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Supporting Information

Triply-bonded Indium≡Phosphorus Molecules: Theoretical Designs and Characterization

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Theoretical Methods

Using the Gaussian 09 program package,[1] all geometries are fully optimized using hybrid density functional theory at the M06-2X,[2] B3LYP,[3,4] and B3PW91[4,5] levels, in conjunction with the Def2-TZVP[6] and LANL2DZ+dp[7] basis sets. These DFT calculations are signified as M06-2X/Def2-TZVP, B3PW91/Def2-TZVP and B3LYP/LANL2DZ+dp, respectively. In order to confirm that the reactants and products have no imaginary frequencies and that the transition states possess only one imaginary frequency, frequency calculations were performed for all structures. Thermodynamic corrections to 298 K, heat capacity corrections and entropy corrections (ΔS) are applied to the three levels of DFT. The relative free energy (ΔG) at 298 K is also computed at the same levels of theory.

Next, $SiMe(Si\textit{t}Bu_3)_2$–In≡P–$SiMe(Si\textit{t}Bu_3)_2$, $Si\textit{i}PrDis_2$–In≡P–$Si\textit{i}PrDis_2$, and NHC–In≡P–NHC are the model reactants for this study. It is known that the B3LYP functional fails to describe nonvalent interactions, such as the London dispersion correctly. As a result, for large ligands, calculations were performed using dispersion-corrected B97-D3 method.[8-10] Because of the limitations of the available memory size and CPU time, frequencies are not computed at the B97-D3/LANL2DZ+dp level of theory for the triply bonded R´In≡PR´ systems that have bulky ligands (R´), so the zero-point energies and the Gibbs free energies that are derived using B97-D3/LANL2DZ+dp cannot be used for these systems.

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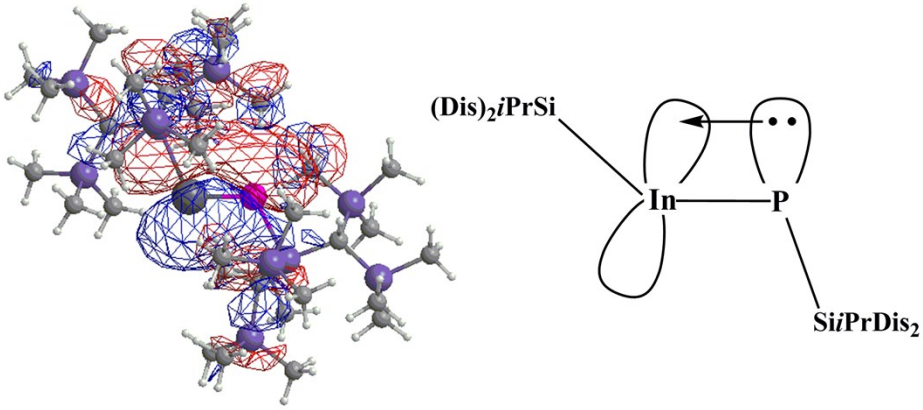
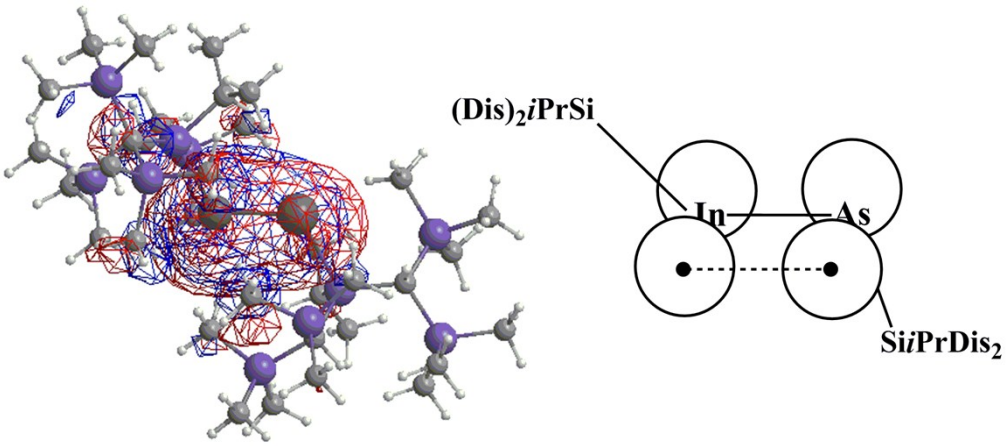
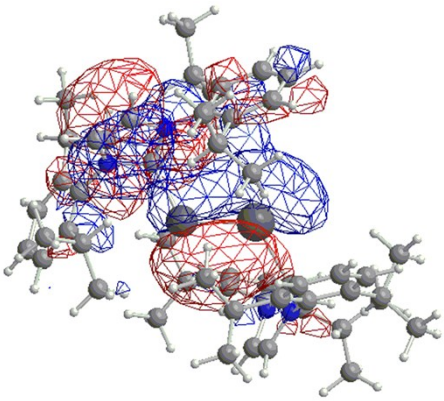


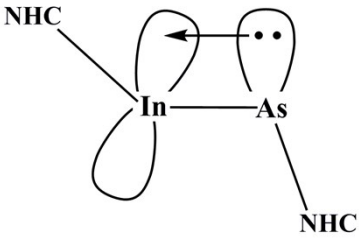
(i) $\pi_{\perp}$



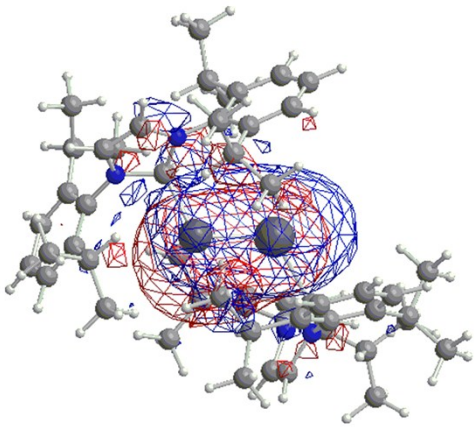
(ii) $\pi_{\parallel}$

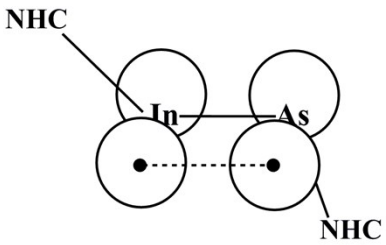
Figure S1: The natural In≡P π bonding orbitals ((i) and (ii)) of (Si*i*PrDis$_2$)In≡P(Si*i*PrDis$_2$)). For comparison, also see Figure 2.





(i) $\pi_{\perp}$





(ii) $\pi_{||}$

Figure S2: The natural In≡P π bonding orbitals ((i) and (ii)) of ((NHC)In≡P(NHC)). For comparison, also see Figure 2.

M06-2X/Def2-TZVP

F2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-0.145842	-2.241631	0.000000
In	0.000000	0.201819	0.000000
F	-1.454650	1.489751	0.000000
F	1.697720	1.147506	0.000000

Energy = -731.0860 hartree
ZPVE = -458763.7953 kcal/mol
Number of imaginary frequency (0)

F2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-2.082366	0.473293	-0.004329
In	0.292798	0.105611	0.003739
F	2.182814	0.424440	-0.010047
F	-0.306324	-1.788255	-0.003092

Energy = -731.081221 hartree
ZPVE = -458760.776989 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -103.4371

-1	-0.05	0.57	0.00
-2	-0.06	-0.18	-0.00
-3	-0.15	0.44	0.00
-4	0.59	-0.29	0.01

F-In-P-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.784822	-1.738703	0.000000
In	0.000000	0.543575	0.000000
F	-0.622667	2.378880	0.000000

F	-0.685370	-2.440503	0.000000

Energy = -731.134049 hartree
ZPVE = -459497.728056 kcal/mol
Number of imaginary frequency (0)

In-PF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.78848874	0.60488054	-0.10692636
F	2.40403774	-0.83149346	0.19566164
F	-1.18906174	1.66272746	0.13411636
In	-0.55641874	-0.25892354	-0.03445964

Energy = -731.090491 hartree
ZPVE = -458766.594007 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -98.0654

-1	-0.27	0.02	0.06
-2	0.23	0.31	0.01
-3	0.87	0.03	-0.01
-4	-0.11	-0.06	-0.02

In-PF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.589204	0.000538	0.605444
F	1.598532	1.212431	-0.500574
F	1.612487	-1.207027	-0.502360
In	-1.076270	-0.001157	-0.001128

Energy = -731.1731 hartree
ZPVE = -428245.0379 kcal/mol
Number of imaginary frequency (0)

(OH)2In-P

Atomic Coordinates (Angstroms)

Number	X	Y	Z
P	0.015704	-2.282083	0.000000
In	0.000000	0.190369	0.000000
O	1.540619	1.455178	0.000000
H	2.427202	1.089791	0.000000
O	-1.682475	1.247012	0.000000
H	-1.527925	2.195864	0.000000

Energy = -682.987580 hartree
ZPVE = -459449.581587 kcal/mol
Number of imaginary frequency (0)

(OH)2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.965864	-0.527288	0.010451
In	-0.338713	-0.146742	-0.003329
O	-2.223304	0.095724	0.030427
H	-2.812949	-0.665641	-0.051255
O	0.827674	1.620118	-0.113553
H	1.086987	2.038567	0.722598

Energy = -682.982388 hartree
ZPVE = -428578.278293 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -123.4234

-1	-0.05	0.36	-0.01
-2	-0.05	-0.09	0.00
-3	-0.08	0.17	-0.00
-4	-0.17	0.19	-0.00
-5	0.51	-0.21	0.02
-6	0.64	-0.22	0.01

HO-In-P-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.817757	-0.590541	0.029727
O	-2.444617	0.957292	0.116981

H	-2.724979	1.266808	-0.749311
O	2.485306	0.329776	-0.034291
H	2.943291	0.413025	0.806347
In	0.545358	-0.063638	-0.023764

Energy = -683.043873 hartree
ZPVE = -428616.860746 kcal/mol
Number of imaginary frequency (0)

In-P(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.66449249	0.58168864	-0.10195262
In	0.66862849	-0.31271664	-0.02080038
O	-2.67149649	-0.64329336	0.20742338
H	-2.49676749	-1.44948136	-0.29641062
O	1.03945149	1.67781736	0.17216062
H	0.87576349	2.40926136	-0.43113138

Energy = -683.010949 hartree
ZPVE = -428596.200606 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -146.9071

-1	0.02	-0.12	0.08
-2	-0.08	0.06	0.02
-3	-0.03	-0.17	-0.13
-4	-0.22	-0.05	-0.44
-5	0.58	-0.04	-0.11
-6	0.56	-0.06	-0.13

In-P(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.002004	-0.000115	-0.010746
P	1.605253	0.000205	-0.599323
O	1.304377	-1.291969	0.474237
H	2.080087	-1.587589	0.964253
O	1.303222	1.292211	0.474198
H	2.078514	1.588222	0.964669

Energy = -683.090404 hartree
ZPVE = -428646.059414 kcal/mol
Number of imaginary frequency (0)

H2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.000035	1.912138	0.000000
In	0.000035	-0.530303	0.000000
H	1.527530	-1.351075	0.000000
H	-1.529797	-1.346175	0.000000

Energy = -532.473565 hartree
ZPVE = -334132.486773 kcal/mol
Number of imaginary frequency (0)

H2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.817207	-0.062718	0.000004
In	-0.515935	0.002029	-0.000004
H	-1.946935	-0.932099	0.000106
H	-0.030374	1.773431	0.000058

Energy = -532.475986 hartree
ZPVE = -334134.005974 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -568.0845

-1 -0.04 0.03 0.00
-2 0.00 -0.01 -0.00
-3 -0.18 0.30 -0.00
-4 0.92 -0.19 0.00

H-In-P-H

Atomic Number	Coordinates (Angstroms) X	Y	Z

H	-1.702659	1.340499	0.000086
P	-1.777529	-0.084648	0.000268
In	0.533006	-0.002196	-0.000197
H	2.248299	0.036833	0.005534

Energy = -532.556766 hartree
ZPVE = -334184.696232 kcal/mol
Number of imaginary frequency (0)

In-PH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.611937	-0.028918	0.001416
H	0.148437	1.728185	-0.164948
P	-1.890897	-0.032936	-0.083293
H	-1.769897	0.182843	1.344960

Energy = -532.496903 hartree
ZPVE = -334147.131601 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -918.7268

-1	-0.01	0.00	-0.00
-2	0.99	0.16	0.02
-3	0.00	-0.02	0.00
-4	-0.00	0.01	0.00

In-PH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.683553	0.000005	-0.000276
P	1.972669	-0.000054	-0.115068
H	1.952332	1.024557	0.869480
H	1.951722	-1.023978	0.870063

Energy = -532.598490 hartree
ZPVE = -334210.87845 kcal/mol
Number of imaginary frequency (0)

(CH3)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	1.298599	-1.883898	-0.003957
H	1.550950	-2.148818	1.022865
H	0.725622	-2.695203	-0.447053
H	2.223669	-1.750827	-0.563426
C	1.259787	1.906431	0.000220
H	0.725573	2.662693	0.571762
H	1.365492	2.256613	-1.026767
H	2.252338	1.768430	0.426227
P	-2.251099	-0.013574	-0.001080
In	0.195358	-0.000500	0.001123

Energy = -611.047229 hartree
ZPVE = -383438.246669 kcal/mol
Number of imaginary frequency (0)

(CH3)2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.233254	-0.035127	-0.000825
P	2.074392	-0.712472	0.000880
C	0.153100	2.150818	0.000765
H	1.210217	2.416681	-0.016650
H	-0.335407	2.573358	-0.877731
H	-0.305580	2.564438	0.900254
C	-2.234655	-0.852459	0.001358
H	-2.231280	-1.942841	-0.018807
H	-2.758749	-0.512358	0.896445
H	-2.776321	-0.481153	-0.869010

Energy = -611.046050 hartree
ZPVE = -383437.506831 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -93.6555

-1	49	-0.04	-0.08	0.00
-2	15	0.00	0.28	-0.00
-3	6	0.38	-0.11	-0.00

-4	1	0.41	-0.24	0.01
-5	1	0.44	-0.08	-0.02
-6	1	0.41	-0.08	0.00
-7	6	-0.11	0.14	-0.00
-8	1	-0.19	0.14	-0.01
-9	1	-0.08	0.17	0.00
-10	1	-0.08	0.19	0.00

H3C-In-P-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.516019	-0.042590	-0.001425
P	1.719256	-0.701659	0.002148
C	-2.639456	0.319668	0.005666
H	-3.153095	-0.507566	-0.483903
H	-2.857712	1.236287	-0.541418
H	-3.009194	0.415691	1.024851
C	2.629119	0.957513	-0.000143
H	3.682122	0.691796	0.102153
H	2.519634	1.506530	-0.932721
H	2.376370	1.605970	0.835511

Energy = -611.114169 hartree
ZPVE = -383480.252189 kcal/mol
Number of imaginary frequency (0)

In-P(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.564609	0.007767	-0.808057
In	-0.813714	-0.363722	0.044492
C	-0.610531	1.992023	0.105465
H	-1.381767	2.209762	0.851698
H	-0.922595	2.336527	-0.886908
H	0.333806	2.459787	0.393483
C	2.379255	-0.123880	0.882618
H	2.934142	-1.075598	0.908692
H	1.699692	-0.107267	1.750793
H	3.127231	0.673822	0.994509

Energy = -611.056701 hartree

ZPVE = -383444.190444 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -386.8666

-1	-0.03	0.16	0.04
-2	-0.04	-0.05	0.01
-3	0.41	0.03	-0.16
-4	0.45	-0.42	0.02
-5	0.10	-0.01	-0.07
-6	0.26	0.37	-0.24
-7	0.01	0.03	-0.01
-8	-0.04	-0.01	-0.21
-9	-0.01	-0.18	-0.02
-10	0.02	-0.02	0.17

In-P(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.081429	-0.000183	0.021676
P	-1.445455	0.000153	-0.748706
C	-1.713894	-1.392138	0.480628
H	-1.046482	-1.380395	1.354937
H	-2.732977	-1.332900	0.866887
H	-1.599816	-2.353413	-0.020794
C	-1.712135	1.392823	0.480518
H	-2.731991	1.336326	0.865110
H	-1.046166	1.379030	1.355899
H	-1.594578	2.353912	-0.020460

Energy = -611.152355 hartree
ZPVE = -383504.214286 kcal/mol
Number of imaginary frequency (0)

(SiH3)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.000155	0.089183	0.004966
P	-0.005657	2.494255	-0.005054
Si	-2.267959	-1.185945	-0.003043
H	-3.389192	-0.331909	0.442751

H	-2.552776	-1.660637	-1.375728
H	-2.183783	-2.361154	0.891751
Si	2.272505	-1.177940	-0.003278
H	3.402395	-0.314160	0.400847
H	2.534940	-1.694468	-1.365898
H	2.202049	-2.327090	0.927262

Energy = -1113.820298 hartree
ZPVE = -698933.375197 kcal/mol
Number of imaginary frequency (0)

(SiH3)2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.006590	2.513734	-0.017850
In	-0.000113	0.103683	0.015728
Si	2.262594	-1.213919	-0.013615
H	2.353670	-2.062137	1.204448
H	2.291422	-2.100538	-1.204893
H	3.441930	-0.314549	-0.060515
Si	-2.267882	-1.204945	-0.013634
H	-2.365004	-2.047691	1.207745
H	-3.443385	-0.300920	-0.066930
H	-2.297898	-2.096539	-1.201271

Energy = -1113.819750 hartree
ZPVE = -698933.03132 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -76.7579

-1	15	0.53	-0.00	-0.00
-2	49	-0.16	0.00	-0.00
-3	14	0.03	0.25	-0.00
-4	1	0.12	0.27	0.01
-5	1	0.09	0.23	0.01
-6	1	-0.05	0.35	-0.03
-7	14	0.03	-0.25	0.00
-8	1	0.12	-0.28	-0.01
-9	1	-0.05	-0.35	0.04
-10	1	0.09	-0.23	-0.01

H3Si-In-P-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.698679	-1.071221	-0.003162
In	-0.436940	-0.183776	0.001664
Si	2.730231	0.924828	-0.000720
H	3.265886	1.273518	-1.342031
H	1.920785	2.099758	0.441039
H	3.892305	0.837629	0.923012
Si	-2.936197	0.447743	-0.000531
H	-3.671843	-0.685400	-0.610309
H	-3.430127	0.663188	1.378072
H	-3.163623	1.668620	-0.806369

Energy = -1113.905122 hartree
ZPVE = -698986.603106 kcal/mol
Number of imaginary frequency (0)

In-P(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.166596	-0.168177	-1.074344
In	0.835948	-0.754163	0.143768
Si	1.334911	1.873234	-0.012321
H	2.318261	2.024424	-1.101312
H	0.224678	2.823950	-0.184068
H	1.983254	2.157253	1.286055
Si	-2.682431	0.339247	0.483269
H	-2.505285	-0.352548	1.779816
H	-2.564619	1.803555	0.683256
H	-4.053547	0.045253	0.013502

Energy = -1113.858832 hartree
ZPVE = -698957.555668 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -137.1348

-1	-0.05	-0.11	-0.09
-2	-0.07	0.07	0.01
-3	0.32	-0.04	0.02
-4	-0.08	0.08	-0.15
-5	0.29	-0.19	0.40

-6	0.61	-0.00	-0.27
-7	-0.01	-0.13	0.03
-8	0.02	-0.04	0.12
-9	0.02	-0.10	-0.07
-10	-0.07	-0.19	0.07

In-P(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-1.640496	1.623592	-0.315505
H	-0.960460	1.576478	-1.647010
H	-3.099538	1.549649	-0.572330
H	-1.321274	2.944690	0.279729
Si	-1.644311	-1.621822	-0.315483
H	-1.295894	-2.942740	0.265266
H	-3.109030	-1.567306	-0.543575
H	-0.990985	-1.556287	-1.660043
In	1.456220	-0.000797	-0.068240
P	-0.972688	0.000653	1.070370

Energy = -1113.950963 hartree
ZPVE = -699015.368792 kcal/mol
Number of imaginary frequency (0)

B3PW91/Def2-TZVP

F2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-0.147513	-2.224791	0.000000
In	0.000000	0.198385	0.000000
F	-1.456606	1.485075	0.000000
F	1.702461	1.142816	0.000000

Energy = -731.228035 hartree
ZPVE = -458852.904242 kcal/mol
Number of imaginary frequency (0)

F2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-2.082366	-0.473293	0.004329
In	0.292798	-0.105611	-0.003739
F	2.182814	-0.424440	0.010047
F	-0.306324	1.788255	0.003092

Energy = -731.225700 hartree
ZPVE = -458851.439007 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -124.1566

-1	0.09	0.55	0.00
-2	0.07	-0.15	-0.00
-3	0.13	0.29	0.00
-4	-0.69	-0.29	0.01

F-In-P-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.747432	-1.738221	0.000000
In	0.000000	0.544868	0.000000
F	-0.539731	2.406959	0.000000
F	-0.705990	-2.476427	0.000000

Energy = -731.285512 hartree
ZPVE = -458888.971635 kcal/mol
Number of imaginary frequency (0)

In-PF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.611937	-0.028918	0.001416
H	0.148437	1.728185	-0.164948
P	-1.890897	-0.032936	-0.083293
H	-1.769897	0.182843	1.344960

Energy = -731.249037 hartree

ZPVE = -458866.083207 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -150.4181

-1	0.04	0.24	-0.26
-2	-0.15	0.21	0.34
-3	0.78	0.05	0.25
-4	-0.12	-0.11	-0.03

In-PF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.567513	-0.000195	0.600680
F	1.716486	1.227665	-0.473832
F	1.717803	-1.226785	-0.474326
In	-1.110639	-0.000102	-0.009730

Energy = -731.323942 hartree
ZPVE = -458913.086844 kcal/mol
Number of imaginary frequency (0)

(OH)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-0.041010	-2.249870	0.000000
In	0.000000	0.178434	0.000000
O	1.573275	1.407294	0.000000
H	2.423769	0.959549	0.000000
O	-1.627999	1.317637	0.000000
H	-1.370823	2.245791	0.000000

Energy = -683.138186 hartree
ZPVE = -428676.043096 kcal/mol
Number of imaginary frequency (0)

(OH)2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z

P	2.136741	-0.468211	0.005895
In	-0.248833	-0.077918	-0.000865
O	-2.128259	-0.681852	0.020049
H	-2.230816	-1.634486	-0.059788
O	-0.066628	1.941971	-0.110684
H	-0.068378	2.394687	0.738846

Energy = -683.134537 hartree
ZPVE = -428673.753312 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -140.1353

-1	-0.05	0.33	-0.00
-2	-0.05	-0.08	-0.00
-3	-0.07	0.13	0.01
-4	-0.14	0.15	-0.05
-5	0.48	-0.19	0.01
-6	0.70	-0.23	0.03

HO-In-P-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.804078	-0.590186	0.001732
O	-2.493514	0.929080	0.118912
H	-2.722155	1.265261	-0.753566
O	2.492425	0.323442	-0.086665
H	2.918584	0.376101	0.775524
In	0.548438	-0.057321	-0.006243

Energy = -683.203945 hartree
ZPVE = -428717.307526 kcal/mol
Number of imaginary frequency (0)

In-P(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.43656980	0.50051894	0.15594148
In	-0.86985800	-0.37304700	0.02113300
O	2.47646080	-0.72697906	-0.29732852

H	2.29628980	-1.57833706	0.14848548
O	-1.11637300	1.56949000	-0.24538600
H	-0.81593200	2.30952400	0.30928600

Energy = -683.169969 hartree
ZPVE = -428695.987247 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -124.3837

-1	0.00	0.10	0.15
-2	-0.06	-0.05	0.02
-3	-0.09	0.15	-0.21
-4	-0.24	0.02	-0.53
-5	0.49	0.03	-0.18
-6	0.46	0.09	-0.24

In-P(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.024989	-0.007684	-0.001123
P	-1.561146	0.010494	-0.604893
O	-1.356151	1.319089	0.466916
H	-2.188226	1.656101	0.816264
O	-1.434967	-1.299653	0.471387
H	-2.290109	-1.592495	0.805740

Energy = -683.246252 hartree
ZPVE = -428743.855592 kcal/mol
Number of imaginary frequency (0)

H2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.000038	1.870171	0.000000
In	0.000038	-0.516470	0.000000
H	-1.492874	-1.370344	0.000000
H	1.490471	-1.375172	0.000000

Energy = -532.645668 hartree
ZPVE = -334240.483126 kcal/mol

Number of imaginary frequency (0)

H2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.855922	-0.027872	-0.000048
In	-0.515249	-0.004889	0.000013
H	-1.830827	-1.077402	0.000046
H	-0.760805	1.735067	0.000021

Energy = -532.645671 hartree
ZPVE = -334240.485009 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -211.8792

-1	-0.04	0.03	0.00
-2	0.01	-0.01	-0.00
-3	-0.36	0.47	0.00
-4	0.79	0.14	-0.00

H-In-P-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-1.678233	1.348212	0.000001
P	-1.770560	-0.083828	0.000008
In	0.530666	-0.002865	-0.000005
H	2.234008	0.049587	0.000153

Energy = -532.730064 hartree
ZPVE = -334293.442460 kcal/mol
Number of imaginary frequency (0)

In-PH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.611937	-0.028918	0.001416
H	0.148437	1.728185	-0.164948

P	-1.890897	-0.032936	-0.083293
H	-1.769897	0.182843	1.344960

Energy = -532.677593 hartree
ZPVE = -334260.516383 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -801.3588

-1	-0.01	0.00	-0.00
-2	0.99	0.16	0.02
-3	0.00	-0.02	0.00
-4	-0.01	-0.00	0.00

In-PH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.680049	0.000001	-0.000104
P	1.961047	-0.000004	-0.115877
H	1.953410	1.030451	0.871605
H	1.953309	-1.030435	0.871625

Energy = -532.771817 hartree
ZPVE = -334319.642885 kcal/mol
Number of imaginary frequency (0)

(CH3)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	1.338314	-1.836534	-0.002360
H	1.629123	-2.062038	1.024607
H	0.761963	-2.667260	-0.405116
H	2.233543	-1.677581	-0.603564
C	1.325012	1.845096	0.001521
H	0.722001	2.691128	0.324612
H	1.686649	2.021010	-1.012523
H	2.176732	1.716574	0.669705
P	-2.222016	-0.003937	-0.000247
In	0.166128	-0.000289	0.000225

Energy = -611.231291 hartree

ZPVE = -383553.747415 kcal/mol
Number of imaginary frequency (0)

(CH3)2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.190011	-0.053629	-0.000592
P	2.134941	-0.495037	0.000632
C	-0.325056	2.157321	0.000658
H	0.647339	2.642273	-0.017586
H	-0.900510	2.433250	-0.883222
H	-0.867668	2.434629	0.904693
C	-2.073983	-1.100212	0.000974
H	-1.921953	-2.177851	-0.022404
H	-2.626943	-0.828765	0.901012
H	-2.649616	-0.792837	-0.872769

Energy = -611.230977 hartree
ZPVE = -383553.550377 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -61.1564

-1	-0.03	-0.09	0.00
-2	0.00	0.28	-0.00
-3	0.37	-0.02	0.00
-4	0.43	-0.15	0.02
-5	0.43	0.03	-0.02
-6	0.39	0.02	-0.00
-7	-0.14	0.15	0.00
-8	-0.26	0.14	-0.00
-9	-0.12	0.20	-0.00
-10	-0.11	0.21	0.00

H3C-In-P-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.519678	-0.026282	-0.000779
P	1.702648	-0.703666	0.001239
C	-2.641725	0.282948	0.004235
H	-3.125774	-0.549926	-0.508356

H	-2.874023	1.206875	-0.526746
H	-3.014320	0.347228	1.026326
C	2.673861	0.915081	-0.000276
H	3.719926	0.608814	0.090530
H	2.574879	1.474780	-0.930471
H	2.450970	1.566881	0.844550

Energy = -611.302201 hartree
ZPVE = -383598.244149 kcal/mol
Number of imaginary frequency (0)

In-P(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.557863	0.003207	-0.795149
In	-0.793970	-0.370210	0.045953
C	-0.666600	1.988449	0.081872
H	-1.479472	2.181334	0.778368
H	-0.915200	2.316085	-0.925740
H	0.260312	2.436670	0.425796
C	2.339040	-0.073771	0.877647
H	2.881571	-1.024103	0.939176
H	1.661309	-0.018766	1.737686
H	3.093434	0.712905	0.963158

Energy = -611.250597 hartree
ZPVE = -383565.862123 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -298.1055

-1	-0.04	0.17	0.03
-2	-0.04	-0.05	0.01
-3	0.40	0.06	-0.16
-4	0.50	-0.29	0.05
-5	0.07	0.02	-0.08
-6	0.33	0.32	-0.31
-7	-0.00	0.02	-0.00
-8	-0.03	-0.01	-0.21
-9	-0.02	-0.20	-0.00
-10	-0.00	-0.01	0.18

In-P(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.133011	-0.000023	0.033516
P	-1.401068	-0.000005	-0.699653
C	-1.876508	-1.423708	0.419493
H	-1.412290	-1.412656	1.413422
H	-2.961652	-1.418431	0.566663
H	-1.618934	-2.366273	-0.070554
C	-1.876257	1.423835	0.419444
H	-2.961222	1.418010	0.567642
H	-1.411112	1.413437	1.412900
H	-1.619713	2.366347	-0.071156

Energy = -611.337606 hartree
ZPVE = -383620.461141 kcal/mol
Number of imaginary frequency (0)

(SiH3)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.294252	2.103662	0.005558
In	-0.009389	0.162216	-0.004733
Si	1.477516	-1.981622	0.003262
H	1.126737	-2.779758	1.213050
H	1.153385	-2.775720	-1.216391
H	2.935860	-1.687252	0.019535
Si	-2.549994	-0.249112	0.003742
H	-3.307027	1.023618	-0.147861
H	-2.915057	-1.165364	-1.112194
H	-2.932923	-0.888783	1.294347

Energy = -1113.993663 hartree
ZPVE = -699042.163469 kcal/mol
Number of imaginary frequency (0)

(SiH3)2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.197378	2.482117	0.001101

In	0.004637	0.149655	-0.000796
Si	2.077508	-1.406880	0.000660
H	2.018783	-2.285760	1.200613
H	2.037722	-2.256001	-1.219608
H	3.354789	-0.647830	0.020935
Si	-2.257762	-1.110697	0.000657
H	-2.322809	-1.987296	1.202246
H	-3.418358	-0.182215	0.017891
H	-2.334458	-1.959678	-1.218039

Energy = -1113.993402 hartree
ZPVE = -699041.999689 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -246.5637

-1	-0.01	0.09	-0.02
-2	0.02	-0.01	0.00
-3	0.01	0.01	0.01
-4	0.01	-0.01	-0.01
-5	-0.01	-0.01	0.01
-6	0.04	0.02	-0.01
-7	-0.09	-0.07	-0.00
-8	0.59	-0.08	-0.38
-9	0.03	0.44	0.47
-10	-0.20	-0.14	-0.01

H3Si-In-P-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.673745	-1.063431	0.004629
In	-0.453576	-0.160046	-0.003711
Si	2.819623	0.874479	0.000662
H	3.327642	1.222076	-1.356765
H	2.107375	2.087581	0.508184
H	4.015749	0.682050	0.872297
Si	-2.960829	0.427512	0.006326
H	-3.689921	-0.707330	-0.619115
H	-3.458173	0.619918	1.392431
H	-3.206747	1.661559	-0.782454

Energy = -1114.073960 hartree
ZPVE = -699092.550631 kcal/mol
Number of imaginary frequency (0)

In-P(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.166596	-0.168177	1.074344
In	-0.835948	-0.754163	-0.143768
Si	-1.334911	1.873234	0.012321
H	-2.318261	2.024424	1.101312
H	-0.224678	2.823950	0.184068
H	-1.983254	2.157253	-1.286055
Si	2.682431	0.339247	-0.483269
H	2.505285	-0.352548	-1.779816
H	2.564619	1.803555	-0.683256
H	4.053547	0.045253	-0.013502

Energy = -1114.032710 hartree
ZPVE = -699066.665854 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -205.5336

-1	-0.05	0.12	-0.01
-2	-0.02	-0.04	-0.02
-3	0.12	0.01	0.06
-4	0.53	0.03	0.42
-5	0.15	0.07	-0.47
-6	-0.39	-0.12	0.28
-7	0.01	0.02	0.02
-8	0.04	-0.04	0.04
-9	0.05	0.01	-0.05
-10	-0.02	-0.01	0.09

In-P(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	1.741221	-1.677694	-0.271621
H	1.391301	-1.616177	-1.724122
H	3.227313	-1.731725	-0.181763
H	1.195067	-2.961166	0.256556
Si	1.739806	1.678386	-0.271585
H	1.200313	2.961991	0.263427

H	3.226719	1.727727	-0.189518
H	1.382055	1.622051	-1.722659
In	-1.514907	-0.000268	-0.071161
P	0.924885	0.000050	0.959325

Energy = -1114.114601 hartree
ZPVE = -699118.053273 kcal/mol
Number of imaginary frequency (0)

B3LYP/LANL2DZ+dp

F2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-0.006609	-2.247811	0.000000
In	0.000000	0.236883	0.000000
F	1.581954	1.219794	0.000000
F	-1.570939	1.236862	0.000000

Energy = -208.138334 hartree
ZPVE = -130608.885968 kcal/mol
Number of imaginary frequency (0)

F2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.014296	-1.875170	0.000000
In	0.000000	0.323724	-0.000000
F	-0.131852	2.164789	-0.000000
F	-1.558641	-0.802001	0.000000

Energy = -208.132179 hartree
ZPVE = -130605.023644 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -113.5721

-1	0.54	0.06	-0.00
-2	-0.12	-0.11	0.00
-3	0.32	-0.06	-0.00

-4 -0.47 0.60 -0.00

F-In-P-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.781243	-1.753608	0.000000
In	0.000000	0.560793	0.000000
F	-0.541978	2.334760	0.000000
F	-0.760093	-2.465284	0.000000

Energy = -208.156488 hartree
ZPVE = -130620.277784 kcal/mol
Number of imaginary frequency (0)

In-PF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.49519352	0.53712528	-0.15776102
F	2.38744452	-0.79609572	0.23572298
F	-0.99843600	1.57054900	0.18678700
In	-0.83161700	-0.35206500	-0.02240000

Energy = -208.120679 hartree
ZPVE = -130597.807279 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -136.6004

-1 0.03 0.19 -0.25
-2 -0.16 0.23 0.35
-3 0.77 0.04 0.28
-4 -0.11 -0.10 -0.04

In-PF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.598758	-0.000003	-0.634571
F	-1.698933	1.262965	0.509972

F	-1.698927	-1.262962	0.509976
In	1.113512	0.000001	0.006919

Energy = -208.170457 hartree
ZPVE = -130629.043472 kcal/mol
Number of imaginary frequency (0)

(OH)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-2.272751	0.013004	0.000000
In	0.223547	0.000485	0.000000
O	1.359374	1.555918	0.000000
H	0.991847	2.449204	0.000000
O	1.144827	-1.681693	0.000000
H	2.112029	-1.661843	0.000000

Energy = -160.032875 hartree
ZPVE = -100422.229391 kcal/mol
Number of imaginary frequency (0)

(OH)2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.965864	-0.527287	0.010451
In	-0.338713	-0.146742	-0.003329
O	-2.223304	0.095723	0.030427
H	-2.812949	-0.665642	-0.051255
O	0.827674	1.620118	-0.113553
H	1.086987	2.038567	0.722598

Energy = -160.040204 hartree
ZPVE = -100426.828412 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -121.1239

-1	-0.04	0.43	-0.01
-2	-0.06	-0.11	0.00
-3	-0.01	0.27	0.00
-4	-0.15	0.38	-0.01

-5 0.51 -0.28 0.02
-6 0.41 -0.23 0.02

HO-In-P-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.833167	-0.607866	0.049549
O	-2.470539	0.993897	0.112001
H	-2.782549	1.257899	-0.766242
O	2.431554	0.356732	-0.000575
H	2.911150	0.491588	0.829314
In	0.564914	-0.070133	-0.034647

Energy = -160.065404 hartree
ZPVE = -100442.641664 kcal/mol
Number of imaginary frequency (0)

In-P(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.654027	0.682753	-0.183301
O	2.682709	-0.544473	0.285603
H	2.444837	-1.412713	-0.084856
O	-1.084786	1.416540	0.125511
H	-1.779914	1.849175	0.640555
In	-0.780790	-0.360292	-0.022349

Energy = -160.033973 hartree
ZPVE = -100422.918397 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -205.4985

-1 -0.01 0.09 -0.09
-2 -0.05 0.15 0.14
-3 -0.20 0.05 0.46
-4 0.47 0.05 0.14
-5 0.60 0.20 0.20
-6 -0.06 -0.05 -0.02

In-P(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.961784	0.000036	-0.029575
P	1.673907	-0.000044	-0.584642
O	1.148817	-1.319593	0.494275
H	1.817320	-1.559221	1.155076
O	1.149162	1.319490	0.494305
H	1.817688	1.558951	1.155122

Energy = -160.091451 hartree
ZPVE = -100458.986417 kcal/mol
Number of imaginary frequency (0)

H2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-0.000003	1.921013	0.000000
In	-0.000003	-0.532634	0.000000
H	-1.525508	-1.358285	0.000000
H	1.525726	-1.357858	0.000000

Energy = -9.473917 hartree
ZPVE = -5944.977656 kcal/mol
Number of imaginary frequency (0)

H2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.817207	0.062718	0.000004
In	0.515935	-0.002029	-0.000004
H	1.946935	0.932099	0.000106
H	0.030374	-1.773431	0.000058

Energy = -9.475280 hartree
ZPVE = -5945.832952 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -504.3146

-1 -0.04 0.03 -0.00
-2 0.00 -0.01 0.00
-3 -0.19 0.31 -0.00
-4 0.91 -0.18 -0.00

H-In-P-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	1.724392	1.363183	0.000013
P	1.795117	-0.087187	0.000020
In	-0.538520	-0.001518	-0.000015
H	-2.263667	0.019027	0.000424

Energy = -9.546803 hartree
ZPVE = -5990.714350 kcal/mol
Number of imaginary frequency (0)

In-PH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.611937	-0.028918	0.001416
H	0.148437	1.728185	-0.164948
P	-1.890897	-0.032936	-0.083293
H	-1.769897	0.182843	1.344960

Energy = -682.4513 hartree
ZPVE = -428245.0379 kcal/mol
Number of imaginary frequency (0)

Imaginary frequency - -749.7189

-1 -0.01 0.00 -0.00
-2 0.99 0.15 0.02
-3 0.00 -0.02 0.00
-4 -0.02 -0.00 0.00

In-PH2

Atomic Coordinates (Angstroms)

Number	X	Y	Z
In	-0.688157	0.000000	-0.000078
P	1.984197	-0.000002	-0.117299
H	1.978404	1.044308	0.881658
H	1.978343	-1.044302	0.881667

Energy = -9.585914 hartree
ZPVE = -6015.256894 kcal/mol
Number of imaginary frequency (0)

(CH3)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.282160	1.877346	-0.000052
H	-1.584823	2.118353	1.028798
H	-0.680005	2.707664	-0.387495
H	-2.188928	1.776717	-0.611786
C	-1.282386	-1.877254	0.003768
H	-0.641709	-2.734506	0.240973
H	-1.729438	-2.037013	-0.987624
H	-2.094505	-1.823713	0.741900
P	2.262452	-0.000361	0.001292
In	-0.196533	-0.000054	-0.001356

Energy = -88.074058 hartree
ZPVE = -55267.352135 kcal/mol
Number of imaginary frequency (0)

(CH3)2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.183921	-0.067765	0.021076
P	-2.168381	-0.405928	-0.023152
C	0.444462	2.076041	-0.023873
H	-0.480262	2.662647	-0.012987
H	1.065971	2.355047	0.839202
H	0.998623	2.292195	-0.947673
C	2.024778	-1.097274	-0.039099
H	1.922672	-2.190800	-0.035504
H	2.538823	-0.792527	-0.961657

H	2.652324	-0.789762	0.810981

Energy = -88.070792 hartree
ZPVE = -55265.302687 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -72.5403

-1	0.02	-0.10	0.00
-2	0.01	0.28	0.00
-3	-0.35	-0.02	-0.01
-4	-0.42	-0.13	-0.00
-5	-0.37	0.05	-0.02
-6	-0.39	0.04	-0.03
-7	0.16	0.17	0.01
-8	0.29	0.16	-0.02
-9	0.14	0.25	0.02
-10	0.11	0.22	0.03

H3C-In-P-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.530821	-0.012964	-0.000081
P	-1.718853	-0.724326	0.000101
C	-2.730566	0.908699	0.000048
H	-2.573543	1.520925	-0.895494
H	-2.572544	1.521730	0.894862
H	-3.781390	0.587028	0.000782
C	2.661168	0.256098	0.000308
H	3.149698	-0.728537	-0.015532
H	2.985111	0.791778	0.902015
H	2.981616	0.818450	-0.886329

Energy = -88.129376 hartree
ZPVE = -55302.064733 kcal/mol
Number of imaginary frequency (0)

In-P(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.564609	-0.007767	-0.808057

In	0.813714	0.363722	0.044492
C	0.610530	-1.992023	0.105465
H	1.381766	-2.209763	0.851698
H	0.922594	-2.336527	-0.886908
H	-0.333807	-2.459787	0.393483
C	-2.379255	0.123880	0.882618
H	-2.934142	1.075598	0.908692
H	-1.699692	0.107267	1.750793
H	-3.127231	-0.673821	0.994509

Energy = -88.081800 hartree
ZPVE = -55272.210318 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -287.8019

-1	-0.04	0.16	-0.04
-2	-0.04	-0.05	-0.01
-3	0.39	0.05	0.15
-4	0.52	-0.27	-0.08
-5	0.02	-0.02	0.05
-6	0.32	0.32	0.36
-7	-0.00	0.02	0.00
-8	-0.02	-0.00	0.19
-9	-0.01	-0.18	0.00
-10	-0.01	-0.00	-0.16

In-P(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.183019	-0.000017	0.039340
P	-1.397117	-0.000018	-0.678135
C	-2.008743	-1.449501	0.390886
H	-1.684364	-1.410178	1.442558
H	-3.108684	-1.469751	0.380083
H	-1.661054	-2.397024	-0.045582
C	-2.008541	1.449600	0.390844
H	-3.108477	1.470589	0.379301
H	-1.684935	1.409837	1.442752
H	-1.659965	2.397034	-0.045149

Energy = -88.160116 hartree
ZPVE = -55321.354391 kcal/mol
Number of imaginary frequency (0)

(SiH3)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-1.828241	-1.725817	0.247127
H	-1.206724	-2.981706	-0.251192
H	-1.621850	-1.681096	1.722605
H	-3.292552	-1.804492	0.008242
Si	-1.828038	1.725923	0.247076
H	-1.183727	2.978809	-0.228520
H	-1.648862	1.665531	1.725087
H	-3.286349	1.824290	-0.017056
In	1.577022	-0.000026	0.069925
P	-0.923074	-0.000102	-0.886957

Energy = -19.671909 hartree
ZPVE = -12344.319616 kcal/mol
Number of imaginary frequency (0)

(SiH3)2In-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.552851	-1.903139	0.022551
In	0.096092	-0.176038	-0.019433
Si	2.657636	0.216150	0.018471
H	3.057482	0.685484	1.369498
H	3.385848	-1.040033	-0.285237
H	3.047826	1.248915	-0.973899
Si	-1.605026	1.881785	0.009629
H	-0.846438	3.048811	-0.512181
H	-2.827344	1.700408	-0.798804
H	-1.969683	2.158257	1.421193

Energy = -19.673017 hartree
ZPVE = -12345.014897 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -96.7808

-1	-0.12	0.18	0.01
-2	0.05	-0.04	0.01

-3	0.03	0.06	-0.02
-4	0.04	0.03	-0.02
-5	0.04	0.07	-0.06
-6	-0.01	0.08	-0.01
-7	-0.10	-0.10	-0.00
-8	0.13	-0.04	0.46
-9	0.18	0.09	-0.46
-10	-0.54	-0.34	-0.07

H3Si-In-P-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.000033	0.092553	-0.008173
P	-0.002109	2.519577	0.008685
Si	2.278935	-1.196437	0.005854
H	3.402450	-0.344743	-0.458676
H	2.571949	-1.656056	1.388860
H	2.189209	-2.388320	-0.877050
Si	-2.277233	-1.199277	0.005873
H	-3.403495	-0.346201	-0.449674
H	-2.564716	-1.667735	1.387181
H	-2.189193	-2.385710	-0.884636

Energy = -19.742977 hartree
ZPVE = -12388.915497 kcal/mol
Number of imaginary frequency (0)

In-P(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.172255	-0.018739	1.181635
In	-0.750995	-0.798969	-0.136949
Si	-1.453425	1.821200	-0.031282
H	-2.284985	1.926631	1.190977
H	-0.385284	2.841993	-0.018615
H	-2.298920	2.058704	-1.226940
Si	2.559522	0.393464	-0.549824
H	2.162698	-0.207378	-1.866234
H	2.585889	1.880653	-0.704495
H	3.950168	-0.075332	-0.253232

Energy = -19.707693 hartree
ZPVE = -12366.774434 kcal/mol
Number of imaginary frequency (1)

Imaginary frequency - -162.7559

-1	-0.08	0.20	-0.03
-2	-0.03	-0.07	-0.02
-3	0.20	0.05	0.11
-4	-0.24	-0.17	-0.17
-5	-0.00	0.25	0.54
-6	0.59	-0.04	-0.19
-7	-0.01	0.03	-0.01
-8	0.01	-0.05	0.02
-9	0.09	0.01	-0.12
-10	-0.06	-0.05	0.10

In-P(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.472855	-0.130569	-0.007559
P	1.673276	-1.055624	0.009686
Si	2.929924	0.824136	0.002228
H	4.314438	0.363932	0.291766
H	2.577428	1.842370	1.031209
H	2.965207	1.533482	-1.305215
Si	-3.019552	0.393688	0.010720
H	-3.434093	0.938811	1.326568
H	-3.346389	1.375598	-1.051609
H	-3.751048	-0.871464	-0.248877

Energy = -19.781815 hartree
ZPVE = -12413.286730 kcal/mol
Number of imaginary frequency (0)

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(SiMe(SitBu3)2)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z

In	-0.078378	-0.238833	-0.686614
P	-0.269887	-1.265627	-2.802888
Si	2.324314	-0.166564	0.453808
Si	-2.406867	0.229725	0.494109
Si	3.932699	-1.670377	-1.110465
Si	3.255276	2.145237	1.389577
Si	-3.788617	1.800077	-1.200994
Si	-3.346518	-2.065854	1.435725
C	2.236011	-1.179813	2.027584
H	1.488553	-1.963466	1.939930
H	1.951946	-0.577060	2.890618
H	3.185678	-1.659386	2.262285
C	-2.280985	1.253194	2.031099
H	-3.253263	1.436377	2.486748
H	-1.843811	2.224450	1.826481
H	-1.666384	0.780342	2.796218
C	-5.651752	2.336926	-0.411511
C	-2.653905	3.601945	-1.458562
C	-4.029410	0.953597	-3.104131
C	-5.064227	1.727164	-3.950916
H	-6.074408	1.637118	-3.544296
H	-5.103695	1.324339	-4.970674
H	-4.831346	2.789071	-4.038191
C	-2.691623	0.947654	-3.866819
H	-2.418114	1.943963	-4.221445
H	-2.746931	0.310506	-4.757532
H	-1.879339	0.576290	-3.245536
C	-4.528426	-0.491237	-2.988567
H	-5.521907	-0.543574	-2.538492
H	-3.840738	-1.085274	-2.395692
H	-4.603566	-0.966660	-3.973851
C	-3.184842	4.439612	-2.641770
H	-4.249280	4.660554	-2.561906
H	-3.014798	3.948465	-3.602025
H	-2.661723	5.402683	-2.691834
C	-1.183890	3.261248	-1.752911
H	-1.049630	2.745627	-2.704847
H	-0.765647	2.630240	-0.977719
H	-0.575536	4.172124	-1.801036
C	-2.733164	4.460324	-0.180774
H	-3.717889	4.918352	-0.061533
H	-2.012960	5.286306	-0.221762
H	-2.518364	3.886373	0.719248
C	-6.264398	3.550710	-1.147311
H	-7.289377	3.731053	-0.799694
H	-6.315986	3.410573	-2.227765

H	-5.707879	4.470514	-0.952601
C	-6.625029	1.151813	-0.575741
H	-7.516067	1.280668	0.049187
H	-6.158352	0.205233	-0.310234
H	-6.977101	1.055451	-1.606961
C	-5.536827	2.732267	1.074461
H	-6.526306	2.944046	1.497313
H	-4.933582	3.630240	1.221891
H	-5.092415	1.951134	1.680486
C	-3.877091	-3.357544	-0.086651
C	-1.751975	-2.945478	2.540625
C	-4.936379	-1.779520	2.772373
C	-5.242146	-2.928131	-0.661451
H	-5.298144	-1.850591	-0.801862
H	-6.065734	-3.209358	0.002493
H	-5.438915	-3.410123	-1.625793
C	-2.807656	-3.352452	-1.201259
H	-2.522621	-2.345488	-1.499573
H	-3.170232	-3.874544	-2.094485
H	-1.890062	-3.861669	-0.896616
C	-4.029119	-4.815607	0.405966
H	-4.739567	-4.909338	1.229302
H	-3.083052	-5.245128	0.739635
H	-4.392872	-5.457192	-0.406269
C	-6.017621	-0.896996	2.137683
H	-6.818752	-0.671232	2.851442
H	-6.489000	-1.373687	1.275901
H	-5.590446	0.045880	1.819753
C	-4.451466	-1.090247	4.065321
H	-5.300395	-0.838666	4.712827
H	-3.917838	-0.160450	3.862260
H	-3.797335	-1.734052	4.655774
C	-5.614906	-3.116291	3.145885
H	-6.391355	-2.954122	3.903834
H	-4.920324	-3.848299	3.557090
H	-6.112776	-3.572018	2.285799
C	-2.266449	-4.044008	3.493588
H	-2.864213	-3.634998	4.310152
H	-1.425494	-4.569139	3.963286
H	-2.863918	-4.797501	2.975417
C	-0.743928	-3.594918	1.577208
H	-0.420842	-2.904060	0.797794
H	-1.145924	-4.485662	1.092061
H	0.144236	-3.928077	2.126332
C	-1.028643	-1.869932	3.373327
H	-1.698462	-1.345657	4.057269
H	-0.553678	-1.125905	2.733124

H	-0.235339	-2.319249	3.982680
C	3.111524	-3.643314	-1.143904
C	1.837368	-3.678542	-2.005741
H	1.402736	-4.685652	-2.015052
H	2.028061	-3.409384	-3.045269
H	1.075612	-3.013018	-1.601084
C	4.125786	-4.654976	-1.716434
H	3.655296	-5.636718	-1.851874
H	4.968646	-4.812473	-1.039909
H	4.519719	-4.355497	-2.688227
C	2.729382	-4.099832	0.275785
H	2.427995	-5.154407	0.277697
H	1.875814	-3.535592	0.639994
H	3.537941	-3.994188	0.998381
C	4.031971	-0.924351	-3.068508
C	5.876291	-1.832540	-0.324211
C	2.648845	-0.471739	-3.561801
H	1.982596	-1.323507	-3.689296
H	2.720876	0.011300	-4.544066
H	2.185499	0.247775	-2.885140
C	4.554663	-1.997931	-4.049867
H	3.857109	-2.832531	-4.153040
H	5.523176	-2.403295	-3.752169
H	4.680262	-1.574073	-5.053916
C	4.972621	0.288951	-3.149445
H	4.638264	1.080514	-2.484770
H	4.986346	0.708694	-4.162842
H	6.005153	0.033584	-2.908311
C	6.857432	-2.467717	-1.334043
H	6.538013	-3.452892	-1.674400
H	7.847546	-2.592585	-0.878287
H	7.000989	-1.840943	-2.217471
C	6.402703	-0.433771	0.006887
H	5.637915	0.133636	0.524994
H	6.687328	0.129733	-0.883914
H	7.292884	-0.478365	0.644636
C	5.884302	-2.685200	0.960156
H	5.686354	-3.738826	0.750943
H	5.153644	-2.339784	1.691549
H	6.867497	-2.649996	1.445127
C	3.762828	3.378825	-0.211262
C	4.798101	1.927076	2.813040
C	1.592127	3.039157	2.416906
C	6.167478	2.360522	2.251719
H	6.453448	1.829986	1.348464
H	6.963613	2.178270	2.984345
H	6.182167	3.433954	2.034999

C	4.576479	2.820497	4.053115
H	3.680366	2.536463	4.607597
H	4.529633	3.879521	3.784138
H	5.410780	2.717417	4.759271
C	4.864558	0.476487	3.323681
H	3.943673	0.193905	3.842867
H	5.684906	0.350328	4.040521
H	5.036585	-0.234942	2.519748
C	5.175628	3.068966	-0.742838
H	5.372313	2.000814	-0.768200
H	5.955877	3.539752	-0.139700
H	5.310469	3.460043	-1.758515
C	3.756804	4.863608	0.210420
H	2.754987	5.222589	0.454384
H	4.123221	5.498431	-0.605678
H	4.405442	5.039234	1.075446
C	2.758534	3.176703	-1.367711
H	1.733978	3.408396	-1.078037
H	2.769656	2.149603	-1.735591
H	3.003394	3.827341	-2.215695
C	1.962043	4.325412	3.187042
H	1.077074	4.957857	3.332493
H	2.709099	4.932995	2.677317
H	2.321884	4.116285	4.196421
C	0.530048	3.420929	1.381130
H	-0.367127	3.807470	1.875575
H	0.248853	2.552011	0.792428
H	0.864082	4.210319	0.706673
C	0.997955	2.009925	3.398557
H	0.185366	2.456416	3.983621
H	1.740716	1.630196	4.104564
H	0.576632	1.154777	2.868111

Energy = -2005.045286 hartree

SiMe(SitBu3)2-In-P-SiMe(SitBu3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.550573	-0.159407	0.448076
P	-1.434456	-0.412524	1.719169
Si	-3.603390	-0.206595	0.935248
Si	3.060046	0.018774	-0.481423
C	2.578642	0.072997	-2.364235
H	1.589903	0.524818	-2.529073

H	2.545269	-0.938044	-2.786686
H	3.301900	0.656095	-2.949934
H	-5.834481	0.264652	2.783711
H	-4.031665	0.976329	3.470300
H	-4.490368	-0.991786	3.680817
Si	-4.032193	2.124560	-0.310813
Si	3.838430	2.374600	0.125122
Si	4.258586	-2.242809	-0.210538
C	-5.956551	2.587355	-0.575873
C	-3.246441	3.432762	0.971874
C	-3.089785	2.310556	-2.089937
C	-6.591976	1.891168	-1.803538
H	-7.675205	2.119212	-1.823616
H	-6.491282	0.801623	-1.774140
H	-6.171636	2.254077	-2.751869
C	-6.135464	4.112186	-0.801985
H	-7.207839	4.319301	-0.982273
H	-5.582451	4.483948	-1.673044
H	-5.836043	4.705142	0.070834
C	-6.824719	2.217986	0.651167
H	-7.861733	2.561089	0.471180
H	-6.480374	2.694064	1.576780
H	-6.868687	1.135777	0.825415
C	-4.203574	3.772417	2.139333
H	-5.054159	4.392874	1.826371
H	-3.640306	4.353194	2.893949
H	-4.594577	2.878782	2.644411
C	-2.854401	4.772963	0.307369
H	-3.694028	5.268356	-0.197770
H	-2.033724	4.652320	-0.412637
H	-2.489169	5.455464	1.097315
C	-1.964772	2.884015	1.624030
H	-1.241572	2.509948	0.892729
H	-2.164148	2.049334	2.306476
H	-1.473421	3.685198	2.208603
C	-3.366037	3.669056	-2.795678
H	-4.393526	3.718660	-3.185543
H	-2.692442	3.755388	-3.670475
H	-3.196358	4.550015	-2.168310
C	-3.466369	1.243450	-3.142868
H	-4.538802	1.217250	-3.369791
H	-3.147812	0.243971	-2.841791
H	-2.941894	1.477764	-4.090080
C	-1.562598	2.180399	-1.884265
H	-1.145855	2.976696	-1.257520
H	-1.048989	2.228585	-2.863596
H	-1.306321	1.213887	-1.420360

C	-5.671544	-2.301422	-0.980203
C	-6.336573	-3.652063	-1.322310
H	-7.186034	-3.440000	-1.990475
H	-6.727597	-4.158108	-0.430232
H	-5.666134	-4.352410	-1.835770
C	-6.695178	-1.443597	-0.218810
H	-7.459611	-1.097886	-0.926716
H	-6.221104	-0.562775	0.235841
H	-7.189922	-1.995917	0.584401
C	-5.371986	-1.573727	-2.296544
H	-6.327923	-1.336518	-2.785009
H	-4.778527	-2.180466	-2.990634
H	-4.833748	-0.638162	-2.114290
C	-4.358142	-3.564026	1.426272
C	-4.382900	-5.058426	1.021724
H	-5.130717	-5.295380	0.254149
H	-4.634762	-5.628311	1.929916
H	-3.408838	-5.412757	0.662781
C	-3.238528	-3.392362	2.469850
H	-2.945648	-2.345910	2.624395
H	-2.328792	-3.926860	2.178958
H	-3.595342	-3.800263	3.425221
C	-5.708857	-3.270268	2.108243
H	-6.547961	-3.675024	1.525902
H	-5.888620	-2.199637	2.265287
H	-5.703516	-3.766193	3.088672
C	-2.736857	-3.037025	-1.062683
C	-1.568086	-3.520644	-0.189774
H	-1.331737	-2.806655	0.607811
H	-0.689339	-3.611118	-0.839984
H	-1.760473	-4.502525	0.259786
C	-3.123961	-4.216798	-1.989637
H	-3.821830	-3.924741	-2.785712
H	-3.566431	-5.064586	-1.450238
H	-2.194829	-4.571012	-2.464965
C	-2.202146	-1.908536	-1.954649
H	-2.899820	-1.661494	-2.758813
H	-1.260009	-2.242166	-2.412971
H	-2.007276	-0.994821	-1.375047
C	2.882675	-3.665177	-0.498476
C	1.889315	-3.749750	0.684394
H	1.431580	-2.783658	0.949738
H	2.358966	-4.164332	1.586809
H	1.062740	-4.428219	0.414216
C	2.054229	-3.387659	-1.774378
H	1.420037	-2.494734	-1.668819
H	1.377749	-4.240800	-1.965879

H	2.682448	-3.260439	-2.669656
C	3.464626	-5.106557	-0.642618
H	3.807514	-5.319880	-1.660760
H	2.660826	-5.831860	-0.420379
H	4.292024	-5.321316	0.045378
C	4.935753	-2.390654	1.635556
C	3.854368	-1.917920	2.640248
H	3.551993	-0.877185	2.454453
H	4.267169	-1.957971	3.665237
H	2.949926	-2.535244	2.630373
C	5.325646	-3.846836	1.990690
H	5.792539	-3.866624	2.993333
H	6.059492	-4.262579	1.281516
H	4.459198	-4.521533	2.022289
C	6.188465	-1.517232	1.899033
H	6.113082	-0.519818	1.454321
H	7.105963	-1.984097	1.522812
H	6.316757	-1.385185	2.988627
C	5.698025	-2.401062	-1.605928
C	5.491768	-1.384092	-2.752388
H	5.484748	-0.342302	-2.406113
H	4.557412	-1.567362	-3.300733
H	6.321592	-1.482977	-3.477162
C	5.742233	-3.791872	-2.282189
H	5.936693	-4.604347	-1.568679
H	6.568144	-3.796458	-3.017777
H	4.820163	-4.019759	-2.833090
C	7.120929	-2.183109	-1.039840
H	7.262392	-1.203660	-0.570826
H	7.844346	-2.254237	-1.873316
H	7.391822	-2.961229	-0.310804
C	3.829291	2.611581	2.083875
C	5.647376	2.642640	-0.620242
C	2.601487	3.700231	-0.687555
C	5.011468	1.877548	2.755477
H	4.929241	1.986162	3.853216
H	5.987558	2.290544	2.464562
H	5.010477	0.804595	2.534689
C	3.940300	4.103062	2.496478
H	3.062134	4.692835	2.203556
H	4.832776	4.591713	2.081798
H	4.017317	4.164005	3.598207
C	2.540564	2.046300	2.730536
H	1.620139	2.501721	2.345068
H	2.565482	2.235868	3.819867
H	2.463049	0.955206	2.603346
C	6.555202	1.438912	-0.298017

H	6.807828	1.379955	0.767850
H	7.506481	1.526764	-0.855473
H	6.089144	0.490067	-0.588729
C	6.362917	3.903003	-0.073507
H	5.805557	4.830429	-0.255258
H	7.343689	4.005267	-0.575960
H	6.562562	3.829164	1.005129
C	5.596476	2.761273	-2.163541
H	5.078586	3.668622	-2.502893
H	5.110178	1.894325	-2.634991
H	6.629342	2.809312	-2.556571
C	2.179810	3.342195	-2.132665
H	1.643432	4.202943	-2.573443
H	1.485692	2.494245	-2.146978
H	3.023619	3.106314	-2.792381
C	1.288757	3.823841	0.115084
H	0.592853	4.493442	-0.422188
H	1.428274	4.247738	1.117725
H	0.778967	2.855691	0.227489
C	3.236879	5.115742	-0.742800
H	2.465647	5.834327	-1.079007
H	4.063542	5.176032	-1.464172
H	3.604605	5.467452	0.229725
C	-4.630506	0.032077	2.987771
Si	-4.118907	-2.413847	0.002805

Energy = -2005.091504 hartree

In-P(SiMe(SitBu3)2)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

P	0.006515	0.011152	-0.457413
In	-0.126139	-0.437200	-2.772409
Si	-2.268527	0.118571	0.542529
Si	2.297173	-0.025055	0.550075
Si	-3.907769	1.765233	-0.863056
Si	-3.123110	-2.246121	1.399223
Si	3.924103	-1.755747	-0.754340
Si	3.140122	2.416256	1.229699
C	-2.057066	1.096747	2.118329
H	-1.655410	2.082098	1.896627
H	-1.374872	0.619719	2.814931
H	-2.995481	1.235608	2.651400
C	2.114065	-0.830094	2.228579

H	3.057687	-0.870067	2.769806
H	1.740764	-1.845876	2.142074
H	1.420393	-0.287804	2.865244
C	5.704967	-2.144259	0.349291
C	2.873710	-3.624695	-0.846254
C	4.482401	-1.215775	-2.709467
C	5.603471	-2.126899	-3.258319
H	6.543060	-1.993048	-2.719894
H	5.817683	-1.885690	-4.307157
H	5.343740	-3.184990	-3.226767
C	3.293053	-1.301711	-3.675357
H	2.867117	-2.303199	-3.733669
H	3.593365	-1.030047	-4.695104
H	2.521897	-0.594615	-3.381019
C	4.998623	0.228349	-2.757331
H	5.894099	0.370365	-2.151136
H	4.225581	0.917843	-2.425354
H	5.265463	0.518353	-3.781120
C	3.538589	-4.606056	-1.833863
H	4.588199	-4.791510	-1.605184
H	3.473611	-4.255490	-2.866490
H	3.030463	-5.578015	-1.805404
C	1.438050	-3.380081	-1.329363
H	1.406910	-3.064151	-2.372612
H	0.937508	-2.622294	-0.730859
H	0.846957	-4.301202	-1.267688
C	2.830096	-4.284379	0.545346
H	3.800138	-4.684044	0.844806
H	2.136397	-5.133738	0.551972
H	2.505423	-3.592158	1.318684
C	6.361010	-3.480517	-0.069854
H	7.338976	-3.592202	0.415318
H	6.532406	-3.549724	-1.144693
H	5.771593	-4.346910	0.232768
C	6.728119	-1.025369	0.064364
H	7.488922	-0.975416	0.851647
H	6.254176	-0.049974	-0.017892
H	7.266011	-1.190691	-0.873351
C	5.405585	-2.236142	1.857778
H	6.320921	-2.456612	2.420318
H	4.689649	-3.025470	2.094492
H	5.009320	-1.309160	2.259130
C	3.559721	3.476396	-0.507853
C	1.553401	3.365409	2.266506
C	4.780361	2.453216	2.531026
C	4.986255	3.135888	-0.983499
H	5.200293	2.073493	-0.884835

H	5.746576	3.667926	-0.403669
H	5.135414	3.422622	-2.030695
C	2.536949	3.110510	-1.605693
H	2.508143	2.039077	-1.810064
H	2.779255	3.615995	-2.547887
H	1.524247	3.414044	-1.332924
C	3.508396	5.004170	-0.286186
H	4.165899	5.327725	0.524646
H	2.502268	5.361574	-0.061731
H	3.830052	5.533145	-1.191890
C	5.908874	1.563749	2.009692
H	6.738464	1.504978	2.724316
H	6.330111	1.929309	1.071618
H	5.536192	0.558967	1.861164
C	4.381025	1.938470	3.929908
H	5.266278	1.802811	4.563328
H	3.867604	0.974855	3.882122
H	3.740368	2.649221	4.456323
C	5.364717	3.877478	2.672830
H	6.193540	3.881682	3.391722
H	4.637615	4.605608	3.029444
H	5.768973	4.250047	1.728679
C	1.995845	4.678565	2.938097
H	2.646617	4.496045	3.796454
H	1.126388	5.223952	3.325774
H	2.512211	5.350559	2.250530
C	0.440407	3.679755	1.265762
H	0.160299	2.773673	0.728092
H	0.728637	4.437145	0.536373
H	-0.449341	4.065867	1.776560
C	0.976005	2.439374	3.350754
H	1.713033	2.121008	4.087151
H	0.549114	1.547138	2.902639
H	0.168465	2.938153	3.900232
C	-2.733953	3.075528	-2.085188
C	-2.351051	2.397790	-3.411710
H	-1.510679	2.914959	-3.890206
H	-3.164931	2.408146	-4.139078
H	-2.065518	1.363794	-3.260061
C	-3.490632	4.372949	-2.434574
H	-2.905901	4.977945	-3.138966
H	-3.662456	5.005515	-1.563152
H	-4.453633	4.174964	-2.910714
C	-1.454255	3.434638	-1.328787
H	-0.854596	4.161844	-1.888692
H	-0.831679	2.550842	-1.180207
H	-1.677876	3.878441	-0.358068

C	-5.220773	0.786690	-2.156624
C	-4.987792	3.000453	0.507283
C	-4.461279	-0.281653	-2.970263
H	-3.861584	0.158082	-3.770627
H	-5.157603	-0.975877	-3.455122
H	-3.788433	-0.865172	-2.343883
C	-5.895037	1.758336	-3.153553
H	-5.186780	2.213474	-3.844798
H	-6.432063	2.566497	-2.654764
H	-6.626446	1.223741	-3.772667
C	-6.354969	0.121816	-1.362693
H	-5.955746	-0.542049	-0.607594
H	-7.000311	-0.476658	-2.016586
H	-6.998408	0.853432	-0.868200
C	-6.101479	3.786591	-0.222102
H	-5.730652	4.386049	-1.051969
H	-6.597816	4.478586	0.469710
H	-6.880703	3.122778	-0.605138
C	-5.681097	2.164523	1.597702
H	-4.977272	1.563750	2.169974
H	-6.446054	1.507613	1.179112
H	-6.194221	2.815361	2.316716
C	-4.041045	4.005628	1.196987
H	-3.590069	4.707580	0.495701
H	-3.235741	3.511217	1.737977
H	-4.589385	4.610343	1.929819
C	-3.445547	-3.560957	-0.185552
C	-4.838854	-2.100757	2.598931
C	-1.587455	-3.048945	2.637318
C	-5.925416	-1.312123	1.863094
H	-5.502308	-0.408123	1.441602
H	-6.742813	-1.025146	2.534594
H	-6.377333	-1.890660	1.054365
C	-5.433748	-3.488001	2.927905
H	-4.736942	-4.138541	3.454613
H	-5.765018	-4.015333	2.029958
H	-6.315328	-3.382304	3.572410
C	-4.517966	-1.371457	3.919393
H	-3.880742	-1.973122	4.571231
H	-5.434670	-1.172991	4.488022
H	-4.029653	-0.409764	3.749931
C	-4.817091	-3.312308	-0.837005
H	-4.933603	-2.273595	-1.126432
H	-5.643001	-3.576808	-0.172652
H	-4.937455	-3.917474	-1.743652
C	-3.428470	-5.035247	0.276655
H	-2.446618	-5.353782	0.628514

H	-3.686722	-5.702142	-0.555394
H	-4.149184	-5.227602	1.074852
C	-2.354273	-3.368680	-1.254391
H	-1.359219	-3.567047	-0.857924
H	-2.356840	-2.353707	-1.651478
H	-2.506922	-4.049502	-2.100049
C	-2.090496	-4.236853	3.479055
H	-1.252244	-4.732137	3.984673
H	-2.593832	-4.996848	2.879616
H	-2.772410	-3.912445	4.268766
C	-0.427109	-3.525018	1.753809
H	0.420162	-3.839563	2.373143
H	-0.091090	-2.718454	1.102414
H	-0.686036	-4.381834	1.132002
C	-1.043815	-1.976842	3.597243
H	-0.317263	-2.409748	4.295493
H	-1.819278	-1.497668	4.194723
H	-0.519432	-1.203004	3.043315

Energy = -2004.982581 hartree

(SiiPrDis2)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.041731	0.053082	-0.650539
Si	-2.397228	0.070981	0.522762
C	-3.364769	1.320024	-0.537471
H	-3.175347	0.995379	-1.561193
C	-2.718277	-1.813293	0.287670
H	-1.699568	-2.194992	0.430267
C	-1.999528	0.761034	2.294717
H	-1.098156	1.345892	2.105310
C	-1.617654	-0.241687	3.373099
H	-2.495972	-0.643892	3.885112
H	-1.001603	0.237407	4.143136
H	-1.051714	-1.067063	2.960526
C	-3.009301	1.721141	2.931951
H	-2.591038	2.160981	3.845566
H	-3.933366	1.214773	3.217082
H	-3.270027	2.552512	2.283073
Si	-3.082736	-2.425949	-1.480336
Si	-3.623815	-2.770687	1.638297
Si	-5.243353	1.338256	-0.405852
Si	-2.687161	3.120444	-0.592069

C	-1.756085	-3.752336	-1.903630
H	-1.642306	-4.451634	-1.071601
H	-0.804239	-3.259702	-2.111094
H	-2.060813	-4.306756	-2.795832
C	-2.977484	-1.206757	-2.913799
H	-3.857570	-0.562212	-2.959455
H	-2.939708	-1.759775	-3.858487
H	-2.083177	-0.592519	-2.866220
C	-4.721977	-3.323753	-1.813252
H	-4.623263	-4.395946	-1.624644
H	-4.989084	-3.213182	-2.869502
H	-5.549997	-2.933392	-1.223618
C	-4.510829	-4.383130	1.133662
H	-3.870582	-5.005346	0.503594
H	-5.458162	-4.175609	0.633144
H	-4.749304	-4.957988	2.034809
C	-4.907363	-1.823467	2.624160
H	-5.862724	-1.781685	2.095171
H	-4.596070	-0.805041	2.841564
H	-5.089236	-2.326358	3.579417
C	-2.326177	-3.492742	2.869458
H	-2.210987	-2.857834	3.747745
H	-1.362933	-3.618842	2.369841
H	-2.660750	-4.474122	3.219235
C	-1.076128	3.493256	0.299150
H	-0.718097	4.479784	-0.012149
H	-0.291749	2.777116	0.077372
H	-1.222364	3.536389	1.380812
C	-2.401947	3.535641	-2.435350
H	-2.013268	4.553312	-2.532708
H	-3.340290	3.463496	-2.991235
H	-1.679807	2.841768	-2.871370
C	-3.798898	4.512368	0.081955
H	-4.794847	4.530812	-0.357089
H	-3.328788	5.475589	-0.143966
H	-3.890417	4.445436	1.168556
C	-5.987543	2.339621	-1.872480
H	-5.752701	3.401716	-1.825325
H	-7.076399	2.231111	-1.864363
H	-5.605184	1.935884	-2.814766
C	-6.087882	-0.321351	-0.697240
H	-5.912120	-0.665637	-1.718164
H	-7.170050	-0.216020	-0.569162
H	-5.745591	-1.067085	0.012069
C	-5.973986	1.981000	1.193146
H	-5.542214	2.928551	1.514084
H	-5.845215	1.252412	1.996993

H	-7.050828	2.138259	1.071928
P	0.074283	0.687574	-2.923912
Si	2.401814	-0.144067	0.558598
C	3.251918	1.533763	0.332854
H	4.281723	1.301608	0.581894
C	3.518185	-1.675917	0.183758
H	3.417677	-2.233641	1.117499
C	1.911088	-0.559106	2.510028
H	1.149441	0.182755	2.748470
C	3.095903	-0.442041	3.474031
H	2.748623	-0.523537	4.510186
H	3.619828	0.507546	3.380713
H	3.828021	-1.240172	3.313570
C	1.297697	-1.956085	2.686674
H	0.864130	-2.052724	3.688562
H	2.038145	-2.756234	2.599444
H	0.511477	-2.146218	1.955288
Si	5.397642	-1.519236	0.180282
Si	2.834908	-2.944716	-1.023902
Si	3.428678	2.144726	-1.456275
Si	2.929339	2.959425	1.527202
C	6.119689	-3.139696	0.968489
H	5.472200	-3.476891	1.782126
H	7.116437	-2.934056	1.369303
H	6.214940	-3.925078	0.217593
C	6.169950	-0.197029	1.296082
H	5.592102	-0.047077	2.207709
H	6.280285	0.754186	0.770033
H	7.177655	-0.507537	1.590987
C	6.231927	-1.348556	-1.495330
H	6.277506	-0.300603	-1.803302
H	5.724062	-1.921033	-2.274415
H	7.263277	-1.710901	-1.435048
C	3.992610	-4.445346	-1.300327
H	4.208954	-4.937127	-0.348535
H	4.922859	-4.147637	-1.788600
H	3.490081	-5.170501	-1.948291
C	2.409354	-2.365814	-2.743982
H	3.295569	-2.009180	-3.274413
H	1.657830	-1.578175	-2.739794
H	1.998266	-3.196601	-3.327193
C	1.314454	-3.793299	-0.261850
H	0.500147	-3.085446	-0.116572
H	1.573249	-4.240140	0.701845
H	0.969136	-4.593738	-0.922375
C	1.631644	2.763420	2.863358
H	1.425194	3.733495	3.327838

H	1.954570	2.098404	3.665575
H	0.695649	2.401273	2.445543
C	4.599226	3.246074	2.465510
H	4.481443	4.072018	3.172329
H	5.383151	3.497843	1.746176
H	4.889108	2.346346	3.011401
C	2.565148	4.675699	0.803937
H	3.359981	5.017417	0.138172
H	2.493970	5.402105	1.620417
H	1.611547	4.687561	0.275163
C	5.103282	3.085500	-1.564594
H	5.115781	3.949062	-0.897125
H	5.261830	3.432519	-2.589650
H	5.920093	2.412532	-1.289270
C	3.592936	0.828075	-2.783604
H	2.616952	0.469794	-3.105835
H	4.089381	1.243229	-3.666562
H	4.179259	-0.016450	-2.442207
C	2.096519	3.304445	-2.101931
H	2.351303	4.351553	-1.922997
H	1.125465	3.095173	-1.654363
H	1.992769	3.187311	-3.185680

Energy = -1397.153540 hartree

(SiiPrDis2)-In-P-(SiiPrDis2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.929460	0.644053	-0.382456
Si	3.156892	-0.260068	-0.573633
C	4.094442	1.368121	-0.376179
H	3.728074	1.820802	0.547490
C	2.967484	-1.556862	0.771723
H	1.947676	-1.914381	0.595354
C	3.023470	-0.869389	-2.435693
H	2.871946	0.046412	-3.014320
C	1.782708	-1.718670	-2.734478
H	1.810091	-2.118179	-3.754126
H	0.878938	-1.107647	-2.668761
H	1.661400	-2.554956	-2.046670
C	4.284736	-1.505780	-3.021213
H	4.085262	-1.953475	-4.001077
H	4.716134	-2.275728	-2.382644
H	5.052314	-0.747396	-3.186781

Si	2.846467	-0.898382	2.543586
Si	3.916717	-3.170862	0.644420
Si	5.960862	1.252900	-0.189883
Si	3.641062	2.685616	-1.705226
C	1.431458	-1.872909	3.424981
H	1.160104	-1.357353	4.350761
H	1.757396	-2.882923	3.678236
H	0.552416	-1.930512	2.780281
C	2.340083	0.909108	2.755123
H	3.194322	1.575875	2.618349
H	1.968539	1.069306	3.772558
H	1.546093	1.194863	2.066125
C	4.358807	-1.129245	3.652794
H	4.052069	-1.548878	4.616250
H	4.832665	-0.165656	3.857477
H	5.109430	-1.794176	3.225142
C	3.656636	-4.323628	2.159722
H	2.591969	-4.535726	2.287883
H	4.060445	-3.892350	3.076920
H	4.173140	-5.271474	1.978278
C	5.766566	-3.053376	0.415504
H	6.266133	-2.732480	1.332294
H	6.029960	-2.367253	-0.386756
H	6.175286	-4.035021	0.154494
C	3.231100	-4.288903	-0.742380
H	3.482100	-3.919027	-1.735021
H	2.144741	-4.374371	-0.650054
H	3.660211	-5.291236	-0.645637
C	1.826851	2.754395	-2.247924
H	1.700878	3.551188	-2.988437
H	1.178849	2.992869	-1.400993
H	1.498054	1.824076	-2.713941
C	3.903406	4.432093	-0.957952
H	3.278741	5.155113	-1.491228
H	4.941122	4.754671	-1.054045
H	3.616615	4.435012	0.097260
C	4.650878	2.584681	-3.292450
H	5.696293	2.853019	-3.121820
H	4.250801	3.286296	-4.031377
H	4.611038	1.583915	-3.728010
C	6.794814	2.972325	-0.050098
H	6.832142	3.470542	-1.021222
H	7.824162	2.846970	0.300162
H	6.260602	3.595952	0.671548
C	6.437125	0.481339	1.464248
H	6.015780	1.065352	2.286160
H	7.525134	0.467536	1.579269

H	6.080337	-0.541182	1.526500
C	6.906406	0.360238	-1.534130
H	6.733460	0.799471	-2.518429
H	6.651425	-0.697623	-1.578077
H	7.981524	0.423124	-1.335870
In	-0.734238	-0.776946	-0.025828
Si	-3.066095	0.408175	-0.406543
C	-3.539757	1.283443	1.210588
H	-4.616881	1.446640	1.197789
C	-4.390277	-0.602502	-1.358212
H	-4.359953	-0.182081	-2.368442
C	-2.477111	1.764529	-1.909103
H	-1.819101	2.463478	-1.390309
C	-3.672046	2.499865	-2.527312
H	-3.320902	3.349090	-3.124103
H	-4.359004	2.884130	-1.775574
H	-4.248656	1.855285	-3.198401
C	-1.683531	1.085494	-3.032095
H	-1.355079	1.830879	-3.765365
H	-2.286881	0.345607	-3.564895
H	-0.786478	0.589824	-2.661483
Si	-6.174487	-0.298982	-0.858033
Si	-3.953708	-2.400813	-1.700874
Si	-3.259514	0.231138	2.794070
Si	-2.794261	3.017228	1.491962
C	-7.398009	-0.924068	-2.198828
H	-6.982766	-0.760435	-3.196671
H	-8.336743	-0.366697	-2.120605
H	-7.632756	-1.979988	-2.057484
C	-6.649411	1.544774	-0.815669
H	-6.543321	1.978396	-1.813837
H	-6.056995	2.128274	-0.113971
H	-7.699451	1.639397	-0.520762
C	-6.710696	-1.081545	0.751474
H	-6.262854	-0.576427	1.608109
H	-6.449431	-2.142121	0.789042
H	-7.797109	-1.005968	0.863572
C	-5.313615	-3.355416	-2.649915
H	-5.663161	-2.780035	-3.510275
H	-6.147434	-3.597283	-1.987240
H	-4.899615	-4.299331	-3.018717
C	-3.566949	-3.502045	-0.243705
H	-4.389335	-3.515923	0.474689
H	-2.649002	-3.208020	0.263389
H	-3.422250	-4.532444	-0.585758
C	-2.504835	-2.503892	-2.941186
H	-1.601925	-2.027671	-2.562915

H	-2.788882	-2.021291	-3.880743
H	-2.275503	-3.553236	-3.150133
C	-3.501628	4.322488	0.304539
H	-3.396503	5.317731	0.748414
H	-4.565090	4.145735	0.126574
H	-2.959398	4.338662	-0.641474
C	-3.311739	3.763513	3.180476
H	-3.034663	4.822055	3.207129
H	-2.807969	3.270209	4.013013
H	-4.395395	3.689808	3.306194
C	-0.926317	3.125395	1.405642
H	-0.606008	4.162670	1.547289
H	-0.545548	2.796846	0.438178
H	-0.448833	2.529413	2.184303
C	-4.626249	0.703101	4.058229
H	-4.382813	1.631166	4.577262
H	-4.719075	-0.088094	4.808110
H	-5.586423	0.817689	3.548477
C	-3.484632	-1.626242	2.600875
H	-2.599987	-2.083899	2.158169
H	-3.623360	-2.088427	3.583724
H	-4.361549	-1.860010	2.002233
C	-1.603635	0.442624	3.663402
H	-1.499252	1.427369	4.123295
H	-0.772195	0.292663	2.973353
H	-1.508786	-0.299033	4.463157

Energy = -1397.217405 hartree

In-P(Sii PrDis2)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

P	-0.213874	-0.514884	-0.062785
Si	2.346711	-0.081942	-0.687284
C	2.928944	1.689417	-0.325545
H	2.427926	1.993262	0.596398
C	2.987247	-1.581157	0.389244
H	2.146751	-2.263235	0.261767
C	2.147178	-0.528134	-2.603669
H	1.421564	0.207519	-2.940946
C	1.483918	-1.866250	-2.936654
H	2.154677	-2.544848	-3.468289
H	0.654081	-1.696794	-3.632407
H	1.088000	-2.384413	-2.064449

C	3.399304	-0.323547	-3.457094
H	3.201275	-0.581174	-4.503793
H	4.238871	-0.932186	-3.116160
H	3.719919	0.718366	-3.448696
Si	3.006489	-1.322643	2.271208
Si	4.376873	-2.679938	-0.234594
Si	4.804883	2.013156	0.021251
Si	2.485264	3.089814	-1.613587
C	1.945632	-2.695040	3.114329
H	2.240045	-2.788348	4.163999
H	2.096766	-3.656991	2.620144
H	0.889321	-2.426747	3.089954
C	2.259469	0.290913	2.863998
H	2.943409	1.134491	2.774334
H	1.973085	0.215098	3.917388
H	1.368445	0.513469	2.282071
C	4.663695	-1.508585	3.186883
H	4.651318	-2.413223	3.803155
H	4.814397	-0.659754	3.860769
H	5.526509	-1.577876	2.525644
C	4.780786	-4.109446	0.996394
H	3.858930	-4.600284	1.317656
H	5.334900	-3.754858	1.865268
H	5.405591	-4.850272	0.487598
C	6.008357	-1.878982	-0.658430
H	6.550460	-1.550766	0.230143
H	5.870938	-1.032709	-1.329520
H	6.653362	-2.598677	-1.173603
C	3.883779	-3.710789	-1.757800
H	4.042601	-3.146413	-2.676140
H	2.845502	-4.041390	-1.681501
H	4.516186	-4.602301	-1.819383
C	1.123249	2.699527	-2.804880
H	0.520704	3.581894	-3.038464
H	0.502860	1.964987	-2.316854
H	1.493381	2.290142	-3.748643
C	1.865938	4.611861	-0.633920
H	0.788358	4.531357	-0.472400
H	2.056562	5.524034	-1.206726
H	2.362909	4.693667	0.334376
C	3.832105	3.738901	-2.785038
H	4.617809	4.291537	-2.268952
H	3.373638	4.435961	-3.495192
H	4.277270	2.931081	-3.369424
C	5.062140	3.834999	0.644260
H	4.853359	4.576435	-0.126212
H	6.103697	3.954986	0.957729

H	4.414121	4.011879	1.507368
C	5.592322	1.124455	1.468570
H	5.074331	1.324701	2.406426
H	6.626884	1.460317	1.597079
H	5.629258	0.064398	1.267343
C	5.972766	1.737803	-1.427845
H	6.265082	2.683743	-1.890652
H	5.534053	1.097779	-2.192343
H	6.894445	1.258701	-1.082077
In	-0.537262	-2.791426	0.507331
Si	-2.438361	0.643266	-0.351344
C	-2.850073	1.419658	1.339042
H	-3.894224	1.726048	1.294220
C	-3.931617	-0.286326	-1.219415
H	-3.994677	0.279723	-2.151486
C	-2.065598	1.984373	-1.840916
H	-1.233619	2.564690	-1.441448
C	-3.232721	2.928912	-2.152385
H	-2.872455	3.789933	-2.726601
H	-3.721988	3.304228	-1.255964
H	-4.002557	2.443744	-2.761151
C	-1.684485	1.272290	-3.155107
H	-1.314691	1.997122	-3.888232
H	-2.538402	0.777063	-3.627243
H	-0.917036	0.510383	-3.002305
Si	-5.685320	0.067819	-0.593350
Si	-3.679516	-1.993447	-1.922837
Si	-2.790351	0.206455	2.810620
Si	-1.931815	3.014926	1.780363
C	-7.026421	-0.538086	-1.834215
H	-6.771022	-0.234231	-2.852028
H	-7.987876	-0.086334	-1.570665
H	-7.139647	-1.622387	-1.772404
C	-6.102109	1.923816	-0.512150
H	-6.038993	2.366667	-1.509363
H	-5.455224	2.479604	0.164907
H	-7.131390	2.045539	-0.159438
C	-6.202227	-0.702371	1.027673
H	-5.794921	-0.153362	1.875949
H	-5.906311	-1.751197	1.092460
H	-7.292420	-0.667283	1.126368
C	-4.808639	-2.252702	-3.482458
H	-4.888373	-1.317869	-4.042993
H	-5.797249	-2.608895	-3.190991
H	-4.354810	-3.012941	-4.125567
C	-4.104537	-3.431878	-0.806392
H	-5.155018	-3.397091	-0.504408

H	-3.495015	-3.465913	0.095406
H	-3.950865	-4.376069	-1.339113
C	-1.997178	-2.231163	-2.731332
H	-1.210345	-1.750425	-2.159876
H	-1.989912	-1.790006	-3.732940
H	-1.762154	-3.294689	-2.833270
C	-2.375338	4.492181	0.679676
H	-2.028022	5.417149	1.151663
H	-3.458560	4.569215	0.556178
H	-1.889170	4.431903	-0.294383
C	-2.419279	3.686605	3.506195
H	-2.040797	4.707366	3.618757
H	-1.979833	3.081994	4.302362
H	-3.507192	3.710366	3.610930
C	-0.077743	2.868802	1.790774
H	0.277237	2.372446	2.693573
H	0.385026	3.859131	1.777306
H	0.261285	2.312885	0.917904
C	-4.036142	0.822597	4.147598
H	-3.559834	1.529804	4.828517
H	-4.386475	-0.027873	4.739856
H	-4.896185	1.298806	3.669750
C	-3.380829	-1.551951	2.473951
H	-2.677971	-2.278451	2.891681
H	-4.347037	-1.739613	2.950006
H	-3.479789	-1.738562	1.410665
C	-1.148876	0.008510	3.683766
H	-0.770034	0.945261	4.095399
H	-0.421054	-0.406598	2.990418
H	-1.246091	-0.694486	4.517444

Energy = -1397.170904 hartree

(NHC)2In-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.464814	-0.334450	-0.756791
P	1.533457	-0.930987	-2.774220
C	1.657134	-0.181279	1.126197
N	1.316882	-1.110030	2.267535
C	2.514065	-1.524589	2.853370
C	3.564870	-1.119893	2.134208
N	3.151082	-0.351514	1.056322

H	1.464874	0.850934	1.423138
H	2.512719	-2.091787	3.772654
H	4.613904	-1.302566	2.311754
C	0.187310	-0.894271	3.076635
C	-2.107613	-0.528296	4.711724
C	-0.801853	-1.918281	3.178896
C	0.045818	0.273319	3.892502
C	-1.120317	0.441705	4.670261
C	-1.936197	-1.702044	3.994764
H	-1.252289	1.332807	5.280224
H	-2.699555	-2.473223	4.085827
H	-2.990082	-0.387327	5.329186
C	3.866833	-0.244007	-0.142860
C	5.239816	0.015625	-2.613705
C	4.191391	-1.401727	-0.927833
C	4.319460	1.030759	-0.589265
C	4.964926	1.133606	-1.842233
C	4.882731	-1.239388	-2.146786
H	5.291793	2.104198	-2.211883
H	5.153419	-2.101071	-2.751397
H	5.757925	0.119070	-3.562895
C	-0.715059	-3.323655	2.571137
H	-1.739185	-3.724991	2.557904
C	0.098648	-4.259940	3.470275
H	1.157052	-3.988145	3.492422
H	0.031646	-5.292760	3.110778
H	-0.271951	-4.243286	4.501157
C	-0.255378	-3.439478	1.122999
H	-0.440573	-4.452229	0.746417
H	0.813238	-3.254359	1.000493
H	-0.814091	-2.749543	0.490439
C	1.144850	1.325775	4.061093
H	2.028650	1.036693	3.496784
C	1.624925	1.422471	5.516305
H	0.850781	1.812721	6.185137
H	2.488842	2.092460	5.589284
H	1.931200	0.440032	5.892679
C	0.716232	2.702009	3.544695
H	-0.108940	3.121963	4.129118
H	0.393649	2.647392	2.500559
H	1.551451	3.408978	3.597157
C	3.865005	-2.833738	-0.486592
H	3.084769	-2.812259	0.276125
C	5.110099	-3.504747	0.106994
H	4.858223	-4.488114	0.518772
H	5.550713	-2.908886	0.911491
H	5.887601	-3.650540	-0.651713

C	3.295495	-3.730503	-1.596067
H	4.036511	-3.968908	-2.365715
H	2.440631	-3.261695	-2.085900
H	2.953035	-4.682352	-1.174118
C	4.244573	2.340133	0.199406
H	5.064987	2.971462	-0.174177
C	4.521573	2.248493	1.700086
H	4.729432	3.245390	2.105982
H	5.392447	1.618095	1.908074
H	3.668168	1.861854	2.256539
C	2.960623	3.110576	-0.090938
H	2.071319	2.573029	0.241011
H	2.856245	3.296522	-1.164945
H	2.970465	4.082323	0.414488
C	-1.600604	0.518716	-0.881224
N	-1.704129	1.845774	-1.597583
C	-2.769459	1.780061	-2.489922
C	-3.231364	0.528173	-2.584983
N	-2.519492	-0.312729	-1.741991
H	-3.147234	2.667181	-2.975385
H	-4.061011	0.157515	-3.169027
C	-2.985806	-1.572791	-1.344017
C	-3.808495	-4.166077	-0.552809
C	-3.975127	-1.740245	-0.337224
C	-2.493924	-2.731477	-2.016748
C	-2.915324	-4.010411	-1.601865
C	-4.343125	-3.043086	0.061185
H	-2.563412	-4.904224	-2.110249
H	-5.090442	-3.191331	0.837590
H	-4.122496	-5.159523	-0.244947
C	-1.239831	3.054830	-1.065405
C	-0.188538	5.451879	0.060633
C	-0.260028	3.822537	-1.767338
C	-1.768247	3.596656	0.145429
C	-1.200933	4.763990	0.703310
C	0.247642	5.005044	-1.174761
H	-1.583642	5.172935	1.635942
H	0.998455	5.599724	-1.693148
H	0.221882	6.359447	0.493542
C	-1.585891	-2.619940	-3.243079
H	-1.121216	-1.630173	-3.266653
C	-2.408400	-2.764494	-4.527265
H	-3.207361	-2.016514	-4.571650
H	-2.875801	-3.752956	-4.599585
H	-1.773780	-2.628214	-5.409576
C	-0.431535	-3.629765	-3.237209
H	0.097268	-3.616405	-2.279046

H	0.288857	-3.388761	-4.026715
H	-0.773333	-4.654220	-3.417948
C	-4.747542	-0.571115	0.264914
H	-4.370396	0.367412	-0.137443
C	-6.230294	-0.622836	-0.123839
H	-6.740230	-1.491136	0.306943
H	-6.347893	-0.670707	-1.212229
H	-6.750613	0.274343	0.229214
C	-4.591352	-0.492451	1.782215
H	-5.133973	0.370791	2.181330
H	-3.536743	-0.378317	2.044285
H	-4.972919	-1.382616	2.292253
C	0.273479	3.557070	-3.180895
H	1.188434	4.158739	-3.288038
C	0.739785	2.143349	-3.499105
H	1.250906	2.121212	-4.468751
H	-0.082136	1.428138	-3.563369
H	1.458922	1.805072	-2.749323
C	-0.681940	4.080656	-4.256869
H	-0.991337	5.110675	-4.048311
H	-1.582716	3.470791	-4.343499
H	-0.192648	4.074117	-5.237423
C	-3.026760	3.055819	0.822001
H	-3.403338	2.199447	0.268088
C	-4.168688	4.080922	0.795224
H	-3.948297	4.964081	1.404069
H	-5.091167	3.635270	1.183766
H	-4.366170	4.418990	-0.228218
C	-2.754621	2.592844	2.252172
H	-2.408429	3.406586	2.897196
H	-1.990766	1.811430	2.255884
H	-3.660594	2.183464	2.708856
H	-1.990076	0.579206	0.138027

Energy = -2328.523706 hartree

NHC-In-P-NHC

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.581777	-0.537376	1.189166
P	0.788892	1.202161	1.087367
C	2.561442	0.809729	0.598770
N	2.656466	-0.590768	0.115159
C	2.362835	-0.526434	-1.252606

C	2.484094	0.729628	-1.713346
N	2.823488	1.554808	-0.661930
H	3.285337	1.071570	1.370136
H	2.067363	-1.404445	-1.799454
H	2.354543	1.108235	-2.715307
C	2.864058	-1.767066	0.860474
C	2.546011	-4.349996	2.048637
C	3.332746	-2.959788	0.210108
C	2.552252	-1.904495	2.257245
C	2.364599	-3.202473	2.799074
C	3.074006	-4.228668	0.781676
H	2.089727	-3.345414	3.840445
H	3.365241	-5.136408	0.255770
H	2.384070	-5.329530	2.488172
C	2.994562	2.941206	-0.647220
C	3.356979	5.746993	-0.371701
C	1.900378	3.838199	-0.816494
C	4.295064	3.492868	-0.434279
C	4.440311	4.889761	-0.275585
C	2.107043	5.227342	-0.663893
H	5.422126	5.326215	-0.101282
H	1.282563	5.925306	-0.790590
H	3.493311	6.818723	-0.259666
C	4.346179	-3.031636	-0.952101
H	5.027019	-3.845318	-0.650535
C	5.316002	-1.857871	-1.107665
H	4.867093	-0.996852	-1.600362
H	6.169648	-2.156126	-1.727799
H	5.712198	-1.540715	-0.137676
C	3.776015	-3.495906	-2.294332
H	3.088286	-4.338137	-2.170142
H	4.588458	-3.830716	-2.949916
H	3.252386	-2.705272	-2.832808
C	2.537716	-0.751328	3.270107
H	2.114966	0.135491	2.816364
C	3.978202	-0.440501	3.698169
H	4.421361	-1.281214	4.244391
H	4.007413	0.437848	4.351973
H	4.621642	-0.236239	2.836390
C	1.673981	-0.949252	4.529562
H	2.107565	-1.679621	5.221036
H	0.660156	-1.273860	4.274091
H	1.590146	-0.004756	5.079842
C	0.502187	3.381748	-1.226360
H	0.432150	2.293886	-1.191655
C	0.220640	3.796503	-2.675786
H	-0.755082	3.429119	-3.003535

H	0.976724	3.386082	-3.354417
H	0.218806	4.885020	-2.799395
C	-0.591906	3.908564	-0.289878
H	-0.745445	4.987724	-0.392516
H	-0.353820	3.702830	0.758858
H	-1.545049	3.423625	-0.516695
C	5.611765	2.709439	-0.475301
H	6.422591	3.435369	-0.317305
C	5.886113	2.111127	-1.857634
H	6.894317	1.684115	-1.897356
H	5.817927	2.878326	-2.636970
H	5.184883	1.315320	-2.114775
C	5.806004	1.681742	0.633730
H	5.260635	0.758564	0.437220
H	5.496591	2.078339	1.606092
H	6.863702	1.403948	0.709487
C	-2.328367	-0.422218	-0.193926
N	-2.674543	-1.753757	-0.790704
C	-4.039108	-1.959689	-0.679367
C	-4.588320	-1.001217	0.078451
N	-3.619058	-0.096515	0.503132
H	-4.529693	-2.772485	-1.191183
H	-5.628045	-0.851556	0.329742
C	-3.910142	1.243927	0.818931
C	-4.415116	3.929349	1.553625
C	-4.345835	2.186580	-0.156249
C	-3.802483	1.658210	2.180230
C	-4.048771	3.002639	2.518691
C	-4.578278	3.521614	0.236664
H	-3.986220	3.335193	3.551689
H	-4.915487	4.258926	-0.488454
H	-4.609988	4.960977	1.833532
C	-1.800544	-2.482825	-1.601362
C	0.128744	-3.861438	-3.173572
C	-1.319843	-3.766680	-1.197550
C	-1.365647	-1.964564	-2.860588
C	-0.386464	-2.653888	-3.607031
C	-0.348376	-4.417298	-1.997753
H	-0.037575	-2.259797	-4.558820
H	0.040764	-5.391058	-1.704364
H	0.872281	-4.386253	-3.766117
C	-3.528925	0.657563	3.304925
H	-3.159155	-0.282390	2.885542
C	-4.827188	0.325669	4.048179
H	-5.585770	-0.061949	3.358979
H	-5.248175	1.206534	4.545478
H	-4.649415	-0.437558	4.813503

C	-2.454094	1.133446	4.290882
H	-1.546340	1.450842	3.767226
H	-2.180947	0.322298	4.975099
H	-2.796802	1.972317	4.905531
C	-4.648934	1.809708	-1.605179
H	-4.346162	0.781506	-1.796514
C	-6.154002	1.876518	-1.887231
H	-6.542264	2.897375	-1.803420
H	-6.713383	1.248132	-1.185391
H	-6.371265	1.521203	-2.900464
C	-3.874620	2.661961	-2.613651
H	-4.040782	2.295723	-3.632760
H	-2.801988	2.610004	-2.411866
H	-4.172395	3.714985	-2.590824
C	-1.791676	-4.598967	0.002462
H	-1.024960	-5.371900	0.163519
C	-1.885823	-3.918909	1.364168
H	-2.109827	-4.659575	2.141139
H	-2.672033	-3.165305	1.417494
H	-0.929830	-3.462111	1.630873
C	-3.073553	-5.373514	-0.320270
H	-2.985694	-5.910351	-1.271307
H	-3.947296	-4.723530	-0.383281
H	-3.278412	-6.115613	0.459646
C	-1.988286	-0.728983	-3.509245
H	-2.780347	-0.335460	-2.873684
C	-2.680165	-1.070163	-4.836161
H	-1.969865	-1.391565	-5.605096
H	-3.211895	-0.194772	-5.225395
H	-3.413262	-1.872922	-4.698966
C	-0.959988	0.385834	-3.710574
H	-0.162405	0.096070	-4.402670
H	-0.491816	0.658587	-2.760478
H	-1.439088	1.280443	-4.121129
H	-2.107640	0.324060	-0.961399

Energy = -2328.549429 hartree

In-P(NHC)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

P	0.557399	-0.327236	-0.324177
In	1.899929	-1.441416	-1.912210
C	1.265069	0.425630	1.218924

N	0.686464	-0.134777	2.498248
C	1.715143	-0.286491	3.424179
C	2.899387	-0.080437	2.846568
N	2.739395	0.236943	1.504879
H	1.056526	1.494085	1.167065
H	1.502833	-0.522827	4.456710
H	3.876665	-0.118783	3.300901
C	-0.606190	0.159810	2.940430
C	-3.233851	0.685056	3.867044
C	-1.535556	-0.904090	3.112821
C	-0.985186	1.472120	3.359045
C	-2.307428	1.710898	3.784852
C	-2.844001	-0.608460	3.555682
H	-2.616022	2.707834	4.091427
H	-3.568626	-1.411446	3.681847
H	-4.244714	0.884280	4.210708
C	3.789279	0.230170	0.587155
C	5.860359	0.138387	-1.367027
C	4.526896	-0.985990	0.335264
C	4.220814	1.415976	-0.071368
C	5.211447	1.328320	-1.079144
C	5.549402	-0.996639	-0.637825
H	5.522937	2.222238	-1.617817
H	6.121854	-1.899227	-0.834303
H	6.640400	0.108565	-2.122412
C	-1.224838	-2.401031	2.989683
H	-2.152330	-2.880178	2.649402
C	-0.903932	-2.980453	4.375457
H	0.007630	-2.539839	4.792775
H	-0.758576	-4.064857	4.319034
H	-1.716213	-2.794921	5.086805
C	-0.161124	-2.861347	1.996867
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H	0.856694	-2.691697	2.355599
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C	0.013274	2.622419	3.498048
H	1.014695	2.265533	3.270655
C	0.100346	3.138701	4.941367
H	-0.823700	3.629480	5.264181
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H	0.307765	2.318783	5.638044
C	-0.278105	3.771224	2.534598
H	-1.230194	4.263020	2.756768
H	-0.312305	3.409699	1.503977
H	0.507629	4.532349	2.593222
C	4.292210	-2.289681	1.117969
H	3.311584	-2.256218	1.598995

C	5.371270	-2.455532	2.198429
H	5.139403	-3.308483	2.845586
H	5.462420	-1.569899	2.832590
H	6.357588	-2.634079	1.754426
C	4.265374	-3.570714	0.266301
H	5.241620	-3.805555	-0.169824
H	3.542750	-3.502899	-0.548301
H	3.977544	-4.427925	0.886134
C	3.824821	2.849671	0.287605
H	4.669674	3.486698	-0.016644
C	3.690256	3.155120	1.777925
H	3.677241	4.238668	1.943148
H	4.530397	2.743353	2.347112
H	2.765607	2.767021	2.196250
C	2.633591	3.349020	-0.516985
H	1.748961	2.729662	-0.372823
H	2.868766	3.345447	-1.586306
H	2.377656	4.377144	-0.239863
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N	-1.302902	1.129450	-1.914649
C	-1.980841	0.595916	-3.006045
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N	-1.816893	-1.150276	-1.592320
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H	-2.822057	-1.352668	-3.482328
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C	-3.760424	-2.034665	-0.292083
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C	-0.856415	-3.905465	-1.975440
H	-0.393357	-2.998537	-2.360363
C	-1.440680	-4.634748	-3.192761
H	-2.214002	-4.030410	-3.679919

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H	-0.658787	-4.836318	-3.933037
C	0.258409	-4.748709	-1.344001
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H	-0.086349	-5.745144	-1.049729
C	-4.659326	-0.825434	-0.536612
H	-4.068636	-0.024660	-0.970526
C	-5.742719	-1.170710	-1.568189
H	-6.434092	-1.933186	-1.192419
H	-5.300931	-1.551629	-2.495372
H	-6.331560	-0.282057	-1.820490
C	-5.311556	-0.260494	0.727529
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C	-3.408398	2.660749	-0.326138
H	-3.238524	1.624608	-0.063803
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H	-4.200430	2.209232	-2.320348
C	-3.959468	3.302735	0.957046
H	-4.391193	4.292833	0.774082
H	-3.180636	3.407680	1.713843
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