2.53105700	0.88968900
H	-2.00786400	2.21943000	2.62436400

C	-0.63050000	-0.18983100	2.54224800
H	0.36650300	0.24553600	2.64110300
H	-1.13389100	-0.07156300	3.50230500
H	-0.52245400	-1.25655200	2.34426700

PH.neutral

-904.63800607 a.u.

C	0.61409300	0.29035600	-0.07937700
P	1.64671300	1.77517900	-0.06049200
C	3.13634300	0.78023000	-0.21024400
C	2.82783200	-0.52268900	-0.06623600
C	1.40203200	-0.80107600	-0.00344400
H	1.00298200	-1.80481400	0.08539400
H	3.56792900	-1.31105600	-0.00058900
H	4.13875800	1.17879100	-0.25600000
H	1.46596200	2.21133600	-1.39206900
C	-0.88439900	0.31745200	-0.02887600
C	-2.90961000	-0.92768600	-0.12667300
N	-1.48618800	-0.90316000	-0.54087000
C	-1.49448500	0.43380400	1.39462500
C	-2.94307700	0.00847900	1.10449200
H	-3.39997200	-0.47543000	1.96977400
H	-3.54069000	0.89384700	0.87510100
H	-1.23132400	1.20098200	-0.60199500
C	-1.23293500	-1.16669600	-1.94081000
H	-1.56832300	-0.35301700	-2.60160200
H	-0.16571900	-1.31020200	-2.10241200
H	-1.74308600	-2.08245900	-2.24194700
C	-3.30134900	-2.36032400	0.22262000
H	-4.35037300	-2.41177700	0.52167600
H	-3.16379600	-3.01909800	-0.63738900
H	-2.68458200	-2.73320600	1.04036700
C	-3.86048800	-0.38653700	-1.20120000
H	-3.90986300	-1.04367200	-2.07072800
H	-4.86632800	-0.30286200	-0.78626600
H	-3.55303700	0.60709600	-1.53514700
C	-1.42216900	1.85006100	1.94903100
H	-1.97565300	1.91447800	2.88860100
H	-0.39089100	2.14690000	2.14764200
H	-1.85633500	2.57020000	1.25162500
C	-0.83239500	-0.53717100	2.37016100
H	0.19411200	-0.23965800	2.58864800
H	-1.39000200	-0.54976300	3.30890900
H	-0.81348100	-1.54933300	1.96425200

SbH₂.cation

-803.76083153 a.u.

C	-0.10492700	-0.47891400	-0.05955300
Sb	1.05598000	1.22452500	-0.46384400

C	2.72028800	-0.01615300	-0.33823400	C	-3.57314500	-1.66565200	0.04711000
C	2.24047500	-1.23101600	-0.06261700	N	-2.17243500	-1.73005400	-0.41396300
C	0.78219400	-1.47100400	0.06416700	C	-2.13755100	-0.14162400	1.37886300
H	0.42646600	-2.47659700	0.26293400	C	-3.40529800	-1.02687500	1.43099300
H	2.90965700	-2.07410800	0.07079000	H	-3.26755000	-1.81708200	2.17134400
H	3.75868300	0.25287500	-0.44497200	H	-4.29091000	-0.45689700	1.71891200
H	1.03535600	2.46654200	0.65705700	H	-1.85898600	0.33044800	-0.71892500
H	0.79620400	1.93566100	-1.95730400	C	-1.99661300	-2.05453200	-1.81588100
C	-1.59687900	-0.53741100	0.06637600	H	-2.32231600	-1.24190600	-2.48278100
C	-3.45558600	-1.95244500	0.54114300	H	-0.94575700	-2.25048600	-2.02236500
N	-2.08926700	-1.88680000	-0.05974700	H	-2.56226500	-2.95245800	-2.06394200
C	-2.11129300	-0.07627600	1.46201000	C	-2.46883700	1.34544400	1.47895500
C	-3.51725600	-0.69383200	1.43560200	H	-1.57175700	1.95658100	1.34688800
H	-3.86707900	-0.92645900	2.44201000	H	-3.19736700	1.64339500	0.72239800
H	-4.21756800	0.02573300	1.00598100	H	-2.88589800	1.57868900	2.46089700
H	-2.03454400	0.13897100	-0.69516200	C	-1.20435000	-0.52813700	2.52470100
C	-1.95256900	-2.47641000	-1.37794600	H	-0.87778300	-1.56445200	2.42701000
H	-2.46017300	-1.89928700	-2.16272300	H	-0.31644400	0.10654400	2.55975600
H	-0.90145000	-2.56310200	-1.65199400	H	-1.73325300	-0.42127500	3.47444200
H	-2.36898400	-3.48274600	-1.37062600	C	-4.47081800	-0.79939300	-0.84949200
C	-4.57101800	-1.87955900	-0.50523400	H	-4.58602900	-1.24076500	-1.84061500
H	-4.60610800	-2.77107100	-1.13161200	H	-5.46364300	-0.71795500	-0.40457000
H	-5.53175300	-1.79433200	0.00380300	H	-4.07655200	0.21101200	-0.97112600
H	-4.45876500	-1.00461700	-1.14969900	C	-4.16647000	-3.06531000	0.15071200
C	-3.58202000	-3.24742500	1.33507600	H	-5.13379900	-3.02483200	0.65537900
H	-4.58088900	-3.33658400	1.76481800	H	-4.32799000	-3.51021500	-0.83261600
H	-3.41796700	-4.11154800	0.68866600	H	-3.49840500	-3.71096500	0.72126900
H	-2.85146800	-3.28176000	2.14297200				
C	-1.27512500	-0.67120300	2.59400600	Se.neutral			
H	-0.28625600	-0.21035900	2.65547600	-2964.29116245 a.u.			
H	-1.77567700	-0.49896400	3.54742900	C	0.93875800	-0.32465200	0.12579000
H	-1.14192700	-1.74572300	2.46659000	Se	2.47343500	0.27360300	-0.75919500
C	-2.16575700	1.44006500	1.59459900	C	3.47263700	-0.66160400	0.49884300
H	-1.16743900	1.88144100	1.67119400	C	2.67371600	-1.29614200	1.38938100
H	-2.69430400	1.90006900	0.75663100	C	1.27263800	-1.11065400	1.18043500
H	-2.69099500	1.71862900	2.50961800	H	0.51176900	-1.56051000	1.80512200
				H	3.06911800	-1.89907800	2.19575200
SbH.neutral				H	4.54968500	-0.66002100	0.46612600
-803.44173943 a.u.				C	-0.43245500	0.08896600	-0.31741800
C	-0.04058800	-0.52581300	-0.07635500	C	-2.77288300	-0.28131000	-0.13510900
Sb	1.24670000	1.19285600	-0.11776300	N	-1.43745400	-0.91214300	-0.00098300
C	2.73847000	-0.32572200	-0.15789400	C	-0.98430700	1.36625400	0.36872700
C	2.16725700	-1.53053000	-0.03905200	C	-2.47848600	1.22880700	0.03498900
C	0.70300900	-1.63729400	-0.00934900	H	-3.10513800	1.67929300	0.80686100
H	0.23459900	-2.61556100	0.06038400	H	-2.69104500	1.75075300	-0.90096800
H	2.75759500	-2.44002400	0.02918200	H	-0.39923700	0.28955100	-1.40589500
H	3.81008300	-0.18474900	-0.16927100	C	-1.26564400	-2.18082800	-0.67591700
H	1.14023400	1.39568300	-1.81645700	H	-1.25260400	-2.08898900	-1.77222000
C	-1.53893400	-0.47463500	-0.03114500	H	-0.32641000	-2.63720400	-0.36685600

H	-2.07454300	-2.85778400	-0.39897400	H	-3.43681700	0.96907700	-0.93097800
C	-3.41670400	-0.52105800	-1.50594900	C	-0.51061700	0.15495700	2.51327600
H	-3.68948200	-1.56742500	-1.65078300	H	0.39313700	0.76671900	2.53770800
H	-4.32535800	0.07751000	-1.58919700	H	-1.01680800	0.25755900	3.47580600
H	-2.74501500	-0.22338100	-2.31442500	H	-0.21255400	-0.88760000	2.39088500
C	-3.68984400	-0.82108900	0.95823500	C	-1.74937900	2.07511000	1.51910800
H	-4.68604800	-0.38104500	0.87831700	H	-2.13100400	2.30970900	2.51505100
H	-3.79303700	-1.90503900	0.87536300	H	-0.84067700	2.66323800	1.36447000
H	-3.28231600	-0.59112700	1.94270400	H	-2.49193800	2.39793300	0.78662600
C	-0.76332700	1.33499300	1.87969300				
H	-1.13057900	0.40294200	2.31078800				
H	0.29510600	1.42946300	2.12585000	SiH.anion			
H	-1.29780000	2.16629500	2.34396200	-852.79109320 a.u.			
C	-0.38215800	2.63814200	-0.21224100	C	0.65347900	0.24726300	0.21253600
H	-0.87328000	3.51702900	0.21109600	Si	1.86680300	1.64292700	0.49527100
H	0.68299100	2.70850400	0.01760900	C	3.28603300	0.44767000	0.35827100
H	-0.50304300	2.67380800	-1.29746100	C	2.80253900	-0.72078300	-0.16475900
				C	1.36607900	-0.83042400	-0.24151700
SiH ₂ .neutral				H	0.89204900	-1.70737400	-0.68144700
-853.37114952 a.u.				H	3.43369600	-1.51890100	-0.55278400
C	0.60618900	0.21733400	-0.09397900	H	4.35487900	0.62556800	0.41794100
Si	1.82344900	1.64222400	-0.16306600	H	1.74001400	2.12504500	1.92143600
C	3.30486500	0.51533900	-0.16113600	C	-0.84394100	0.28683300	0.24923200
C	2.82330900	-0.73503800	-0.11896700	C	-2.95334500	-0.58837800	-0.43572200
C	1.34982400	-0.89875300	-0.08992200	N	-1.52618200	-0.49957400	-0.78878700
H	0.90780200	-1.89049400	-0.06062100	C	-1.49027400	-0.27184400	1.54293700
H	3.45521500	-1.61784800	-0.10548100	C	-2.95790000	-0.40397100	1.10391300
H	4.36428200	0.72681800	-0.18077400	H	-3.46323200	-1.23273400	1.60731100
H	1.75582800	2.54402400	1.01015800	H	-3.49983700	0.51024800	1.36117100
H	1.67867900	2.46583700	-1.38439000	H	-1.16237000	1.34529200	0.17366200
C	-0.89071800	0.26035100	-0.02977600	C	-1.22888600	-0.07592900	-2.13645000
C	-2.93147500	-0.91483700	0.07160900	H	-1.49188500	0.97716400	-2.32855500
N	-1.53706500	-0.98934900	-0.40954700	H	-0.15942400	-0.18261200	-2.31100500
C	-1.45786900	0.58212900	1.39331900	H	-1.76515400	-0.70087500	-2.85569200
C	-2.74282700	-0.27701300	1.45419700	C	-3.49149700	-1.95716600	-0.85000000
H	-2.61849600	-1.06733000	2.19672600	H	-4.55174200	-2.05315000	-0.59948300
H	-3.61564300	0.31143300	1.74406700	H	-3.38249200	-2.10397500	-1.92735200
H	-1.22163600	1.07205100	-0.70371100	H	-2.93477600	-2.74410700	-0.34047100
C	-1.38747700	-1.30562000	-1.81627300	C	-3.81445000	0.50678600	-1.08289500
H	-1.71576400	-0.48533800	-2.47245100	H	-3.88120400	0.38141100	-2.16569000
H	-0.34259700	-1.51107900	-2.04272200	H	-4.82681300	0.46965200	-0.67361700
H	-1.96594700	-2.19613400	-2.06171500	H	-3.40118700	1.49630700	-0.87586100
C	-3.53372500	-2.31013000	0.18129400	C	-1.31695100	0.68796000	2.71127500
H	-4.49494100	-2.26302000	0.69698500	H	-1.81833300	0.30613600	3.60593900
H	-3.70972900	-2.75356800	-0.80028100	H	-0.25550400	0.81963500	2.93110300
H	-2.86384400	-2.96083300	0.74394100	H	-1.73548700	1.66999100	2.47603700
C	-3.83511200	-0.04001500	-0.81073300	C	-0.91198500	-1.63589400	1.91326600
H	-3.96544200	-0.47540300	-1.80258600	H	0.13580900	-1.54084700	2.19917200
H	-4.82184200	0.04440800	-0.35296500	H	-1.47456000	-2.06294900	2.74937500
				H	-0.96334600	-2.32116000	1.06553700

S.neutral

-960.91020044 a.u.

C	0.63941600	0.26438600	0.04838700
S	1.55456900	1.70934200	0.20467500
C	3.03961900	0.87295500	0.07505200
C	2.84120800	-0.46285300	-0.09291500
C	1.46318700	-0.81084500	-0.10929900
H	1.08110300	-1.81387200	-0.23812600
H	3.64686400	-1.17401100	-0.20434400
H	3.97317800	1.40874500	0.12434700
C	-0.85749600	0.29007500	0.12657000
C	-2.88764200	-0.87813400	-0.26297300
N	-1.46728600	-0.75934600	-0.67207200
C	-1.44614300	0.03963200	1.53847400
C	-2.90163300	-0.28973500	1.16928000
H	-3.35199700	-0.97902100	1.88583300
H	-3.49621400	0.62671000	1.18265900
H	-1.19995800	1.29170800	-0.19901800
C	-1.22178200	-0.66242500	-2.09498700
H	-1.55760000	0.29158000	-2.52828600
H	-0.15497200	-0.76243400	-2.29042400
H	-1.73504900	-1.47306500	-2.61341000
C	-3.29200100	-2.34892400	-0.29024400
H	-4.33876300	-2.46652000	-0.00232500
H	-3.16990300	-2.76458300	-1.29262200
H	-2.67217900	-2.92545800	0.39643300
C	-3.83899100	-0.07029000	-1.15342900
H	-3.89974400	-0.48112400	-2.16231600
H	-4.84157500	-0.08758000	-0.72283300
H	-3.52305000	0.97311800	-1.22311800
C	-0.78071800	-1.15165200	2.22479200
H	0.25450300	-0.92893300	2.48665400
H	-1.32083800	-1.39260500	3.14266600
H	-0.78676100	-2.03022500	1.57863800
C	-1.34063700	1.27034900	2.42823700
H	-1.85168700	1.09749000	3.37780400
H	-0.29704800	1.50513900	2.64834600
H	-1.79526200	2.14262200	1.95314600

SnH₂.neutral

-778.08799552 a.u.

C	-0.10700200	-0.45714300	-0.06582200
Sn	1.28206600	1.18803900	-0.14604400
C	2.77102900	-0.34325900	-0.13240200
C	2.11927600	-1.51034100	-0.08342600
C	0.63595900	-1.56973500	-0.05561700
H	0.16416800	-2.54868900	-0.01512100
H	2.65096100	-2.45827500	-0.06150400

H	3.85084100	-0.29992100	-0.14744200
H	1.27372900	2.22317200	1.22664600
H	1.19086900	2.14745000	-1.56731500
C	-1.60406300	-0.42279000	0.00298200
C	-3.64186700	-1.60037300	0.15568900
N	-2.25078400	-1.68540500	-0.33331400
C	-2.16568000	-0.05524600	1.41791300
C	-3.44695600	-0.91650300	1.51493500
H	-3.31467400	-1.68130400	2.28239000
H	-4.32025200	-0.32209000	1.79092100
H	-1.94362100	0.36405100	-0.69603700
C	-2.11339500	-2.04173200	-1.73187300
H	-2.44696800	-1.23962400	-2.40770100
H	-1.07104500	-2.25452100	-1.96233900
H	-2.69526700	-2.93785900	-1.94701400
C	-4.23733000	-2.99377000	0.31618300
H	-5.19522700	-2.93382400	0.83675100
H	-4.41779500	-3.47034000	-0.64889900
H	-3.56054100	-3.62245600	0.89530400
C	-4.55618500	-0.75911900	-0.74819600
H	-4.69278800	-1.22821000	-1.72367500
H	-5.53942000	-0.66301000	-0.28524200
H	-4.16294500	0.24681800	-0.90608500
C	-2.46445400	1.43959200	1.49746000
H	-1.55864300	2.02956100	1.32966100
H	-3.20659400	1.73771000	0.75427700
H	-2.84873900	1.70274100	2.48521000
C	-1.21349100	-0.44169700	2.54864400
H	-0.90327100	-1.48343200	2.45391700
H	-0.31649100	0.18062300	2.55887700
H	-1.72074800	-0.31826100	3.50816900

SnH.anion

-777.54374622 a.u.

C	-0.08258300	-0.40942400	-0.00645400
Sn	1.35821400	1.30453900	-0.14041600
C	2.74984000	-0.42083100	-0.10382300
C	2.06386100	-1.57430200	-0.17176900
C	0.59184900	-1.56577000	-0.12824800
H	0.07487500	-2.52656800	-0.19049500
H	2.55177900	-2.54774100	-0.26166800
H	3.83618900	-0.46006100	-0.14901500
H	1.44003800	1.66052800	1.63147400
C	-1.58041300	-0.35665300	0.08007900
C	-3.69277400	-1.48427200	0.09544000
N	-2.30356000	-1.54481600	-0.39691400
C	-2.12089100	-0.20247400	1.52589400
C	-3.60305400	-0.55865800	1.33237900
H	-4.02804400	-1.03068200	2.22226700

H	-4.17398400	0.35529200	1.14688900	C	-4.55705600	-1.00972600	-1.04700900
H	-1.92869700	0.53111800	-0.48542700	H	-4.63663100	-1.58632200	-1.96971900
C	-2.15289000	-1.79944300	-1.81002400	H	-5.54635300	-0.97242400	-0.58790300
H	-2.50093100	-0.96467800	-2.44049100	H	-4.26777200	0.01248000	-1.30145900
H	-1.10135300	-1.96310900	-2.03606500	C	-1.39121400	-1.44900300	2.38053200
H	-2.71051000	-2.69603000	-2.09366400	H	-1.39035700	-2.42458300	1.89296000
C	-4.15369600	-2.89387100	0.46374400	H	-0.35589700	-1.16578400	2.57483400
H	-5.18507000	-2.88688700	0.82734100	H	-1.90667400	-1.54046400	3.33882700
H	-4.10416400	-3.55363600	-0.40607800	C	-2.00915400	0.95958500	2.18989700
H	-3.50710700	-3.30421900	1.23980000	H	-0.97148900	1.23950500	2.38224600
C	-4.67971900	-0.88114300	-0.91548300	H	-2.46825500	1.73545600	1.57229200
H	-4.81847400	-1.52723700	-1.78474800	H	-2.53049700	0.94188500	3.14952600
H	-5.65238100	-0.74192500	-0.43804900	CAAC.neutral			
H	-4.33103200	0.09410100	-1.26226300	-409.09927986 a.u.			
C	-1.94439200	1.21396200	2.05631900	C	-1.24057500	0.01579000	-0.11617100
H	-0.88534700	1.45613900	2.16199900	N	-0.66627100	-0.05869500	1.24492000
H	-2.39825600	1.94325500	1.38010000	C	0.64061100	0.56214000	1.19751400
H	-2.42045400	1.31600600	3.03654600	C	1.24851000	0.01221300	-0.09389700
C	-1.44237000	-1.19189500	2.47192100	C	0.01755300	0.01486100	-1.02520700
H	-1.48501100	-2.20519400	2.06818000	H	0.02295600	0.91136200	-1.64895400
H	-0.39201700	-0.93069900	2.60566000	H	0.02640300	-0.84567000	-1.69696000
H	-1.94059100	-1.17566100	3.44595600	C	-2.05024800	1.29717100	-0.34965300
Te.neutral				H	-2.34592800	1.36256100	-1.39800300
-830.64210261 a.u.				H	-2.95756200	1.31470000	0.25675100
C	-0.04403700	-0.41045000	-0.03322000	H	-1.45945500	2.18509400	-0.11206500
Te	1.11348700	1.30090800	-0.06718000	C	-2.12597500	-1.20153600	-0.35921200
C	2.64607600	-0.06229500	-0.13994300	H	-2.96154300	-1.22479700	0.34348100
C	2.16975000	-1.32613000	-0.13777100	H	-2.53950600	-1.18127300	-1.36961500
C	0.74549700	-1.50833600	-0.08544100	H	-1.54658500	-2.11661600	-0.23360400
H	0.29965400	-2.49668900	-0.09185100	C	2.38034300	0.88393600	-0.62056600
H	2.83604500	-2.17980700	-0.17648600	H	3.21558500	0.90498500	0.08349400
H	3.68658600	0.21962700	-0.17241800	H	2.75576400	0.49800300	-1.57087600
C	-1.54163000	-0.38903900	0.06859100	H	2.04409200	1.91041900	-0.78084100
C	-3.56269100	-1.63721700	-0.06275600	C	1.74842700	-1.41431900	0.13364000
N	-2.15662400	-1.56360600	-0.52831600	H	2.08079700	-1.85888700	-0.80700100
C	-2.09692200	-0.40422100	1.51843400	H	2.59203000	-1.42228700	0.82783400
C	-3.55317700	-0.81518800	1.24801000	H	0.95477400	-2.03508400	0.55088200
H	-3.97186000	-1.37926900	2.08350600	H	1.22276400	0.30076900	2.08579500
H	-4.16556600	0.08088500	1.12241200	H	0.57942400	1.66540200	1.15117500
H	-1.91190400	0.53690400	-0.41327100	C	-1.49840200	0.39472800	2.33336000
C	-1.95627900	-1.69530500	-1.95568600	H	-2.47104900	-0.09784800	2.29722800
H	-2.32364800	-0.82856400	-2.52524400	H	-1.02675200	0.12863500	3.28071800
H	-0.89489500	-1.81016300	-2.16991700	H	-1.66337400	1.48347700	2.33279000
H	-2.47006100	-2.58604100	-2.31908300	cAAc1.BH.neutral			
C	-3.93313400	-3.09866400	0.17094700	-508.26475751 a.u.			
H	-4.96929200	-3.18563300	0.50461200	C	-0.36165700	-3.77645000	-1.00237300
H	-3.82623900	-3.67592600	-0.74980000	B	0.77622900	-4.87262500	-1.18662000
H	-3.28273600	-3.53839000	0.92707700	C	0.21179300	-5.92969700	-2.19551800
				C	-1.09181200	-5.64404000	-2.26351500

H	-1.14677600	-7.06391800	-1.18924900	B	2.38871600	1.79531500	-0.26419300
H	1.34720300	-7.30925600	-0.55769400	H	2.96256400	-1.98664500	1.40491100
H	1.94103100	-4.84952300	1.05889000	H	4.72560700	0.04863800	1.63977700
C	-0.25355600	-2.63019200	0.34016300	H	4.43568200	2.22762600	0.69762900
C	-1.52870500	-1.81510000	0.00376900	H	2.23674900	2.85682200	-0.78880300
C	-0.98039200	-0.39727700	0.14156000	C	-0.47517100	1.95176100	-1.56332400
C	0.37979700	-0.45348200	-0.02655400	H	0.28006200	2.71511800	-1.72771200
N	0.82734100	-1.73487900	-0.12667000	H	-0.96240300	1.70924700	-2.51061500
B	-1.67272500	0.93070100	0.30721600	H	-1.24353800	2.31254400	-0.87473900
C	-0.77931900	2.24723800	0.34051000	C	-0.23721000	-2.33319200	0.88139200
C	0.55072100	2.21037800	0.14211300	H	-0.53247800	-1.71111300	1.72413500
B	1.22775200	0.86198500	-0.21164200	H	-1.11932200	-2.89263600	0.56004800
H	-2.85737200	1.02460900	0.43424300	H	0.53215300	-3.03821500	1.20670400
H	-1.24890100	3.21431400	0.51417000	C	0.72652600	-2.39554700	-1.41721400
H	1.12146400	3.13534900	0.15234700	H	-0.12294800	-2.99126400	-1.76751700
H	2.32433700	0.82373900	-0.67596300	H	1.10306900	-1.80266000	-2.25485200
C	2.20782400	-2.12657000	-0.00663900	H	1.52183200	-3.07237100	-1.09625700
H	2.46242100	-2.40083600	1.02374100	H	-1.09998400	-0.76400500	-1.77915400
H	2.41963500	-2.98365400	-0.64957600				
H	2.84409100	-1.30353200	-0.32112100				
C	-1.98244100	-1.96614800	-1.45742900	cAAc3.neutral			
H	-1.13152000	-1.88767300	-2.13635700	-456.36320686 a.u.			
H	-2.49498200	-2.90589900	-1.65573100	C	-0.16510700	-2.68735300	0.07509900
H	-2.67703200	-1.15619200	-1.68708700	C	-1.46324000	-1.86717800	-0.09025300
C	-2.67646500	-2.12873100	0.95400400	C	-0.94198200	-0.44037400	0.04863200
H	-3.00215000	-3.16717100	0.85961600	C	0.42507200	-0.46680900	-0.07840200
H	-2.38413000	-1.95252000	1.99031100	N	0.90206400	-1.73149600	-0.20960700
H	-3.52998800	-1.48607900	0.73289700	B	-1.65733000	0.86813000	0.23792500
H	-0.17317000	-2.63747100	1.44448700	C	-0.78791400	2.20201300	0.29554000
				C	0.55014700	2.19424400	0.15041800
cAAc3.CH.anion				B	1.27127000	0.86267200	-0.16885800
-648.70772455 a.u.				H	-2.84320200	0.93909900	0.37072300
C	-1.90615400	-0.04099000	0.02084400	H	-1.28252400	3.15945600	0.45386000
C	-3.24059300	-0.04332700	-0.43533600	H	1.09981700	3.13107100	0.18941200
C	-4.03992400	0.55886500	0.54652100	H	2.40672400	0.83966600	-0.52930700
C	-3.19700600	0.95315200	1.60710300	C	2.27246600	-2.14829300	-0.06902700
C	-1.88227000	0.58984300	1.28381500	H	2.49151700	-2.45431100	0.96132800
H	-0.99867000	0.76424000	1.88603200	H	2.47004400	-2.99833200	-0.72409600
H	-3.51360800	1.43567800	2.52273700	H	2.93896300	-1.33452100	-0.34248200
H	-5.11361000	0.68571900	0.50624700	C	-2.03055900	-2.06048500	-1.50069900
H	-3.57319200	-0.44374000	-1.38601300	H	-1.27091000	-1.83924500	-2.25309400
C	-0.72986900	-0.43759900	-0.79943000	H	-2.37689200	-3.08751200	-1.64627600
C	0.30695600	-1.48114300	-0.25762500	H	-2.87320300	-1.38547100	-1.66043700
C	1.49713600	-0.61962600	0.14536200	C	-2.51287000	-2.24123000	0.94927700
C	1.30575400	0.65029400	-0.39831600	H	-2.81232100	-3.28756900	0.84580800
N	0.13739800	0.75815200	-1.03102000	H	-2.13161500	-2.08759300	1.95971100
B	2.73036400	-0.91929400	0.90516900	H	-3.40234400	-1.62147000	0.82629000
C	3.81318200	0.24482000	1.07246100	H	-0.05019900	-3.05426500	1.10522500
C	3.66021100	1.47912200	0.54670900	H	-0.10857300	-3.54503300	-0.60017900
				NHC1.BH.neutral			

-484.99252708 a.u.			H	-2.66167900	-0.94043600	-1.86399600	
C	-0.97129700	0.01459400	-0.12589700	C	1.14584200	-2.07706400	2.15294200
B	-2.10997100	0.90927000	-0.76948700	H	1.93078700	-2.27863800	1.41508100
C	-3.44718000	0.40234200	-0.10595200	H	1.41710600	-1.16097700	2.67997500
C	-3.09557300	-0.62154700	0.67705300	H	1.09919000	-2.89316100	2.87915300
C	-1.60363700	-0.86182000	0.65828200				
H	-1.12410300	-1.65398100	1.22264600	NHC1.neutral			
H	-3.76315200	-1.23471300	1.27222900	-305.97862582 a.u.			
H	-4.46661700	0.73683300	-0.23233400	C	0.51791700	-0.04003200	-0.37200000
H	-1.97772200	1.73805400	-1.61166900	N	1.40080600	-1.19857200	-0.34641300
C	0.50566700	0.05415200	-0.35451200	C	2.62963800	-0.67667100	0.11597900
H	0.69786500	0.20420500	-1.44765300	H	3.43059300	-1.33550700	0.40879000
N	1.18181900	1.13315500	0.37543600	N	1.42408000	1.07688600	-0.60378700
C	2.48975600	0.65133100	0.58030100	C	2.64317000	0.64673100	-0.03370000
H	3.26455800	1.30551100	0.94575900	H	3.45793100	1.33800900	0.10640800
N	1.22696400	-1.13955900	0.08364400	C	0.85778300	-2.34502500	0.34559000
C	2.51779900	-0.66931800	0.41483000	H	1.59535300	-3.14664400	0.35846500
H	3.32022500	-1.36124800	0.61118400	H	0.57576200	-2.10550500	1.38223500
C	1.02355400	2.44542900	-0.20624400	H	-0.02653500	-2.70646700	-0.18027100
H	1.32537400	2.46780700	-1.26453900	C	0.90590100	2.35965700	-0.18655400
H	-0.01873600	2.75924900	-0.13824900	H	0.02786700	2.61231000	-0.78188000
H	1.62852200	3.16212800	0.34779700	H	0.62146100	2.36345200	0.87675100
C	1.15060900	-2.24846400	-0.84305700	H	1.65953700	3.12884100	-0.35134400
H	0.11560400	-2.57726100	-0.93754000	H	0.02207600	0.07750900	0.62232900
H	1.52410000	-1.97460000	-1.84108800	H	-0.24802100	-0.11964500	-1.14511900
H	1.74211100	-3.08079600	-0.46314900				
				NHC2.BH.neutral			
NHC1.CH.anion				-638.65043165 a.u.			
-498.31403594 a.u.				C	1.65642900	-5.04341900	-1.36116500
C	0.88744400	-0.43028700	-0.20356600	B	2.54110200	-6.35557100	-1.29554500
C	1.52836900	0.82512500	-0.19495100	C	2.13396300	-7.18275300	-2.57438400
C	2.61680200	0.77320800	-1.07953900	C	1.16032300	-6.48268300	-3.16298800
C	2.65227500	-0.51953100	-1.63979200	C	0.86491800	-5.19660400	-2.42585600
C	1.58967500	-1.26346400	-1.10332500	H	0.09819300	-4.49769500	-2.74187200
H	1.34473500	-2.29267300	-1.33273100	H	0.61892600	-6.76097200	-4.06015700
H	3.37576100	-0.87854900	-2.36131500	H	2.49543600	-8.13187900	-2.94247100
H	3.30566700	1.58000900	-1.29372500	H	3.30150200	-6.66110300	-0.43428000
H	1.21879100	1.67643500	0.40100900	C	1.62862100	-3.87218700	-0.43018300
C	-0.31380900	-0.75863100	0.61375400	C	2.20509100	-1.66324300	-0.27829600
H	-0.58544800	0.12945200	1.19476500	C	0.80958700	-1.75360000	-0.17503600
N	-1.51997900	-1.20776900	-0.15362600	C	0.05368900	-0.66890100	0.20882400
C	-1.51237500	-2.61311500	-0.09279300	C	0.71746500	0.53529400	0.47896800
H	-2.15116900	-3.19812800	-0.73590700	C	2.09258800	0.62509000	0.37592300
N	-0.16286300	-1.91241000	1.55791700	C	2.86134800	-0.48433000	0.00004300
C	-0.72447700	-3.02221000	0.90088500	N	2.69294600	-2.89971900	-0.70416300
H	-0.56183000	-4.02334800	1.26852800	N	0.42212200	-3.05196100	-0.52707800
C	-1.71091700	-0.59377000	-1.44993700	H	-1.02157200	-0.73995800	0.30605600
H	-1.76152700	0.48943700	-1.32883600	H	0.14288500	1.39982400	0.78324600
H	-0.89731100	-0.81021600	-2.15165500	H	2.58869700	1.55982000	0.60061800

H	3.93898500	-0.41205600	-0.06213100	C	1.56812600	-0.71852100	0.16934000
H	1.73974300	-4.24437400	0.61566000	C	2.72252400	-1.41024500	-0.12123100
C	4.03352200	-3.29427400	-0.35348000	C	3.91030900	-0.67958700	-0.26157300
H	4.29239200	-4.21711500	-0.87283300	C	3.91844200	0.69573100	-0.12739400
H	4.73536400	-2.52564200	-0.67258900	C	2.73914200	1.39935200	0.15288100
H	4.15041300	-3.45397600	0.72809000	N	0.27741500	1.09634200	0.61417100
C	-0.76694700	-3.59897900	0.08426100	N	0.26398400	-1.17328600	0.39273900
H	-1.62819000	-2.98343500	-0.17154300	H	2.71787100	-2.48532700	-0.24324300
H	-0.94217200	-4.60303500	-0.30003300	H	4.82908300	-1.20289600	-0.49008900
H	-0.68077300	-3.64641000	1.17891600	H	4.84354500	1.24253800	-0.25150900
NHC2.CH.anion				H	2.74722000	2.47772400	0.24096300
-651.98596529 a.u.				C	-0.14931600	2.41570200	0.21884400
C	1.64614900	-5.06429300	-1.36030200	H	-1.16233200	2.59180200	0.58050000
C	1.86454400	-6.38605900	-0.91589000	H	0.50143100	3.16359000	0.66928800
C	1.75843500	-7.23849600	-2.02309200	H	-0.13421000	2.54609700	-0.87276300
C	1.47404200	-6.44427100	-3.15403000	C	-0.17773000	-2.38622800	-0.24972600
C	1.40436300	-5.10468700	-2.74923100	H	-1.19312000	-2.61709000	0.07228600
H	1.20268500	-4.24620000	-3.37573500	H	-0.16298500	-2.30324900	-1.34596300
H	1.33341200	-6.80776100	-4.16408800	H	0.46374700	-3.21464900	0.04681200
H	1.87393800	-8.31433000	-2.01276200	H	-0.90690000	0.09929000	-0.83716200
H	2.07621300	-6.67320000	0.10746700	H	-1.47863500	-0.06241800	0.85505700
C	1.67487300	-3.87608500	-0.48965700	NHC3.BH.neutral			
C	2.19278800	-1.63726500	-0.31777100	-612.09930588 a.u.			
C	0.80391000	-1.78399800	-0.07169600	C	1.65524600	-5.08381500	-1.37355800
C	0.06863500	-0.74271900	0.45271000	B	2.55791500	-6.38572400	-1.36793200
C	0.72448900	0.47478200	0.71569500	C	2.16568000	-7.15376500	-2.68774900
C	2.07556100	0.61752000	0.47631700	C	1.18705300	-6.43659100	-3.24717100
C	2.83524400	-0.45043300	-0.03746600	C	0.87269800	-5.19139400	-2.45002600
N	2.65129600	-2.82137900	-0.84706500	H	0.10181400	-4.48450900	-2.73750500
N	0.44291800	-3.05469100	-0.45579100	H	0.65473300	-6.67661600	-4.16073700
H	-0.98752700	-0.85941000	0.66046800	H	2.53997500	-8.07925400	-3.10058100
H	0.15959700	1.30269100	1.12593800	H	3.32256900	-6.72016000	-0.52137900
H	2.56598200	1.55692100	0.69958400	C	1.60905900	-3.96237500	-0.38275300
H	3.89945300	-0.34311000	-0.20538800	C	2.18554300	-1.74692300	-0.18525100
H	1.89470900	-4.21158400	0.55105300	C	0.82240300	-1.81931500	-0.11226300
C	4.04083900	-3.17146200	-0.81778300	B	-0.02089500	-0.58156500	0.19953300
H	4.15517700	-4.13180400	-1.32112500	C	0.74120100	0.77271700	0.49026300
H	4.62809700	-2.41898000	-1.34718600	C	2.07784200	0.85030300	0.41014700
H	4.42710300	-3.25669600	0.21052800	B	2.93228300	-0.41216200	0.02554600
C	-0.75229100	-3.67784800	0.03144200	N	2.68158300	-2.98271000	-0.56500000
H	-1.62405300	-3.07950600	-0.23946000	N	0.42292300	-3.11866300	-0.45728300
H	-0.83374100	-4.65887300	-0.43721400	H	-1.21198900	-0.61917200	0.22556500
H	-0.74024300	-3.80261900	1.12605400	H	0.17632000	1.66439700	0.75348900
NHC2.neutral				H	2.56775600	1.80052100	0.60871600
-459.63675374 a.u.				H	4.11483100	-0.33364900	-0.09778000
C	-0.58920100	-0.00615800	0.22443300	H	1.69572400	-4.40141200	0.64400400
C	1.57638700	0.67808200	0.30560100	C	4.02345100	-3.42148200	-0.28979300
				H	4.10888400	-3.84980700	0.71927200

H	4.32538400	-4.18432100	-1.01000000
H	4.70602300	-2.57951000	-0.37455900
C	-0.78123600	-3.68119700	0.10646300
H	-1.59796800	-2.97029200	0.00354700
H	-1.04611800	-4.59641700	-0.42302600
H	-0.65409000	-3.92098400	1.17232300

NHC3.CH.anion

-625.43410052 a.u.

C	1.65615500	-5.12282000	-1.32833300
C	1.89264300	-6.45279900	-0.92480700
C	1.76524200	-7.27668100	-2.05285500
C	1.44980600	-6.45543400	-3.15454200
C	1.38178200	-5.12661900	-2.71161000
H	1.16013400	-4.25297200	-3.31010400
H	1.28714800	-6.79270800	-4.17034600
H	1.88701700	-8.35170000	-2.07372500
H	2.13012200	-6.76587200	0.08503100
C	1.69911000	-3.95030700	-0.43334400
C	2.17846800	-1.68711700	-0.31822500
C	0.82674900	-1.83884400	-0.05100500
B	-0.00854100	-0.67215200	0.46405100
C	0.70708200	0.72955900	0.67028700
C	2.01274200	0.87718700	0.41012900
B	2.87705600	-0.34612200	-0.11181200
N	2.65674500	-2.88562200	-0.78857500
N	0.47467400	-3.13141400	-0.36053900
H	-1.17109900	-0.78780800	0.71899000
H	0.13642200	1.58856600	1.02155100
H	2.47560800	1.85260000	0.55535000
H	4.04442500	-0.20050200	-0.32579000
H	1.94335200	-4.30837100	0.60061800
C	4.04251700	-3.24662600	-0.83571800
H	4.14812500	-4.11723500	-1.48390600
H	4.63046300	-2.41874100	-1.22978000
H	4.42684100	-3.50996800	0.16280100
C	-0.71306900	-3.78131400	0.10838000
H	-1.56964400	-3.11754300	-0.00185000
H	-0.86641300	-4.68433200	-0.48345200
H	-0.62506400	-4.07213500	1.16765200

NHC3.neutral

-433.08529407 a.u.

C	-0.60160400	-0.00166400	0.19740900
C	1.58155900	0.66759600	0.24701300
C	1.57376900	-0.69451600	0.13196900
B	2.87400100	-1.48569700	-0.08235400
C	4.21512800	-0.66721600	-0.21705700
C	4.22277000	0.66921200	-0.10420300

B	2.89088100	1.46870600	0.16702200
N	0.28504200	1.10121000	0.52634200
N	0.27214100	-1.15408600	0.33584300
H	2.88043800	-2.67557500	-0.14806200
H	5.15231500	-1.18791600	-0.39995700
H	5.16598400	1.20253100	-0.19810000
H	2.91089700	2.65260600	0.30174500
C	-0.17060200	2.41953500	0.16593100
H	-1.09725900	2.64775200	0.69397900
H	0.57786400	3.15566900	0.44987300
H	-0.35721100	2.50369300	-0.91472900
C	-0.19809200	-2.38800900	-0.24018200
H	-1.12779200	-2.69103600	0.24297700
H	-0.38459700	-2.28756300	-1.31946800
H	0.54169300	-3.16979400	-0.08446300
H	-0.97243500	0.08914800	-0.85263000
H	-1.46554400	-0.05311300	0.86503300

Compounds in D₀

AlH2.anion

-805.72354910 a.u.

C	0.55786900	-0.33530500	0.03347300
Al	2.00257700	1.11896200	-0.15283200
C	3.39694300	-0.30319800	-0.15074900
C	2.74485300	-1.49445100	0.00758000
C	1.31691500	-1.54053200	0.10202700
H	0.86903400	-2.51864000	0.25321100
H	3.27135900	-2.45025200	0.07194700
H	4.48219000	-0.33896600	-0.21563600
H	2.07993300	2.14510700	1.11128000
H	1.88889300	1.98723700	-1.52565100
C	-0.81216300	-0.34408300	0.05087300
C	-2.90468400	0.58223200	-0.51016200
N	-1.62371200	0.80284100	0.15999100
C	-1.76959800	-1.54497700	-0.01094900
C	-3.15943900	-0.88414200	-0.14785100
H	-3.78775600	-1.38604000	-0.88809700
H	-3.68291500	-0.91567300	0.81122600
C	-1.01937000	2.10875000	0.05093800
H	-0.25736200	2.22391400	0.82019500
H	-0.53622500	2.27349300	-0.92020200
H	-1.78084600	2.87416600	0.20735800
C	-2.78772800	0.79662900	-2.02584500
H	-3.69959400	0.47786700	-2.53686800
H	-2.62264900	1.85266100	-2.25010000
H	-1.94073600	0.23783500	-2.42602300
C	-4.00682700	1.47634100	0.04928900

H	-4.97865100	1.13242400	-0.31356000
H	-4.00328300	1.43289400	1.13962600
H	-3.88777300	2.51593600	-0.26054400
C	-1.51046400	-2.45669900	-1.21685300
H	-0.50234300	-2.86353800	-1.20999300
H	-2.22446600	-3.28674200	-1.21020500
H	-1.63683300	-1.91084900	-2.15250800
C	-1.72701100	-2.36536600	1.28432400
H	-1.87483800	-1.70855700	2.14345100
H	-2.52361700	-3.11748700	1.28128300
H	-0.77319600	-2.87404800	1.41205800

AlH.neutral

-805.08884901 a.u.

C	0.57956400	-0.28903000	-0.02735800
Al	2.00028600	1.05832100	0.00027600
C	3.42252300	-0.21620500	-0.04259200
C	2.77014100	-1.43124100	-0.07595100
C	1.35062500	-1.49582200	-0.06750600
H	0.90078000	-2.47800200	-0.10834400
H	3.31094100	-2.37446800	-0.11163200
H	4.50440800	-0.20590600	-0.04931300
H	1.98596300	2.63430500	0.05308500
C	-0.80277300	-0.29623700	-0.03266700
C	-2.99277700	0.61483900	-0.28709800
N	-1.56683100	0.82500400	-0.00030400
C	-1.73705500	-1.51046500	-0.09257800
C	-3.14036600	-0.87797000	0.02021700
H	-3.85940200	-1.35785900	-0.64526400
H	-3.50839200	-0.99117800	1.04173000
C	-0.99510700	2.14090600	-0.05718000
H	-0.35359600	2.32150100	0.80825400
H	-0.38275000	2.27551100	-0.95711000
H	-1.78710400	2.88550200	-0.05857100
C	-3.29340500	0.95537600	-1.74879000
H	-4.34369100	0.76201500	-1.97293800
H	-3.09599200	2.01084100	-1.94662700
H	-2.67819500	0.36291900	-2.42531800
C	-3.88332800	1.44958600	0.62910800
H	-3.84976000	2.51186500	0.38424400
H	-4.91836500	1.12208400	0.51814700
H	-3.58870500	1.31822300	1.67083300
C	-1.58770300	-2.26211300	-1.42178800
H	-0.58515100	-2.66387100	-1.55042100
H	-2.29837800	-3.09118700	-1.44989300
H	-1.79315400	-1.61205000	-2.27222300
C	-1.53812500	-2.47068200	1.08611400
H	-0.61369300	-3.03791800	1.02255500
H	-1.53379600	-1.92207700	2.02918700

H	-2.36777300	-3.18154500	1.10853300
---	-------------	-------------	------------

AsH2.cation

-2798.90806276 a.u.

C	0.20665400	-0.57575600	-0.12596100
As	1.36378300	0.89896800	0.22855900
C	2.89289300	-0.17531500	0.22943400
C	2.46839200	-1.45267600	-0.03401600
C	1.08941400	-1.68650600	-0.20752700
H	0.73100600	-2.67560000	-0.43967100
H	3.17566200	-2.26782500	-0.11696600
H	3.90371200	0.16485100	0.37349300
H	1.39516100	2.04664700	-0.74855000
H	1.05029900	1.58772700	1.53284500
C	-1.18928000	-0.61393000	-0.11822200
C	-3.44962500	0.13131300	-0.13311300
N	-1.99714400	0.42940800	-0.27264100
C	-2.01509000	-1.88611400	0.05851600
C	-3.40918200	-1.31054700	0.38475500
H	-4.20239300	-1.91701300	-0.05107900
H	-3.55019300	-1.30733500	1.46664100
C	-1.56591600	1.74851900	-0.68295500
H	-1.09676300	2.30182500	0.13561300
H	-0.88075500	1.67155900	-1.52828200
H	-2.43041100	2.32383200	-1.00071100
C	-4.15255200	0.26124700	-1.48330800
H	-5.20181700	-0.00855700	-1.36363000
H	-4.12284400	1.28428800	-1.85972500
H	-3.71461400	-0.39548800	-2.23309900
C	-4.08084500	1.07775400	0.88221100
H	-4.11273700	2.10586200	0.51894900
H	-5.10869400	0.76555400	1.06947600
H	-3.53854700	1.05196900	1.82809700
C	-2.03269000	-2.68176900	-1.25564900
H	-1.04723200	-3.06590700	-1.51401700
H	-2.70484200	-3.53349300	-1.14355400
H	-2.38417800	-2.07879500	-2.09182300
C	-1.55015500	-2.77316600	1.21516700
H	-0.63697400	-3.32059900	0.99610900
H	-1.39152500	-2.18696900	2.12138200
H	-2.32984000	-3.50795900	1.42158300

AsH.neutral

-2798.55014316 a.u.

C	0.19337100	-0.59636900	-0.06232100
As	1.37297500	0.94318800	-0.49304000
C	2.83190000	-0.31008200	-0.55003400
C	2.41389900	-1.54663600	-0.16610900
C	1.03383300	-1.72495300	0.08504100

H	0.66804500	-2.68729400	0.40721600	H	-3.56260000	-1.43220500	-0.40315000
H	3.10199700	-2.37608000	-0.04177200	H	-3.18011600	-0.80469600	1.20383000
H	3.86104200	-0.03962600	-0.73070000	C	-0.83528400	2.19739900	-0.32813500
H	1.05074900	0.96352300	-1.99295000	H	0.04398700	2.45490100	0.25233000
C	-1.18509600	-0.61910300	0.03482300	H	-0.53590300	2.19236700	-1.38452300
C	-3.37083500	0.14242800	-0.41971700	H	-1.60170700	2.96009100	-0.17452700
N	-2.02907900	0.46228300	0.09292800	C	-2.82582400	0.66219500	-1.88330900
C	-2.04536500	-1.88887100	0.06531000	H	-3.76012900	0.20825300	-2.22265200
C	-3.48457200	-1.33141000	-0.02374400	H	-2.81374800	1.70277900	-2.21468000
H	-4.09604300	-1.89250000	-0.73184600	H	-1.98833900	0.15340100	-2.36197900
H	-3.96562900	-1.39417600	0.95415000	C	-3.75391900	1.48338100	0.28656300
C	-1.58433300	1.83217700	0.11798500	H	-4.75224000	1.08639000	0.08382700
H	-0.83276200	1.96270800	0.89366800	H	-3.60138500	1.52097900	1.36611300
H	-1.15866900	2.16571600	-0.83601500	H	-3.71672800	2.50058800	-0.10707500
H	-2.42937000	2.47501400	0.35587400	C	-1.30986400	-2.40801700	-1.08573500
C	-3.41561400	0.34864200	-1.93633100	H	-0.28884500	-2.74785500	-1.24051000
H	-4.38608200	0.04842500	-2.33541100	H	-1.95076000	-3.28223800	-0.92719600
H	-3.25931500	1.40049700	-2.18454300	H	-1.63481600	-1.91738500	-2.00346800
H	-2.63834800	-0.23551100	-2.43050600	C	-1.16826900	-2.24081800	1.41391700
C	-4.45994400	0.97202600	0.25005700	H	-0.19158600	-2.72057700	1.41687700
H	-4.47538400	2.00301400	-0.10522800	H	-1.20740000	-1.56109400	2.26694700
H	-5.43224000	0.53412000	0.01902500	H	-1.93704600	-3.01062500	1.54541600
H	-4.32995700	0.97090200	1.33329700				
C	-1.76259100	-2.82271100	-1.11646100	BH.neutral			
H	-0.73767600	-3.18645400	-1.11755200	-587.52452842 a.u.			
H	-2.43266100	-3.68368800	-1.06402600	C	1.82168100	-0.05838200	-0.04405200
H	-1.93541300	-2.31828600	-2.06759700	B	2.89432200	1.08548300	-0.04348600
C	-1.89519100	-2.64723500	1.39102600	C	4.24333300	0.34343800	-0.03740000
H	-0.92536500	-3.12789300	1.49608900	C	3.97923500	-1.01485600	-0.04664000
H	-2.03066100	-1.96736200	2.23366800	C	2.59533400	-1.27102700	-0.03504300
H	-2.66211100	-3.42352200	1.45151400	H	2.19939200	-2.27510800	-0.06979300
				H	4.71882900	-1.80611500	-0.06407600
BH2.anion				H	5.25233800	0.73481500	-0.02733200
-588.14594019 a.u.				H	2.74426900	2.26366800	0.00380900
C	0.86575600	-0.21037800	-0.04946500	C	0.43731300	-0.05258000	0.01787600
B	1.97770100	1.03070000	-0.04727300	C	-1.79052500	0.81132100	-0.01800600
C	3.33986200	0.17826100	-0.07017100	N	-0.34569100	1.01523900	-0.21529700
C	3.04785800	-1.15257700	-0.06483700	C	-0.46578200	-1.24832700	0.33431900
C	1.64332000	-1.40347100	-0.04358200	C	-1.82076400	-0.57613000	0.63097200
H	1.26156000	-2.41704900	-0.01722900	H	-2.65870500	-1.17506800	0.27176700
H	3.77259000	-1.96549500	-0.07164700	H	-1.93456700	-0.46227700	1.71076700
H	4.36921800	0.52896400	-0.08478700	C	0.14357900	2.29080300	-0.68086000
H	1.89616800	1.70855100	0.97700100	H	0.57144000	2.87891000	0.13250000
H	1.88843800	1.78017300	-1.01216400	H	0.92293200	2.13582000	-1.42686900
C	-0.51094600	-0.22748800	0.00528700	H	-0.67821500	2.84727700	-1.12677500
C	-2.70080500	0.58220400	-0.35331400	C	-2.53770200	0.85020000	-1.35296400
N	-1.34935100	0.91595700	0.10121500	H	-3.59972400	0.66791000	-1.18247500
C	-1.41901500	-1.45892200	0.11727200	H	-2.44320100	1.82398900	-1.83501300
C	-2.83451500	-0.84942600	0.16762000	H	-2.16351400	0.09167600	-2.03874800

C	-2.35868800	1.87511200	0.91930200	H	-0.05562900	-2.84159800	1.24021200
H	-2.34662100	2.86525800	0.46124800	H	-0.96843900	-1.70019100	2.22486500
H	-3.39441300	1.63217700	1.16236100	H	-1.78296700	-3.09368100	1.49702200
H	-1.78456900	1.91225400	1.84590200				
C	-0.56573800	-2.17193000	-0.88760100	CH.anion			
H	0.39373900	-2.62939500	-1.12135900	-600.78965017 a.u.			
H	-1.28576200	-2.96766700	-0.68424100	C	0.85754100	-0.31494800	-0.19321600
H	-0.89592800	-1.62983600	-1.77345400	C	1.73455000	0.74939700	0.17026100
C	-0.03220800	-2.04500700	1.56698400	C	3.05340400	0.29895400	0.06246400
H	0.84619700	-2.65893800	1.38921900	C	3.02566600	-1.04381500	-0.37488800
H	0.18748400	-1.37579200	2.39987000	C	1.69012300	-1.42340400	-0.52836700
H	-0.84910100	-2.70691400	1.86458700	H	1.34521200	-2.37988500	-0.89852900
				H	3.88878600	-1.66496000	-0.57704800
CH2.neutral				H	3.94109400	0.87545200	0.28945700
-601.36978960 a.u.				H	1.42020100	1.71111900	0.55413500
C	0.87220500	-0.24862800	-0.07721800	C	-0.57543400	-0.31173700	-0.15714500
C	1.80753700	0.95770900	0.00616500	C	-2.74141200	0.60550900	-0.00447700
C	3.17972800	0.35328900	-0.00751900	N	-1.30916400	0.91254900	-0.11918500
C	3.07531000	-0.99430200	-0.08768100	C	-1.41044800	-1.41043500	0.48432200
C	1.70812000	-1.38689400	-0.12349800	C	-2.71387700	-0.66995700	0.84556900
H	1.38693200	-2.41202800	-0.19005200	H	-3.60764300	-1.28168500	0.69380100
H	3.90481000	-1.68705900	-0.12144100	H	-2.68164700	-0.38165500	1.89965500
H	4.08986200	0.93206100	0.03022000	C	-0.96934600	1.88334300	-1.14008700
H	1.63365100	1.52560700	0.92660300	H	0.07863500	2.15384800	-1.05331500
H	1.68282700	1.65585700	-0.82446300	H	-1.12068500	1.48372300	-2.15515100
C	-0.50866100	-0.24646500	-0.02923300	H	-1.57844500	2.78225800	-1.01701200
C	-2.74364000	0.52146100	-0.22728700	C	-3.40617900	0.35877100	-1.36909600
N	-1.32835300	0.87281200	-0.00271600	H	-4.39784700	-0.07909200	-1.23496300
C	-1.37006100	-1.50071500	0.10211700	H	-3.52253000	1.29319800	-1.92280700
C	-2.78333900	-0.91644600	0.29014800	H	-2.80060500	-0.31667400	-1.97424800
H	-3.54569100	-1.51129700	-0.21523800	C	-3.48324400	1.72815500	0.71591900
H	-3.02777400	-0.89668200	1.35427800	H	-4.52094200	1.43701400	0.90223000
C	-0.89258800	2.15562900	-0.51274400	H	-2.99690400	1.94074100	1.66842000
H	-0.11434700	2.58700500	0.10965300	H	-3.49681700	2.64436800	0.12149100
H	-0.52116400	2.07983500	-1.54180200	C	-1.68218400	-2.59648900	-0.45408800
H	-1.73528200	2.84355400	-0.50233300	H	-0.74136300	-3.05497500	-0.75831000
C	-3.10700700	0.62441400	-1.71343600	H	-2.28750700	-3.35640300	0.05423800
H	-4.10803900	0.22609800	-1.88547600	H	-2.20946700	-2.28284000	-1.35536000
H	-3.10138500	1.66427400	-2.04498400	C	-0.74522500	-1.95494200	1.75589000
H	-2.40106100	0.07203700	-2.33305500	H	0.18660500	-2.46398000	1.50752400
C	-3.67414900	1.41367800	0.58846600	H	-0.49893900	-1.13228500	2.42963100
H	-4.69267100	1.02494400	0.53042200	H	-1.41309700	-2.65292900	2.27353700
H	-3.36472700	1.42618200	1.63368700				
H	-3.69588800	2.43896200	0.21647300	GaH2.anion			
C	-1.31256900	-2.38834400	-1.14955700	-2488.14133213 a.u.			
H	-0.30231100	-2.73877900	-1.35031900	C	0.12013200	-0.58595100	0.04555200
H	-1.95464800	-3.26070900	-1.00533600	Ga	1.57659500	0.90481400	-0.23844500
H	-1.65920900	-1.85927200	-2.03602300	C	2.96519400	-0.57738400	-0.20113600
C	-1.01266300	-2.33477200	1.33854900	C	2.30709000	-1.75201700	0.01531000

H	-3.67256300	1.42880900	-2.09645300
H	-3.10619400	-0.20736100	-2.43445100
C	-4.34764900	1.07924500	0.52662800
H	-4.35693700	2.11645100	0.18892400
H	-5.36997100	0.70395500	0.45336600
H	-4.04181500	1.05271800	1.57281100
C	-1.96731700	-2.68653900	-1.27466500
H	-0.95838100	-3.06101800	-1.43121300
H	-2.64247300	-3.54234100	-1.20182600
H	-2.24487500	-2.11341900	-2.15844500
C	-1.79075800	-2.71292500	1.23327600
H	-0.84043000	-3.23648700	1.16933900
H	-1.77826600	-2.10136000	2.13664900
H	-2.58160800	-3.46001200	1.33626800

GeH.anion

-2639.69055653 a.u.

C	0.15764600	-0.58480600	0.01171100
Ge	1.52492300	0.93855400	0.35001200
C	2.87010800	-0.50919200	0.47096500
C	2.33689100	-1.68205400	0.00762000
C	0.94001900	-1.74606900	-0.22963500
H	0.52814600	-2.66232800	-0.64009700
H	2.94209000	-2.56503000	-0.20331100
H	3.94307600	-0.42189900	0.61463800
H	1.20699600	1.22859900	1.90132700
C	-1.21811700	-0.60421400	-0.01373000
C	-3.29351000	0.19379200	0.73634100
N	-2.08050500	0.51400400	-0.01972200
C	-2.12991300	-1.84078400	-0.02183200
C	-3.52698300	-1.24998500	0.28285500
H	-4.13258200	-1.23260500	-0.62705600
H	-4.06825500	-1.83161100	1.03338400
C	-1.54844600	1.84845600	0.10264800
H	-1.05257400	2.02989600	1.06466700
H	-0.80906400	2.01646800	-0.67734200
H	-2.35734500	2.57050000	-0.02297600
C	-4.46827800	1.08322000	0.34386400
H	-5.39446200	0.66600300	0.74661900
H	-4.36443500	2.09655300	0.73563300
H	-4.54996900	1.13363900	-0.74344600
C	-3.04983300	0.29191100	2.24862800
H	-2.89435200	1.33164500	2.54459700
H	-3.90402900	-0.09783100	2.80810000
H	-2.15513200	-0.26831700	2.52482800
C	-2.15981000	-2.50870300	-1.40307900
H	-1.20331100	-2.96437600	-1.65359200
H	-2.93093700	-3.28680100	-1.43199200
H	-2.39065800	-1.76497300	-2.16805800

C	-1.76295000	-2.87309400	1.05028500
H	-2.46581700	-3.71157700	1.00858200
H	-0.75329600	-3.25396100	0.91798100
H	-1.81877000	-2.43263100	2.04678600

lnH2.anion

-753.33472817 a.u.

C	0.63612500	0.50901800	-0.00843300
ln	2.31828100	-0.96062100	0.50673900
C	3.48108500	0.91189000	0.69769700
C	2.64936300	1.94853400	0.39284800
C	1.26404200	1.78008200	0.05697900
H	0.73013800	2.69503600	-0.18870400
H	3.00994700	2.98075300	0.38820600
H	4.51214800	1.16028600	0.93752200
H	2.78890200	-2.08574200	-0.81928700
H	2.00454500	-1.88886900	2.01946600
C	-0.71349300	0.37419300	-0.19556000
C	-2.71300400	-0.83092100	0.09871200
N	-1.37699200	-0.83293300	-0.49748400
C	-1.80931300	1.45172800	-0.12770700
C	-3.11843000	0.62842700	-0.13508300
H	-3.83208100	0.97765500	0.61535300
H	-3.60049100	0.70129600	-1.11342100
C	-0.64565100	-2.07358700	-0.52352400
H	0.19640500	-1.98380400	-1.20726700
H	-0.24807800	-2.36278300	0.45891100
H	-1.29817100	-2.86982600	-0.88495700
C	-2.65725900	-1.18302400	1.59137000
H	-3.63379100	-1.04297200	2.06149400
H	-2.35909500	-2.22464800	1.72835400
H	-1.92260700	-0.55912600	2.10262100
C	-3.66536600	-1.78130000	-0.61926300
H	-4.69154000	-1.58154800	-0.30135700
H	-3.59732800	-1.63219100	-1.69832300
H	-3.44748000	-2.82684600	-0.39469200
C	-1.73498200	2.29906100	1.14702600
H	-0.78944800	2.83035700	1.22590900
H	-2.55067500	3.02926200	1.15224600
H	-1.83416200	1.67349700	2.03520400
C	-1.77965700	2.35987600	-1.36374700
H	-2.65784700	3.01492600	-1.37297900
H	-0.88702800	2.98259800	-1.38878300
H	-1.79292900	1.75208000	-2.27035100

lnH.neutral

-752.70390120 a.u.

C	-0.18171900	-0.74278400	-0.04032100
ln	1.34478300	0.83934000	-0.02507500

C	2.76040200	-0.74585800	-0.07668400	N	-1.36132200	0.74878500	-0.19629400
C	2.02724800	-1.90427600	-0.09320000	C	-1.32284900	-1.59424200	0.09066100
C	0.60209500	-1.92888900	-0.07527200	C	-2.73348000	-1.04999100	0.39753700
H	0.14978200	-2.91062700	-0.10167400	H	-3.50760400	-1.67832700	-0.04177600
H	2.52346300	-2.87237000	-0.12302500	H	-2.88514800	-1.04333000	1.47807600
H	3.84057600	-0.79905800	-0.09150000	C	-0.98110200	2.04703100	-0.71476000
H	1.28354700	2.56383900	0.02338100	H	-0.41212000	2.63969800	0.00558800
C	-1.56274000	-0.76809600	-0.04350300	H	-0.42390900	1.94602300	-1.65169500
C	-3.77139900	0.09181900	-0.32129300	H	-1.87803600	2.61801300	-0.93432000
N	-2.35838900	0.33898100	0.00025300	C	-3.45006300	0.47798700	-1.51225300
C	-2.47379700	-2.00365600	-0.10511800	H	-4.48422600	0.13997000	-1.44662800
C	-3.89034900	-1.40082700	-0.00710100	H	-3.46964100	1.50275700	-1.88465700
H	-4.59438300	-1.89944100	-0.67502300	H	-2.93417100	-0.14356100	-2.24240300
H	-4.26395600	-1.51474400	1.01239900	C	-3.53246400	1.30611400	0.84737200
C	-1.83621200	1.67471500	-0.05521200	H	-3.58555700	2.33262200	0.48149300
H	-1.19976500	1.87985000	0.80848600	H	-4.55658800	0.95458900	0.97727000
H	-1.24001500	1.84302300	-0.96110900	H	-3.04256500	1.30232600	1.82135800
H	-2.65754300	2.38677300	-0.04580200	C	-1.29159400	-2.40047900	-1.21560700
C	-4.04377700	0.41582000	-1.79264500	H	-0.28539900	-2.75111400	-1.44396600
H	-5.08073200	0.18757900	-2.04459700	H	-1.93601200	-3.27461000	-1.11285400
H	-3.87542600	1.47645100	-1.99025300	H	-1.64191900	-1.81740100	-2.06585300
H	-3.39107200	-0.15852900	-2.44937800	C	-0.85232300	-2.46744000	1.25584600
C	-4.70885100	0.90685600	0.56576000	H	0.08608200	-2.97809500	1.05279100
H	-4.70889900	1.96678900	0.30870300	H	-0.73529100	-1.87881400	2.16674700
H	-5.72914100	0.54141900	0.43749400	H	-1.60579100	-3.23378900	1.44371000
H	-4.43186000	0.79774000	1.61489000				
C	-2.30404600	-2.76416200	-1.42697500	NH.neutral			
H	-1.29340900	-3.14619800	-1.55049500	-617.43488240 a.u.			
H	-2.99731400	-3.60818500	-1.44930100	C	0.85193400	-0.33597300	-0.11238700
H	-2.52132400	-2.12666900	-2.28388200	N	1.58938100	0.82112400	0.05725100
C	-2.26759100	-2.95141500	1.08309100	C	2.93044300	0.54259800	0.01710100
H	-1.33318100	-3.50338700	1.03263200	C	3.07306700	-0.80132900	-0.21414500
H	-2.28070100	-2.39458500	2.02128900	C	1.77856500	-1.36231000	-0.29666000
H	-3.08518900	-3.67631600	1.10486300	H	1.53684800	-2.38996900	-0.50969700
				H	4.00910700	-1.32191700	-0.32857700
NH2.cation				H	3.66522700	1.31889300	0.14292200
-617.78797580 a.u.				H	1.18564100	1.68094900	0.38595900
C	0.85282200	-0.27523400	-0.07505600	C	-0.56529200	-0.35175300	-0.06685400
N	1.63431300	0.99705200	0.09466400	C	-2.74206300	0.56637900	0.09928400
C	3.05823500	0.59510100	0.12830100	N	-1.31683800	0.81705300	-0.21281400
C	3.11084400	-0.74759100	-0.00766200	C	-1.40518700	-1.49286100	0.45687200
C	1.81602800	-1.29550600	-0.12605100	C	-2.67621000	-0.74081900	0.90335500
H	1.60200500	-2.33746200	-0.27737800	H	-3.57910900	-1.34023400	0.77502000
H	4.02729300	-1.31611000	-0.03169600	H	-2.58580600	-0.49898600	1.96468400
H	3.80184400	1.36516300	0.22658800	C	-1.05101800	1.69435500	-1.34079100
H	1.46543200	1.66606900	-0.66015100	H	0.00557900	1.94117700	-1.39586000
H	1.36386900	1.45682100	0.96852500	H	-1.32835900	1.22928000	-2.29447900
C	-0.52922800	-0.30313200	-0.06808300	H	-1.61411400	2.62089200	-1.22460800
C	-2.80626600	0.38738100	-0.12832900	C	-3.29711200	1.71162800	0.94100800

C	3.12723200	0.08247000	-0.57779500	N	-2.32857800	0.24658300	-0.26862800
C	2.82455900	-1.20325000	-0.23404200	C	-2.37473400	-2.07110800	0.04564000
C	1.46349500	-1.45929900	0.03256000	C	-3.76060600	-1.47981300	0.37835600
H	1.12994600	-2.43962400	0.33262300	H	-4.56252900	-2.07248600	-0.06065400
H	3.57229900	-1.98330700	-0.15075000	H	-3.89996300	-1.48304300	1.46050600
H	4.12285800	0.45299800	-0.76859800	C	-1.88139000	1.56831900	-0.64234300
H	1.34234000	1.31327300	-1.78315100	H	-1.42943000	2.10443800	0.19956500
C	-0.77428300	-0.37300600	0.03000100	H	-1.17769600	1.50810100	-1.47436000
C	-2.96473000	0.39218100	-0.38508600	H	-2.73416500	2.15760700	-0.96710600
N	-1.62340900	0.69969700	0.13549600	C	-4.48880300	0.11709600	-1.47451600
C	-1.62259700	-1.64839800	0.01159600	H	-5.54234200	-0.13515000	-1.35384300
C	-3.06650600	-1.09890600	-0.05347700	H	-4.44193700	1.14214400	-1.84398400
H	-3.67331200	-1.63333300	-0.78577200	H	-4.06412700	-0.54184900	-2.22995800
H	-3.54730200	-1.20849700	0.92041300	C	-4.40100200	0.91097700	0.89796300
C	-1.18916600	2.07059400	0.23555800	H	-4.42526700	1.94236800	0.54339600
H	-0.42305000	2.15878100	1.00236200	H	-5.43080900	0.60703800	1.08802700
H	-0.78272100	2.46509600	-0.70287300	H	-3.85441700	0.87225200	1.84102900
H	-2.03491000	2.68951100	0.52844200	C	-2.40669800	-2.85443700	-1.27569800
C	-3.01684700	0.66251800	-1.89142700	H	-1.42849000	-3.25356400	-1.53868400
H	-3.98766300	0.37525000	-2.29915500	H	-3.09387800	-3.69516800	-1.17152000
H	-2.86576500	1.72457500	-2.09554300	H	-2.74771100	-2.23710300	-2.10574400
H	-2.23949400	0.10250500	-2.41273000	C	-1.92372900	-2.97591000	1.19395100
C	-4.05685400	1.18494900	0.32306400	H	-1.01846500	-3.53464100	0.97080600
H	-4.07832100	2.23050300	0.01352000	H	-1.75721600	-2.40024700	2.10550600
H	-5.02723000	0.75217000	0.07503000	H	-2.71442800	-3.70090700	1.39331200
H	-3.92436200	1.13699000	1.40496500				
C	-1.33183900	-2.53297300	-1.20545200	SbH.neutral			
H	-0.30317400	-2.88626600	-1.21923200	-802.82119646 a.u.			
H	-1.99344000	-3.40185400	-1.18720300	C	-0.16448600	-0.78388700	-0.16785800
H	-1.50898000	-1.99335000	-2.13635200	Sb	1.18759100	0.91877100	-0.34643900
C	-1.46217500	-2.45738600	1.30583300	C	2.61566700	-0.59905900	-0.67713200
H	-0.48587700	-2.92927700	1.38929200	C	2.03842900	-1.82244100	-0.52020300
H	-1.60443400	-1.81375300	2.17535000	C	0.64713400	-1.94013500	-0.27676500
H	-2.21911000	-3.24516400	1.33578700	H	0.23916900	-2.93172100	-0.14992900
				H	2.62999600	-2.73247000	-0.57175100
SbH2.cation				H	3.67726300	-0.46859600	-0.82831600
-803.16665404 a.u.				H	0.80120400	1.22094400	-1.99999800
C	-0.13455700	-0.78125900	-0.12652900	C	-1.54057400	-0.82098400	-0.06298400
Sb	1.17480200	0.80003600	0.26182600	C	-3.72576000	0.03898700	-0.32233700
C	2.70623200	-0.55606800	0.21235200	N	-2.37214000	0.23596000	0.22042800
C	2.12541700	-1.76678700	-0.06222300	C	-2.42176700	-2.06150700	-0.27540400
C	0.72650800	-1.90497500	-0.21861100	C	-3.85369100	-1.48190300	-0.22258800
H	0.33023000	-2.87833000	-0.45989400	H	-4.48655600	-1.88602200	-1.01394800
H	2.74782400	-2.64720000	-0.17227900	H	-4.31729900	-1.73070900	0.73391300
H	3.75889800	-0.36483200	0.33061100	C	-1.90208800	1.57122500	0.47422900
H	0.88332800	1.57129700	1.73015500	H	-1.14616400	1.55628100	1.25761200
H	1.25954100	2.09088400	-0.81702200	H	-1.47844400	2.05514500	-0.41581600
C	-1.52939600	-0.80858400	-0.12030900	H	-2.73193700	2.18217200	0.82328600
C	-3.78330000	-0.03358700	-0.12786900	C	-4.79205700	0.73141100	0.51850300

H	-4.79722000	1.81278100	0.37650800	C	-1.56771600	-2.87144100	1.14170400
H	-5.77449700	0.36074500	0.22190500	H	-0.65769400	-3.43149600	0.94064100
H	-4.64585900	0.51218900	1.57715900	H	-1.41200600	-2.28971300	2.05120700
C	-3.79119600	0.54241500	-1.76695800	H	-2.36845800	-3.59208100	1.32444300
H	-4.76920200	0.32974000	-2.20211200				
H	-3.63350600	1.62233500	-1.80487200	SiH2.neutral			
H	-3.02454000	0.06670000	-2.37959800	-852.75629864 a.u.			
C	-2.17302300	-2.73622000	-1.62901000	C	0.60603500	-0.32244200	-0.06372300
H	-1.15456000	-3.10477100	-1.72568600	Si	1.86555600	1.08118500	0.09205600
H	-2.85636200	-3.58101900	-1.74089200	C	3.31744700	-0.05236500	0.08710600
H	-2.35348300	-2.04542200	-2.45304300	C	2.82366200	-1.32515700	-0.01806200
C	-2.26679900	-3.07785600	0.86427600	C	1.41636500	-1.49843300	-0.08599700
H	-1.30888900	-3.59203200	0.84898300	H	1.01442200	-2.49599200	-0.17184000
H	-2.37146900	-2.58230700	1.83076100	H	3.46632000	-2.19960600	-0.05196200
H	-3.05258300	-3.83289100	0.78097500	H	4.37703400	0.14972100	0.14069700
				H	1.86340200	2.07268700	-1.01040200
Se.neutral				H	1.70480200	1.86201000	1.34544700
-2963.65726630 a.u.				C	-0.77310300	-0.34018200	-0.05506400
C	0.24656000	-0.63046200	0.00543100	C	-3.00017500	0.47238100	-0.30142100
Se	1.20840200	0.96309700	0.46238500	N	-1.57719400	0.76685400	-0.07580400
C	2.75592700	-0.07484000	0.56132500	C	-1.66285400	-1.58519900	0.00023900
C	2.49491700	-1.38189400	0.28167000	C	-3.07736400	-0.98863600	0.14662400
C	1.15704300	-1.69718500	-0.01899900	H	-3.81944100	-1.54951300	-0.42342200
H	0.86043400	-2.69327000	-0.30891800	H	-3.37455600	-1.01725300	1.19679800
H	3.27675200	-2.13024700	0.26913300	C	-1.07346200	2.07949700	-0.40242100
H	3.70950500	0.37636500	0.77793800	H	-0.38078700	2.43657400	0.35965900
C	-1.13514800	-0.69849200	-0.15720000	H	-0.56554000	2.08261700	-1.37145600
C	-3.39792500	0.05242600	-0.30422900	H	-1.90158400	2.78320500	-0.43950000
N	-1.96692200	0.35105200	-0.45106800	C	-3.36638800	0.66393200	-1.77660900
C	-1.97204700	-1.96178300	-0.01961200	H	-4.40403000	0.37282100	-1.94712700
C	-3.36634500	-1.36914900	0.27474000	H	-3.26096100	1.71023300	-2.06946900
H	-4.16507600	-1.99188600	-0.13120600	H	-2.72658300	0.06690800	-2.42532100
H	-3.50321000	-1.31664400	1.35679700	C	-3.89700400	1.35275600	0.56498000
C	-1.53901300	1.63693200	-0.94381900	H	-3.89848400	2.39247800	0.23496300
H	-1.26372300	2.33060100	-0.14303800	H	-4.92490000	0.99048700	0.50561200
H	-0.68260300	1.51736100	-1.60666100	H	-3.57468900	1.31480900	1.60583400
H	-2.34900800	2.09119000	-1.51266900	C	-1.55849800	-2.41440400	-1.28745800
C	-4.13222500	0.10803800	-1.64758300	H	-0.55159300	-2.79272600	-1.44851800
H	-5.17353400	-0.18401700	-1.50383500	H	-2.23862400	-3.26691900	-1.22339100
H	-4.13231500	1.11469600	-2.06714000	H	-1.83298000	-1.82969600	-2.16460000
H	-3.68340800	-0.56674900	-2.37472800	C	-1.37369700	-2.46839600	1.21929900
C	-4.04673500	1.03756500	0.66760300	H	-0.42918900	-3.00063900	1.14326100
H	-4.04867800	2.05092900	0.26102500	H	-1.34881800	-1.86624600	2.12868000
H	-5.08274600	0.75065400	0.85710500	H	-2.17104600	-3.20875700	1.32023900
H	-3.50738900	1.04414500	1.61556400				
C	-1.96620400	-2.76351100	-1.32907000	SiH.anion			
H	-0.96984500	-3.15321900	-1.53930200	-852.15892506 a.u.			
H	-2.65453000	-3.60926400	-1.25555400	C	0.61921800	-0.32740800	0.03473100
H	-2.26478700	-2.14850300	-2.17732900	Si	1.92073900	1.10498800	0.13257600

C	3.30735900	-0.10054200	-0.05534400
C	2.80067300	-1.36952100	0.14820000
C	1.39981000	-1.51388200	0.19905500
H	0.97906000	-2.48778900	0.41554100
H	3.43257700	-2.24476400	0.29927400
H	4.37772700	0.07326500	-0.05669800
H	1.81793000	1.90750000	-1.14413500
C	-0.76215200	-0.34097900	-0.01624800
C	-2.87625600	0.45302900	-0.68268800
N	-1.61447200	0.79112200	-0.01592600
C	-1.66985200	-1.57598600	0.00543000
C	-3.08096100	-0.98054000	-0.19028900
H	-3.69029100	-1.56978200	-0.88046200
H	-3.60417500	-0.94254700	0.76869200
C	-1.06121300	2.09085100	-0.31111300
H	-0.31710300	2.35442300	0.43945000
H	-0.57080300	2.12614100	-1.29201900
H	-1.85600700	2.83767400	-0.27858900
C	-2.74560100	0.52958700	-2.21082200
H	-3.62513600	0.10262800	-2.69880700
H	-2.64736200	1.56786100	-2.53545300
H	-1.85714000	-0.00850800	-2.54407100
C	-4.02211400	1.34886300	-0.22205200
H	-4.97339400	0.93446900	-0.56549800
H	-4.03452100	1.40327700	0.86761600
H	-3.93982400	2.36076600	-0.62260800
C	-1.62072100	-2.29294400	1.36235600
H	-2.39492200	-3.06703700	1.40802600
H	-0.65474900	-2.75942300	1.54385500
H	-1.80125300	-1.57485500	2.16435900
C	-1.36777500	-2.57160800	-1.12324700
H	-0.33384800	-2.90683800	-1.09950700
H	-2.02520300	-3.44275800	-1.03275800
H	-1.54412100	-2.11787300	-2.09925800

S.neutral

-960.27358557 a.u.

C	0.65896000	-0.36322900	-0.03691100
S	1.63885700	1.08591200	0.15910600
C	3.11177700	0.20500600	0.13065400
C	2.88796800	-1.13360700	-0.01374200
C	1.52854400	-1.46816800	-0.10372200
H	1.18952200	-2.48116300	-0.23570500
H	3.68409300	-1.86298900	-0.06322700
H	4.05188100	0.72495400	0.20675400
C	-0.74098000	-0.38706300	-0.05023100
C	-2.98466600	0.32776200	-0.28223100
N	-1.57743800	0.71348900	-0.06629500
C	-1.56644500	-1.66210200	0.08242300

C	-2.99221500	-1.10257000	0.25918100
H	-3.74066400	-1.72250100	-0.23646800
H	-3.23628400	-1.07081700	1.32300000
C	-1.15716500	2.00685500	-0.56698000
H	-0.50082100	2.51445000	0.13701400
H	-0.64146300	1.92025600	-1.52914000
H	-2.03498300	2.63483100	-0.69958200
C	-3.35179600	0.39881400	-1.76909800
H	-4.34488500	-0.02263800	-1.93185400
H	-3.36856800	1.43246300	-2.11855500
H	-2.63592000	-0.14903000	-2.38073100
C	-3.93016900	1.21486500	0.52149200
H	-3.96244700	2.23578200	0.13849400
H	-4.94323900	0.81220200	0.46377400
H	-3.62482100	1.24301600	1.56755300
C	-1.48726900	-2.55809900	-1.16341700
H	-0.47117900	-2.89553600	-1.35751800
H	-2.11461000	-3.44052200	-1.01546200
H	-1.83779800	-2.04188600	-2.05553900
C	-1.19768200	-2.48295000	1.32453800
H	-0.22944900	-2.97004600	1.23257100
H	-1.17084300	-1.84429400	2.20847200
H	-1.95180400	-3.25800800	1.48160600

SnH2.neutral

-777.47204375 a.u.

C	-0.15446000	-0.78342500	-0.09952700
Sn	1.24172900	0.82295800	0.30497600
C	2.71143500	-0.69469200	0.36079600
C	2.06864100	-1.87003700	0.10141000
C	0.65940700	-1.94448200	-0.11237800
H	0.24733600	-2.91941600	-0.33297700
H	2.62461600	-2.80270100	0.04578600
H	3.77995700	-0.65674000	0.51177700
H	1.42175800	2.03256200	-0.91243700
H	0.91161100	1.65502500	1.78078800
C	-1.53098100	-0.80412000	-0.17492900
C	-3.76892200	0.04428200	-0.33998100
N	-2.32245800	0.29384700	-0.36033500
C	-2.43828300	-2.03278100	-0.08249000
C	-3.82462000	-1.40316700	0.16181500
H	-4.62018700	-1.97112000	-0.32296600
H	-4.02809700	-1.39829600	1.23455200
C	-1.81018900	1.59340800	-0.70683000
H	-1.35338800	2.10330100	0.14859000
H	-1.06908800	1.51380000	-1.50491400
H	-2.62495900	2.22244500	-1.05890200
C	-4.38099200	0.20393400	-1.73479500
H	-5.44807900	-0.02074400	-1.69741200

H	-4.27219100	1.22602500	-2.10107100
H	-3.91235900	-0.46679200	-2.45312300
C	-4.47015500	0.99114700	0.63318400
H	-4.44329500	2.02426700	0.28231500
H	-5.51797700	0.70361500	0.73667800
H	-3.99828000	0.94379900	1.61524100
C	-2.41219800	-2.81855200	-1.40086000
H	-1.42528900	-3.23680200	-1.59314300
H	-3.12964800	-3.64126600	-1.35364300
H	-2.67164800	-2.18651200	-2.24960000
C	-2.11222200	-2.96383700	1.08808200
H	-1.21220700	-3.55095500	0.92654400
H	-1.98136400	-2.39257000	2.00818900
H	-2.94373100	-3.65852600	1.23037700

SnH.anion

-776.91585307 a.u.

C	1.51048600	0.18950400	0.24662000
Sn	3.04378400	1.83400300	-0.24832300
C	4.34874500	0.06623100	-0.25586400
C	3.68161300	-1.01554000	0.24244800
C	2.27872400	-0.97962800	0.48748700
H	1.83651400	-1.87815800	0.90953200
H	4.19549000	-1.95111200	0.47653500
H	5.42540400	-0.01079300	-0.38794600
H	2.63470700	1.89915900	-2.01483000
C	0.13956100	0.16430400	0.25168100
C	-1.91197200	0.99057800	-0.53908600
N	-0.71747300	1.28501900	0.25558500
C	-0.78225700	-1.06738800	0.21117200
C	-2.16567900	-0.46218000	-0.12609300
H	-2.68319800	-1.02320000	-0.90814400
H	-2.80176600	-0.46378800	0.76288900
C	-0.17157300	2.61520100	0.18087000
H	0.54943700	2.75587900	0.98340400
H	0.34426100	2.81952500	-0.76725000
H	-0.97487300	3.34309300	0.30675700
C	-3.09076900	1.87896800	-0.15675300
H	-2.96852000	2.90098600	-0.51954400
H	-4.00802500	1.47970000	-0.59623900
H	-3.20357000	1.90238700	0.92868000
C	-1.62617400	1.12198600	-2.04113300
H	-2.46976500	0.75563800	-2.63150500
H	-1.45144500	2.16632300	-2.30849300
H	-0.73025900	0.55946000	-2.30864200
C	-0.38614000	-2.08228300	-0.86636700
H	0.60964100	-2.48537800	-0.69867600
H	-1.10444600	-2.90843900	-0.87372400
H	-0.38913500	-1.61934900	-1.85413400

C	-0.85962900	-1.75731500	1.57939900
H	-1.63942600	-2.52699700	1.57109300
H	0.08305400	-2.22936900	1.85112100
H	-1.10638500	-1.02473000	2.35016400

Te.neutral

-830.01142185 a.u.

C	-0.10052900	-0.83541200	-0.01239800
Te	1.00367300	0.87392400	0.56756600
C	2.56450900	-0.46207900	0.62331900
C	2.14744400	-1.71053600	0.27305000
C	0.79195100	-1.91905100	-0.05388600
H	0.46366300	-2.89162300	-0.39121700
H	2.85073800	-2.53417400	0.22130400
H	3.57730500	-0.17364900	0.85282900
C	-1.47801800	-0.90319000	-0.17524500
C	-3.74289700	-0.14456100	-0.30020200
N	-2.31150800	0.14758100	-0.45679800
C	-2.32280700	-2.16617900	-0.05033700
C	-3.71259700	-1.57272000	0.26113100
H	-4.51625600	-2.18791700	-0.14653100
H	-3.84143500	-1.53279500	1.34469400
C	-1.88281900	1.44300800	-0.91867400
H	-1.62524500	2.12596700	-0.10136200
H	-1.01738600	1.33885800	-1.57250900
H	-2.68609100	1.90639500	-1.49001800
C	-1.91674800	-3.09517700	1.09461600
H	-1.01263100	-3.65920800	0.87955400
H	-1.74992100	-2.52769600	2.01115500
H	-2.72246200	-3.81147700	1.27279800
C	-2.32935300	-2.94495100	-1.37322500
H	-1.33885700	-3.34260000	-1.59494300
H	-3.02693700	-3.78396600	-1.31086000
H	-2.62468400	-2.31227100	-2.20957400
C	-4.37707200	0.83170600	0.69021900
H	-4.38146000	1.84976200	0.29551700
H	-5.41151700	0.54511500	0.88832800
H	-3.82711700	0.82581300	1.63218600
C	-4.48856500	-0.06717100	-1.63600000
H	-5.53222600	-0.34703700	-1.48521300
H	-4.47930900	0.94344900	-2.04603800
H	-4.05559300	-0.74096100	-2.37361100

CAAC.neutra

-408.44835912 a.u.

C	-1.24218900	-0.00349800	-0.08633000
N	-0.71546300	-0.44781100	1.21733600
C	0.61657600	-0.08535600	1.30779700
C	1.24043700	-0.02048900	-0.05919000

C	0.00181500	-0.17670900	-0.97764200	H	-3.01011500	-1.45451000	-1.51436200
H	0.00424800	0.53713500	-1.80303600	H	-1.49219800	-1.98764500	-2.24983200
H	-0.01017500	-1.18079500	-1.40687700	C	-2.35474000	-2.01856000	1.12852600
C	-1.70157000	1.45695600	-0.02668000	H	-3.20550300	-1.33918300	1.04966800
H	-1.96443000	1.81146000	-1.02444900	H	-2.73071200	-3.03735300	1.19400400
H	-2.58321300	1.56324600	0.60854000	H	-1.81951100	-1.79271300	2.05093100
H	-0.91228500	2.09362800	0.37560200				
C	-2.39070800	-0.89194300	-0.54506600	cAAc1.CH.anion			
H	-3.27980000	-0.75366600	0.07270600	-520.95523862 a.u.			
H	-2.66281900	-0.64256400	-1.57231400	C	-0.06968400	-4.06624600	0.11549900
H	-2.09634900	-1.94115500	-0.50620300	C	1.02271500	-4.83884600	0.62781100
C	1.96825300	1.30869000	-0.29017100	C	0.67166000	-6.18903700	0.59378200
H	2.75976100	1.44185100	0.45005300	C	-0.63302300	-6.29442200	0.06268900
H	2.42363700	1.33132700	-1.28388300	C	-1.09027000	-5.00953600	-0.22874800
H	1.28475700	2.15356000	-0.20441000	H	-2.04914200	-4.77176700	-0.66567300
C	2.23147800	-1.17039600	-0.27933500	H	-1.18142800	-7.21319800	-0.09971500
H	2.60688600	-1.17013100	-1.30622400	H	1.28983700	-7.01129200	0.93031300
H	3.08719400	-1.07432700	0.39243400	H	1.94161200	-4.44620800	1.03686600
H	1.75094100	-2.13099900	-0.08699100	C	-0.15965700	-2.65633100	-0.01660200
H	1.16332400	-0.36209600	2.20140100	C	-1.42783200	-1.80969500	-0.06084400
C	-1.54114400	-0.31343000	2.39386200	C	-0.85557400	-0.41106100	0.06337900
H	-1.07816000	-0.85841700	3.21675600	C	0.48007200	-0.48248400	0.18419300
H	-1.65892600	0.73380500	2.70165600	N	0.93204700	-1.77881500	0.17848500
H	-2.52579000	-0.74391400	2.21369000	C	2.30140900	-2.11427000	-0.11679700
				H	2.83717500	-2.49638900	0.75609600
cAAc1.BH.neutral				H	2.33035700	-2.88708200	-0.88743400
-507.68416524 a.u.				H	2.82002200	-1.22347300	-0.47805500
C	0.00927900	-3.99903600	0.12259500	H	1.19650600	0.32346700	0.26928400
B	1.25465800	-4.95075600	0.26022800	H	-1.45235100	0.48898500	0.08387300
C	0.65072300	-6.36450200	0.27801800	C	-2.22637500	-1.94669900	-1.37431000
C	-0.72522400	-6.24240800	0.16793600	H	-2.66964200	-2.93823300	-1.46959700
C	-1.11934200	-4.89781800	0.07731200	H	-3.03142000	-1.20358800	-1.40066900
H	-2.15510000	-4.60808300	-0.01454900	H	-1.57059200	-1.77786200	-2.22872400
H	-1.43482300	-7.06053700	0.15090500	C	-2.36986700	-2.13504500	1.11685100
H	1.13918800	-7.32670400	0.35855600	H	-3.24413600	-1.47509600	1.10148600
H	2.40991900	-4.68928800	0.33635000	H	-2.70165600	-3.17309600	1.06218500
C	-0.13337800	-2.63112200	0.04980600	H	-1.84420900	-1.99567200	2.06212300
C	-1.43473900	-1.82482100	-0.08556200				
C	-0.92977500	-0.40285800	-0.11133500	cAAc1.neutral			
C	0.39154200	-0.41410500	-0.01047200	-328.60878443 a.u.			
N	0.88063400	-1.72415000	0.08566800	C	-0.19962100	-2.58638100	0.07165900
C	2.28444800	-2.02817600	0.20679000	C	-1.44244600	-1.73302900	0.05209700
H	2.48149900	-2.57187500	1.13137900	C	-0.82248000	-0.34886600	0.06051200
H	2.61587800	-2.65105100	-0.62473500	C	0.50590500	-0.45129700	-0.05371600
H	2.84025500	-1.09324700	0.20710800	N	0.90063500	-1.78045300	-0.12719000
H	1.09507400	0.40403100	0.00591700	C	2.25922600	-2.23550300	0.00745200
H	-1.56748600	0.46206100	-0.19883200	H	2.51960500	-2.43058100	1.05289900
C	-2.16225500	-2.13285200	-1.40234400	H	2.39351700	-3.15720400	-0.55978700
H	-2.53163900	-3.15573200	-1.43192800	H	2.93608600	-1.48241600	-0.39322500

H	1.25494500	0.32535000	-0.09958300
H	-1.39034600	0.56790800	0.09488800
C	-2.26259400	-1.95525200	-1.23529500
H	-2.64634500	-2.97747400	-1.26894600
H	-3.11236000	-1.26946000	-1.27145600
H	-1.64304500	-1.78601700	-2.11627500
C	-2.34491000	-1.98185400	1.26934000
H	-3.20738900	-1.31119600	1.24983100
H	-2.71256100	-3.01030700	1.26573700
H	-1.79284700	-1.81594500	2.19380600
H	-0.14948400	-3.63379000	-0.19274700

cAAc2.BH.neutral
-661.33719822 a.u.

C	0.02250100	-3.97554400	0.11685800
B	1.24702000	-4.90536400	0.44824600
C	0.65403400	-6.32320600	0.46167900
C	-0.70121600	-6.22136600	0.18629200
C	-1.09202600	-4.88730300	-0.00370700
H	-2.11124400	-4.61425700	-0.23121700
H	-1.39785200	-7.04808400	0.12094800
H	1.13371200	-7.27464800	0.64989700
H	2.37225800	-4.61630000	0.69238200
C	-0.12003000	-2.61122500	0.02385600
C	-1.43506800	-1.81846200	-0.07243700
C	-0.94563500	-0.39081400	-0.01947100
C	0.44289900	-0.38897800	0.03009100
N	0.90524900	-1.70934200	0.01455400
C	-1.64265300	0.79684100	-0.02700500
C	-0.93301400	1.99732700	0.02484700
C	0.45279100	1.98520300	0.08381700
C	1.16791300	0.78934600	0.08939500
H	-2.72569500	0.80253700	-0.06989900
H	-1.46413000	2.93939200	0.02445200
H	0.99423100	2.92094000	0.13177300
H	2.24699200	0.79816200	0.15169700
C	2.30757600	-2.03986500	-0.04562600
H	2.69459300	-2.32982700	0.93220800
H	2.45130200	-2.87418400	-0.72969400
H	2.85471300	-1.17549300	-0.41388200
C	-2.13635400	-2.05710800	-1.41916400
H	-1.45624500	-1.84807500	-2.24540300
H	-2.49125800	-3.08021500	-1.51838000
H	-2.99133100	-1.38385900	-1.50263700
C	-2.36827100	-2.09774200	1.11080300
H	-2.72650200	-3.12466000	1.11103600
H	-1.85314200	-1.91586500	2.05417700
H	-3.23006800	-1.43011600	1.05726100

cAAc2.CH.anion
-674.61683797 a.u.

C	-0.07189700	-4.03777700	0.08854800
C	1.00400900	-4.73145600	0.73060000
C	0.68873600	-6.08868500	0.78493400
C	-0.57492000	-6.27521100	0.17855200
C	-1.04362200	-5.03326200	-0.24579300
H	-1.97016000	-4.85745600	-0.77425000
H	-1.08556500	-7.22092300	0.05360600
H	1.29995000	-6.86287600	1.22978500
H	1.87533300	-4.26844100	1.17272900
C	-0.18471800	-2.64494800	-0.15028500
C	-1.46654400	-1.81694900	-0.14300600
C	-0.92039700	-0.40952100	0.01285600
C	0.48530900	-0.46126900	0.08775300
N	0.90963600	-1.75125000	0.01001600
C	-1.56813700	0.80049100	0.06365100
C	-0.82768500	1.98672400	0.17897900
C	0.55904100	1.92574900	0.22920600
C	1.23876800	0.71108900	0.17957900
H	-2.65132200	0.84015800	0.00427400
H	-1.33260300	2.94297900	0.22129300
H	1.13021600	2.84347800	0.31136700
H	2.31954500	0.67810900	0.23127100
C	2.27424700	-2.07367800	-0.31556500
H	2.92234200	-2.05725400	0.56648700
H	2.30067800	-3.07314400	-0.74231300
H	2.66321900	-1.35209800	-1.04325500
C	-2.27389200	-1.93516100	-1.44819700
H	-1.64676600	-1.68221800	-2.30356600
H	-2.64009500	-2.95369400	-1.57806100
H	-3.13178600	-1.25453700	-1.43021700
C	-2.37497400	-2.18128500	1.04405100
H	-2.69339000	-3.22111100	0.96513100
H	-1.83135500	-2.06563300	1.98230100
H	-3.25514900	-1.53108900	1.06528400

cAAc2.neutral
-482.26202251 a.u.

C	-0.19490900	-2.55427500	-0.03663400
C	-1.47755600	-1.76472700	-0.03040600
C	-0.92447100	-0.34975500	0.00728600
C	0.47617100	-0.39210000	0.01997500
N	0.89598600	-1.70582200	-0.00605300
C	-1.57167100	0.86473400	0.02882400
C	-0.81842100	2.04183200	0.06313100
C	0.56883400	1.98289400	0.07529400
C	1.24301500	0.76479300	0.05394800
H	-2.65499500	0.91120200	0.01934500

H	-1.31665800	3.00154100	0.08026700	C	-2.34306800	-2.08626100	1.17381400
H	1.14136300	2.90125100	0.10190800	H	-2.72051600	-3.10557900	1.22672300
H	2.32454200	0.72601400	0.06358600	H	-1.80296000	-1.87489800	2.09718800
C	2.27605600	-2.10309400	-0.00188100	H	-3.19240800	-1.40400400	1.10910100
H	2.78303100	-1.74657100	0.89896800				
H	2.33061500	-3.18881600	-0.02634200	cAAc3.CH.anion			
H	2.80016300	-1.70575300	-0.87544000	-648.14640142 a.u.			
C	-2.31502900	-2.00611000	-1.29759200	C	-0.02539300	-4.06677500	0.11327600
H	-1.73348300	-1.77865400	-2.19068600	C	1.13451300	-4.91450600	0.30184900
H	-2.63329600	-3.04955200	-1.34592300	C	0.72164900	-6.22219700	0.31289500
H	-3.20744200	-1.37574600	-1.29298100	C	-0.69593000	-6.25737200	0.12935800
C	-2.33824600	-2.06364300	1.20866700	C	-1.14799100	-4.96880500	0.01455600
H	-2.65699000	-3.10804500	1.20312500	H	-2.17584200	-4.68449900	-0.13259600
H	-1.77340500	-1.87772800	2.12187600	H	-1.30679900	-7.14797200	0.08792700
H	-3.23063500	-1.43327900	1.21651800	H	1.36370600	-7.08187700	0.44426000
H	-0.06958400	-3.62351600	-0.05877900	H	2.15380900	-4.60217500	0.44034100
				C	-0.12545300	-2.67128200	0.05196000
				C	-1.42262900	-1.86409600	-0.04598400
				C	-0.93249500	-0.42904900	-0.02809600
				C	0.43384400	-0.42876100	0.04038100
				N	0.88106600	-1.79169400	0.07459600
				B	-1.72129500	0.87429800	-0.08604400
				C	-0.89757500	2.17359200	-0.05241700
				C	0.47256100	2.15819200	0.02205300
				B	1.27703600	0.85387400	0.07662100
				H	-2.92525600	0.88235700	-0.15522300
				H	-1.39162400	3.14631700	-0.08708300
				H	0.99166300	3.11814500	0.04329200
				H	2.47716600	0.85347800	0.14729800
				C	2.28089300	-2.13212800	0.10966100
				H	2.54624200	-2.58575700	1.06721500
				H	2.51267500	-2.84065600	-0.68684800
				H	2.85234300	-1.22016000	-0.02726800
				C	-2.15318200	-2.13025700	-1.37112400
				H	-1.47943200	-1.95655700	-2.21133600
				H	-2.53464900	-3.14811000	-1.43941500
				H	-2.98344000	-1.42650700	-1.45267600
				C	-2.34367700	-2.11658000	1.15438600
				H	-2.72111700	-3.13819500	1.17796500
				H	-1.80710900	-1.92629700	2.08490300
				H	-3.18222200	-1.42013900	1.09906300
				cAAc3.neutral			
				-455.74333709 a.u.			
				C	-0.19054500	-2.57234600	-0.03083600
				C	-1.46549300	-1.79446600	-0.02345400
				C	-0.94601300	-0.37328800	0.00671900
				C	0.43394600	-0.40143200	0.01427700
				N	0.82473200	-1.77935000	-0.00974200

B	-1.68411400	0.96044000	0.02788100
C	-0.78530400	2.21751200	0.05682000
C	0.58000400	2.15606200	0.06365900
B	1.34228600	0.82053500	0.04295200
H	-2.88136900	1.01774200	0.02179500
H	-1.24096500	3.20680600	0.07282100
H	1.12991200	3.09551100	0.08461300
H	2.53620800	0.73132000	0.04813300
C	2.22078400	-2.18747600	-0.00935000
H	2.69751100	-1.79043300	0.88405400
H	2.28332500	-3.27215900	-0.02958300
H	2.70781100	-1.75691100	-0.88142000
C	-2.28149500	-2.08607000	-1.29410700
H	-1.69936700	-1.87092400	-2.19011200
H	-2.61461100	-3.12560700	-1.32154000
H	-3.15594500	-1.43532300	-1.29395400
C	-2.29614800	-2.13414500	1.22559200
H	-2.62932200	-3.17390000	1.20948300
H	-1.72452000	-1.95344800	2.13585300
H	-3.17068500	-1.48367600	1.24008800
H	-0.06763500	-3.64790100	-0.05064200

NHC1.BH.neutral
-484.43617847 a.u.

C	-0.92026700	0.07053800	-0.00451300
B	-1.87132500	1.18966900	0.51150700
C	-3.28193700	0.60750100	0.27940300
C	-3.13490200	-0.63576400	-0.29327600
C	-1.76158700	-0.97314800	-0.45651200
H	-1.43849300	-1.89085200	-0.93166900
H	-3.93620300	-1.29652000	-0.60119100
H	-4.25455200	1.03194000	0.49290300
H	-1.57884700	2.23297700	1.01003100
C	0.48388700	0.01282000	-0.01123500
N	1.29022600	-1.08827200	0.05210500
C	2.61788800	-0.70597700	0.03096800
H	3.41565100	-1.42503100	0.07243000
N	1.33741900	1.07392700	-0.06910500
C	2.64544700	0.63649500	-0.03749000
H	3.47292200	1.32139800	-0.07412300
C	0.84270300	-2.44721100	0.27211200
H	1.64215700	-2.99645000	0.76507600
H	-0.03940100	-2.42995300	0.90980300
H	0.59326000	-2.94228300	-0.66607900
C	0.93849500	2.45786400	-0.21788200
H	0.06954300	2.50742200	-0.87188900
H	0.66929400	2.89323700	0.74261900
H	1.76940700	3.00746600	-0.65532100

NHC1.CH.anion
-497.67892375 a.u.

C	0.80058600	-0.21385100	0.02225400
C	0.10859400	0.79001700	0.74694700
C	0.82603000	1.98795000	0.63329900
C	1.96872300	1.74209600	-0.15657800
C	1.96052300	0.39132900	-0.52619900
H	2.73493400	-0.12901900	-1.07614400
H	2.72935400	2.46665200	-0.41799300
H	0.54499800	2.94000500	1.06565300
H	-0.83655500	0.64477600	1.25511000
C	0.40257200	-1.60091200	-0.08729200
N	0.07405300	-2.24809000	-1.31723300
C	-0.63188900	-3.39894100	-1.00770100
H	-0.90622000	-4.11096000	-1.76970900
N	-0.47743400	-2.19717800	0.86545800
C	-0.96621800	-3.37174600	0.29135400
H	-1.58697000	-4.05197200	0.85158200
C	0.99953100	-2.19583600	-2.41411800
H	0.55336300	-2.67260500	-3.28908000
H	1.21923300	-1.15305500	-2.64047800
H	1.94651000	-2.70087800	-2.16289700
C	-0.03720500	-2.22681200	2.24138600
H	0.23581000	-1.21708700	2.54253100
H	-0.84705000	-2.59058400	2.87748600
H	0.84239100	-2.87920500	2.35706800

NHC1.neutral
-305.34038288 a.u.

C	0.49432100	0.04396000	0.25991900
N	1.32518400	-1.08312400	0.41615500
C	2.61360700	-0.70950600	0.06237800
H	3.41216300	-1.42912400	0.00305200
N	1.38198700	1.13369700	0.16201900
C	2.64782300	0.62511900	-0.09055000
H	3.48139000	1.27136600	-0.30640100
C	0.80630900	-2.40897700	0.19126200
H	1.56269900	-3.14473000	0.46139200
H	-0.06967400	-2.56720500	0.82032200
H	0.51359100	-2.55271700	-0.85510700
C	0.92951800	2.39883000	-0.35990700
H	0.63839700	2.31682200	-1.41335700
H	0.06630700	2.73929900	0.21197300
H	1.72368800	3.13740700	-0.25877300
H	-0.36424300	0.14196100	0.92283500

NHC2.BH.neutral
-638.08506728 a.u.

C	1.62894400	-5.44853100	0.03946000
---	------------	-------------	------------

B	2.23664200	-6.40719600	1.10576300	N	0.64354300	-3.24780100	-0.56301600
C	1.85852600	-7.81213200	0.59346000	H	-0.55097300	-0.74583900	-1.36124800
C	1.16446900	-7.65850500	-0.58929700	H	0.55995600	1.40743100	-0.66614800
C	1.00519800	-6.29049800	-0.92372200	H	2.62863500	1.40887600	0.60348600
H	0.53387000	-5.96152000	-1.84096500	H	3.72590500	-0.74246200	1.32574100
H	0.78343900	-8.45803400	-1.21264800	C	3.76930000	-3.65407900	1.13278100
H	2.06387900	-8.78633000	1.01774800	H	3.96938800	-4.68293000	0.84197300
H	2.81059700	-6.11976700	2.10952100	H	4.55650900	-2.99442700	0.76034900
C	1.60618300	-4.05651600	-0.00095000	H	3.74718400	-3.58926600	2.22414400
C	2.17654100	-1.90137300	0.35111700	C	-0.61285000	-3.65445400	-1.13154900
C	1.01277100	-1.91777500	-0.42138300	H	-0.59037500	-3.60357100	-2.22364300
C	0.40625100	-0.74692200	-0.83864700	H	-0.81946300	-4.67825600	-0.82777600
C	1.00144800	0.45062100	-0.45401000	H	-1.39583200	-2.98515900	-0.76750300
C	2.16036600	0.46737100	0.31699500				
C	2.76865100	-0.71171000	0.73600100				
N	2.52168900	-3.21987300	0.58194500	NHC2.neutral			
N	0.67904900	-3.24733800	-0.61317600	-458.99625419 a.u.			
H	-0.48709600	-0.75665900	-1.44803700	C	-0.59707700	0.03117900	-0.07132400
H	0.55428400	1.38566400	-0.76259400	C	1.56311400	0.69653400	0.15105700
H	2.59695600	1.41559900	0.59949900	C	1.54680700	-0.70914500	0.04808900
H	3.66077800	-0.69400800	1.34666700	C	2.72069700	-1.43369300	-0.03587800
C	3.75534600	-3.63324100	1.21216900	C	3.92573200	-0.72137500	0.00677900
H	4.09551700	-4.55704000	0.74944500	C	3.94175500	0.65975500	0.10794900
H	4.49730200	-2.85109400	1.05910200	C	2.75355200	1.39830100	0.17157100
H	3.61812800	-3.80841200	2.27848600	N	0.25441900	1.11754500	0.18604400
C	-0.59169800	-3.67673000	-1.15349100	N	0.22868700	-1.10044900	0.02357400
H	-0.53231900	-3.86274500	-2.22636600	H	2.71183200	-2.51063200	-0.13711500
H	-0.90109700	-4.58878000	-0.64781000	H	4.86028800	-1.26276500	-0.05338500
H	-1.32645600	-2.89478200	-0.96721600	H	4.88865500	1.18242300	0.12572900
				H	2.76970900	2.47841300	0.22834100
				C	-0.15211000	2.48819200	0.03996600
NHC2.CH.anion				H	-1.21029800	2.57249700	0.28121500
-651.35076858 a.u.				H	0.41199500	3.11624400	0.72963900
C	1.57235900	-5.51832800	0.01232800	H	0.00576800	2.84949000	-0.98144400
C	2.02090000	-6.35984700	1.06967400	C	-0.20911800	-2.42543400	-0.31996100
C	1.84317300	-7.68654600	0.67492000	H	0.33920500	-3.16012000	0.26986200
C	1.28792500	-7.69297800	-0.62291700	H	-1.26936700	-2.51956000	-0.09174400
C	1.11849200	-6.37026700	-1.03434900	H	-0.05793000	-2.63759000	-1.38338700
H	0.76456400	-6.04019600	-2.00179300	H	-1.56210400	0.00540100	0.43343500
H	1.04744600	-8.57138000	-1.20636400				
H	2.07817100	-8.55902100	1.26938900	NHC3.BH.neutral			
H	2.37693300	-6.01984200	2.03289600	-611.54157774 a.u.			
C	1.57685600	-4.09182600	0.00334500	C	1.63020500	-5.50542200	0.03833500
C	2.18034400	-1.93034000	0.35638400	B	2.27308900	-6.46856000	1.08154300
C	0.98706000	-1.93117900	-0.37692300	C	1.89161000	-7.87309300	0.57104600
C	0.35456800	-0.74564600	-0.77215400	C	1.16535400	-7.71695600	-0.58977300
C	1.00531300	0.46044000	-0.38420700	C	0.98869500	-6.34575600	-0.91083500
C	2.17726900	0.46124900	0.33349400	H	0.48694800	-6.01978300	-1.81224900
C	2.82035800	-0.74395200	0.73665700	H	0.77109900	-8.51387200	-1.20838200
N	2.51550100	-3.24666100	0.55909300	H	2.11627400	-8.84799300	0.98387800

H	2.87534300	-6.19123400	2.07123600
C	1.60079000	-4.10720000	0.00148300
C	2.17296000	-1.94879000	0.33012000
C	1.00054600	-1.96283800	-0.38107100
B	0.31540600	-0.66525800	-0.84028800
C	1.00290900	0.68404000	-0.41391300
C	2.14601800	0.70002100	0.29169400
B	2.84427700	-0.62908000	0.75824600
N	2.52717800	-3.25929100	0.55186600
N	0.66018500	-3.28598600	-0.56837800
H	-0.67560700	-0.67339200	-1.49737000
H	0.55187300	1.63020800	-0.70225500
H	2.58780500	1.65827800	0.55284500
H	3.83078900	-0.60952000	1.42077400
C	3.74736500	-3.69484600	1.20038700
H	4.14124700	-4.55864900	0.66732400
H	4.45929100	-2.87479900	1.17443900
H	3.55537600	-3.98755200	2.23079000
C	-0.58938700	-3.73698600	-1.14630500
H	-0.46626700	-4.00735700	-2.19469700
H	-0.94029300	-4.60650000	-0.59332600
H	-1.31291900	-2.93009300	-1.07009800

NHC3.CH.anion

-624.90861695 a.u.

C	1.57232300	-5.53699600	0.01262500
C	2.09541500	-6.37775400	1.03692500
C	1.88398100	-7.69595300	0.65945600
C	1.24708400	-7.70207200	-0.60647100
C	1.04400700	-6.38752300	-1.00087400
H	0.61825600	-6.06315600	-1.93912000
H	0.97596100	-8.57993500	-1.17608100
H	2.14958400	-8.56812100	1.24030300
H	2.52328300	-6.04405200	1.97092600
C	1.57680000	-4.10971200	0.00349800
C	2.17734400	-1.95521000	0.34499900
C	0.98987800	-1.95599900	-0.36555200
B	0.28885200	-0.66789600	-0.80464600
C	1.00202200	0.61984300	-0.38246800
C	2.18148700	0.62066300	0.32898800
B	2.88652300	-0.66605800	0.76761400
N	2.51213100	-3.29761600	0.54494700
N	0.64657900	-3.29870700	-0.54830000
H	-0.73400000	-0.67637300	-1.43472200
H	0.57599400	1.58853900	-0.64802100
H	2.61363700	1.58996200	0.58216000
H	3.90931700	-0.67294800	1.39780400
C	3.74644600	-3.73475300	1.15285300
H	4.04840400	-4.68198500	0.71032100

H	4.49716200	-2.96779800	0.97495200
H	3.63107500	-3.86914600	2.23006200
C	-0.59052000	-3.73574400	-1.15059300
H	-0.47606300	-3.88462900	-2.22599300
H	-0.89846100	-4.67530100	-0.69599000
H	-1.33634300	-2.96182800	-0.98253400

NHC3.neutral

-432.51865580 a.u.

C	-0.50439200	0.02208200	-0.01686700
C	1.61013500	0.69671100	0.03256800
C	1.59702000	-0.69314200	-0.05313900
B	2.87237000	-1.53970200	-0.10057000
C	4.15474100	-0.71007100	-0.04467400
C	4.16771100	0.66438500	0.04007800
B	2.90122900	1.51855800	0.08801200
N	0.27562800	1.09338300	0.05205900
N	0.25527000	-1.06404500	-0.08098600
H	2.83442400	-2.73358800	-0.17428600
H	5.11942300	-1.21421500	-0.07215700
H	5.14173200	1.14986100	0.07361600
H	2.88582100	2.71295900	0.16155900
C	-0.17318600	2.46905900	0.13513200
H	-1.26045600	2.49679000	0.13311700
H	0.20833900	2.91741500	1.05048900
H	0.21438200	3.02607600	-0.71574500
C	-0.21942300	-2.43082700	-0.16697000
H	0.15223200	-2.99522000	0.68614100
H	-1.30701800	-2.43763100	-0.17149600
H	0.15890200	-2.88641600	-1.08008200
H	-1.58158000	0.03245400	-0.02022700