Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A Possible Target: the Triply Bonded Indium≡Antimony Molecules With High Stability

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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 (DS) are applied to the three levels of DFT. The relative free energy (DG) at 298 K is also computed at the same levels of theory.

Next, Si*i*PrDis$_2$–In≡Sb–Si*i*PrDis$_2$, Tbt–In≡Sb–Tbt, and Ar*–In≡Sb–Ar* 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 the dispersion-corrected M06-2X method.[2] Because of the limitations of the available memory size and CPU time, frequencies are not computed at the dispersion-corrected M06-2X/Def2-TZVP level of theory for the triply bonded R´In≡SbR´ systems that have bulky ligands (R´), so the zero-point energies and the Gibbs free energies that are derived using the dispersion-corrected M06-2X/Def2-TZVP cannot be used for these systems.

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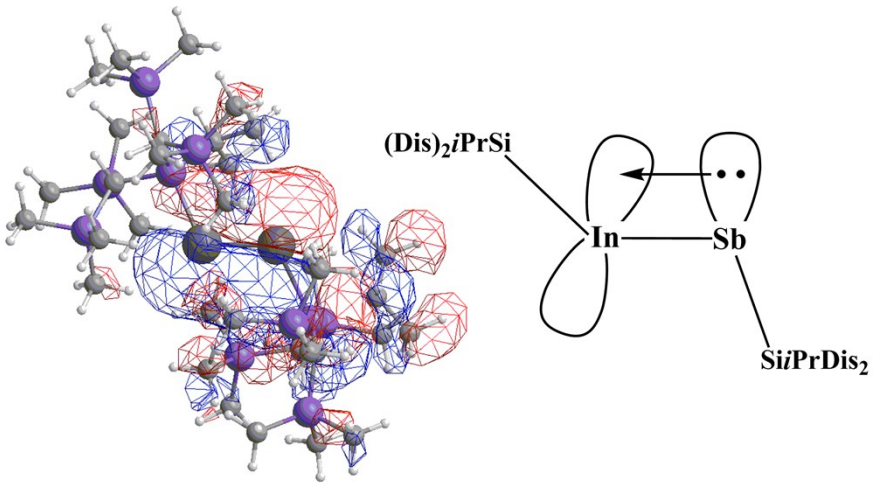
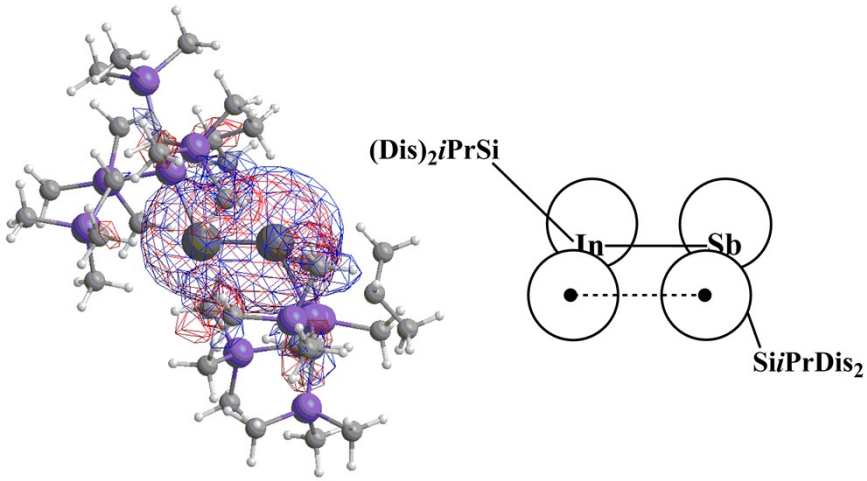
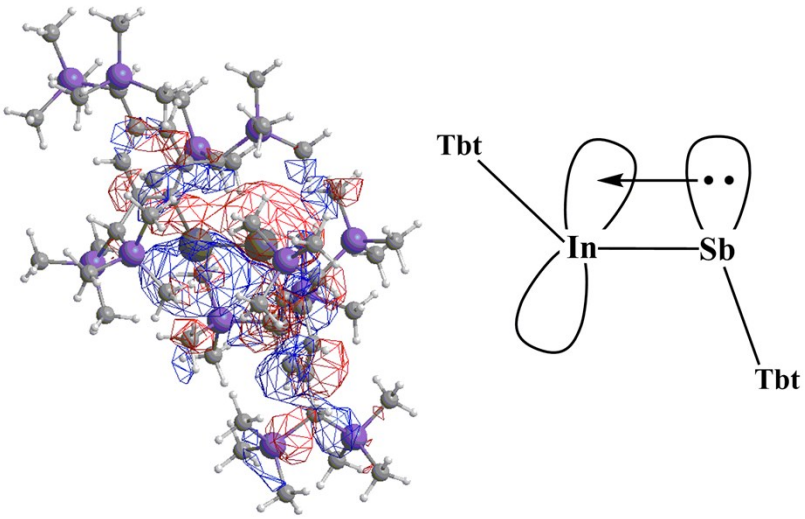


(I) $\pi_{\perp}$

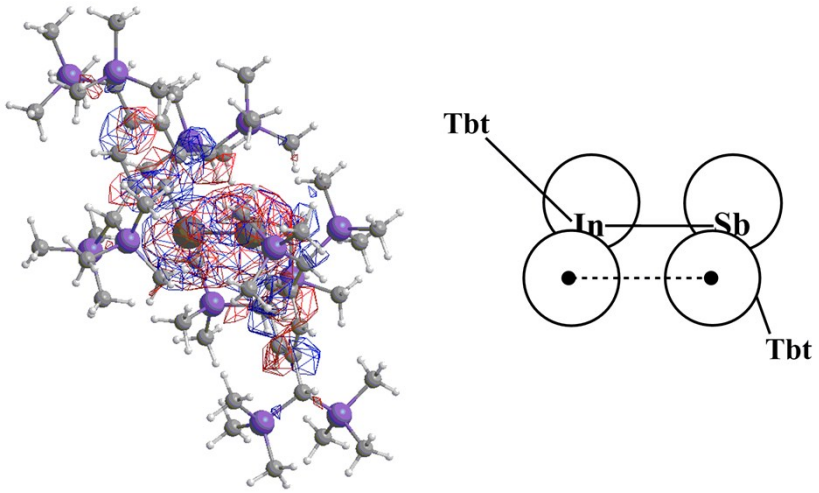


(II) $\pi_{\parallel}$

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

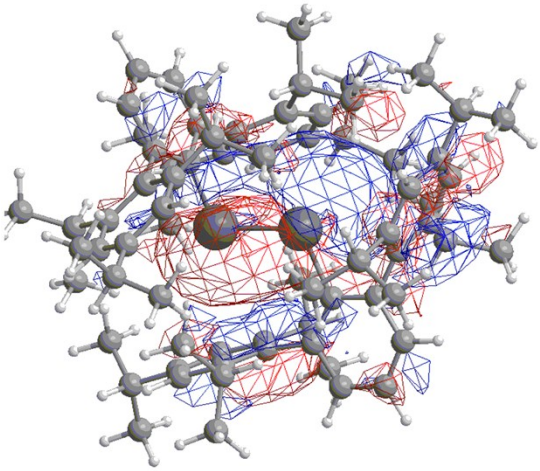


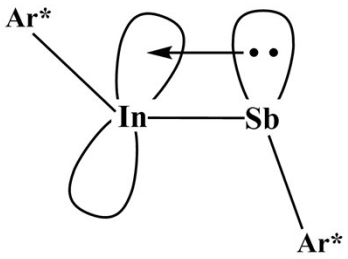
(I) $\pi_{\perp}$



(II) $\pi_{\parallel}$

Figure S2: The natural In≡Sb π bonding orbitals ((I) and (II)) of ((Tbt)In≡Sb(Tbt)). For comparison, also see Figure 2.





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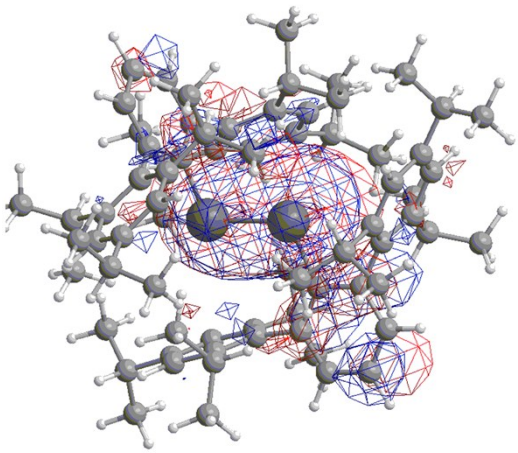

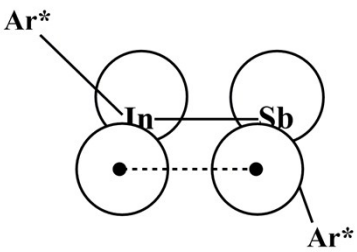

(II) $\pi_{\parallel}$

Figure S3: The natural In≡Sb π bonding orbitals ((I) and (II)) of ((Ar*)In≡Sb(ASr*)). For comparison, also see Figure 2.

Table S1

The charge decomposition analysis (CDA) results[a] for R′In≡SbR′ (R′ = Si*i*PrDis$_2$) system based on M06-2X orbitals, where X term indicates the number of electrons donated from R′–In fragment to R′–Sb fragment, Y term indicates the number of electrons back donated from R′–Sb fragment to R′–In fragment and W term indicates the number of electrons involved in repulsive polarization. Significant X and Y terms are bolded for easier comparison.

	Orbital	**Occupancy**	**X**	**Y**	**X − Y**	**W**
	229	2.000000	0.000927	0.002795	-0.001868	-0.008366
	230	2.000000	0.000600	0.003078	-0.002478	-0.021809
	231	2.000000	0.000062	0.000108	-0.000046	-0.001249
	232	2.000000	0.000292	0.001328	-0.001036	-0.004728
	233	2.000000	0.000888	0.000119	0.000768	-0.008861
	234	2.000000	-0.000202	0.002138	-0.002339	-0.006618
	235	2.000000	0.000037	0.000628	-0.000586	-0.003490
	236	2.000000	0.001950	0.003845	-0.001896	-0.012107
	237	2.000000	0.007635	0.095074	-0.087439	-0.184157
	238	2.000000	0.049394	0.021612	0.027782	0.014692
HOMO	239	2.000000	-0.011601	0.045300	-0.056901	-0.035802
LUMO	240	0.000000	0.000000	0.000000	0.000000	0.000000
	241	0.000000	0.000000	0.000000	0.000000	0.000000
sum		478.000000	0.091132	0.299681	-0.208548	-0.058494

[a] For clearness, only list the X, Y, and W terms for HOMO(No.239)–11 ~ LUMO+2. [b] Summation of contributions from all unoccupied and occupied orbitals.

Table S2

The charge decomposition analysis (CDA) results[(a)] for R′In≡SbR′ (R′ = Tbt) system based on M06-2X orbitals, where X term indicates the number of electrons donated from R′−In fragment to R′−Sb fragment, Y term indicates the number of electrons back donated from R′−Sb fragment to R′−In fragment and W term indicates the number of electrons involved in repulsive polarization. Significant X and Y terms are bolded for easier comparison.

	Orbital	**Occupancy**	**X**	**Y**	**X − Y**	**W**
	317	2.000000	0.001587	0.004426	-0.002839	-0.032876
	318	2.000000	0.000782	0.005472	-0.004690	-0.020200
	319	2.000000	0.000638	0.000396	0.000242	-0.001135
	320	2.000000	-0.000023	0.001347	-0.001370	-0.001716
	321	2.000000	0.007725	0.044663	-0.036938	-0.072492
	322	2.000000	0.002593	0.016524	-0.013932	0.024335
	323	2.000000	0.004348	0.000459	0.003899	-0.008902
	324	2.000000	0.001434	0.000257	0.001177	-0.001815
	325	2.000000	-0.000046	0.000170	-0.000216	-0.000806
	326	2.000000	0.029045	0.034207	-0.005162	-0.133137
HOMO	327	2.000000	-0.028250	0.018059	-0.046308	0.012909
LUMO	328	0.000000	0.000000	0.000000	0.000000	0.000000
	329	0.000000	0.000000	0.000000	0.000000	0.000000
sum		654.000000	0.095378	0.312044	-0.216666	-0.023572

[(a)] For clearness, only list the X, Y, and W terms for HOMO(No.327)−11 ~ LUMO+2. [(b)] Summation of contributions from all unoccupied and occupied orbitals.

Table S3

The charge decomposition analysis (CDA) results[(a)] for R′In≡SbR′ (R′ = Ar*) system based on M06-2X orbitals, where X term indicates the number of electrons donated from R′−In fragment to R′−Sb fragment, Y term indicates the number of electrons back donated from R′−Sb fragment to R′−In fragment and W term indicates the number of electrons involved in repulsive polarization. Significant X and Y terms are bolded for easier comparison.

	Orbital	**Occupancy**	**X**	**Y**	**X − Y**	**W**
	277	2.000000	0.000937	0.000915	-0.005380	0.003691
	278	2.000000	0.001264	0.003194	0.000349	-0.005783
	279	2.000000	0.001306	0.001661	-0.001888	0.001655
	280	2.000000	0.001948	0.001661	0.000287	-0.007474
	281	2.000000	0.000926	0.004704	-0.003777	-0.007299
	282	2.000000	0.003710	0.002940	0.000770	0.002088
	283	2.000000	0.001000	0.007000	-0.006000	0.001636
	284	2.000000	0.001958	0.004082	-0.002123	-0.014169
	285	2.000000	0.004133	0.008109	-0.003976	-0.043184
	286	2.000000	0.117233	0.017853	0.099380	-0.276903
HOMO	287	2.000000	0.015823	0.130839	-0.115016	-0.086797
LUMO	288	0.000000	0.000000	0.000000	0.000000	0.000000
	289	0.000000	0.000000	0.000000	0.000000	0.000000
sum		574.000000	0.299237	0.390445	-0.091208	-0.420759

[(a)] For clearness, only list the X, Y, and W terms for HOMO(No.287)−11 ~ LUMO+2. [(b)] Summation of contributions from all unoccupied and occupied orbitals.

M06-2X/Def2-TZVP

F2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.002055	-0.001449	-0.000019
Sb	1.718497	-0.001548	0.000005
F	-2.154789	-1.574611	0.000037
F	-2.127726	1.591272	0.000036

F2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.032517	-0.106600	-0.000555
Sb	-1.645205	-0.108926	0.000182
F	2.880872	-0.678932	0.001544
F	0.820474	1.876560	0.000447

F-In-Sb-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.234926	-0.040865	-0.000006
Sb	1.472605	-0.282355	0.000003
F	1.545268	1.666548	0.000000
F	-3.166542	0.155952	0.000020

In-SbF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.550727	-0.340754	-0.000646

Sb	1.400051	0.308391	-0.000975
F	-1.410116	1.661006	0.004525
F	1.919339	-1.553338	0.004513

In-SbF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	1.297766	-0.002909	-0.334870
F	1.017263	-1.497360	1.044202
F	1.042386	1.501786	1.037721
In	-1.729039	0.002214	-0.033856

(OH)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.996342	-0.000008	-0.000019
Sb	1.729207	0.000014	0.000025
O	-2.081188	-1.679341	-0.000256
H	-3.034237	-1.564596	0.001879
O	-2.081330	1.679286	-0.000279
H	-3.034426	1.564713	0.002079

(OH)2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.032711	-0.086351	-0.021127
Sb	-1.666853	-0.118630	0.008250
O	0.829861	1.922299	-0.023461
H	1.519047	2.508507	0.294816
O	2.902635	-0.739338	0.057750
H	3.027638	-1.690865	0.045339

HO-In-Sb-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.232196	-0.062673	-0.016448
Sb	-1.466989	-0.292981	0.006925
O	-1.616831	1.701207	0.105817
H	-1.771647	2.085985	-0.759968
O	3.185533	0.241712	-0.050715
H	3.660841	0.383670	0.771937

In-Sb(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.551269	-0.420726	-0.000480
Sb	-1.411467	0.362911	0.007711
O	-2.365913	-1.346717	-0.114484
H	-2.135861	-1.966234	0.582905
O	1.813538	1.595147	0.041565
H	2.527500	2.085923	-0.369292

In-Sb(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.724245	-0.001791	-0.008534
Sb	1.249154	0.000666	-0.350952
O	1.067645	-1.537169	0.983992
H	1.932022	-1.821279	1.301241
O	1.049714	1.542458	0.980191
H	1.910226	1.832806	1.302022

H2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.343002	0.000000	0.000019
H	-2.169558	1.530064	0.000030
Sb	1.375417	0.000000	-0.000019
H	-2.169586	-1.530048	0.000030

H2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.314509	0.005632	0.000000
Sb	1.341413	0.010792	0.000000
H	-2.744509	0.950265	0.000000
H	-1.256611	-1.776604	0.000000

H-In-Sb-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.308093	-0.008159	0.000001
H	-3.034319	0.111796	0.000002
Sb	1.297390	-0.027138	-0.000001
H	0.964030	1.672017	0.000003

In-SbH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.437067	-0.031636	0.007148
H	1.044227	1.616153	-0.713472
Sb	-1.384622	-0.017590	-0.019922
H	-0.844793	0.831103	1.379238

In-SbH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.537648	0.000003	-0.004914
Sb	-1.433463	-0.000062	-0.039902
H	-1.118505	-1.219249	1.139349
H	-1.119667	1.222247	1.136452

(CH3)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.010612	-0.000303	-0.002965
Sb	1.740577	-0.000683	0.000780
C	-2.116162	-1.886466	0.005025
H	-2.760687	-1.928470	-0.873370
H	-1.459340	-2.753311	0.000647
H	-2.748950	-1.928682	0.891854
C	-2.110356	1.889999	0.002705
H	-3.074564	1.757693	-0.487121
H	-2.287804	2.202322	1.032394
H	-1.558995	2.678963	-0.505292

(CH3)2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.011923	-0.032949	-0.001154
Sb	-1.649923	-0.175343	0.000343
C	0.835674	2.195089	0.001244
H	-0.184822	2.581483	0.007426
H	1.343822	2.570903	0.889041
H	1.334748	2.574289	-0.890170
C	2.895648	-1.090989	0.002736

H	2.741589	-2.166975	0.029543
H	3.459264	-0.834416	-0.893518
H	3.479279	-0.792858	0.872885

H3C-In-Sb-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.193455	-0.011532	-0.002439
Sb	-1.409651	0.374995	0.000939
C	-1.942839	-1.765741	0.000920
H	-3.031809	-1.775696	-0.036846
H	-1.565048	-2.286674	-0.873884
H	-1.624301	-2.268644	0.909126
C	3.353244	-0.173942	0.004725
H	3.728957	-0.351661	-1.001627
H	3.780321	0.754271	0.386720
H	3.662362	-0.993178	0.654276

In-Sb(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.455678	-0.351300	0.107568
Sb	-1.409874	-0.145840	-0.294719
C	-1.252779	0.718976	1.688432
H	-1.829778	1.643319	1.704323
H	-1.710252	0.028225	2.398087
H	-0.228249	0.927986	2.008414
C	1.303501	1.855181	-0.679048
H	1.278647	1.857638	-1.766919
H	0.505317	2.487829	-0.297131
H	2.255366	2.261597	-0.343225

In-Sb(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

In	-1.678837	0.000182	-0.024652
Sb	1.234473	-0.000181	-0.402871
C	1.075438	1.580421	1.119157
H	0.160871	1.539057	1.719911
H	1.918217	1.481271	1.801913
H	1.128576	2.556634	0.639288
C	1.073769	-1.580385	1.119386
H	1.913659	-1.478509	1.805327
H	0.156761	-1.541770	1.716708
H	1.131606	-2.556570	0.639995

(SiH3)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	3.092679	-0.994698	-0.021472
H	3.713799	-0.668815	-1.324231
H	3.905732	-0.423996	1.075463
H	3.015557	-2.464907	0.130925
Si	0.230798	2.556573	-0.010528
H	0.890147	3.154327	1.176420
H	0.895342	3.106275	-1.217695
H	-1.180107	3.000639	-0.022355
In	0.741468	-0.051579	0.019445
Sb	-1.845119	-0.491027	-0.006340

(SiH3)2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.726239	0.013758	-0.004369
Sb	1.974895	-0.264070	0.001217
Si	-2.519587	-1.855878	0.003279
H	-3.155578	-1.923985	1.338625
H	-3.572715	-1.573160	-0.997612
H	-1.939471	-3.182421	-0.296368
Si	-1.228364	2.581484	0.003753
H	-2.036974	2.963748	1.184588
H	0.020019	3.378617	0.037518
H	-1.977864	2.972146	-1.213192

H3Si-In-Sb-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.914780	-0.294707	-0.000395
Sb	-1.689644	-0.489602	0.000208
Si	-1.144321	2.021912	-0.000068
H	-1.623562	2.744477	-1.198406
H	-1.620915	2.743256	1.200030
H	0.350098	2.250692	-0.001459
Si	3.459007	0.182728	0.000666
H	3.834818	0.886675	1.243626
H	4.191505	-1.097904	-0.077188
H	3.810051	1.018212	-1.166204

In-Sb(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.208163	-0.753187	0.332780
Sb	1.362641	-0.225284	-0.580180
Si	-1.735025	1.644756	-0.860616
H	-1.739695	1.500313	-2.332270
H	-3.115079	1.982379	-0.439797
H	-0.875581	2.783136	-0.465357
Si	1.172868	1.073931	1.600939
H	2.031655	0.534865	2.675824
H	1.509866	2.493928	1.361562
H	-0.235706	1.039363	2.118451

In-Sb(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.803008	-0.000053	-0.086116

Sb	1.164145	-0.000013	-0.726973
Si	0.871724	1.710956	1.141617
H	-0.521580	1.652068	1.712994
H	1.765249	1.478571	2.296523
H	1.037944	3.097090	0.654320
Si	0.871977	-1.710767	1.141774
H	1.774528	-1.486114	2.291037
H	-0.517513	-1.643590	1.721424
H	1.025568	-3.097400	0.651498

B3PW91/Def2-TZVP

F2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.000191	0.994208	0.000000
Sb	0.000136	-1.706148	0.000000
F	0.000136	2.127631	1.590841
F	0.000136	2.127631	-1.590841

F2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.016800	-0.093325	-0.000094
Sb	1.653432	-0.097472	0.000030
F	-2.804778	-0.837581	0.000251
F	-1.028758	1.898024	0.000094

F-In-Sb-F

Atomic Number	Coordinates (Angstroms) X	Y	Z

In	1.224717	-0.036355	-0.000576
Sb	-1.449235	-0.287969	0.000237
F	3.155485	0.173158	0.001819
F	-1.611058	1.656600	-0.000026

In-SbF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.502127	-0.318920	-0.000386
Sb	-1.320354	0.290452	-0.000677
F	1.121946	1.682176	0.003022
F	-1.818187	-1.591730	0.002914

In-SbF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.648791	0.064129	-0.090335
Sb	-1.325258	-0.178263	-0.237956
F	-1.305250	1.580616	0.593333
F	-0.161706	-0.919605	1.246910

(OH)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.557720	-0.000032	-0.114521
Sb	1.378101	-0.000193	-0.209904
O	0.297848	-1.429901	0.808916
H	0.636979	-1.608549	1.690567
O	0.298465	1.431491	0.808050
H	0.637657	1.607227	1.690334

(OH)2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.013576	-0.073291	-0.035576
Sb	1.667054	-0.103615	0.013131
O	-1.045136	1.953339	-0.032883
H	-1.712929	2.337636	0.543630
O	-2.812075	-0.903090	0.086217
H	-2.783918	-1.863964	0.103237

HO-In-Sb-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.227471	-0.042744	0.021866
Sb	1.443584	-0.303656	-0.005379
O	1.718094	1.675266	-0.112653
H	1.879281	2.017289	0.771716
O	-3.180963	0.228778	-0.166692
H	-3.653037	0.331278	0.665915

In-Sb(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z

In-Sb(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

In	-0.987501	-0.007848	-0.000795
Sb	1.722300	-0.009815	0.000243
O	-2.322245	-1.494592	0.002183
H	-1.932794	-2.373091	-0.002568
O	-1.999091	1.709892	0.001345
H	-2.946230	1.535842	0.000925

H2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.533417	0.000022	-0.004160
Sb	1.427586	-0.000098	-0.041123
H	1.163545	-1.213642	1.152509
H	1.167003	1.217548	1.148647

H2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.007376	1.300838	0.000000
Sb	0.007376	-1.330409	0.000000
H	1.011257	2.677099	0.000000
H	-1.748878	1.432724	0.000000

H-In-Sb-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.017342	1.299183	0.000000
H	-0.054260	3.017644	0.000000
Sb	0.017342	-1.288692	0.000000
H	-1.679968	-0.954349	0.000000

In-SbH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.416442	-0.030742	0.008837
H	-1.046949	1.569447	-0.768052
Sb	1.363845	-0.018210	-0.020604
H	0.896499	0.865633	1.385801

In-SbH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.000011	1.318031	0.000000
Sb	0.000011	-1.351935	0.000000
H	-0.000566	2.182587	1.493687
H	-0.000566	2.182587	-1.493687

(CH3)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.749741	-0.000349	0.033567
Sb	-1.177101	0.000283	-0.428463
C	-1.406790	1.615298	1.042314
H	-2.428629	1.584178	1.421452
H	-0.718609	1.532157	1.885136
H	-1.249500	2.572680	0.544089
C	-1.410005	-1.614952	1.042112
H	-2.436859	-1.593046	1.408364
H	-1.237302	-2.571756	0.547709
H	-0.733487	-1.523645	1.893565

(CH3)2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.978129	-0.051228	-0.002480
Sb	-1.653399	-0.136187	0.000725
C	1.107815	2.176059	0.002871
H	0.154449	2.700806	-0.005059
H	1.661648	2.447436	0.902373
H	1.676921	2.449015	-0.886511
C	2.812218	-1.180572	0.003111
H	2.676905	-2.130948	-0.512750
H	3.600007	-0.606118	-0.485789
H	3.104907	-1.377394	1.036363

H3C-In-Sb-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.185727	0.013107	0.000703
Sb	1.397158	-0.376469	-0.000268
C	1.952385	1.762919	-0.000154
H	3.043308	1.756311	-0.003261
H	1.602808	2.275236	-0.893282
H	1.607997	2.273011	0.896311
C	-3.336135	0.179652	-0.001143
H	-3.660018	0.808375	-0.831499
H	-3.764575	-0.817602	-0.121669
H	-3.681429	0.606959	0.940403

In-Sb(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.425884	-0.376126	-0.002716
Sb	1.353254	0.006563	-0.355284
C	-1.342256	1.990824	0.083508
H	-0.480869	2.507789	0.495009

H	-1.527273	2.307049	-0.942180
H	-2.217251	2.157696	0.708345
C	1.443361	-0.082433	1.820020
H	1.926232	-1.025667	2.083978
H	2.075781	0.732289	2.173528
H	0.469135	-0.034058	2.312733

In-Sb(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.973308	-0.000131	-0.000384
Sb	1.708836	-0.000762	0.000107
C	-2.118820	1.855818	0.002544
H	-2.514978	2.016221	-1.002244
H	-2.952806	1.750327	0.698307
H	-1.509071	2.711306	0.288456
C	-2.130223	-1.849092	-0.001455
H	-2.165047	-2.245356	1.015171
H	-3.145283	-1.633677	-0.337460
H	-1.677102	-2.593871	-0.655404

(SiH3)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.768211	0.001446	-0.112229
Sb	-1.183889	-0.001639	-0.686924
Si	-0.793227	-1.761887	1.124192
H	-1.598442	-1.574815	2.359591
H	-1.016814	-3.130877	0.588814
H	0.647971	-1.753175	1.596380
Si	-0.799890	1.762488	1.122277
H	-1.606750	1.574649	2.356444
H	0.640807	1.758589	1.596213
H	-1.027100	3.129950	0.584302

(SiH3)2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.666451	-0.077009	-0.003842
Sb	-1.953634	-0.301047	0.001278
Si	1.014526	2.538908	0.002470
H	-0.225232	3.360201	0.046391
H	1.848605	2.891779	1.186172
H	1.772687	2.903699	-1.227271
Si	2.826695	-1.457056	0.003302
H	3.482622	-1.332262	1.332596
H	2.559911	-2.895234	-0.262020
H	3.763571	-0.947235	-1.033574

H3Si-In-Sb-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.917854	-0.264030	0.002519
Sb	1.663923	-0.519117	-0.001236
Si	1.225350	2.021455	0.000229
H	1.770055	2.710144	1.201667
H	1.757445	2.709582	-1.207157
H	-0.250598	2.347042	0.008409
Si	-3.460763	0.181954	-0.003008
H	-4.052277	-0.205130	1.304448
H	-3.714493	1.624642	-0.250595
H	-4.099571	-0.621571	-1.078230

In-Sb(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.141758	-0.705824	-0.450962
Sb	-1.343182	0.482703	-0.453933
Si	-1.229002	-0.941201	1.661077
H	0.176558	-1.465553	1.874217
H	-1.577734	-0.153649	2.873010
H	-2.096986	-2.144781	1.588331

Si	1.915099	1.510114	0.882911
H	2.218275	2.506142	-0.177874
H	1.044893	2.128192	1.914236
H	3.185746	1.132401	1.559959

In-Sb(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.915130	-0.265761	0.005864
Sb	1.667719	-0.514550	-0.002901
Si	-3.457363	0.175478	-0.007179
H	-3.950602	0.463780	1.364658
H	-3.771036	1.324607	-0.895334
H	-4.139309	-1.041447	-0.522066
Si	1.204877	2.021160	0.000612
H	1.738190	2.718826	1.201782
H	1.722472	2.718860	-1.207622
H	-0.277199	2.326783	0.011101

B3LYP/LANL2DZ+dp

F2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.000203	1.049098	0.000000
Sb	-0.000144	-1.744789	0.000000
F	-0.000144	2.087691	1.558743
F	-0.000144	2.087691	-1.558743

F2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z

F-In-Sb-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.271678	-0.063038	-0.000292
Sb	-1.499653	-0.281993	0.000124
F	3.112974	0.220701	0.000954
F	-1.538518	1.720469	-0.000066

In-SbF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.935541	-0.249784	-0.000033
Sb	-1.452536	0.183574	-0.000349
F	0.712895	1.368604	0.001066
F	-3.019804	-1.048924	0.001088

In-SbF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
F	1.358284	1.470282	0.995517
F	1.358340	-1.470263	0.995528
In	-1.867010	-0.000005	0.005049
Sb	1.314389	0.000001	-0.356212

(OH)2In-Sb

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
In	1.606607	0.000021	-0.122115
Sb	-1.515442	-0.000480	-0.140779
O	-0.064528	1.327031	0.640424
H	-0.215308	1.849042	1.451512
O	-0.061594	-1.324023	0.642168
H	-0.211921	-1.849693	1.451135

(OH)2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.239586	-0.175940	0.042577
Sb	1.527677	-0.231537	-0.020851
O	1.152369	1.787406	-0.071016
H	1.338831	2.282030	0.754143
O	-2.987839	0.379322	-0.114823
H	-3.826883	0.813594	-0.290339

HO-In-Sb-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.289573	-0.095178	0.050729
Sb	1.511116	-0.286649	-0.022284
O	1.607970	1.738786	-0.085962
H	1.822500	2.196088	0.753314
O	-3.073698	0.323619	-0.134273
H	-3.974536	0.587516	-0.340680

In-Sb(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z

In	1.857488	-0.285116	0.000002
Sb	-1.388369	0.207772	-0.000109
O	-2.969970	-1.044115	0.000422
H	-2.908386	-2.021840	-0.000139
O	0.703609	1.420256	0.000108
H	0.829200	2.387051	0.001340

In-Sb(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.051263	-0.017674	0.000556
Sb	-1.751286	-0.032129	-0.000164
O	2.340952	-1.395961	-0.005397
H	2.441604	-2.355991	0.024787
O	1.750149	1.736823	0.000212
H	2.633265	2.133705	-0.002158

H2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.594231	0.000019	-0.001319
Sb	1.477113	-0.000062	-0.044610
H	1.391014	-1.231686	1.170972
H	1.393521	1.233884	1.168774

H2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.009056	1.331528	0.000000
Sb	0.009056	-1.357160	0.000000
H	0.861581	2.818268	0.000000
H	-1.767137	1.152068	0.000000

H-In-Sb-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.016580	1.337593	0.000000
H	0.052927	3.070746	0.000000
Sb	0.016580	-1.323697	0.000000
H	-1.710960	-1.104242	0.000000

In-SbH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.475468	-0.027449	0.012645
H	1.008745	1.503350	-0.887481
Sb	-1.414693	-0.021700	-0.022177
H	-1.157342	0.948366	1.398888

In-SbH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.000002	1.367041	0.000000
Sb	0.000002	-1.399418	0.000000
H	-0.000105	2.192659	1.525925
H	-0.000105	2.192659	-1.525925

(CH3)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z

In	-1.830213	-0.000512	0.051905
Sb	1.193393	-0.000093	-0.436564
C	1.576722	-1.626114	1.017229
H	2.655524	-1.666488	1.208244
H	1.055470	-1.467110	1.968379
H	1.263693	-2.587025	0.590180
C	1.571332	1.629208	1.015216
H	2.651294	1.681999	1.197233
H	1.243294	2.587125	0.592151
H	1.059773	1.462765	1.970574

(CH3)2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.019902	-0.053912	-0.002146
Sb	-1.662879	-0.167576	0.000647
C	0.812761	2.165470	0.002275
H	-0.192626	2.603077	0.024085
H	1.355701	2.513830	0.891035
H	1.318777	2.516876	-0.906704
C	2.938520	-0.994460	0.003588
H	2.890103	-1.984676	-0.462904
H	3.659629	-0.375275	-0.544609
H	3.292342	-1.111812	1.036081

H3C-In-Sb-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.221277	0.037228	0.002323
Sb	-1.418864	-0.389364	-0.000829
C	-2.049777	1.750559	-0.000542
H	-3.145412	1.721210	-0.032668
H	-1.738630	2.265532	0.911795
H	-1.687999	2.284941	-0.882558
C	3.362614	0.135598	-0.004649
H	3.742646	0.345044	1.001915
H	3.772137	-0.823552	-0.348834
H	3.699753	0.923240	-0.690050

In-Sb(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.494505	-0.356229	0.017427
Sb	-1.385368	-0.027594	-0.364332
C	-1.527517	-0.019020	1.835935
H	-2.181845	0.803341	2.146549
H	-1.998985	-0.961855	2.145888
H	-0.560122	0.070764	2.347629
C	1.243557	2.000644	0.008613
H	1.193217	2.349134	-1.028785
H	0.454789	2.467985	0.604588
H	2.219763	2.243353	0.443862

In-Sb(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.030103	-0.000211	-0.000474
Sb	-1.752456	-0.000823	0.000123
C	2.100102	-1.878955	-0.000727
H	2.285256	-2.199205	1.033625
H	1.541957	-2.669349	-0.515521
H	3.067934	-1.742883	-0.501198
C	2.091720	1.883799	0.002053
H	2.072004	2.328795	-1.001713
H	1.644823	2.596078	0.705935
H	3.137284	1.709820	0.287891

(SiH3)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.996323	-0.028524	0.128296

Sb	-0.924956	0.003773	-0.779722
Si	-1.537227	-1.901823	0.939017
H	-0.827506	-1.819573	2.248407
H	-2.995890	-1.906913	1.224144
H	-1.176382	-3.210705	0.329921
Si	-1.400970	1.970971	0.914299
H	-2.717611	1.800200	1.581975
H	-0.378728	2.124592	1.993195
H	-1.416231	3.249600	0.155267

(SiH3)2In-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.041780	0.997372	-0.029996
Sb	1.034600	-0.950460	-0.025756
Si	2.916950	0.913986	0.084528
H	3.162407	1.424754	1.458016
H	4.155837	0.218049	-0.363470
H	2.694968	2.083100	-0.806861
Si	-2.990584	-1.050382	0.124307
H	-4.130974	-0.892023	1.088926
H	-2.970925	0.468834	-0.486316
H	-3.597840	-1.790977	-1.030641

H3Si-In-Sb-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	1.035385	-0.148514	0.004082
Sb	-1.565739	-0.668182	-0.001836
Si	-1.962458	1.963298	-0.000022
H	-2.739902	2.360486	-1.203113
H	-2.738333	2.360420	1.204094
H	-0.716344	2.783981	-0.000683
Si	3.604643	0.355638	-0.004600
H	4.292481	-0.498981	-1.007873
H	3.822665	1.781563	-0.363774
H	4.207664	0.101877	1.329722

In-Sb(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.292370	-0.838504	0.095461
Sb	1.259296	0.100810	-0.765685
Si	-1.851198	1.909212	0.117960
H	-2.330019	2.224880	-1.255436
H	-3.006489	2.020838	1.051892
H	-0.866993	2.944894	0.524299
Si	1.815682	0.119224	1.814794
H	2.762223	-0.981349	2.131892
H	2.434826	1.415696	2.189641
H	0.605742	-0.077684	2.671487

In-Sb(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-1.033256	-0.151522	0.005416
Sb	1.568933	-0.666183	-0.002436
Si	-3.602632	0.353175	-0.006049
H	-4.159174	0.363375	1.371662
H	-3.845541	1.680725	-0.629175
H	-4.315236	-0.683091	-0.799309
Si	1.945907	1.969143	0.000048
H	2.708446	2.376185	1.209487
H	2.728287	2.372374	-1.198110
H	0.691326	2.777888	-0.011704

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SiMe(SitBu3)2-In-Sb-SiMe(SitBu3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

Sb	-4.855481	1.796320	-0.013523
In	-2.452345	0.713474	-0.181757
Si	-6.595192	-0.208811	-0.481995
Si	-0.067289	-0.155862	0.416892
C	-6.089153	-1.824723	0.481073
H	-6.031219	-2.689047	-0.183670
H	-5.119808	-1.703525	0.976619
H	-6.827095	-2.064311	1.252197
C	-0.049945	-1.952020	-0.348848
H	0.512554	-2.651451	0.278194
H	-1.051748	-2.367650	-0.483536
H	0.432217	-1.934130	-1.326972
Si	-0.469290	-0.323277	2.972755
Si	1.588090	1.054409	-1.096111
Si	-8.456073	0.733393	1.132630
Si	-6.502005	-0.960614	-3.025920
C	1.809608	2.936551	-0.500363
C	0.538208	3.778223	-0.819752
C	2.024251	3.013271	1.037463
C	3.022450	3.660714	-1.160584
H	0.408676	3.944059	-1.894496
H	-0.381904	3.317420	-0.435773
H	0.628097	4.767454	-0.345091
H	2.960538	2.545494	1.354446
H	2.059996	4.069843	1.346674
H	1.208096	2.537923	1.587455
H	3.046385	4.704639	-0.809724
H	3.978260	3.203971	-0.881871
H	2.962973	3.683959	-2.252326
C	0.847586	1.026834	-2.974452
C	0.948397	-0.378370	-3.641196
C	-0.650687	1.428255	-3.074529
C	1.617977	2.027518	-3.895622
H	1.975901	-0.747153	-3.713006
H	0.347905	-1.128738	-3.115146
H	0.552671	-0.313022	-4.667039
H	-0.875474	2.403305	-2.633200
H	-0.938612	1.478186	-4.137035
H	-1.304733	0.678431	-2.612763
H	1.247886	1.908737	-4.926257
H	1.441103	3.069704	-3.609664
H	2.696834	1.855432	-3.913988
C	3.344232	0.096086	-1.084120
C	4.169304	0.425826	0.192395
C	3.183217	-1.452765	-1.099016
C	4.238355	0.474494	-2.304892
H	4.468041	1.477957	0.240669
H	3.626368	0.177859	1.107125
H	5.092030	-0.175413	0.186119
H	2.621866	-1.819516	-1.963438
H	4.182720	-1.913897	-1.136900
H	2.688646	-1.819694	-0.193471

H	3.825899	0.115945	-3.253594
H	4.405226	1.553309	-2.389299
H	5.223257	-0.002380	-2.179296
C	1.230638	-0.971794	3.777845
C	1.637925	-2.311195	3.094606
C	2.393295	0.034217	3.524341
C	1.175991	-1.204226	5.320874
H	0.865158	-3.084508	3.170242
H	1.866653	-2.160633	2.032055
H	2.548076	-2.704686	3.573073
H	2.411823	0.830023	4.272719
H	3.355374	-0.496437	3.588660
H	2.332013	0.503025	2.539142
H	2.204157	-1.312949	5.700177
H	0.716564	-0.365947	5.859694
H	0.634842	-2.113087	5.590745
C	-0.998332	1.475139	3.727919
C	0.199101	2.222069	4.388250
C	-1.566518	2.423530	2.634338
C	-2.096410	1.377818	4.833774
H	0.592961	1.683505	5.256863
H	1.022042	2.411939	3.695704
H	-0.161014	3.198832	4.746866
H	-2.521762	2.059754	2.234066
H	-1.773794	3.412909	3.072014
H	-0.863187	2.581760	1.808118
H	-2.159437	2.347113	5.352620
H	-3.083033	1.182404	4.409836
H	-1.883250	0.611592	5.590374
C	-1.923926	-1.715364	3.247143
C	-3.370797	-1.139271	3.318596
C	-1.950065	-2.769421	2.103281
C	-1.718074	-2.508447	4.573329
H	-3.593015	-0.714826	4.300002
H	-3.586000	-0.379729	2.558100
H	-4.080647	-1.966541	3.164215
H	-0.974461	-3.217956	1.898012
H	-2.638785	-3.581175	2.385000
H	-2.331438	-2.338432	1.170710
H	-2.590862	-3.163625	4.722988
H	-0.833604	-3.152945	4.541773
H	-1.643749	-1.856524	5.451100
C	-7.788810	0.828716	3.042507
C	-7.460903	-0.572350	3.637898
C	-6.502786	1.676390	3.258702
C	-8.882671	1.476397	3.950482
H	-8.322334	-1.246715	3.655674
H	-6.644625	-1.062303	3.097255
H	-7.129187	-0.444044	4.680964
H	-5.648335	1.290727	2.695994
H	-6.628138	2.725887	2.981298
H	-6.246357	1.648625	4.331409
H	-8.474229	1.573654	4.969332
H	-9.162123	2.482183	3.615358

H	-9.789987	0.872887	4.021461
C	-8.974130	2.553080	0.485326
C	-8.029297	3.683804	0.989944
C	-8.910229	2.579344	-1.067647
C	-10.410751	2.988574	0.906877
H	-8.137043	3.861776	2.066052
H	-6.972587	3.486410	0.779589
H	-8.293973	4.620751	0.473877
H	-7.889237	2.403742	-1.425212
H	-9.565238	1.831191	-1.526226
H	-9.222653	3.569707	-1.435487
H	-10.588863	4.010105	0.534492
H	-11.193329	2.349097	0.486995
H	-10.534907	3.012670	1.996134
C	-10.048360	-0.485019	1.066595
C	-10.688740	-0.394030	-0.346821
C	-9.684567	-1.981140	1.298772
C	-11.168233	-0.157198	2.104426
H	-11.155833	0.578801	-0.532000
H	-9.951925	-0.572513	-1.133188
H	-11.474474	-1.159603	-0.445298
H	-9.310753	-2.167792	2.309209
H	-10.592482	-2.592400	1.169695
H	-8.939061	-2.351329	0.591714
H	-12.086295	-0.691160	1.810361
H	-10.904436	-0.507260	3.108832
H	-11.411514	0.906114	2.167300
C	-8.032674	-2.195637	-3.390307
C	-8.280768	-3.087304	-2.141766
C	-9.360100	-1.441594	-3.695930
C	-7.801382	-3.156078	-4.593236
H	-8.558679	-2.486075	-1.273673
H	-9.109392	-3.784259	-2.344302
H	-7.405353	-3.686666	-1.869008
H	-9.385205	-1.088301	-4.731751
H	-10.207730	-2.132226	-3.564480
H	-9.529952	-0.578870	-3.047185
H	-8.733920	-3.710758	-4.785677
H	-7.537683	-2.624078	-5.515446
H	-7.021484	-3.894307	-4.387373
C	-6.469588	0.641839	-4.241130
C	-7.872552	1.285239	-4.447163
C	-5.567965	1.769710	-3.663186
C	-5.925234	0.319117	-5.665294
H	-8.415085	1.428439	-3.508489
H	-7.737961	2.278023	-4.904909
H	-8.501805	0.698717	-5.123168
H	-4.565629	1.437811	-3.382422
H	-5.459234	2.565585	-4.418294
H	-6.002344	2.224096	-2.768518
H	-6.003238	1.229103	-6.281721
H	-4.869236	0.028790	-5.652883
H	-6.498191	-0.468751	-6.171803
C	-4.787006	-2.010080	-3.336846

C	-3.553852	-1.084433	-3.153976
C	-4.575138	-3.202102	-2.356108
C	-4.672321	-2.631919	-4.777228
H	-3.481576	-0.313639	-3.927655
H	-3.585254	-0.572988	-2.182462
H	-2.632187	-1.687882	-3.197824
H	-5.417037	-3.904048	-2.349545
H	-3.686632	-3.769467	-2.678377
H	-4.393106	-2.870555	-1.329723
H	-5.053383	-3.658088	-4.797884
H	-5.190798	-2.073199	-5.556027
H	-3.607819	-2.678899	-5.059934

In-Sb(SiMe(SitBu3)2)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-0.307287	0.129299	-0.203395
In	2.161273	1.670765	-1.028048
Si	-2.450664	0.225169	-2.107821
Si	-0.427779	0.636216	2.583685
Si	1.468842	-1.125332	3.372957
Si	-0.884403	3.149579	3.331937
Si	-3.295471	-2.372451	-2.350241
Si	-1.879449	1.873930	-4.119832
C	-3.910830	1.144536	-1.233810
H	-3.992014	0.838931	-0.187195
H	-3.742006	2.225144	-1.238340
H	-4.873319	0.947527	-1.719743
C	-2.020412	-0.231551	3.272305
H	-1.832974	-0.672068	4.257179
H	-2.849827	0.467792	3.373699
H	-2.345762	-1.034084	2.605681
C	-1.474401	3.718993	-3.444294
C	-2.767542	4.452475	-2.979081
C	-0.498060	3.725994	-2.237872
C	-0.817368	4.619512	-4.537530
H	-3.311481	3.900237	-2.205505
H	-2.493809	5.430735	-2.553846
H	-3.454961	4.641332	-3.808888
H	0.525457	3.482861	-2.551743
H	-0.462472	4.736699	-1.801566
H	-0.793020	3.025420	-1.453193
H	-0.643567	5.619225	-4.106536
H	0.155516	4.236246	-4.865858
H	-1.448709	4.750011	-5.420447
C	-0.291937	1.155056	-5.082640
C	1.005735	1.397100	-4.263741

C	-0.404705	-0.382694	-5.245508
C	-0.056288	1.759449	-6.499603
H	1.277134	2.455743	-4.203554
H	0.890357	0.995381	-3.245564
H	1.847359	0.865966	-4.734542
H	-0.468805	-0.877587	-4.271929
H	-1.274286	-0.681798	-5.837024
H	0.492836	-0.769374	-5.755128
H	0.888043	1.358982	-6.902997
H	-0.848004	1.484162	-7.204558
H	0.027943	2.850677	-6.491833
C	-3.425955	2.018947	-5.380520
C	-3.560794	0.698607	-6.188334
C	-4.777699	2.266384	-4.643818
C	-3.285157	3.167251	-6.428088
H	-2.732137	0.561410	-6.891485
H	-3.601081	-0.177445	-5.539863
H	-4.490427	0.718225	-6.778267
H	-4.851804	3.283018	-4.246891
H	-5.606971	2.133540	-5.357015
H	-4.944065	1.580088	-3.811461
H	-4.099331	3.068918	-7.165152
H	-3.383472	4.158978	-5.972503
H	-2.340098	3.133151	-6.978752
C	-4.818498	-2.512969	-3.652449
C	-5.680797	-1.222023	-3.597846
C	-4.379805	-2.727425	-5.131226
C	-5.771729	-3.704316	-3.334494
H	-6.028184	-0.990408	-2.585459
H	-5.128771	-0.359730	-3.973249
H	-6.570948	-1.347749	-4.234816
H	-4.113439	-3.773215	-5.315476
H	-5.224048	-2.484003	-5.795282
H	-3.530079	-2.113116	-5.434470
H	-6.480235	-3.816116	-4.170940
H	-5.239749	-4.656604	-3.223242
H	-6.364256	-3.529984	-2.431854
C	-1.750861	-3.568012	-2.835644
C	-1.470862	-3.686895	-4.363613
C	-0.443025	-3.048616	-2.178908
C	-1.950824	-5.033223	-2.341507
H	-2.198002	-4.334845	-4.861933
H	-1.459846	-2.727269	-4.881894
H	-0.479051	-4.146848	-4.499773
H	-0.122905	-2.089778	-2.600821
H	-0.534318	-2.903409	-1.101327
H	0.367313	-3.774601	-2.356679
H	-1.117279	-5.644307	-2.723157
H	-1.933999	-5.111980	-1.249966
H	-2.881419	-5.481727	-2.712419
C	-4.002662	-2.893276	-0.533444
C	-2.860636	-2.797335	0.511304
C	-5.151751	-1.954747	-0.062376
C	-4.579343	-4.344609	-0.403663

H	-2.109431	-3.581413	0.368163
H	-2.339012	-1.835218	0.481485
H	-3.282229	-2.931230	1.520401
H	-6.020319	-1.986868	-0.730778
H	-5.495840	-2.286705	0.930530
H	-4.831532	-0.915651	0.033280
H	-4.704564	-4.556871	0.670525
H	-5.562840	-4.448125	-0.865089
H	-3.930191	-5.119594	-0.811669
C	1.784224	-0.872726	5.333373
C	2.485489	0.498869	5.563515
C	0.446197	-0.904296	6.131220
C	2.696758	-1.941811	6.017727
H	3.544327	0.452211	5.284911
H	2.023281	1.313378	5.001431
H	2.440412	0.763631	6.630742
H	-0.333106	-0.269755	5.702139
H	0.047153	-1.921767	6.193465
H	0.624371	-0.561533	7.162594
H	2.987041	-1.563848	7.011649
H	2.169940	-2.887085	6.178161
H	3.615956	-2.154847	5.466476
C	0.836612	-3.004978	3.037029
C	-0.544380	-3.306510	3.692385
C	0.677208	-3.329232	1.523579
C	1.841674	-4.057068	3.606660
H	-0.585796	-3.061958	4.758516
H	-1.355964	-2.776199	3.188451
H	-0.749619	-4.384859	3.595099
H	0.160973	-2.535065	0.975269
H	1.641957	-3.502847	1.038144
H	0.092996	-4.257772	1.421040
H	1.814428	-4.113530	4.698823
H	1.554454	-5.049097	3.223484
H	2.878247	-3.876281	3.297106
C	3.182024	-0.764904	2.397831
C	3.196103	-1.357738	0.958378
C	3.400488	0.768465	2.274646
C	4.448395	-1.345659	3.100473
H	4.030954	-0.910526	0.392785
H	3.365174	-2.439905	0.972272
H	2.268995	-1.178033	0.402905
H	3.539321	1.252777	3.244865
H	4.299188	0.971065	1.670747
H	2.543968	1.257403	1.793431
H	5.322824	-1.156215	2.457205
H	4.652076	-0.878580	4.068976
H	4.383965	-2.429884	3.247174
C	-1.220050	3.320782	5.299775
C	-2.554170	2.624590	5.700032
C	-0.106515	2.658197	6.151170
C	-1.292807	4.803555	5.780376
H	-3.431230	3.101480	5.250716
H	-2.563138	1.563472	5.424596

H	-2.676227	2.682095	6.793446
H	0.860419	3.156048	6.041537
H	-0.384845	2.712248	7.216317
H	0.026082	1.609159	5.898158
H	-2.067539	5.389126	5.280184
H	-1.519930	4.808054	6.859163
H	-0.335055	5.321281	5.652760
C	-2.548456	3.722827	2.362708
C	-2.247478	4.039717	0.873320
C	-3.656159	2.631044	2.336639
C	-3.197428	4.999819	2.981295
H	-1.591330	4.906035	0.744897
H	-1.796828	3.181237	0.366464
H	-3.193313	4.273115	0.359130
H	-3.967424	2.306482	3.334167
H	-4.546047	3.041020	1.832650
H	-3.336225	1.753366	1.767090
H	-2.499086	5.837281	3.072922
H	-4.019483	5.326339	2.323908
H	-3.632988	4.807006	3.967361
C	0.616975	4.358315	2.812225
C	1.827917	4.224656	3.781122
C	1.151773	3.996230	1.399793
C	0.224375	5.867065	2.780493
H	1.612934	4.637580	4.772237
H	2.148890	3.184075	3.903939
H	2.681884	4.787873	3.371668
H	1.541830	2.972355	1.400762
H	0.388265	4.068765	0.622228
H	1.978248	4.673369	1.131210
H	1.118919	6.461668	2.534097
H	-0.530403	6.086051	2.018832
H	-0.152381	6.226505	3.742883

(SiiPrDis2)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	0.505730	0.052076	0.680876
Sb	2.330673	0.045867	2.780878
Si	1.531944	0.335351	-1.776263
Si	-2.124333	-0.104257	1.087732
C	2.845778	-1.146026	-1.944454
H	2.160148	-1.988259	-1.732451
C	2.271635	2.170645	-2.036699
H	3.356331	1.947888	-2.020862
C	-2.912621	-1.731141	0.295860
C	-2.509937	0.093809	3.013546

H	-3.465584	-0.447701	3.146325
Si	-2.934495	1.888763	3.672911
Si	-1.334546	-0.802920	4.289391
Si	-4.859393	-1.894608	0.375570
Si	4.171634	-1.398803	-0.534793
Si	3.592256	-1.647143	-3.663078
Si	2.191486	3.618608	-0.695042
Si	2.068389	3.032186	-3.783981
C	-2.913293	1.478730	0.166380
C	-3.895903	1.268437	-1.034653
C	-1.895698	2.605009	-0.185070
H	-3.521897	1.886654	0.972585
H	-3.969900	0.232003	-1.372118
H	-4.913148	1.593963	-0.778484
H	-3.583179	1.859623	-1.903715
H	-0.997645	2.592187	0.445318
H	-1.557100	2.528867	-1.221531
H	-2.359867	3.597286	-0.069176
C	0.160348	-0.138386	-3.110272
C	-1.180295	0.622978	-3.012043
C	-0.213213	-1.646081	-3.131112
H	0.609622	0.107715	-4.083298
H	-1.746509	0.286444	-2.139256
H	-1.061392	1.703387	-2.941357
H	-1.799577	0.415489	-3.899452
H	0.644877	-2.319550	-3.185326
H	-0.790579	-1.904596	-2.234708
H	-0.854640	-1.857798	-4.000372
H	-2.736355	-1.524268	-0.778616
Si	-2.100862	-3.481309	0.486044
C	-5.494443	-3.485873	1.213012
H	-5.153346	-4.401392	0.717709
H	-5.212695	-3.541487	2.271018
H	-6.592976	-3.473950	1.162499
C	-5.713119	-0.508442	1.364175
H	-6.770438	-0.449367	1.070723
H	-5.682579	-0.732612	2.438850
H	-5.271612	0.478565	1.216520
C	-5.541029	-1.945760	-1.418294
H	-5.916047	-2.950770	-1.655225
H	-6.375303	-1.242904	-1.545921
H	-4.781767	-1.694123	-2.169192
C	-2.407829	-4.261645	2.200881
H	-1.530101	-4.840451	2.515599
H	-2.597560	-3.508882	2.972576
H	-3.267079	-4.939797	2.175478
C	-2.833550	-4.659837	-0.841730
H	-3.624442	-4.195881	-1.443349
H	-2.047201	-4.990013	-1.533978
H	-3.255732	-5.560741	-0.376388
C	-0.222553	-3.527955	0.134927
H	-0.022567	-3.484598	-0.941656
H	0.363906	-2.738390	0.620203
H	0.176077	-4.484894	0.503049

C	-0.266857	-2.281226	3.703337
H	-0.561891	-3.178740	4.261434
H	-0.326802	-2.518188	2.641819
H	0.795793	-2.098202	3.914818
C	-2.432816	-1.535076	5.663560
H	-1.851124	-1.681871	6.584642
H	-3.294885	-0.905717	5.905172
H	-2.807572	-2.520042	5.351251
C	-0.041177	0.365241	5.077500
H	-0.460112	1.120961	5.749884
H	0.666405	-0.235457	5.664849
H	0.536752	0.942050	4.326670
C	-1.565547	3.174857	3.352803
H	-0.620715	2.909352	3.840750
H	-1.359826	3.333249	2.291328
H	-1.890198	4.141633	3.764672
C	-3.249100	1.883610	5.556227
H	-2.375532	1.632517	6.164308
H	-3.573345	2.894632	5.842158
H	-4.059175	1.193372	5.823504
C	-4.594383	2.637235	3.072740
H	-5.440986	2.049171	3.451512
H	-4.665214	3.642883	3.514144
H	-4.726672	2.753677	1.993311
C	3.595634	-2.771247	0.673540
H	3.456293	-2.401306	1.695850
H	2.646921	-3.233202	0.376213
H	4.358749	-3.561461	0.702887
C	5.889832	-2.048073	-1.054497
H	6.486004	-2.104678	-0.131381
H	5.829753	-3.063168	-1.461235
H	6.432012	-1.416062	-1.763052
C	4.582631	0.237489	0.360707
H	5.214156	0.863088	-0.288092
H	3.711258	0.864123	0.610982
H	5.163203	0.045788	1.273898
C	5.099749	-0.542300	-4.052193
H	5.104252	-0.238311	-5.105346
H	5.078455	0.371604	-3.444429
H	6.043639	-1.059280	-3.846993
C	4.069510	-3.504252	-3.545737
H	3.689585	-4.042030	-4.424871
H	5.153298	-3.662636	-3.503245
H	3.628615	-3.977310	-2.657103
C	2.453938	-1.636858	-5.200587
H	1.940264	-0.695837	-5.408537
H	3.092444	-1.861463	-6.067990
H	1.694256	-2.424723	-5.143244
C	3.944147	4.397846	-0.687113
H	4.702926	3.670051	-1.006269
H	4.034064	5.278881	-1.329584
H	4.196181	4.702997	0.337625
C	0.834117	4.930292	-1.053687
H	0.231815	4.746943	-1.947875

H	0.146749	4.962907	-0.197764
H	1.279365	5.929869	-1.148211
C	1.918287	3.369549	1.171696
H	1.942537	4.398102	1.569240
H	0.963027	2.936987	1.479577
H	2.702117	2.807876	1.683631
C	0.291676	3.287094	-4.430555
H	0.342298	4.023429	-5.245310
H	-0.148462	2.372095	-4.838755
H	-0.396631	3.687133	-3.676913
C	3.043511	2.115022	-5.128396
H	2.856203	2.599790	-6.096895
H	4.120417	2.175987	-4.928395
H	2.781486	1.060580	-5.227818
C	2.840940	4.780312	-3.814745
H	2.313038	5.503865	-3.185939
H	3.896569	4.773071	-3.520882
H	2.787081	5.144229	-4.850798

(SiiPrDis2)-In-Sb-(SiiPrDis2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-0.438188	-1.032893	-1.734214
In	0.819116	-0.139563	0.394423
Si	3.079863	-0.041605	1.811382
Si	-3.081342	-1.403205	-1.563739
C	-3.902914	-0.476633	-0.039506
H	-4.947408	-0.312512	-0.353795
C	-3.916742	-1.055190	-3.320552
H	-4.413207	-2.031093	-3.479924
C	3.068146	1.518242	2.984680
H	4.061330	1.480432	3.464277
C	4.670883	-0.376246	0.697606
H	4.755479	-1.461864	0.896965
Si	4.420124	-0.444816	-1.233176
Si	6.444825	0.180599	1.265631
Si	1.904883	1.530841	4.560883
Si	3.087975	3.256405	2.120668
Si	-4.118862	-1.514196	1.598128
Si	-3.278058	1.324604	0.357070
Si	-5.456047	0.130188	-3.430224
Si	-2.822344	-0.949919	-4.936760
C	2.892087	-1.693067	2.843723
C	4.010265	-1.890833	3.901052
C	2.765994	-2.969424	1.970209
H	1.942747	-1.599605	3.380863

H	4.087335	-1.042255	4.593261
H	3.811780	-2.791295	4.501614
H	4.990097	-2.028950	3.424432
H	1.928201	-2.910171	1.261246
H	3.676343	-3.173021	1.391109
H	2.587247	-3.844718	2.611908
C	-3.299965	-3.342375	-1.332459
C	-2.268654	-4.220765	-2.086127
C	-4.725329	-3.849427	-1.695002
H	-3.137264	-3.520797	-0.259561
H	-1.238692	-3.988433	-1.792214
H	-2.452568	-5.284740	-1.871006
H	-2.349232	-4.091560	-3.174171
H	-5.526696	-3.219015	-1.295685
H	-4.853217	-3.907436	-2.784339
H	-4.876109	-4.867251	-1.304848
C	3.469872	-2.048773	-1.629851
H	2.603341	-2.244829	-0.989628
H	3.097646	-2.024661	-2.663196
H	4.148917	-2.909624	-1.538970
C	6.038243	-0.627333	-2.226488
H	5.766510	-0.908525	-3.254485
H	6.618647	0.298653	-2.280118
H	6.688693	-1.419473	-1.834882
C	3.525887	1.055606	-1.996834
H	4.202841	1.913085	-2.103737
H	3.180325	0.780175	-3.003025
H	2.641069	1.397214	-1.444354
C	7.322442	1.446860	0.135435
H	7.996215	0.939778	-0.565427
H	6.633860	2.065580	-0.448685
H	7.933020	2.123900	0.748656
C	7.489008	-1.417469	1.263164
H	7.492014	-1.900586	0.277488
H	8.532809	-1.200829	1.530416
H	7.104900	-2.146492	1.990620
C	6.566354	0.876261	3.036423
H	6.191159	1.904069	3.109386
H	6.041169	0.260631	3.775532
H	7.628780	0.894985	3.319891
C	4.412114	3.387443	0.768094
H	5.424658	3.361604	1.186190
H	4.329735	2.598353	0.017413
H	4.295209	4.350986	0.250966
C	3.579135	4.601304	3.382875
H	3.747862	5.548401	2.850420
H	2.827955	4.788609	4.157198
H	4.520353	4.337705	3.885401
C	1.442264	3.723871	1.285597
H	1.225453	3.074707	0.425584
H	0.583306	3.695581	1.962639
H	1.522257	4.749749	0.897681
C	0.565255	2.893151	4.583841
H	0.079868	2.854074	5.570382

H	0.946284	3.910500	4.448226
H	-0.215097	2.714971	3.833472
C	3.060013	1.826930	6.047205
H	3.607007	2.773756	5.951527
H	2.486513	1.864282	6.983836
H	3.800490	1.020778	6.143391
C	0.878858	-0.027939	4.965633
H	0.232829	-0.352991	4.139555
H	1.487323	-0.879003	5.288777
H	0.216753	0.238569	5.802569
C	-2.048656	1.375830	1.834163
H	-1.682695	0.383360	2.127104
H	-1.187805	2.005937	1.574694
H	-2.518651	1.820992	2.721215
C	-4.787736	2.372515	0.875062
H	-4.463000	3.393112	1.124548
H	-5.524977	2.452629	0.065177
H	-5.298502	1.961631	1.752785
C	-2.435617	2.264103	-1.080455
H	-2.930787	3.232888	-1.233100
H	-1.380534	2.452263	-0.851697
H	-2.454020	1.719019	-2.028167
C	-2.504451	-2.366815	2.173452
H	-1.647171	-2.124823	1.534008
H	-2.259519	-2.071830	3.203669
H	-2.615525	-3.459771	2.163449
C	-4.736836	-0.441885	3.055259
H	-5.730905	-0.020529	2.856594
H	-4.831376	-1.097607	3.933625
H	-4.064733	0.377046	3.326801
C	-5.487386	-2.836764	1.465542
H	-5.173694	-3.734148	0.925718
H	-5.767534	-3.142527	2.484077
H	-6.391682	-2.445118	0.980331
C	-6.290406	0.052611	-5.147886
H	-6.661691	-0.952411	-5.385962
H	-7.158279	0.727865	-5.128142
H	-5.638542	0.378698	-5.966468
C	-6.841871	-0.419420	-2.231252
H	-6.883081	-1.510830	-2.120931
H	-6.745847	0.018982	-1.230456
H	-7.810449	-0.093029	-2.635940
C	-5.119352	1.978722	-3.139704
H	-4.940638	2.217990	-2.088603
H	-4.261099	2.342665	-3.714959
H	-6.003601	2.546356	-3.464075
C	-3.749040	-1.880645	-6.328612
H	-3.372746	-1.550609	-7.308455
H	-3.535062	-2.956484	-6.245258
H	-4.833266	-1.752619	-6.325114
C	-1.129732	-1.835090	-4.989969
H	-0.308665	-1.215844	-4.616562
H	-1.104478	-2.788597	-4.450695
H	-0.929981	-2.054399	-6.050573

C	-2.467719	0.851118	-5.445005
H	-1.781815	0.856381	-6.303904
H	-3.367438	1.407712	-5.734247
H	-1.975339	1.395822	-4.628285

In-Sb(SiiPrDis2)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-0.813816	-0.362072	-0.551513
In	1.114729	-0.089270	1.657568
Si	0.414761	0.264995	-2.947240
Si	-3.524255	-0.336631	-0.043326
C	1.711319	-1.217450	-3.148090
H	1.027576	-2.060059	-2.934359
C	1.247497	2.056563	-3.150720
H	2.322634	1.796659	-3.096510
C	-4.366829	-2.000251	-0.683453
C	-3.829188	-0.073083	1.897032
H	-4.766292	-0.646920	2.036780
Si	-4.293141	1.716782	2.552203
Si	-2.642865	-0.894962	3.206218
Si	-6.322901	-2.134417	-0.534603
Si	3.059608	-1.471863	-1.765487
Si	2.436866	-1.734446	-4.884487
Si	1.098901	3.459825	-1.785177
Si	1.138316	2.927456	-4.914988
C	-4.432881	1.126088	-1.012526
C	-5.177035	0.732380	-2.322592
C	-3.576663	2.406697	-1.207185
H	-5.227977	1.402596	-0.313350
H	-4.616485	0.058328	-2.975415
H	-6.135530	0.252026	-2.106802
H	-5.397374	1.637145	-2.907648
H	-2.592228	2.191624	-1.633564
H	-4.093145	3.107850	-1.881003
H	-3.408998	2.928362	-0.260115
C	-0.968165	-0.069613	-4.265892
C	-2.207490	0.819055	-4.044368
C	-1.440360	-1.546940	-4.293989
H	-0.532317	0.172184	-5.246664
H	-2.696282	0.521794	-3.116579
H	-1.971457	1.881869	-3.962063
H	-2.932906	0.695442	-4.862812
H	-0.629986	-2.254952	-4.487112
H	-1.896158	-1.819626	-3.333134
H	-2.198675	-1.686842	-5.079157
H	-4.240797	-1.855824	-1.774790

Si	-3.603054	-3.778304	-0.462340
C	-6.975281	-3.677424	0.381010
H	-6.659828	-4.618576	-0.080888
H	-6.689792	-3.699331	1.439051
H	-8.073944	-3.641381	0.334343
C	-7.193821	-0.715694	0.396933
H	-8.277141	-0.823668	0.239805
H	-7.015015	-0.784279	1.478544
H	-6.911996	0.288341	0.071054
C	-7.057325	-2.264381	-2.302335
H	-7.279098	-3.312230	-2.544136
H	-8.000407	-1.704999	-2.376912
H	-6.382169	-1.879525	-3.075103
C	-3.896540	-4.499678	1.287385
H	-3.023078	-5.085878	1.602644
H	-4.064812	-3.725026	2.044090
H	-4.766070	-5.165523	1.297660
C	-4.447517	-4.931007	-1.749130
H	-5.205197	-4.423811	-2.357482
H	-3.686768	-5.323659	-2.437467
H	-4.928274	-5.792392	-1.266362
C	-1.757091	-3.989886	-0.871720
H	-1.549635	-3.713052	-1.913196
H	-1.077540	-3.404630	-0.248569
H	-1.519062	-5.059134	-0.753740
C	-1.539216	-2.348998	2.643931
H	-1.479164	-3.066366	3.475823
H	-1.901955	-2.884035	1.767609
H	-0.509702	-2.040052	2.419837
C	-3.701508	-1.642758	4.604803
H	-3.062276	-1.859002	5.473757
H	-4.510524	-0.986521	4.938984
H	-4.145775	-2.594768	4.281542
C	-1.416967	0.357730	3.975136
H	-1.880964	1.027432	4.706215
H	-0.619357	-0.189343	4.496568
H	-0.953165	1.002027	3.214769
C	-2.871062	2.964341	2.282304
H	-2.293533	3.104367	3.204997
H	-2.174934	2.638697	1.500937
H	-3.272600	3.945205	1.991470
C	-4.687347	1.703612	4.426935
H	-3.859682	1.400061	5.074468
H	-4.966254	2.730095	4.708268
H	-5.548963	1.061234	4.653154
C	-5.927843	2.482442	1.913201
H	-6.790749	1.911423	2.290545
H	-5.991374	3.495145	2.345429
H	-6.038255	2.586314	0.828491
C	2.469156	-2.849395	-0.574950
H	1.886840	-2.487378	0.281178
H	1.823202	-3.564038	-1.103855
H	3.335860	-3.401910	-0.182940
C	4.785000	-2.088682	-2.305684

H	5.390444	-2.155104	-1.389255
H	4.760784	-3.088668	-2.750467
H	5.302743	-1.412446	-2.992922
C	3.482129	0.157695	-0.870045
H	4.128837	0.766862	-1.517725
H	2.611639	0.776688	-0.627849
H	4.044075	-0.039176	0.053344
C	4.005399	-0.738798	-5.336985
H	3.998490	-0.471391	-6.400733
H	4.086223	0.193063	-4.764118
H	4.910120	-1.328224	-5.148578
C	2.879476	-3.600613	-4.772681
H	2.579369	-4.105837	-5.700957
H	3.954628	-3.769384	-4.641364
H	2.358692	-4.101040	-3.944789
C	1.273901	-1.698330	-6.402597
H	0.761465	-0.752409	-6.592732
H	1.895891	-1.919815	-7.283066
H	0.511329	-2.483102	-6.339221
C	2.758199	4.418828	-1.764134
H	3.606096	3.737550	-1.924406
H	2.821495	5.213333	-2.511520
H	2.892809	4.879103	-0.775541
C	-0.378922	4.621636	-2.134442
H	-1.225726	4.084193	-2.580768
H	-0.732450	5.051179	-1.185955
H	-0.117419	5.454896	-2.799996
C	0.911084	3.047947	0.066141
H	0.961451	4.014424	0.591205
H	-0.037673	2.567543	0.310186
H	1.737212	2.436173	0.455105
C	-0.595511	3.269178	-5.628937
H	-0.457058	3.932558	-6.495189
H	-1.104771	2.367811	-5.983029
H	-1.259794	3.786016	-4.927247
C	2.104923	1.984202	-6.251884
H	1.939700	2.491994	-7.213339
H	3.182359	2.008097	-6.048564
H	1.809536	0.941366	-6.374785
C	1.980324	4.643930	-4.952327
H	1.472840	5.397615	-4.341602
H	3.033494	4.605819	-4.651812
H	1.945780	4.990253	-5.995751

(NHC)2In-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z

In	-0.426952	-1.612632	1.836010
Sb	1.204382	-2.439713	-0.380402
C	-2.582383	-2.094354	1.513087
N	-3.052968	-1.893653	0.086138
C	-4.277904	-1.233794	0.104973
C	-4.557819	-0.809696	1.340324
N	-3.550306	-1.193320	2.211490
H	-4.873527	-1.134447	-0.789837
H	-5.427875	-0.273917	1.690207
C	-3.622449	-1.014156	3.589351
C	-3.775297	-0.565030	6.373695
C	-4.145845	-2.015418	4.448873
C	-3.248955	0.246328	4.140638
C	-3.333256	0.444820	5.530369
C	-4.185843	-1.777618	5.837233
H	-3.068222	1.404174	5.967989
H	-4.566614	-2.538172	6.515332
H	-3.830905	-0.395412	7.445454
C	-2.695592	-2.758646	-0.952361
C	-1.798405	-4.526266	-2.981892
C	-1.967165	-2.259492	-2.072207
C	-3.094769	-4.129704	-0.956328
C	-2.610533	-4.993124	-1.961836
C	-1.508174	-3.172420	-3.051173
H	-2.889914	-6.044257	-1.968290
H	-0.936318	-2.815521	-3.906358
H	-1.439972	-5.203637	-3.751642
C	-4.132089	-4.696551	0.015284
H	-4.461402	-3.920994	0.706342
C	-5.402144	-5.139039	-0.724935
H	-5.218994	-5.990119	-1.389391
H	-5.806714	-4.320517	-1.330833
H	-6.176435	-5.439789	-0.010467
C	-3.581570	-5.844658	0.863638
H	-3.260207	-6.696577	0.255898
H	-4.344428	-6.208009	1.560254
H	-2.724416	-5.511734	1.454789
C	-1.728964	-0.783037	-2.422296
H	-0.855782	-0.759804	-3.091177
C	-2.910951	-0.245155	-3.241088
H	-3.828294	-0.197607	-2.647887
H	-3.112702	-0.876955	-4.113318
H	-2.700019	0.765080	-3.608902
C	-1.367896	0.209727	-1.319591
H	-0.500411	-0.128839	-0.754121
H	-2.189474	0.409020	-0.630058
H	-1.095913	1.176165	-1.761253
C	-2.833646	1.422036	3.251603
H	-2.661852	1.075784	2.227573
C	-3.946465	2.473286	3.191696
H	-4.129126	2.929227	4.171050
H	-4.888877	2.032037	2.849848
H	-3.681204	3.275942	2.495058

C	-1.515944	2.065626	3.687662
H	-0.725801	1.313737	3.731736
H	-1.585740	2.544915	4.669156
H	-1.206463	2.832794	2.969359
C	-4.754834	-3.310935	3.919361
H	-4.767313	-3.295079	2.828653
C	-3.935292	-4.527096	4.343026
H	-2.905802	-4.430843	3.987500
H	-4.353736	-5.445561	3.919165
H	-3.909131	-4.648790	5.430763
C	-6.221920	-3.472842	4.336476
H	-6.662900	-4.349068	3.848320
H	-6.810190	-2.595862	4.044196
H	-6.334411	-3.608845	5.417147
C	0.451022	-2.365903	3.750506
N	1.044788	-3.747115	3.614958
C	2.397165	-3.696792	3.944095
C	2.772059	-2.445309	4.220347
N	1.686668	-1.590238	4.129255
H	-0.310909	-2.316362	4.530207
H	2.989733	-4.599204	3.987024
H	3.742910	-2.087218	4.529575
C	1.751428	-0.224661	4.414504
C	2.038389	2.533608	5.013270
C	1.315868	0.294140	5.671783
C	2.368136	0.668359	3.482181
C	2.490129	2.035730	3.801752
C	1.471443	1.670772	5.940540
H	2.967806	2.725960	3.110646
H	1.174151	2.091443	6.897192
H	2.153284	3.588297	5.247629
C	0.303903	-4.917976	3.833340
C	-1.205859	-7.294781	4.154278
C	0.202499	-5.867480	2.773818
C	-0.259194	-5.250205	5.097052
C	-1.032159	-6.425086	5.221508
C	-0.570039	-7.032417	2.950554
H	-1.484054	-6.687847	6.175529
H	-0.658999	-7.763032	2.150219
H	-1.793779	-8.200068	4.276550
C	0.788623	-0.609189	6.786363
H	0.235269	-1.427112	6.328812
C	1.945948	-1.191784	7.603956
H	2.643680	-1.755538	6.978834
H	1.570371	-1.873694	8.374683
H	2.518355	-0.401778	8.103420
C	-0.213377	0.055921	7.741796
H	0.272674	0.761838	8.424004
H	-0.706465	-0.700464	8.362563
H	-0.987767	0.596589	7.192232
C	2.962898	0.190453	2.155050
H	2.658617	-0.841001	1.961027
C	4.494664	0.203503	2.207443
H	4.868244	-0.394736	3.045024

H	4.889996	1.218640	2.324020
H	4.914376	-0.213107	1.285361
C	2.468313	1.009013	0.953729
H	1.375512	1.073081	0.938346
H	2.791732	0.542412	0.016670
H	2.861537	2.030971	0.956960
C	0.030573	-4.457186	6.369653
H	0.678387	-3.612037	6.140442
C	-1.241494	-3.889512	7.000373
H	-0.998618	-3.275885	7.874325
H	-1.929700	-4.674417	7.330290
H	-1.772055	-3.256567	6.284929
C	0.809518	-5.296758	7.390674
H	1.099038	-4.682182	8.250224
H	1.725381	-5.701842	6.945939
H	0.220451	-6.138015	7.770933
C	0.995324	-5.710230	1.474902
H	1.471113	-4.726768	1.445514
C	2.124822	-6.743704	1.399865
H	2.776587	-6.678131	2.278037
H	2.743003	-6.574267	0.511507
H	1.739756	-7.767885	1.346081
C	0.114346	-5.790474	0.229230
H	-0.663110	-5.025264	0.275543
H	-0.371917	-6.764413	0.116542
H	0.705997	-5.614164	-0.675563
H	-2.725542	-3.130100	1.828274

NHC-In-Sb-NHC

Atomic Number	Coordinates (Angstroms) X	Y	Z
In	-0.956846	-1.998087	4.253012
Sb	-1.560623	-2.674538	1.532932
C	-3.252241	-1.460138	0.890280
N	-3.608577	-1.553438	-0.545569
C	-4.912703	-2.007206	-0.671652
C	-5.461182	-2.166851	0.540524
N	-4.518212	-1.910032	1.524245
H	-3.017863	-0.426944	1.144433
H	-5.361276	-2.145282	-1.643622
H	-6.470340	-2.454434	0.792467
C	-4.802354	-1.692618	2.875037
C	-5.316298	-1.318480	5.634316
C	-4.930331	-2.813634	3.749460
C	-4.990563	-0.384466	3.404305
C	-5.218964	-0.224344	4.786751
C	-5.194603	-2.600024	5.116770

H	-5.354228	0.768040	5.211461
H	-5.318765	-3.438860	5.796695
H	-5.515575	-1.173734	6.692603
C	-2.629018	-1.550229	-1.539725
C	-0.539270	-1.539627	-3.455878
C	-2.176280	-0.323823	-2.105827
C	-2.063916	-2.776388	-2.011175
C	-1.029681	-2.740818	-2.968635
C	-1.110158	-0.348974	-3.033709
H	-0.598310	-3.660110	-3.356022
H	-0.733143	0.579789	-3.459005
H	0.264580	-1.532577	-4.186592
C	-2.581437	-4.144986	-1.559939
H	-3.141539	-4.041021	-0.626631
C	-3.528469	-4.729198	-2.614128
H	-3.007159	-4.931627	-3.556637
H	-4.353271	-4.044902	-2.836530
H	-3.961863	-5.671929	-2.262948
C	-1.466944	-5.154349	-1.251985
H	-0.938974	-5.483236	-2.153009
H	-1.891445	-6.051101	-0.787428
H	-0.727240	-4.732884	-0.564011
C	-2.770491	1.065429	-1.855344
H	-2.571587	1.649360	-2.766959
C	-4.289704	1.149737	-1.707483
H	-4.630478	0.825047	-0.724072
H	-4.798873	0.555466	-2.473336
H	-4.621561	2.188376	-1.821744
C	-2.056862	1.803841	-0.723738
H	-0.985032	1.892802	-0.930021
H	-2.168274	1.294974	0.234537
H	-2.454488	2.818287	-0.610450
C	-5.029303	0.865396	2.527303
H	-4.918541	0.586193	1.479288
C	-6.383958	1.580494	2.610461
H	-6.573880	1.996631	3.605371
H	-7.203305	0.893225	2.371745
H	-6.422953	2.409097	1.894705
C	-3.887401	1.829128	2.864545
H	-2.916130	1.325308	2.815191
H	-3.990445	2.252103	3.869601
H	-3.868637	2.663746	2.155244
C	-4.832930	-4.251550	3.233988
H	-4.318130	-4.259314	2.266983
C	-4.011259	-5.173344	4.145286
H	-3.033849	-4.735917	4.368558
H	-3.847329	-6.140333	3.657179
H	-4.513156	-5.378825	5.096403
C	-6.231910	-4.842460	3.032338
H	-6.167881	-5.846124	2.598243
H	-6.835369	-4.226057	2.359139
H	-6.776064	-4.921968	3.980326
C	1.098045	-2.613584	4.855903
N	1.399509	-4.065748	4.879207

C	2.634602	-4.287035	4.290861
C	3.108486	-3.142415	3.780918
N	2.195842	-2.112143	3.982242
H	1.195724	-2.192405	5.857398
H	3.099169	-5.260668	4.306615
H	4.052007	-2.958354	3.288852
C	2.563653	-0.758433	3.996009
C	3.207818	1.993659	3.928850
C	3.169633	-0.136405	5.123058
C	2.345959	0.009909	2.814258
C	2.675273	1.378269	2.805020
C	3.458984	1.243240	5.070074
H	2.534538	1.976711	1.908618
H	3.913331	1.743629	5.922552
H	3.456240	3.051212	3.905766
C	0.584652	-5.022848	5.487161
C	-1.182932	-6.897920	6.670892
C	-0.020700	-6.052017	4.701037
C	0.341283	-5.006355	6.890862
C	-0.570426	-5.927013	7.448650
C	-0.888761	-6.976219	5.317898
H	-0.785062	-5.913710	8.514929
H	-1.345409	-7.777363	4.742278
H	-1.863178	-7.613383	7.124458
C	3.587090	-0.904585	6.376059
H	3.343537	-1.962832	6.270383
C	5.105570	-0.857136	6.587792
H	5.634922	-1.220808	5.699988
H	5.393938	-1.491965	7.432867
H	5.463403	0.155856	6.800058
C	2.851369	-0.401698	7.622314
H	3.134574	0.623676	7.882741
H	3.082465	-1.036206	8.484938
H	1.766405	-0.419255	7.473622
C	1.824770	-0.635788	1.529230
H	1.405449	-1.621738	1.752121
C	2.968823	-0.847856	0.533442
H	3.767131	-1.454923	0.974222
H	3.411325	0.102472	0.214734
H	2.609688	-1.366622	-0.362061
C	0.689665	0.159054	0.876984
H	-0.112308	0.363175	1.594237
H	0.261189	-0.408239	0.044074
H	1.031685	1.116875	0.472087
C	1.099262	-4.089721	7.850634
H	1.873519	-3.544044	7.307993
C	0.166846	-3.066322	8.504229
H	0.736923	-2.369700	9.128122
H	-0.581919	-3.545381	9.144399
H	-0.369224	-2.479925	7.751213
C	1.863587	-4.880334	8.922496
H	2.490093	-4.206854	9.517962
H	2.519455	-5.628066	8.462758
H	1.193333	-5.400412	9.614697

C	0.267850	-6.220775	3.206977
H	0.745660	-5.318842	2.814185
C	1.221757	-7.399385	2.979255
H	2.138357	-7.294591	3.568235
H	1.508185	-7.465065	1.923966
H	0.759490	-8.352956	3.258545
C	-0.989951	-6.404112	2.350423
H	-1.675690	-5.562981	2.477902
H	-1.533330	-7.324597	2.584652
H	-0.716556	-6.454934	1.292219

In-Sb(NHC)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-0.385416	-1.995372	1.746670
In	1.375177	-2.447267	-0.496885
C	-2.545064	-2.176160	1.472578
N	-3.030418	-2.000764	0.061542
C	-4.213582	-1.276422	0.074110
C	-4.423323	-0.774677	1.294643
N	-3.394323	-1.149190	2.152926
H	-4.828997	-1.187836	-0.808357
H	-5.256629	-0.184409	1.646176
C	-3.525979	-1.072338	3.542121
C	-3.776293	-0.788014	6.343059
C	-4.249596	-2.033635	4.297680
C	-3.003734	0.078355	4.205404
C	-3.135413	0.193377	5.601409
C	-4.339873	-1.878744	5.695819
H	-2.756503	1.064682	6.128461
H	-4.881510	-2.606964	6.295666
H	-3.870366	-0.683786	7.420411
C	-2.654211	-2.826670	-0.993645
C	-1.725721	-4.515734	-3.074094
C	-1.957926	-2.277380	-2.108822
C	-2.997535	-4.210965	-1.018545
C	-2.489720	-5.036938	-2.043027
C	-1.493693	-3.149529	-3.122304
H	-2.722841	-6.099191	-2.061831
H	-0.949778	-2.750962	-3.977424
H	-1.356818	-5.162661	-3.864849
C	-4.009107	-4.828852	-0.051418
H	-4.389404	-4.064580	0.626559
C	-5.247301	-5.351705	-0.793788
H	-5.013664	-6.202524	-1.442453
H	-5.691050	-4.566092	-1.415599
H	-6.009656	-5.682627	-0.079745

C	-3.397427	-5.934177	0.809122
H	-2.997194	-6.757551	0.208826
H	-4.145503	-6.355962	1.488250
H	-2.583616	-5.536011	1.419806
C	-1.711770	-0.786822	-2.388851
H	-0.775712	-0.736464	-2.964704
C	-2.820419	-0.239506	-3.299187
H	-3.796235	-0.262746	-2.803881
H	-2.905139	-0.823232	-4.222510
H	-2.612597	0.797749	-3.583988
C	-1.483813	0.179530	-1.224865
H	-0.807532	-0.232253	-0.476980
H	-2.411622	0.477956	-0.733210
H	-1.029222	1.105971	-1.596437
C	-2.389388	1.234135	3.409511
H	-1.968743	0.841230	2.476593
C	-3.456896	2.277240	3.062285
H	-3.879617	2.732995	3.965073
H	-4.286175	1.840000	2.500035
H	-3.028646	3.078882	2.450692
C	-1.229131	1.928324	4.125195
H	-0.527008	1.189102	4.509985
H	-1.564031	2.545128	4.965937
H	-0.694973	2.589318	3.434337
C	-5.021240	-3.183934	3.655869
H	-4.928959	-3.135973	2.571115
C	-4.475821	-4.545397	4.084602
H	-3.416972	-4.628919	3.825125
H	-5.011300	-5.353601	3.575724
H	-4.575762	-4.712957	5.161754
C	-6.525819	-3.089101	3.939337
H	-7.069392	-3.858373	3.379698
H	-6.920038	-2.113095	3.634976
H	-6.757958	-3.229441	5.000264
C	0.484146	-2.272329	3.739899
N	0.936662	-3.687000	3.947530
C	2.313905	-3.720410	4.094112
C	2.820561	-2.486497	4.013911
N	1.816025	-1.550751	3.784248
H	-0.197078	-1.917868	4.516561
H	2.832586	-4.644103	4.302562
H	3.844436	-2.169894	4.151459
C	1.931453	-0.241942	4.289020
C	2.340677	2.411432	5.221105
C	1.861251	0.058330	5.681026
C	2.242257	0.815781	3.383307
C	2.436175	2.125706	3.868807
C	2.062041	1.388398	6.115141
H	2.678537	2.936832	3.186202
H	2.017813	1.634366	7.173870
H	2.497765	3.424674	5.579573
C	0.109132	-4.808029	4.048229
C	-1.459923	-7.168699	4.274838
C	0.130492	-5.808170	3.025857

C	-0.672073	-5.056695	5.218135
C	-1.447969	-6.234060	5.298235
C	-0.664202	-6.966078	3.160541
H	-2.034332	-6.458754	6.184944
H	-0.647992	-7.741086	2.398163
H	-2.056877	-8.071781	4.364966
C	1.624569	-0.998206	6.755363
H	1.451276	-1.966004	6.290261
C	2.853665	-1.173587	7.653808
H	3.744190	-1.403895	7.058570
H	2.699455	-1.998634	8.357785
H	3.067491	-0.274108	8.240895
C	0.377882	-0.692686	7.593460
H	0.481575	0.228220	8.176356
H	0.181090	-1.504218	8.301602
H	-0.502976	-0.585915	6.952688
C	2.420914	0.572456	1.888566
H	2.205781	-0.472590	1.663829
C	3.868602	0.816775	1.450486
H	4.562788	0.204824	2.037261
H	4.163989	1.864698	1.569665
H	4.000351	0.553948	0.395243
C	1.448667	1.410353	1.051208
H	0.413026	1.231509	1.358969
H	1.533543	1.152036	-0.009737
H	1.642281	2.484323	1.141188
C	-0.579313	-4.174863	6.463686
H	-0.422689	-3.145714	6.148419
C	-1.846174	-4.131435	7.329557
H	-1.777880	-3.320029	8.062761
H	-1.995387	-5.058965	7.892767
H	-2.735655	-3.959765	6.719852
C	0.604904	-4.616126	7.332093
H	0.702543	-3.973805	8.213555
H	1.550048	-4.569189	6.783190
H	0.480533	-5.647243	7.682468
C	1.049841	-5.721257	1.805838
H	1.488247	-4.722839	1.745865
C	2.206220	-6.721401	1.923992
H	2.756679	-6.586948	2.860672
H	2.914223	-6.589648	1.098516
H	1.852304	-7.757959	1.895321
C	0.310960	-5.934548	0.479521
H	-0.493553	-5.203323	0.369555
H	-0.126132	-6.934036	0.392622
H	0.995309	-5.810906	-0.366748
H	-2.794300	-3.174314	1.840226
