Supporting Information

Triply Bonded Gallium≡Phosphorus Molecules: Theoretical Designs and Characterization

Jia-Syun Lu,[1] Ming-Chung Yang,[1] and Ming-Der Su[1,2]*

[1]Department of Applied Chemistry, National Chiayi University, Chiayi 60004, Taiwan

[2]Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 80708, Taiwan

*Email: midesu@mail.ncyu.edu.tw

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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,[3-5] and B3PW91[5,6] levels, in conjunction with the Def2-TZVP[7] and LANL2DZ+dp[8-12] 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, Si*i*PrDis$_2$–Ga≡P–Si*i*PrDis$_2$, Tbt–Ga≡P–Tbt, and Ar*–Ga≡P–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 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′Ga≡PR′ 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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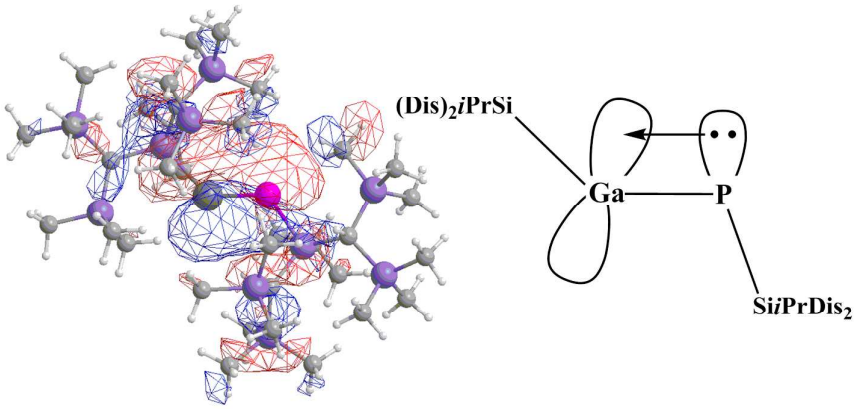
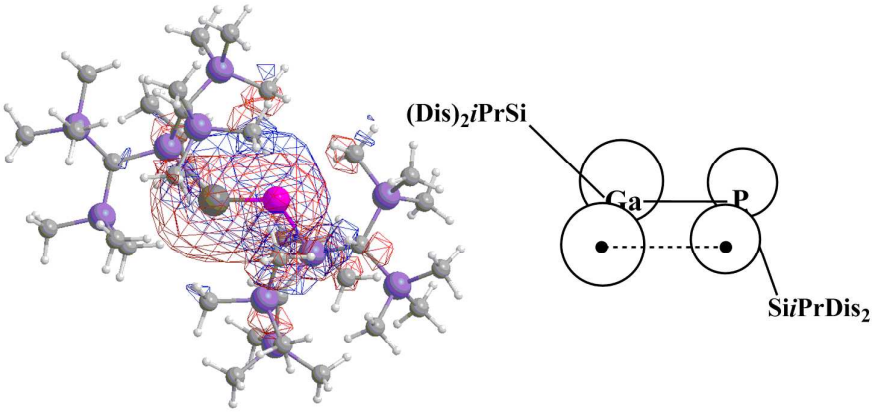
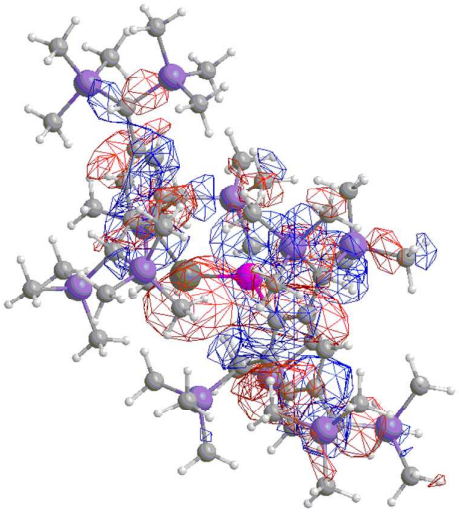


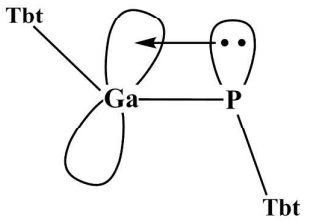
(i) $\pi_{\perp}$



(ii) $\pi_{\parallel}$

Figure S1: The natural Ga≡P π bonding orbitals ((i) and (ii)) of (Si*i*PrDis$_2$)–Ga≡P–(Si*i*PrDis$_2$)). For comparison, also see Figure 1.





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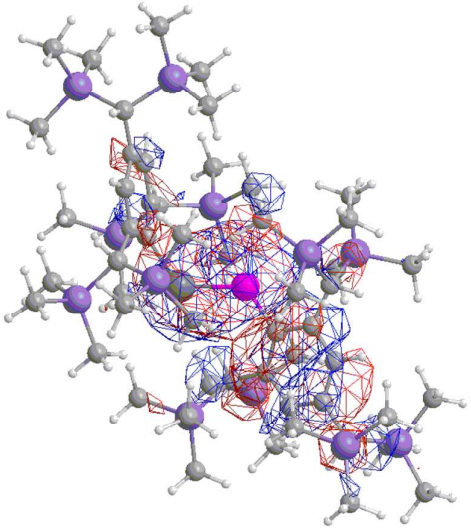
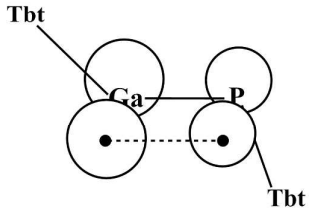
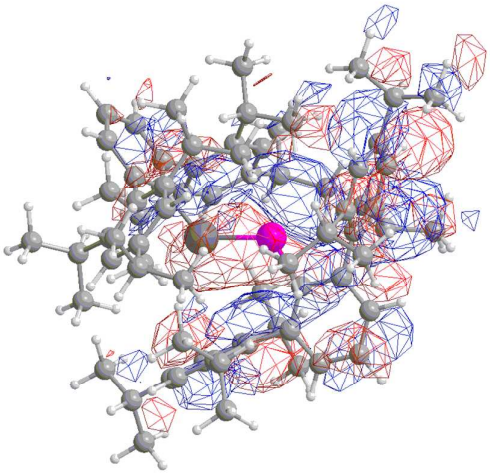
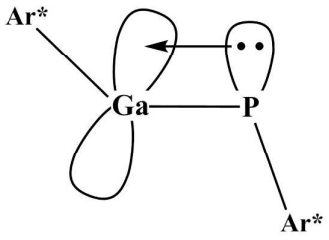




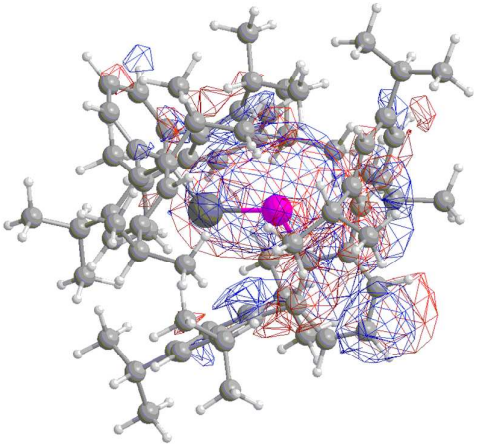
(ii) $\pi_{\parallel}$

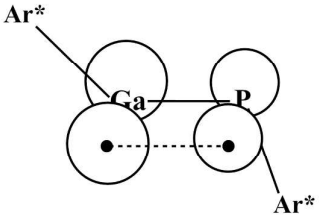
Figure S2: The natural Ga≡P π bonding orbitals ((i) and (ii)) of ((Tbt)–Ga≡P–(Tbt)). For comparison, also see Figure 1.





(i) $\pi_{\perp}$





(ii) $\pi_{\parallel}$

Figure S3: The natural Ga≡P π bonding orbitals ((i) and (ii)) of ((Ar*)–Ga≡P–(Ar*)). For comparison, also see Figure 1.

Table S1

The charge decomposition analysis (CDA) results[(a)] for R′Ga≡PR′ (R′ = Si*i*PrDis$_2$) system based on M06-2X orbitals, where X term indicates the number of electrons donated from R′–Ga fragment to R′–P fragment, Y term indicates the number of electrons back donated from R′–P fragment to R′–Ga 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**
	230	2.000000	0.000213	0.003839	-0.003626	-0.011171
	231	2.000000	0.000253	0.000054	0.000199	0.000091
	232	2.000000	0.000626	0.000027	0.000599	-0.001521
	233	2.000000	-0.000191	0.002037	-0.002228	-0.003677
	234	2.000000	0.002294	0.004102	-0.001808	-0.036031
	235	2.000000	-0.002471	0.000316	0.002155	-0.004660
	236	2.000000	0.000147	0.000367	-0.000220	-0.002126
	237	2.000000	0.000203	0.001237	-0.001034	-0.004032
	238	2.000000	0.002482	0.059719	-0.057237	0.124325
	239	2.000000	0.089724	0.065805	0.023919	-0.196128
HOMO	240	2.000000	0.014293	0.141141	-0.126848	-0.062298
LUMO	241	0.000000	0.000000	0.000000	0.000000	0.000000
	242	0.000000	0.000000	0.000000	0.000000	0.000000
sum[(b)]		480.000000	0.193341	0.376603	-0.183262	-0.196628

[(a)] For clearness, only list the X, Y, and W terms for HOMO(No.240)–10 ~ LUMO+2. [(b)] Summation of contributions from all unoccupied and occupied orbitals.

Table S2

The charge decomposition analysis (CDA) results[(a)] for R′Ga≡PR′ (R′ = Tbt) system based on M06-2X orbitals, where X term indicates the number of electrons donated from R′–Ga fragment to R′–P fragment, Y term indicates the number of electrons back donated from R′–P fragment to R′–Ga 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**
	278	2.000000	0.002103	0.012975	0.010872	-0.016816
	279	2.000000	0.000115	0.006014	0.005899	-0.001129
	280	2.000000	0.002322	0.000875	-0.001448	-0.010446
	281	2.000000	0.000277	0.008935	0.009213	-0.012516
	282	2.000000	0.005575	0.000678	-0.004897	-0.000538
	283	2.000000	-0.002239	0.001556	-0.000683	-0.004663
	284	2.000000	0.000429	0.012640	0.012211	-0.016421
	285	2.000000	0.001121	0.008650	0.007429	-0.020456
	286	2.000000	0.001374	0.003856	0.002481	-0.028605
	287	2.000000	0.010718	0.037254	0.026537	-0.139838
HOMO	288	2.000000	-0.019981	0.004145	0.024127	-0.013132
LUMO	289	0.000000	0.000000	0.000000	0.000000	0.000000
	290	0.000000	0.000000	0.000000	0.000000	0.000000
sum[(b)]		576.000000	0.113977	0.310706	-0.196730	-0.049265

[(a)] For clearness, only list the X, Y, and W terms for HOMO(No.288)–10~LUMO+2. [(b)] Summation of contributions from all unoccupied and occupied orbitals.

Table S3

The charge decomposition analysis (CDA) results[(a)] for R′Ga≡PR′ (R′ = Ar*) system based on M06-2X orbitals, where X term indicates the number of electrons donated from R′–Ga fragment to R′–P fragment, Y term indicates the number of electrons back donated from R′–P fragment to R′–Ga 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**
	318	2.000000	0.001436	0.011433	-0.009997	-0.027046
	319	2.000000	0.000220	0.001704	-0.001484	-0.006777
	320	2.000000	0.000435	0.009562	-0.009127	-0.022739
	321	2.000000	0.002033	0.000403	0.001630	-0.005120
	322	2.000000	-0.000001	0.003818	-0.003819	-0.005202
	323	2.000000	0.003814	0.025317	-0.021503	-0.038208
	324	2.000000	0.000718	0.004041	-0.003323	0.000324
	325	2.000000	0.000887	0.000320	0.000567	-0.001882
	326	2.000000	0.002669	0.009197	-0.006528	-0.020040
	327	2.000000	0.020494	0.052231	-0.031737	-0.178493
HOMO	328	2.000000	0.000696	0.036357	-0.035661	-0.063386
LUMO	329	0.000000	0.000000	0.000000	0.000000	0.000000
	330	0.000000	0.000000	0.000000	0.000000	0.000000
sum[(b)]		656.000000	0.192536	0.346257	-0.1537521	-0.214783

[(a)] For clearness, only list the X, Y, and W terms for HOMO(No.328)–10~LUMO+2. [(b)] Summation of contributions from all unoccupied and occupied orbitals.

M06-2X/Def2-TZVP

F2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.265893	0.000043	-0.000012
P	-2.011041	-0.000141	0.000007
F	1.217732	1.467483	0.000014
F	1.218151	-1.467398	0.000014

F2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.365984	-0.130857	0.014425
P	1.818319	-0.450710	-0.010685
F	-2.083014	-0.344148	-0.025268
F	0.313095	1.546062	-0.006611

F-Ga-P-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.518476	-0.584570	0.000000
Ga	0.655608	-0.070128	0.000000
F	-2.086922	0.942293	0.000000
F	2.359509	0.273544	0.000001

Ga-PF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.396573	0.588294	-0.171598
F	2.362406	-0.617849	0.215820
F	-1.219051	1.301879	0.187945
Ga	-1.007703	-0.483248	-0.034191

Ga-PF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.175144	-0.006136	0.605095
F	1.286945	1.196361	-0.490920
F	1.217590	-1.219320	-0.486994
Ga	-1.295741	0.009635	-0.008878

(OH)2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.258876	0.000000	0.000001
P	-2.030308	-0.000002	-0.000012
O	1.139553	1.564213	-0.000004
H	2.098264	1.530795	0.000054
O	1.139561	-1.564209	0.000017
H	2.098272	-1.530784	-0.000029

(OH)2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.685669	0.537080	0.004739
Ga	0.515271	0.152439	0.012271
O	2.258336	-0.149745	-0.115640
H	2.752410	-0.268611	0.699817
O	-1.246416	-1.204566	-0.112417
H	-1.536143	-1.678689	0.673162

HO-Ga-P-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.512086	-0.610339	-0.018218
Ga	-0.657074	-0.077591	0.037183
O	-2.382613	0.295724	-0.163580
H	-2.925674	0.446814	0.614132
O	2.149067	0.940608	-0.115710
H	2.482052	1.222922	0.740800

Ga-P(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.413647	0.679782	-0.117807
O	2.488752	-0.478795	0.206667
H	2.290179	-1.334357	-0.199071
O	-1.431473	1.240226	0.059813

H	-2.224265	1.552015	0.501602
Ga	-0.958995	-0.532447	-0.021525

Ga-P(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	1.213938	-0.177957	0.002478
P	-1.193390	0.154140	0.610446
O	-0.408630	1.286132	-0.437506
H	-0.949427	1.938414	-0.894196
O	-1.621008	-1.009493	-0.508747
H	-2.544686	-0.946969	-0.769289

H2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.680806	-0.000001	0.000009
H	1.426738	-1.390967	0.000020
P	-1.597219	-0.000005	-0.000022
H	1.426561	1.391070	0.000020

H2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.008847	-0.671655	0.000000
P	0.008847	1.571259	0.000000

H	1.149360	-1.748324	0.000000
H	-1.556332	-0.999260	0.000000

H-Ga-P-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.460824	-0.074470	0.000005
Ga	-0.674678	-0.011149	-0.000005
H	-2.233243	0.117926	0.000088
H	1.235896	1.344757	-0.000005

Ga-PH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.771614	-0.042009	0.004584
H	0.372571	1.542541	-0.303729
P	-1.530209	-0.037861	-0.076882
H	-1.339456	0.327660	1.314846

Ga-PH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.867772	0.000001	-0.001001
P	1.587561	-0.000025	-0.113892
H	1.543802	1.025535	0.869538
H	1.543726	-1.025189	0.869872

(CH3)2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.237612	-0.000606	-0.000277
P	2.030940	-0.023576	0.000148
C	-1.179967	1.761126	0.000087
H	-0.501816	2.611489	-0.017354
H	-1.833853	1.819278	-0.871355
H	-1.805156	1.833532	0.891413
C	-1.248531	-1.722584	0.000149
H	-0.605236	-2.599630	-0.012795
H	-1.900934	-1.756068	-0.873742
H	-1.880138	-1.767428	0.888762

(CH3)2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.257717	-0.028842	-0.000024
P	-1.936485	-0.528830	0.000015
C	0.276080	1.995293	0.000020
H	-0.710187	2.473828	0.000077
H	0.824050	2.327333	0.894104
H	0.823965	2.327369	-0.894101
C	1.938563	-1.077475	0.000018
H	1.758452	-2.159336	-0.001175
H	2.537574	-0.823882	-0.886759
H	2.536332	-0.825667	0.888146

H3C-Ga-P-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.425152	-0.713496	-0.000366
Ga	-0.624155	-0.045293	0.000818
C	2.382617	0.919104	-0.000551
H	3.430309	0.628544	0.079853
H	-3.083807	-0.532790	-0.466350
H	2.154650	1.561341	0.846649
C	-2.561988	0.303467	0.001293
H	2.265926	1.479286	-0.925556
H	-2.939161	0.430978	1.015066
H	-2.780152	1.203760	-0.573994

Ga-P(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.223143	-0.020063	-0.814010
C	-1.872701	0.149694	0.913068
H	-2.435786	1.081915	0.985851
H	-2.580549	-0.663137	1.090684
H	-1.122775	0.122302	1.715666
C	1.041616	1.611494	-0.000272
H	1.647525	1.766053	-0.894097
H	0.180767	2.274026	-0.023578
H	1.634494	1.811070	0.890244
Ga	0.839031	-0.537369	0.095762

Ga-P(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.028816	0.001668	-0.744548
Ga	1.278508	-0.003337	0.039477
C	-1.325985	-1.396888	0.470631
H	-1.215690	-2.353324	-0.040787
H	-0.670151	-1.405063	1.352691
H	-2.349795	-1.330732	0.842497
C	-1.307313	1.405238	0.469346
H	-1.177853	2.359540	-0.041542
H	-0.654993	1.401210	1.354144
H	-2.333258	1.356690	0.837561

(SiH3)2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-2.240561	-0.898905	0.000576
H	-2.384254	-1.755614	-1.196545
H	-2.386448	-1.734045	1.212670
H	-3.303043	0.128400	-0.009469
Si	2.070139	-1.184166	0.000594
H	2.094074	-2.034501	1.210741
H	2.092751	-2.047673	-1.200431
H	3.266431	-0.316205	-0.004862
Ga	-0.014221	0.090432	-0.001313
P	0.229817	2.274616	0.000814

(SiH3)2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-0.009604	2.328630	0.000119
Ga	0.000372	0.115879	-0.000178
Si	-2.134741	-1.091474	0.000068
H	-2.193449	-1.962487	-1.201300
H	-2.201009	-1.947427	1.211825
H	-3.304081	-0.181025	-0.009311
Si	2.142244	-1.078906	0.000092
H	2.210344	-1.941453	-1.206873
H	3.306063	-0.161351	0.000914
H	2.209617	-1.942638	1.206254

H3Si-Ga-P-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.355600	-0.382094	-0.001598
P	1.690751	-1.069368	0.001796
Si	1.896183	1.150004	0.000091
H	2.538401	1.722670	1.202653
H	2.547628	1.719621	-1.199003
H	0.505319	1.778129	-0.004931
Si	-2.652573	0.360499	0.001291
H	-2.884093	1.229686	-1.169631
H	-3.534339	-0.821462	-0.070405
H	-2.921126	1.109766	1.244558

Ga-P(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-0.853271	-0.027498	1.249667
Si	1.796988	1.200391	-0.046682
H	2.759035	0.924627	1.046894
H	2.524999	1.348030	-1.332655
H	1.091108	2.476170	0.209617
Si	-2.078461	0.580675	-0.547935
H	-3.343378	-0.190844	-0.595923
H	-2.380084	2.031682	-0.489735
H	-1.356711	0.315582	-1.836385
Ga	0.562733	-1.013797	-0.239425

Ga-P(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-1.564162	-0.001912	-0.098364
P	0.619663	0.000511	1.102728
Si	1.139497	-1.627240	-0.334729
H	0.076474	-1.791678	-1.380888
H	2.399106	-1.367700	-1.061476
H	1.216029	-2.916698	0.381339
Si	1.134199	1.630197	-0.334540
H	2.390416	1.371490	-1.067479
H	0.066282	1.795679	-1.375563
H	1.214025	2.919126	0.382217

B3PW91/Def2-TZVP

F2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.261223	-0.000653	-0.000002
P	1.997865	-0.003227	0.000001
F	-1.221615	-1.465134	0.000002
F	-1.208391	1.472761	0.000002

F2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.000000	0.356901	0.000000
P	0.999742	-1.622831	0.000000
F	-1.511858	-0.612786	0.000000
F	-0.154378	2.088177	0.000000

F-Ga-P-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.651840	-0.076896	-0.000003
P	1.505144	-0.583007	0.000003
F	2.088390	0.945444	0.000000
F	-2.351738	0.291099	0.000006

Ga-PF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.318474	0.600217	-0.193603
F	2.303566	-0.586672	0.243026
F	-1.229137	1.290950	0.210357
Ga	-0.949902	-0.494896	-0.037949

Ga-PF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.162354	-0.000012	0.600547
F	1.300590	1.226355	-0.474428
F	1.298288	-1.227417	-0.474041
Ga	-1.316942	0.000314	-0.015225

(OH)2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.248321	-0.001249	-0.000195
P	-2.021086	0.003437	0.000049
O	1.318491	1.440834	-0.000281
H	0.874442	2.291974	0.003948
O	1.138205	-1.552339	0.000658
H	2.090335	-1.412763	-0.001667

(OH)2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.971382	-0.266059	-0.002109
Ga	-0.276539	-0.035555	0.007898
O	-1.692703	-1.107881	0.006168
H	-1.518695	-2.053963	-0.040293
O	-0.660620	1.723321	-0.116545
H	-0.652757	2.223526	0.710116

HO-Ga-P-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.659686	-0.066971	-0.028543
P	-1.495514	-0.610574	0.020550
O	-2.195589	0.912871	0.118527
H	-2.470140	1.208306	-0.755197
O	2.399571	0.293937	-0.053184
H	2.820746	0.371949	0.809042

Ga-P(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.323942	0.671021	-0.158104
O	2.437932	-0.441428	0.256530
H	2.295701	-1.310927	-0.143362
O	-1.393651	1.240639	0.079381
H	-2.079636	1.519813	0.694439
Ga	-0.917079	-0.537674	-0.027961

Ga-P(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-1.221728	-0.187328	0.002410
P	1.183508	0.150478	-0.609407
O	0.388830	1.296416	0.421918
H	0.924083	1.962013	0.867327
O	1.683645	-0.987582	0.512649
H	2.617084	-0.882666	0.722545

H2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.657469	0.000000	0.000009
H	1.422413	-1.366372	0.000020
P	-1.548423	-0.000001	-0.000022
H	1.422389	1.366385	0.000020

H2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.006788	-0.666767	0.000000
P	0.006788	1.564082	-0.000000
H	1.205686	-1.674313	0.000000
H	-1.517920	-1.117125	0.000000

H-Ga-P-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.674356	-0.004804	0.000000
H	-2.228040	0.039521	0.000001
P	1.453773	-0.082474	-0.000001
H	1.326475	1.346509	0.000000

Ga-PH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.771614	-0.042009	0.004584
H	0.372571	1.542541	-0.303729
P	-1.530209	-0.037861	-0.076882
H	-1.339456	0.327660	1.314846

Ga-PH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.866254	0.000000	-0.000843
P	1.583955	-0.000002	-0.114665
H	1.547284	1.030909	0.873054
H	1.547251	-1.030896	0.873068

(CH3)2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.213007	-0.001242	-0.002668
P	-2.003996	-0.020156	0.001607
C	1.202463	1.728518	0.003268
H	1.784646	1.794432	-0.918472
H	0.545494	2.593535	0.072999
H	1.892033	1.730774	0.850025
C	1.264372	-1.692433	0.000779
H	2.072889	-1.606152	-0.727708
H	1.703205	-1.823355	0.992547
H	0.657458	-2.564899	-0.235086

(CH3)2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.238362	-0.024579	-0.000023
P	-1.971134	-0.397022	0.000014
C	0.550037	1.966275	0.000020
H	-0.364354	2.564709	0.000085
H	1.137387	2.219608	0.890932
H	1.137292	2.219657	-0.890941
C	1.781821	-1.267374	0.000015
H	1.475689	-2.316956	-0.001155
H	2.401026	-1.080772	-0.885469
H	2.399613	-1.082373	0.886826

H3C-Ga-P-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.405437	-0.711548	-0.000951
Ga	-0.627140	-0.028137	0.001694
C	2.419448	0.883805	-0.001028
H	3.458325	0.557352	0.089702
H	-3.055785	-0.521434	-0.551987
H	2.204689	1.539131	0.842879
C	-2.559654	0.280716	0.000086
H	2.326604	1.442918	-0.931981
H	-2.952586	0.312725	1.017146
H	-2.780226	1.227647	-0.498356

Ga-P(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.205894	0.074363	-0.813213
C	-1.921400	0.090123	0.895176
H	-2.505028	1.002874	1.037542
H	-2.621841	-0.747931	0.967278
H	-1.201618	-0.010205	1.721103
C	1.106610	1.592294	0.089689
H	1.807615	1.713555	-0.736320
H	0.293161	2.304281	-0.005763
H	1.612234	1.717967	1.044882
Ga	0.825569	-0.554532	0.072912

Ga-P(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	1.259098	-0.000419	0.033511
P	-1.037223	0.000215	-0.738501
C	-1.280478	-1.413201	0.475315
H	-0.550271	-1.475380	1.299527
H	-2.265140	-1.317408	0.938613
H	-1.249717	-2.357983	-0.069907
C	-1.278180	1.414240	0.475149
H	-2.263392	1.320784	0.937769
H	-0.548424	1.474579	1.299924
H	-1.244807	2.358957	-0.070018

(SiH3)2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-2.139600	-1.027253	0.000177
H	-2.219478	-1.898969	-1.201210
H	-2.227641	-1.881224	1.213692
H	-3.289984	-0.090726	-0.010776
Si	2.076130	-1.132987	0.000160
H	2.122078	-1.984609	1.217715
H	2.106549	-2.013197	-1.197384
H	3.274333	-0.258640	-0.018105
Ga	-0.002696	0.128069	-0.000410
P	0.080421	2.293372	0.000271

(SiH3)2Ga-P (TS1)

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
P	0.079465	2.298570	-0.000252
Ga	-0.001340	0.142827	0.000214
Si	-2.117071	-1.041456	-0.000087
H	-2.183975	-1.897798	-1.212581
H	-2.181465	-1.906330	1.205842
H	-3.277204	-0.117776	0.003990
Si	2.052164	-1.149209	-0.000295
H	2.036553	-2.069673	-1.169230
H	3.261455	-0.291058	-0.075171
H	2.102908	-1.954226	1.249649

H3Si-Ga-P-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.354758	-0.380884	0.000583
P	1.678005	-1.072978	-0.000647
Si	1.891200	1.148958	-0.000049
H	2.546761	1.719909	1.206924
H	2.543297	1.721693	-1.208016
H	0.498938	1.789281	0.002709
Si	-2.636987	0.362294	-0.000437
H	-2.884853	1.222587	-1.184098
H	-3.516610	-0.832617	-0.060990
H	-2.919107	1.123693	1.241923

Ga-P(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z

P	-0.853271	-0.027498	1.249667
Si	1.796988	1.200391	-0.046682
H	2.759035	0.924627	1.046894
H	2.524999	1.348030	-1.332655
H	1.091108	2.476170	0.209617
Si	-2.078461	0.580675	-0.547935
H	-3.343378	-0.190844	-0.595923
H	-2.380084	2.031682	-0.489735
H	-1.356711	0.315582	-1.836385
Ga	0.562733	-1.013797	-0.239425

Ga-P(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-1.499029	-0.001664	-0.066678
P	0.724323	0.000758	1.136389
Si	1.047452	-1.605553	-0.372062
H	-0.154921	-1.668874	-1.302717
H	2.219677	-1.405521	-1.261033
H	1.112554	-2.936145	0.282955
Si	1.043092	1.607907	-0.372017
H	2.214348	1.410138	-1.262793
H	-0.160769	1.669039	-1.301073
H	1.106546	2.938608	0.282938

B3LYP/LANL2DZ+dp

F2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.288609	-0.000248	0.000000
P	-2.012050	-0.001712	0.000000
F	1.176308	1.474522	0.000000
F	1.183009	-1.470814	0.000000

F2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.483167	-0.245466	0.000000
P	1.702775	-0.422192	0.000000
F	0.949523	1.327422	0.000000
F	-2.123238	0.221723	0.000000

F-Ga-P-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.669312	-0.063273	-0.000003
P	-1.524260	-0.616753	0.000002
F	-2.115302	0.973912	0.000000
F	2.350327	0.271948	0.000005

Ga-PF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z

P	1.334132	0.629460	-0.156815
F	2.367511	-0.629646	0.194078
F	-1.226312	1.277589	0.180685
Ga	-0.976864	-0.492690	-0.032924

Ga-PF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.197885	-0.000215	-0.632277
F	1.300168	-1.263635	0.505711
F	1.304920	1.261705	0.506283
Ga	-1.335938	0.000664	0.012136

(OH)2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.282282	0.000011	0.000002
P	-2.031763	-0.000029	-0.000012
O	1.099638	1.563245	0.000024
H	2.065341	1.601174	-0.000034
O	1.099718	-1.563259	-0.000011
H	2.065506	-1.600976	0.000058

(OH)2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z

P	1.902426	-0.491374	0.003858
Ga	-0.340150	-0.086189	0.000335
O	-2.048890	-0.514893	0.013730
H	-2.325450	-1.439893	-0.009392
O	0.063564	1.677328	-0.108945
H	0.216318	2.182885	0.702859

HO-Ga-P-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.673990	-0.085704	-0.042205
P	-1.524842	-0.628744	0.037883
O	-2.173133	0.975403	0.112788
H	-2.488941	1.240039	-0.764070
O	2.376392	0.322026	-0.026055
H	2.841805	0.468508	0.810307

Ga-P(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	1.393991	0.674985	-0.181015
O	2.499164	-0.485595	0.283512
H	2.319547	-1.365039	-0.093291
O	-1.387766	1.226509	0.123217
H	-2.111161	1.609474	0.638662
Ga	-0.968046	-0.525695	-0.034967

Ga-P(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-1.175916	-1.382843	0.432530
H	-2.028520	-1.837017	0.336037
O	-1.765829	1.229022	0.375348
H	-1.337488	1.328429	1.243568
Ga	1.395998	0.055785	0.038069
P	-1.091731	0.000655	-0.614851

H2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.675541	0.000000	0.000009
H	1.418527	-1.394795	0.000020
P	-1.585253	-0.000001	-0.000022
H	1.418494	1.394813	0.000020

H2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.671727	0.003206	-0.000017
H	1.755680	1.137030	0.000233
P	-1.571326	0.021810	0.000009
H	0.990664	-1.563555	0.000170

H-Ga-P-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.686349	-0.003804	0.000000
H	-2.257811	0.029014	0.000001
P	1.477642	-0.084967	-0.000001
H	1.369990	1.363399	0.000000

Ga-PH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.771614	-0.042009	0.004584
H	0.372572	1.542541	-0.303729
P	-1.530209	-0.037861	-0.076882
H	-1.339456	0.327660	1.314846

Ga-PH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.881245	0.000000	-0.000209
P	1.608055	-0.000001	-0.116931
H	1.598895	1.045833	0.880227
H	1.598865	-1.045827	0.880234

(CH3)2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.235286	-0.000036	-0.002359
P	-2.039684	-0.005633	0.001366
C	1.215605	1.741087	0.003124
H	1.797828	1.829224	-0.926314
H	0.558828	2.615560	0.083626
H	1.923173	1.757418	0.845308
C	1.232788	-1.731564	0.000343
H	2.082991	-1.665516	-0.694110
H	1.634265	-1.917098	1.007899
H	0.613949	-2.591118	-0.284578

(CH3)2Ga-P (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.257717	-0.028842	0.000024
P	1.936485	-0.528830	-0.000015
C	-0.276080	1.995293	-0.000020
H	0.710187	2.473828	-0.000077
H	-0.824050	2.327333	-0.894104
H	-0.823965	2.327369	0.894101
C	-1.938563	-1.077475	-0.000018
H	-1.758452	-2.159336	0.001175
H	-2.537574	-0.823882	0.886759
H	-2.536332	-0.825667	-0.888146

H3C-Ga-P-CH3

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
P	1.428074	-0.727553	0.002497
Ga	-0.637327	-0.027034	-0.002633
C	2.447967	0.904180	-0.000080
H	3.485174	0.591640	0.184733
H	-3.092884	-0.511505	-0.562470
H	2.164474	1.606778	0.792510
C	-2.586409	0.281994	0.007052
H	2.414161	1.410796	-0.971978
H	-2.984274	0.291949	1.030773
H	-2.819976	1.244643	-0.471228

Ga-P(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-1.237929	0.017464	-0.827523
C	-1.964301	0.155548	0.910004
H	-2.559001	1.076512	0.976306
H	-2.654171	-0.689188	1.051335
H	-1.229364	0.135267	1.733680
C	1.133904	1.600621	0.028448
H	1.849409	1.702526	-0.798084
H	0.323253	2.321007	-0.100947
H	1.642120	1.779652	0.982714
Ga	0.844486	-0.552411	0.094746

Ga-P(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

Ga	1.372103	-0.000145	0.060219
P	-0.988889	0.000023	-0.710060
C	-1.497410	-1.448699	0.416311
H	-1.042815	-1.442235	1.421141
H	-2.589626	-1.433376	0.548351
H	-1.238313	-2.397383	-0.074847
C	-1.496518	1.449139	0.416207
H	-2.588568	1.433666	0.549442
H	-1.040828	1.443187	1.420527
H	-1.238132	2.397655	-0.075616

(SiH3)2Ga-P

Atomic	Coordinates (Angstroms)		
Number	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
Ga	1.577022	-0.000026	0.069925
P	-0.923074	-0.000102	-0.886957

(SiH3)2Ga-P (TS1)

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

P	-0.009606	2.328630	0.000119
Ga	0.000372	0.115879	-0.000178
Si	-2.134740	-1.091476	0.000068
H	-2.193447	-1.962489	-1.201300
H	-2.201007	-1.947429	1.211825
H	-3.304081	-0.181027	-0.009311
Si	2.142245	-1.078904	0.000092
H	2.210346	-1.941451	-1.206873
H	3.306063	-0.161349	0.000914
H	2.209619	-1.942636	1.206254

H3Si-Ga-P-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	-0.397887	-0.383849	-0.000041
P	1.650018	-1.100973	0.000045
Si	2.032781	1.132249	0.000002
H	2.763947	1.600183	1.205294
H	2.764073	1.600128	-1.205242
H	0.738279	1.916432	-0.000083
Si	-2.690534	0.412002	0.000032
H	-2.945177	1.225842	-1.211684
H	-3.582685	-0.772323	-0.000960
H	-2.945665	1.224161	1.212781

Ga-P(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	-0.853271	-0.027498	1.249667

Si	1.796987	1.200392	-0.046682
H	2.759035	0.924628	1.046894
H	2.524998	1.348031	-1.332655
H	1.091107	2.476170	0.209617
Si	-2.078461	0.580674	-0.547935
H	-3.343378	-0.190845	-0.595923
H	-2.380085	2.031681	-0.489735
H	-1.356711	0.315581	-1.836385
Ga	0.562733	-1.013797	-0.239425

Ga-P(SiH3)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	-1.590606	-0.000688	-0.095850
P	0.631793	0.000245	1.078710
Si	1.155904	-1.678777	-0.330339
H	0.069693	-1.911238	-1.341689
H	2.401664	-1.421037	-1.090860
H	1.278614	-2.930449	0.452517
Si	1.154039	1.679791	-0.330318
H	2.399092	1.422806	-1.092260
H	0.066640	1.912023	-1.340490
H	1.276981	2.931354	0.452675

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(SiMe(SitBu3)2)2Ga-P

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	0.423933	-0.502276	1.395229
P	0.538140	-1.486643	-0.758644
Si	2.208625	1.107930	1.903195
Si	-1.580720	-1.002296	2.738067
Si	4.572657	-0.053942	1.253243
Si	1.643045	3.550761	1.020203
Si	-1.176941	-2.825780	4.680241
Si	-3.702838	-1.396117	1.114723
C	2.543205	1.336226	3.716454
H	3.332903	2.065746	3.895375
H	2.880458	0.398105	4.158062
H	1.671287	1.662134	4.280607
C	-2.073160	0.509454	3.708055
H	-1.214848	0.925682	4.236809
H	-2.827495	0.283195	4.461901
H	-2.478919	1.290580	3.065515
C	5.001792	0.146614	-0.755059
C	6.167468	0.624207	2.473771
C	4.350911	-2.143083	1.682053
C	1.235963	3.609506	-1.024776
C	3.130813	4.949179	1.482464
C	-0.122475	4.126376	2.078029
C	-3.581642	-3.257935	0.173081
C	-3.651237	0.119647	-0.395048
C	-5.556686	-1.165044	2.091481
C	-0.083427	-4.432611	3.898208
C	-2.923362	-3.443033	5.677545
C	-0.029646	-1.788199	6.183484
C	5.714008	-2.863476	1.721387
H	6.320627	-2.555652	2.574502
H	6.298738	-2.704780	0.813729
H	5.571445	-3.946393	1.824714
C	3.483435	-2.825894	0.609075
H	3.976235	-2.868941	-0.363074

H	2.532458	-2.317830	0.482794
H	3.262674	-3.862794	0.889903
C	3.666091	-2.311208	3.045960
H	4.224016	-1.864055	3.868354
H	3.544720	-3.373415	3.285251
H	2.676297	-1.859697	3.036501
C	6.040214	-0.892341	-1.236437
H	6.964585	-0.856441	-0.655187
H	6.312112	-0.707883	-2.283255
H	5.659168	-1.913778	-1.195655
C	3.717125	-0.040183	-1.588569
H	3.901847	0.172626	-2.648015
H	2.920762	0.622988	-1.254007
H	3.333305	-1.061441	-1.532847
C	5.600791	1.535711	-1.044324
H	6.586021	1.664397	-0.589421
H	4.962717	2.329768	-0.672412
H	5.726309	1.694451	-2.121997
C	7.523476	0.140030	1.905229
H	8.345513	0.433757	2.569702
H	7.739061	0.582272	0.929715
H	7.576565	-0.943303	1.797345
C	6.225183	2.156959	2.535220
H	7.031746	2.492399	3.199189
H	5.299963	2.579192	2.929845
H	6.441018	2.586693	1.554831
C	6.034311	0.107422	3.921389
H	6.807545	0.549335	4.562321
H	6.171163	-0.972309	3.990425
H	5.072214	0.364031	4.365884
C	2.531030	3.616677	-1.853671
H	3.097543	4.540810	-1.721760
H	2.312121	3.538135	-2.925602
H	3.169629	2.777627	-1.597194
C	0.404419	2.386037	-1.436996

H	0.880557	1.445261	-1.159093
H	0.244134	2.362709	-2.521453
H	-0.580060	2.421934	-0.974796
C	0.440248	4.878637	-1.411294
H	0.946115	5.797909	-1.111010
H	-0.560078	4.892644	-0.975790
H	0.302830	4.929862	-2.498623
C	-1.339018	3.405743	1.474807
H	-1.166880	2.331052	1.401762
H	-1.595501	3.776715	0.481478
H	-2.226950	3.561016	2.099099
C	-0.355489	5.647257	2.000033
H	0.382573	6.199578	2.586844
H	-1.336182	5.907450	2.417175
H	-0.334540	6.024749	0.976297
C	-0.015135	3.731068	3.561905
H	0.900428	4.089356	4.034630
H	-0.056223	2.650000	3.676286
H	-0.857937	4.136098	4.135011
C	4.468780	4.464413	0.913535
H	5.317855	4.973396	1.383193
H	4.559079	4.638591	-0.161176
H	4.566727	3.398645	1.076937
C	3.263179	5.118451	3.008856
H	4.110935	5.768807	3.256537
H	3.430731	4.167936	3.515869
H	2.378148	5.587789	3.444482
C	2.854412	6.333829	0.857217
H	3.633705	7.047889	1.151684
H	1.902237	6.761763	1.167961
H	2.864439	6.298753	-0.235086
C	1.154190	-4.746295	4.760404
H	1.833550	-3.895425	4.821185
H	1.730704	-5.574586	4.329736
H	0.870206	-5.055015	5.771070

C	-0.912336	-5.730780	3.848718
H	-0.325654	-6.549984	3.414218
H	-1.806199	-5.632099	3.232983
H	-1.205187	-6.056036	4.851483
C	0.398447	-4.111998	2.471483
H	1.037350	-3.230700	2.463698
H	-0.429642	-3.937932	1.782723
H	0.987500	-4.939947	2.059193
C	-2.578712	-4.115873	7.025185
H	-2.186703	-3.404093	7.754493
H	-1.848119	-4.921981	6.902244
H	-3.476622	-4.554574	7.477829
C	-3.709234	-4.480539	4.857756
H	-3.300821	-5.488581	4.957724
H	-3.718057	-4.225552	3.805762
H	-4.749476	-4.552665	5.197058
C	-3.833706	-2.229982	5.953433
H	-3.434522	-1.561381	6.715700
H	-4.818546	-2.548688	6.314757
H	-3.984982	-1.639638	5.054432
C	0.615955	-2.742907	7.212110
H	1.551846	-3.172320	6.847395
H	-0.033734	-3.564938	7.508137
H	0.886499	-2.197279	8.124837
C	1.082385	-1.009591	5.484183
H	1.698502	-0.464095	6.208598
H	0.665903	-0.280871	4.792180
H	1.743678	-1.674042	4.932133
C	-0.917246	-0.784387	6.949081
H	-0.300082	-0.094279	7.537862
H	-1.569941	-1.287311	7.665802
H	-1.532903	-0.175514	6.288015
C	-3.397813	-4.368914	1.214388
H	-2.591129	-4.122247	1.899451
H	-3.150522	-5.325900	0.739739

H	-4.308922	-4.538160	1.791467
C	-4.861350	-3.588509	-0.624758
H	-4.755395	-4.553140	-1.136518
H	-5.087712	-2.848897	-1.392043
H	-5.736661	-3.674423	0.024031
C	-2.374706	-3.301428	-0.782001
H	-1.450748	-3.035222	-0.265631
H	-2.508199	-2.637373	-1.638467
H	-2.236205	-4.308653	-1.193526
C	-5.911497	-2.435052	2.879401
H	-5.118170	-2.693452	3.568603
H	-6.091624	-3.291631	2.225844
H	-6.823056	-2.290953	3.471633
C	-6.703841	-0.935746	1.080169
H	-6.632712	0.032558	0.583101
H	-7.674724	-0.942859	1.591551
H	-6.744781	-1.711559	0.312847
C	-5.530542	0.034470	3.059839
H	-4.839701	-0.124291	3.883992
H	-6.519406	0.190823	3.508031
H	-5.251898	0.968721	2.570944
C	-4.566619	-0.232010	-1.585696
H	-4.170978	-1.073149	-2.161590
H	-4.631375	0.613632	-2.281674
H	-5.585862	-0.474762	-1.287662
C	-4.082132	1.475496	0.197856
H	-3.549992	1.698596	1.123140
H	-5.152529	1.516989	0.404994
H	-3.874345	2.291423	-0.504999
C	-2.232055	0.268831	-0.946982
H	-1.559524	0.629626	-0.174203
H	-2.212793	0.997637	-1.765818
H	-1.837081	-0.661129	-1.350556

SiMe(SitBu3)2-Ga-P-SiMe(SitBu3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.835368	0.157973	-0.618867
P	-1.093800	-0.188750	0.305199
Si	-3.094770	0.620642	-0.354496
Si	3.042086	0.021482	0.401939
C	2.513667	0.742124	2.118312
H	1.476023	0.479165	2.355628
H	2.579188	1.834795	2.117366
H	3.156594	0.368286	2.926994
C	-3.482927	2.583415	0.975838
Si	-2.728687	1.197012	-2.619879
H	-3.987204	1.441550	-3.380555
H	-2.015477	0.076359	-3.282792
H	-1.869869	2.390588	-2.815009
Si	-4.400003	-1.723175	-0.633919
Si	3.383179	-2.437021	0.753388
Si	4.366433	1.835610	-0.687064
C	-6.236903	-1.503396	-1.344783
C	-3.363277	-2.812899	-1.965033
C	-4.448451	-2.704719	1.092255
C	-7.207101	-0.990265	-0.257224
H	-8.192267	-0.784860	-0.717655
H	-6.863112	-0.062113	0.210052
H	-7.367778	-1.735600	0.534091
C	-6.827797	-2.840948	-1.863302
H	-7.868319	-2.660584	-2.194034
H	-6.862450	-3.621877	-1.092358
H	-6.280667	-3.239436	-2.726638
C	-6.291145	-0.503204	-2.524143
H	-7.340683	-0.398613	-2.859129
H	-5.704710	-0.835805	-3.388475

H	-5.936771	0.497034	-2.248589
C	-3.683244	-2.426726	-3.430146
H	-4.698462	-2.713090	-3.735314
H	-2.981810	-2.964448	-4.095770
H	-3.553700	-1.356246	-3.628888
C	-3.680002	-4.324736	-1.829121
H	-4.748057	-4.561780	-1.918235
H	-3.307188	-4.740393	-0.883513
H	-3.154411	-4.858476	-2.643374
C	-1.833801	-2.691461	-1.812625
H	-1.488138	-2.892592	-0.792940
H	-1.472002	-1.694931	-2.084312
H	-1.348912	-3.423280	-2.487325
C	-5.328639	-3.981971	1.041071
H	-6.396917	-3.735010	0.953439
H	-5.203667	-4.526144	1.996605
H	-5.068955	-4.676954	0.235750
C	-5.013079	-1.874779	2.265524
H	-6.035937	-1.517534	2.090948
H	-4.377581	-1.017991	2.498351
H	-5.041048	-2.513527	3.169083
C	-3.014946	-3.113937	1.503816
H	-2.569698	-3.850562	0.822384
H	-3.039862	-3.570599	2.511492
H	-2.335344	-2.249604	1.544417
C	-5.099538	2.664598	1.093989
C	-5.682498	4.004509	1.636862
H	-6.768981	3.869013	1.774111
H	-5.553521	4.836294	0.933814
H	-5.268002	4.301321	2.605621
C	-5.834819	2.429811	-0.256434
H	-6.891226	2.194524	-0.055694
H	-5.413221	1.576218	-0.801770
H	-5.830064	3.292267	-0.925571
C	-5.665261	1.559349	2.010479

H	-6.764226	1.558339	1.942524
H	-5.416972	1.698277	3.066758
H	-5.313785	0.575313	1.692035
C	-2.835680	3.843195	0.151676
C	-2.741348	5.163999	0.978578
H	-3.701982	5.505930	1.377765
H	-2.367249	5.953188	0.303238
H	-2.029922	5.094791	1.808264
C	-1.380391	3.599534	-0.362730
H	-1.157740	2.550714	-0.578828
H	-0.628612	3.947855	0.349986
H	-1.219858	4.167251	-1.292009
C	-3.654681	4.257008	-1.103225
H	-4.590238	4.764498	-0.839801
H	-3.892066	3.421804	-1.770987
H	-3.060050	4.978857	-1.684131
C	-2.720356	2.336418	2.417538
C	-1.183222	2.584384	2.377873
H	-0.690855	2.026573	1.577101
H	-0.754786	2.223380	3.326751
H	-0.921062	3.645337	2.301540
C	-3.225494	3.249731	3.576313
H	-4.249264	3.017431	3.894374
H	-3.167441	4.318436	3.344753
H	-2.572940	3.068432	4.447335
C	-2.854557	0.896834	2.983899
H	-3.847166	0.678650	3.381651
H	-2.146302	0.774551	3.818806
H	-2.595056	0.125237	2.249125
C	3.118985	3.375571	-0.970425
C	2.068292	3.096274	-2.069965
H	1.522733	2.144745	-1.928657
H	2.510897	3.080955	-3.075444
H	1.306700	3.895456	-2.057838
C	2.338527	3.710031	0.320989

H	1.608177	2.929890	0.576418
H	1.770706	4.646436	0.172936
H	3.001164	3.861355	1.186616
C	3.833965	4.689177	-1.416997
H	4.254557	5.238325	-0.568174
H	3.086904	5.355613	-1.886045
H	4.636265	4.533011	-2.148766
C	4.989114	1.208453	-2.442151
C	3.834476	0.495611	-3.191152
H	3.468849	-0.376822	-2.631821
H	4.206128	0.125495	-4.164367
H	2.976880	1.145582	-3.397649
C	5.505511	2.362969	-3.332918
H	5.937135	1.944814	-4.261528
H	6.298593	2.945821	-2.836627
H	4.705274	3.055342	-3.629580
C	6.133754	0.170809	-2.335081
H	5.962043	-0.563539	-1.540783
H	7.107220	0.640902	-2.154653
H	6.212803	-0.382543	-3.288347
C	5.837340	2.383541	0.550060
C	5.523320	1.939945	1.996793
H	5.378278	0.855762	2.082743
H	4.625995	2.433526	2.394460
H	6.369215	2.213136	2.654582
C	6.068989	3.910232	0.614478
H	6.332711	4.342275	-0.360897
H	6.913798	4.105820	1.300721
H	5.199741	4.447966	1.015202
C	7.206605	1.777149	0.164686
H	7.202124	0.682847	0.110793
H	7.946962	2.065614	0.933595
H	7.569434	2.169910	-0.796979
C	3.314466	-3.412464	-0.953967
C	5.142816	-2.617834	1.612605

C	1.984865	-3.166381	1.957984
C	4.573076	-3.158988	-1.812366
H	4.457658	-3.670866	-2.786090
H	5.486743	-3.553606	-1.346276
H	4.725766	-2.094408	-2.021938
C	3.221733	-4.946677	-0.744075
H	2.279262	-5.254813	-0.274127
H	4.049374	-5.342114	-0.139278
H	3.270063	-5.444075	-1.730922
C	2.098281	-2.986852	-1.810779
H	1.138274	-3.110244	-1.297506
H	2.064036	-3.603506	-2.728447
H	2.175276	-1.937695	-2.135495
C	6.187632	-1.753276	0.879559
H	6.415569	-2.134489	-0.123630
H	7.133974	-1.740154	1.451246
H	5.849231	-0.715353	0.776329
C	5.690529	-4.066555	1.630581
H	5.025969	-4.774026	2.142439
H	6.658548	-4.076936	2.166456
H	5.880710	-4.448230	0.617143
C	5.091770	-2.110555	3.074566
H	4.457344	-2.733645	3.718912
H	4.731089	-1.074077	3.146243
H	6.112130	-2.130168	3.500570
C	1.601562	-2.219331	3.121749
H	0.996604	-2.786931	3.852786
H	0.977491	-1.388118	2.771003
H	2.464589	-1.807104	3.659809
C	0.659353	-3.470285	1.222445
H	-0.085435	-3.805608	1.966288
H	0.748138	-4.271852	0.477538
H	0.237089	-2.581055	0.734921
C	2.457865	-4.497694	2.603442
H	1.608886	-4.930959	3.164705

H	3.274555	-4.350286	3.323378
H	2.778812	-5.249641	1.870981

Ga-P(SiMe(SitBu3)2)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.628899	-0.680427	1.675464
Ga	0.653200	-1.633203	-0.539922
Si	2.148284	1.178013	1.795434
Si	-1.339474	-1.327820	2.892508
Si	4.664695	0.278628	1.169297
Si	1.237227	3.553303	0.947482
Si	-0.679997	-3.091886	4.758078
Si	-3.664499	-1.672398	1.363444
C	2.500869	1.463216	3.649742
H	3.195729	2.306771	3.772641
H	2.969288	0.570212	4.080577
H	1.599997	1.682780	4.234074
C	-1.811712	0.197798	3.942105
H	-0.919160	0.636533	4.408830
H	-2.503853	-0.079592	4.749223
H	-2.291715	0.976651	3.336558
C	4.997872	0.473590	-0.770180
C	6.069094	1.240602	2.254711
C	4.801284	-1.637749	1.664181
C	0.771893	3.521505	-0.977637
C	2.543532	5.010406	1.260756
C	-0.375590	3.935070	2.029385
C	-3.674446	-3.428560	0.442422
C	-3.766324	-0.235312	-0.001339
C	-5.295292	-1.509993	2.515525
C	0.378956	-4.560569	3.957207

C	-2.244955	-3.831636	5.731072
C	0.407439	-2.104846	6.103001
C	6.152266	-0.426319	-1.279082
H	7.102426	-0.221746	-0.766514
H	6.313645	-0.228268	-2.355996
H	5.931432	-1.496728	-1.177706
C	5.365102	1.921714	-1.160982
H	6.307654	2.254762	-0.704969
H	4.586128	2.637930	-0.886434
H	5.494701	1.983521	-2.258193
C	3.723831	0.092440	-1.560693
H	3.464724	-0.970247	-1.449370
H	3.881606	0.274948	-2.640507
H	2.853584	0.690004	-1.251378
C	6.259985	-2.163480	1.694712
H	6.848984	-1.722790	2.510273
H	6.802822	-2.001462	0.754674
H	6.237112	-3.255308	1.874145
C	4.013727	-2.546333	0.694391
H	4.076141	-3.594179	1.042711
H	4.399900	-2.522261	-0.333087
H	2.946130	-2.281298	0.680110
C	4.196777	-1.873171	3.061957
H	4.695469	-1.305327	3.854322
H	4.288107	-2.941902	3.322445
H	3.131973	-1.617175	3.068024
C	7.485762	0.993477	1.671458
H	8.227257	1.483108	2.332010
H	7.608040	1.437200	0.673578
H	7.756804	-0.066476	1.609566
C	5.895957	2.769553	2.296143
H	6.667825	3.202798	2.960550
H	4.920853	3.073391	2.695275
H	6.029929	3.229784	1.311433
C	6.095651	0.780709	3.733296

H	6.822266	1.407122	4.284943
H	6.420928	-0.260208	3.851496
H	5.124623	0.899936	4.232060
C	3.893161	4.653350	0.609361
H	4.707594	5.249624	1.058899
H	3.899371	4.859979	-0.467351
H	4.138993	3.600236	0.746536
C	2.133926	6.378574	0.659982
H	2.923976	7.116565	0.899960
H	1.190719	6.774371	1.053763
H	2.059924	6.337615	-0.435337
C	2.785159	5.224929	2.773937
H	3.609241	5.949629	2.913659
H	3.072981	4.301121	3.294930
H	1.902050	5.637099	3.281998
C	2.005550	3.641208	-1.900056
H	2.486685	4.626323	-1.840908
H	1.682920	3.503457	-2.949598
H	2.760600	2.873661	-1.692627
C	-0.192028	4.670045	-1.373825
H	0.216160	5.664802	-1.149354
H	-1.172387	4.587696	-0.886012
H	-0.369442	4.629084	-2.465627
C	0.077239	2.195756	-1.336346
H	0.709585	1.321399	-1.119673
H	-0.162058	2.175196	-2.416750
H	-0.858601	2.069211	-0.789746
C	-0.805440	5.422305	1.979219
H	-0.108846	6.072737	2.526891
H	-1.791288	5.524584	2.472311
H	-0.909089	5.813175	0.958538
C	-1.565090	3.086915	1.542901
H	-1.316351	2.017743	1.507566
H	-1.926477	3.387521	0.551231
H	-2.412210	3.213080	2.242896

C	-0.175057	3.577385	3.520156
H	0.715828	4.038208	3.965258
H	-0.105503	2.493018	3.657829
H	-1.053456	3.923209	4.097778
C	-2.403472	-0.022446	-0.682711
H	-1.628061	0.272166	0.033861
H	-2.493374	0.775335	-1.441793
H	-2.049080	-0.918498	-1.212753
C	-4.160867	1.115982	0.638562
H	-3.556827	1.353784	1.521358
H	-5.218295	1.150187	0.931711
H	-4.004442	1.929189	-0.094117
C	-4.780364	-0.520922	-1.139122
H	-4.439182	-1.328390	-1.802714
H	-4.871416	0.387655	-1.765012
H	-5.786701	-0.771355	-0.781969
C	-2.551261	-3.491460	-0.616441
H	-1.558286	-3.292947	-0.176034
H	-2.703558	-2.789660	-1.447070
H	-2.507548	-4.507924	-1.051082
C	-5.012746	-3.767752	-0.260900
H	-4.915405	-4.755775	-0.750499
H	-5.299155	-3.047029	-1.035099
H	-5.840773	-3.848363	0.457278
C	-3.407329	-4.570947	1.436788
H	-2.555608	-4.344110	2.079971
H	-3.170502	-5.502721	0.889622
H	-4.276893	-4.781112	2.070896
C	-6.568856	-1.228996	1.673706
H	-6.738870	-1.977713	0.888736
H	-6.562488	-0.236601	1.206002
H	-7.445206	-1.260752	2.349178
C	-5.584250	-2.810702	3.296791
H	-4.713678	-3.176004	3.846062
H	-5.937252	-3.616722	2.638516

H	-6.385067	-2.623486	4.036999
C	-5.185095	-0.363964	3.550100
H	-4.424971	-0.563958	4.313688
H	-6.152463	-0.261498	4.077641
H	-4.956184	0.608223	3.095564
C	1.398603	-1.153182	5.412653
H	2.111187	-1.678729	4.771408
H	1.982315	-0.605239	6.177523
H	0.885201	-0.408926	4.795346
C	1.239381	-3.049389	7.008400
H	1.755665	-2.442526	7.777360
H	2.018860	-3.582793	6.446694
H	0.631643	-3.793856	7.538577
C	-0.457657	-1.221698	7.034798
H	0.212767	-0.594808	7.652743
H	-1.072756	-1.807030	7.730890
H	-1.117913	-0.540546	6.481937
C	1.765921	-4.041951	3.538808
H	2.369516	-3.716006	4.393865
H	1.688196	-3.207955	2.828552
H	2.327608	-4.853759	3.038188
C	0.588633	-5.753922	4.921922
H	1.063261	-5.461719	5.867939
H	1.255360	-6.493157	4.437385
H	-0.350005	-6.275373	5.156491
C	-0.258719	-5.126839	2.670900
H	0.427285	-5.873260	2.226930
H	-0.420586	-4.346252	1.912023
H	-1.211143	-5.638083	2.856658
C	-2.956695	-4.925204	4.908338
H	-2.329233	-5.816628	4.771754
H	-3.257179	-4.572548	3.920354
H	-3.872469	-5.248955	5.438465
C	-1.864384	-4.491547	7.081424
H	-1.120408	-5.291341	6.969535

H	-2.773001	-4.950054	7.517308
H	-1.487064	-3.770727	7.817576
C	-3.278944	-2.724212	6.043203
H	-2.921263	-2.020289	6.804518
H	-4.211207	-3.178864	6.428075
H	-3.546632	-2.144220	5.153154

(SiiPrDis2)2Ga-P

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	2.889741	0.986057	6.636651
Si	2.592477	0.939811	4.125930
C	2.887671	-0.872866	3.593744
H	2.202691	-1.412728	4.271856
C	0.766789	1.611729	4.053384
H	0.795597	2.277709	4.940053
C	4.052684	2.047400	3.483965
H	4.764170	1.921954	4.317644
C	3.796017	3.555105	3.354822
H	3.343537	3.790944	2.380855
H	4.748361	4.110375	3.413062
H	3.136353	3.939815	4.133489
C	4.790817	1.576670	2.219351
H	5.708229	2.178974	2.089050
H	4.180005	1.721964	1.316957
H	5.088316	0.523259	2.258433
Si	-0.666233	0.431850	4.621493
Si	0.260243	2.914605	2.729012
Si	2.315306	-1.506267	1.894777
Si	4.573530	-1.677569	4.088112
C	-1.524136	1.271305	6.079284
H	-1.753463	2.329466	5.873844

H	-0.913764	1.223616	6.992231
H	-2.477936	0.756314	6.286742
C	-0.172566	-1.279936	5.243215
H	0.131901	-1.974524	4.447974
H	-1.062509	-1.708166	5.737299
H	0.615972	-1.240812	6.016634
C	-2.053971	0.086984	3.377165
H	-2.871001	0.813660	3.493835
H	-2.465009	-0.911078	3.605344
H	-1.748061	0.083840	2.325801
C	-1.595980	3.027085	2.372645
H	-2.200222	3.096685	3.290826
H	-1.982964	2.200145	1.764005
H	-1.755527	3.960700	1.805621
C	1.090977	2.638539	1.054165
H	0.490178	1.969770	0.417764
H	2.097030	2.205475	1.135634
H	1.181433	3.601821	0.524441
C	0.627429	4.667624	3.368258
H	1.608981	5.054091	3.065202
H	0.565578	4.727474	4.466284
H	-0.134104	5.354348	2.962648
C	5.786530	-0.574163	5.020357
H	6.602763	-1.220562	5.384049
H	5.360212	-0.070896	5.898110
H	6.244584	0.182823	4.368330
C	4.189142	-3.173796	5.166143
H	5.126415	-3.672084	5.468811
H	3.569817	-3.911747	4.632131
H	3.658694	-2.878821	6.087451
C	5.644335	-2.300245	2.651725
H	5.138942	-2.990885	1.963592
H	6.491865	-2.847502	3.101348
H	6.076279	-1.481616	2.055262
C	2.264133	-3.399866	1.936381

H	3.240410	-3.886932	2.064823
H	1.828032	-3.764240	0.989828
H	1.608314	-3.744002	2.753892
C	0.539197	-1.053448	1.469626
H	-0.176938	-1.557942	2.132845
H	0.332625	-1.400003	0.441771
H	0.343380	0.024693	1.501383
C	3.342328	-0.924104	0.427145
H	4.426427	-1.008417	0.571768
H	3.113326	0.122536	0.175027
H	3.072236	-1.537128	-0.449689
P	2.380919	-0.922354	7.569115
Si	3.918943	2.723960	8.090166
C	5.491602	1.899608	8.822658
H	5.691454	2.587070	9.662910
C	2.798239	3.546078	9.442048
H	2.697745	4.540926	8.963141
C	4.293543	4.215115	6.910957
H	4.801991	3.782910	6.036473
C	5.207034	5.296543	7.517669
H	5.478222	6.045212	6.751335
H	6.138938	4.891114	7.931212
H	4.689009	5.838846	8.325451
C	3.013576	4.903942	6.402406
H	3.250976	5.612449	5.590872
H	2.524345	5.489686	7.196649
H	2.270612	4.191314	6.020714
Si	3.516716	4.132560	11.112038
Si	0.938080	3.096018	9.509051
Si	5.297132	0.250023	9.786057
Si	7.186742	2.006056	7.925832
C	2.718558	5.812398	11.503177
H	2.555408	6.416370	10.594902
H	3.384584	6.387536	12.168199
H	1.750737	5.710047	12.013660

C	5.373539	4.511718	11.138704
H	5.729884	4.988274	10.215328
H	6.001694	3.630777	11.335521
H	5.554603	5.224161	11.962424
C	3.193266	2.980123	12.571727
H	3.944136	2.178510	12.636927
H	2.198408	2.510885	12.538610
H	3.253576	3.565627	13.505286
C	-0.019332	4.039919	10.839917
H	0.021202	5.129672	10.694281
H	0.311640	3.811606	11.864021
H	-1.076928	3.733241	10.759878
C	0.506807	1.295439	9.806745
H	0.820118	0.957339	10.805806
H	0.939707	0.611183	9.061949
H	-0.589804	1.185241	9.745780
C	0.140558	3.691429	7.903413
H	0.512463	3.173852	7.008681
H	0.310666	4.770825	7.763568
H	-0.947642	3.527852	7.949157
C	7.188612	2.699467	6.167609
H	8.172790	2.482696	5.718651
H	7.046570	3.788167	6.142788
H	6.428923	2.236894	5.523456
C	8.280156	3.130202	8.983832
H	9.285924	3.213213	8.538241
H	8.395775	2.715388	9.998614
H	7.871196	4.146931	9.086796
C	8.157044	0.389261	7.796907
H	8.389421	-0.047786	8.779083
H	9.118021	0.626324	7.307565
H	7.657455	-0.375917	7.190109
C	6.522188	0.322804	11.229457
H	7.570167	0.389035	10.898105
H	6.424134	-0.592967	11.837995

H	6.323260	1.182858	11.890317
C	3.605368	0.020742	10.588856
H	2.880593	-0.482697	9.922649
H	3.724243	-0.639524	11.466329
H	3.145104	0.953115	10.928253
C	5.631719	-1.349167	8.839187
H	6.685848	-1.654769	8.897526
H	5.335354	-1.292340	7.785736
H	5.021808	-2.149987	9.289606

(SiiPrDis2)-Ga-P-(SiiPrDis2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
P	0.904785	0.854018	-0.141278
Si	2.953470	-0.006268	-0.578938
C	4.130079	1.260836	0.254040
H	3.713247	1.305281	1.281615
C	2.819705	-1.790538	0.153733
H	1.791196	-1.977021	-0.218026
C	3.108269	0.126591	-2.495256
H	3.085685	1.223295	-2.640024
C	1.873744	-0.416726	-3.247927
H	2.032991	-0.357520	-4.339594
H	0.981983	0.172797	-2.995123
H	1.651394	-1.465725	-3.004541
C	4.426599	-0.358828	-3.130919
H	4.352582	-0.327410	-4.232963
H	4.686431	-1.390272	-2.853690
H	5.268233	0.281620	-2.841353
Si	2.462107	-1.937860	2.044251
Si	3.662576	-3.331319	-0.583489
Si	5.962677	0.855765	0.589522

Si	3.930292	3.074880	-0.354049
C	0.930843	-3.055371	2.215287
H	0.327906	-2.752340	3.088149
H	1.212447	-4.111001	2.359968
H	0.274414	-3.011061	1.330223
C	2.057132	-0.338094	2.963482
H	2.939948	0.308069	3.095633
H	1.694572	-0.611403	3.971803
H	1.274966	0.247725	2.460759
C	3.841897	-2.741889	3.071817
H	3.379774	-3.380792	3.844432
H	4.439789	-1.980494	3.593610
H	4.536377	-3.370365	2.496858
C	3.152959	-4.903322	0.346371
H	2.060339	-5.045267	0.316649
H	3.468084	-4.933520	1.398847
H	3.608740	-5.770668	-0.163268
C	5.545775	-3.286671	-0.616876
H	5.977439	-3.399170	0.390189
H	5.944516	-2.355742	-1.043815
H	5.919287	-4.124034	-1.231506
C	3.014750	-3.682114	-2.326762
H	3.319064	-2.954442	-3.089577
H	1.911413	-3.725544	-2.326840
H	3.377723	-4.674615	-2.647260
C	2.230210	3.586910	-0.991141
H	2.300822	4.644648	-1.306273
H	1.473609	3.531235	-0.194642
H	1.850358	3.005406	-1.843325
C	4.211727	4.260874	1.099078
H	3.689992	5.211870	0.894924
H	5.269527	4.494833	1.285372
H	3.789721	3.852301	2.033424
C	5.132199	3.472348	-1.757249
H	6.186406	3.479667	-1.440070

H	4.897249	4.473954	-2.157951
H	5.033964	2.755657	-2.588770
C	6.853219	2.277992	1.466812
H	7.017640	3.154769	0.822500
H	7.845148	1.913751	1.788000
H	6.315907	2.613622	2.367984
C	6.115674	-0.584563	1.786634
H	5.722170	-0.309679	2.778448
H	7.179923	-0.849746	1.914512
H	5.584246	-1.481159	1.450028
C	7.009239	0.470826	-0.930904
H	6.981319	1.278566	-1.677675
H	6.718501	-0.462519	-1.431148
H	8.058246	0.355915	-0.606023
Ga	-0.845092	-0.378452	-0.291779
Si	-3.163202	0.183185	-0.689285
C	-3.468235	1.712411	0.447021
H	-4.555073	1.695100	0.650416
C	-4.407476	-1.279400	-0.563688
H	-4.652666	-1.426834	-1.637392
C	-3.078321	0.613134	-2.576833
H	-2.561328	1.585506	-2.641123
C	-4.460721	0.747636	-3.248461
H	-4.352409	1.161425	-4.266878
H	-5.146593	1.397800	-2.694435
H	-4.944765	-0.237894	-3.352780
C	-2.241373	-0.403329	-3.381753
H	-2.185601	-0.102413	-4.442754
H	-2.692786	-1.407493	-3.351273
H	-1.205145	-0.488278	-3.014586
Si	-6.118791	-0.884866	0.160924
Si	-3.674741	-2.989965	-0.138910
Si	-2.745745	1.702774	2.237387
Si	-3.202712	3.441302	-0.342990
C	-7.403833	-2.174396	-0.359263

H	-7.256964	-2.497516	-1.403529
H	-8.409062	-1.723600	-0.292515
H	-7.400198	-3.074541	0.271728
C	-6.835196	0.725191	-0.529532
H	-7.011041	0.630730	-1.613484
H	-6.219255	1.620097	-0.370362
H	-7.814740	0.906821	-0.053840
C	-6.085326	-0.794983	2.041607
H	-5.468245	0.036592	2.412091
H	-5.693920	-1.724864	2.486054
H	-7.108635	-0.647900	2.428123
C	-4.961756	-4.371704	-0.220409
H	-5.555661	-4.358509	-1.147596
H	-5.660746	-4.340726	0.629557
H	-4.433256	-5.340075	-0.175122
C	-2.889933	-3.150841	1.563339
H	-3.602466	-2.935381	2.374678
H	-2.011690	-2.510002	1.714419
H	-2.553549	-4.194856	1.687785
C	-2.371717	-3.493711	-1.419502
H	-1.503198	-2.817271	-1.494039
H	-2.811531	-3.569212	-2.428291
H	-1.980329	-4.491336	-1.154272
C	-4.359056	3.800136	-1.796334
H	-4.388909	4.895236	-1.934256
H	-5.394123	3.466012	-1.620797
H	-4.014100	3.363220	-2.743440
C	-3.625204	4.810826	0.894634
H	-3.581706	5.777024	0.361454
H	-2.927451	4.873152	1.742208
H	-4.644691	4.704333	1.300385
C	-1.436497	3.717126	-0.923937
H	-1.399196	4.589395	-1.599635
H	-1.009187	2.854657	-1.456777
H	-0.764937	3.926388	-0.079390

C	-4.015273	2.493307	3.399148
H	-3.984818	3.592138	3.358608
H	-3.791913	2.195051	4.438189
H	-5.049294	2.180329	3.179348
C	-2.426727	-0.025451	2.921631
H	-1.516707	-0.488631	2.507874
H	-2.264910	0.064611	4.010327
H	-3.266177	-0.714505	2.765260
C	-1.114414	2.625577	2.449691
H	-1.211067	3.717435	2.357514
H	-0.349293	2.282396	1.736384
H	-0.730693	2.409136	3.462593

Ga-P(SiiPrDis2)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

P	2.561515	1.662443	6.622817
Si	2.317598	1.308722	4.248909
C	3.694682	0.191466	3.450852
H	3.937194	-0.502898	4.279528
C	0.521612	0.538874	4.291377
H	0.056852	1.204461	5.057443
C	2.374621	3.052076	3.453288
H	3.360284	3.395556	3.792519
C	1.349671	4.087178	3.978643
H	0.651376	4.390277	3.190138
H	1.857051	4.996264	4.331644
H	0.744499	3.716967	4.820770
C	2.427076	3.057773	1.911973
H	2.534891	4.090860	1.535539
H	1.512682	2.640156	1.464025
H	3.280033	2.480993	1.530465

Si	0.277168	-1.177893	5.163925
Si	-0.796200	0.831067	2.912427
Si	3.394296	-1.063703	2.019480
Si	5.439131	0.943415	3.058053
C	-0.835710	-0.910111	6.673072
H	-1.229308	-1.884327	7.014774
H	-1.701520	-0.267043	6.445478
H	-0.297114	-0.463084	7.525240
C	1.888033	-1.910970	5.787274
H	2.508418	-2.343754	4.991358
H	1.665928	-2.711169	6.513617
H	2.476314	-1.142260	6.301666
C	-0.611802	-2.549482	4.178743
H	-1.610506	-2.725655	4.610076
H	-0.039218	-3.486356	4.277366
H	-0.746605	-2.370941	3.105243
C	-2.460391	0.068695	3.411501
H	-2.773269	0.383546	4.420759
H	-2.499668	-1.027122	3.372126
H	-3.219165	0.449164	2.705087
C	-0.365422	0.186449	1.194365
H	-0.378228	-0.910456	1.115453
H	0.616179	0.536239	0.847838
H	-1.121222	0.573532	0.488220
C	-1.270431	2.645874	2.681668
H	-0.568441	3.212866	2.056211
H	-1.389908	3.180047	3.636746
H	-2.248558	2.663486	2.169635
C	5.710495	2.690306	3.677355
H	6.782570	2.843745	3.888312
H	5.164027	2.864884	4.603732
H	5.399103	3.451964	2.946331
C	6.768809	-0.116425	3.889901
H	6.927465	0.206531	4.930102
H	7.725843	0.010276	3.354591

H	6.534743	-1.189957	3.907967
C	5.900057	1.093334	1.225394
H	6.035393	0.143035	0.691973
H	6.868721	1.624897	1.203932
H	5.185552	1.704545	0.653999
C	4.886629	-2.232862	1.902777
H	5.846879	-1.758873	1.660065
H	4.671508	-2.972526	1.111119
H	5.017662	-2.794179	2.843677
C	1.991787	-2.289099	2.242545
H	2.128427	-2.954561	3.104844
H	1.969462	-2.924709	1.339042
H	1.014626	-1.809421	2.327895
C	3.122527	-0.275938	0.314807
H	4.034936	-0.327345	-0.297495
H	2.815378	0.777334	0.354173
H	2.335217	-0.830774	-0.220942
Ga	0.327287	2.324858	7.276456
Si	4.117599	2.664183	8.111364
C	4.594086	1.170754	9.215871
H	5.167120	1.617739	10.051057
C	3.727000	4.250197	9.228455
H	4.468614	4.924542	8.749157
C	5.545480	3.386352	7.054740
H	5.856012	2.573441	6.380175
C	6.793268	3.860791	7.826938
H	7.624392	4.048867	7.123778
H	7.143931	3.141320	8.573631
H	6.595395	4.810885	8.348064
C	5.034636	4.573333	6.207874
H	5.797162	4.888019	5.476980
H	4.826717	5.444700	6.849170
H	4.107385	4.342922	5.666361
Si	4.425842	4.334800	11.018187
Si	2.200215	5.375384	8.959366

Si	3.158005	0.295621	10.135079
Si	5.813297	-0.108350	8.489789
C	4.494502	6.125604	11.636009
H	4.939139	6.825844	10.912111
H	5.126711	6.140387	12.541579
H	3.506781	6.514658	11.923161
C	6.238258	3.803021	11.180268
H	6.904601	4.493064	10.639701
H	6.476651	2.782827	10.849191
H	6.502674	3.869715	12.250807
C	3.463814	3.423388	12.357312
H	3.588273	2.333783	12.322646
H	2.386340	3.642476	12.331478
H	3.851143	3.767908	13.332875
C	2.574364	7.200923	9.314980
H	3.576604	7.494176	8.960284
H	2.491200	7.489358	10.371458
H	1.841349	7.802339	8.748311
C	0.701865	4.928425	10.016238
H	0.943610	4.974258	11.091130
H	0.281266	3.931900	9.810807
H	-0.098674	5.663975	9.823247
C	1.723902	5.435785	7.138180
H	1.834965	4.472862	6.626305
H	2.372576	6.155247	6.611526
H	0.682288	5.778201	7.017311
C	7.528466	0.595261	8.116339
H	8.193591	-0.254714	7.882447
H	7.967577	1.122924	8.978967
H	7.550515	1.275690	7.253453
C	6.169244	-1.508387	9.714633
H	6.969696	-2.139662	9.289808
H	5.299710	-2.158412	9.894201
H	6.523608	-1.137153	10.690052
C	5.177834	-0.909497	6.916779

H	4.357884	-1.609169	7.124199
H	5.988478	-1.476041	6.430688
H	4.797129	-0.165188	6.204024
C	3.786504	-0.326506	11.816531
H	4.249616	-1.321558	11.733066
H	2.939486	-0.416131	12.518828
H	4.531893	0.341292	12.278253
C	1.678131	1.438173	10.454004
H	0.774118	1.041757	9.959067
H	1.453773	1.507499	11.530620
H	1.841812	2.461994	10.097951
C	2.422292	-1.191634	9.249318
H	3.142264	-1.991735	9.024500
H	1.954330	-0.875314	8.308790
H	1.635124	-1.621456	9.894350

(Ar*)2Ga-P

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	-0.437832	-0.728589	8.512315
P	-1.920509	0.998079	8.922244
H	-0.198419	-0.924667	3.337157
C	0.270103	-0.501364	4.227804
C	1.449293	0.542639	6.539113
C	-0.067467	-1.056357	5.485174
C	1.176507	0.553520	4.103800
C	1.788027	1.039402	5.261318
C	0.462698	-0.491805	6.694003
H	1.419977	0.970076	3.122505
H	2.545673	1.821961	5.192184
C	-0.967724	-2.264505	5.331612
C	-2.665835	-4.399016	4.475308

C	-2.380946	-2.111228	5.331422
C	-0.406439	-3.490674	4.858845
C	-1.268808	-4.521268	4.437830
C	-3.199966	-3.185974	4.934926
H	-0.839908	-5.456410	4.068470
H	-4.283292	-3.047776	4.934981
C	2.267922	1.172417	7.642083
C	3.960405	2.576659	9.471303
C	1.860120	2.420633	8.201007
C	3.580038	0.686403	7.928519
C	4.375874	1.383293	8.863202
C	2.708318	3.086129	9.103270
H	5.371507	0.986937	9.083510
H	2.383849	4.035429	9.535708
C	-3.035049	-0.756338	5.574466
H	-2.300331	-0.098535	6.064158
C	-4.265732	-0.839429	6.485465
H	-5.071046	-1.442996	6.036709
H	-4.666523	0.168524	6.659686
H	-4.006276	-1.276010	7.459989
C	-3.409782	-0.111235	4.220662
H	-2.532400	-0.024254	3.561709
H	-3.830155	0.896695	4.375018
H	-4.166477	-0.722025	3.699036
C	1.101742	-3.700497	4.707251
H	1.604102	-2.974398	5.359283
C	1.565278	-5.107398	5.127767
H	1.227234	-5.876419	4.412724
H	1.195413	-5.371764	6.123722
H	2.665726	-5.146955	5.150026
C	1.560610	-3.446885	3.252990
H	1.351401	-2.421055	2.924404
H	1.044616	-4.138776	2.565820
H	2.646029	-3.621568	3.160038
C	-3.562136	-5.523926	3.971331

H	-2.912166	-6.396658	3.780775
C	-4.620474	-5.944297	5.010424
H	-5.329071	-5.124181	5.212455
H	-4.150361	-6.225472	5.965464
H	-5.204529	-6.804870	4.642923
C	-4.228797	-5.136987	2.633098
H	-3.472105	-4.866691	1.879219
H	-4.896870	-4.269632	2.764903
H	-4.831620	-5.972715	2.238327
C	0.593697	3.140651	7.746633
H	-0.090204	2.391218	7.320386
C	0.934542	4.156490	6.632184
H	1.606479	4.939449	7.024023
H	0.015339	4.645156	6.267183
H	1.432434	3.675709	5.777854
C	-0.139582	3.863299	8.890196
H	-0.300632	3.201189	9.750342
H	-1.131051	4.193160	8.544069
H	0.413653	4.756415	9.224725
C	4.851002	3.358971	10.429155
H	4.205114	4.103806	10.927844
C	5.934492	4.132557	9.646359
H	5.477407	4.782586	8.883247
H	6.614017	3.433651	9.130386
H	6.538444	4.759586	10.324285
C	5.483185	2.478951	11.523471
H	6.184291	1.745000	11.094324
H	4.713816	1.924662	12.082619
H	6.050202	3.099737	12.237198
C	4.324863	-0.430541	7.178777
H	5.085459	-0.793155	7.891315
C	5.124057	0.176878	5.999325
H	5.793935	-0.583793	5.562956
H	5.736817	1.029302	6.332683
H	4.450035	0.528082	5.204232

C	3.539475	-1.662362	6.706708
H	4.251254	-2.461856	6.443265
H	2.943919	-1.436608	5.814399
H	2.866578	-2.054454	7.480498
H	-0.140810	-4.715992	11.974284
C	-0.539743	-3.727505	11.735950
C	-1.457990	-1.158908	11.130512
C	-0.084075	-3.082349	10.562344
C	-1.447397	-3.108943	12.599925
C	-1.873661	-1.804129	12.312010
C	-0.579376	-1.802399	10.204675
H	-1.781729	-3.615386	13.509759
H	-2.491723	-1.262658	13.030877
C	0.979952	-3.809160	9.803504
C	3.020241	-5.389657	8.631147
C	2.345752	-3.424969	9.952861
C	0.641969	-4.995545	9.105762
C	1.672331	-5.761092	8.527947
C	3.335122	-4.222648	9.352696
H	1.419922	-6.683880	7.997472
H	4.382358	-3.940177	9.465848
C	-1.806260	0.307709	11.051391
C	-2.687980	2.939667	11.807273
C	-3.157437	0.759203	10.690735
C	-0.957109	1.186314	11.857890
C	-1.396336	2.454415	12.187875
C	-3.528482	2.103320	11.100243
H	-0.743740	3.100279	12.779603
H	-4.530713	2.457110	10.849306
C	2.741519	-2.237622	10.840013
H	2.040281	-1.415264	10.628126
C	4.163847	-1.710071	10.596544
H	4.923060	-2.410259	10.983764
H	4.298982	-0.752095	11.120435
H	4.363984	-1.539562	9.534148

C	2.609384	-2.599682	12.337887
H	1.576713	-2.837985	12.619146
H	2.950882	-1.757142	12.962787
H	3.240460	-3.474561	12.569135
C	-0.797184	-5.507037	9.050176
H	-1.432467	-4.772247	9.564608
C	-1.338328	-5.636044	7.618523
H	-0.755229	-6.354940	7.021144
H	-1.315824	-4.672397	7.094439
H	-2.381962	-5.991286	7.637968
C	-0.921900	-6.842532	9.813702
H	-0.528179	-6.756385	10.838853
H	-0.357286	-7.642453	9.306725
H	-1.977161	-7.157891	9.872545
C	4.109959	-6.278944	8.045962
H	3.611806	-7.002325	7.376249
C	5.140598	-5.497781	7.209385
H	5.705497	-4.783906	7.830800
H	4.650098	-4.927648	6.405978
H	5.869191	-6.187817	6.751853
C	4.802594	-7.079571	9.170640
H	5.542967	-7.785293	8.757203
H	4.064422	-7.650550	9.756547
H	5.327592	-6.400223	9.862989
C	-4.312075	-0.205441	10.374297
H	-3.872576	-1.092594	9.895523
C	-5.335947	0.435931	9.417670
H	-5.991023	1.141956	9.953646
H	-5.982482	-0.337313	8.975838
H	-4.833131	0.977840	8.605993
C	-5.062347	-0.656188	11.651284
H	-4.422830	-1.222042	12.339932
H	-5.909064	-1.304971	11.367523
H	-5.474047	0.212505	12.192554
C	-3.122452	4.344963	12.200720

H	-4.168662	4.466297	11.869686
C	-2.271039	5.408803	11.475312
H	-2.325755	5.283347	10.384184
H	-1.210908	5.334072	11.767691
H	-2.621152	6.422954	11.731411
C	-3.082223	4.560520	13.728639
H	-3.692898	3.810436	14.256068
H	-3.466554	5.562638	13.982550
H	-2.052519	4.492962	14.115954
C	0.379658	0.688907	12.405695
H	0.477437	-0.372604	12.150797
C	0.425494	0.789090	13.944710
H	-0.429504	0.267812	14.403813
H	0.403274	1.837937	14.283487
H	1.353727	0.332820	14.326610
C	1.564907	1.419864	11.757595
H	2.516158	1.020580	12.142921
H	1.540448	2.501061	11.967999
H	1.560721	1.296965	10.667929

Ar*-Ga-P-Ar*

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	0.842327	0.353359	-0.497812
P	-0.931567	-0.059239	0.686184
H	0.720110	0.113472	5.486567
C	-0.008813	-0.285611	4.776551
C	-1.872478	-1.299587	2.943195
C	0.146789	0.029287	3.409996
C	-1.072079	-1.078711	5.235674
C	-2.000080	-1.585406	4.310820
C	-0.807340	-0.467293	2.475529

H	-1.179276	-1.293792	6.301917
H	-2.840757	-2.198952	4.644886
C	1.330507	0.863552	3.026735
C	3.643536	2.466751	2.602756
C	1.204646	2.271916	2.877304
C	2.610346	0.256041	2.934356
C	3.740080	1.071153	2.718510
C	2.361411	3.046281	2.667641
H	4.731889	0.610976	2.677441
H	2.260617	4.131976	2.585472
C	-2.896230	-1.803232	1.967763
C	-4.891988	-2.672950	0.132354
C	-4.011021	-0.968794	1.667178
C	-2.779892	-3.079574	1.345414
C	-3.782685	-3.480019	0.441653
C	-4.983961	-1.420205	0.756163
H	-3.687887	-4.465250	-0.025257
H	-5.839632	-0.779495	0.522486
C	-0.148201	2.963515	3.028369
H	-0.914894	2.178786	3.102909
C	-0.500314	3.836562	1.811893
H	0.205595	4.674325	1.692892
H	-1.508052	4.266336	1.929032
H	-0.492005	3.246075	0.886330
C	-0.191946	3.784014	4.335115
H	0.042550	3.153730	5.207851
H	-1.192277	4.224649	4.483043
H	0.539409	4.609424	4.309053
C	2.802306	-1.243587	3.148366
H	1.805930	-1.704088	3.198133
C	3.560419	-1.911086	1.989213
H	4.585596	-1.519696	1.891333
H	3.048898	-1.754906	1.028815
H	3.636384	-2.997292	2.155125
C	3.508545	-1.510603	4.495017

H	2.953127	-1.056894	5.330315
H	4.526394	-1.085592	4.498353
H	3.591908	-2.594153	4.683277
C	4.904980	3.314387	2.472771
H	5.758481	2.614489	2.430615
C	4.918364	4.148125	1.178623
H	4.113119	4.899153	1.185745
H	4.773786	3.508146	0.294533
H	5.876427	4.683827	1.070097
C	5.102173	4.217154	3.709279
H	5.119539	3.622367	4.636435
H	4.283882	4.950970	3.795532
H	6.050243	4.776890	3.636487
C	-4.201639	0.389833	2.342146
H	-3.342010	0.559665	3.005877
C	-5.468913	0.382646	3.222346
H	-6.378146	0.262246	2.609838
H	-5.559891	1.332015	3.776199
H	-5.441712	-0.444092	3.949998
C	-4.238898	1.556004	1.336804
H	-3.308295	1.611752	0.754510
H	-4.367170	2.510376	1.871762
H	-5.078991	1.454349	0.630352
C	-5.996091	-3.156739	-0.800297
H	-6.639604	-2.285488	-1.017186
C	-6.868947	-4.220689	-0.098360
H	-7.275394	-3.834025	0.849786
H	-6.274112	-5.120108	0.132782
H	-7.711893	-4.526083	-0.741597
C	-5.457327	-3.690101	-2.141926
H	-4.855172	-4.601803	-1.997365
H	-4.822422	-2.942663	-2.642143
H	-6.290552	-3.947084	-2.817303
C	-1.694556	-4.121798	1.644383
H	-1.718283	-4.805890	0.778475

C	-2.097071	-4.960790	2.878291
H	-1.393861	-5.799289	3.020121
H	-3.112174	-5.373167	2.761687
H	-2.078968	-4.343744	3.789533
C	-0.238410	-3.636736	1.774987
H	0.436280	-4.505452	1.699211
H	-0.056038	-3.155489	2.744844
H	0.032505	-2.924202	0.984959
H	2.392577	-1.256484	-5.104735
C	1.833288	-0.479494	-4.577159
C	0.320595	1.474266	-3.201659
C	1.737454	-0.534202	-3.172477
C	1.199999	0.551209	-5.290455
C	0.431805	1.507387	-4.607133
C	1.007736	0.463992	-2.474025
H	1.286127	0.596995	-6.379631
H	-0.099096	2.286837	-5.159440
C	2.327026	-1.705001	-2.442071
C	3.461639	-3.983048	-1.181280
C	1.564949	-2.902789	-2.318871
C	3.649841	-1.646816	-1.931218
C	4.193139	-2.792059	-1.316809
C	2.146461	-4.012786	-1.680632
H	5.218516	-2.761185	-0.937045
H	1.562959	-4.932475	-1.591911
C	-0.592567	2.466953	-2.538933
C	-2.364992	4.435263	-1.512372
C	-0.087252	3.715866	-2.098205
C	-1.987048	2.191218	-2.451277
C	-2.843102	3.180124	-1.932129
C	-0.984934	4.676237	-1.594274
H	-3.914573	2.972570	-1.877529
H	-0.605022	5.650091	-1.271848
C	0.166207	-3.035789	-2.922948
H	-0.105725	-2.063447	-3.358264

C	-0.903569	-3.382509	-1.870873
H	-0.690226	-4.348546	-1.385724
H	-1.896114	-3.459620	-2.343426
H	-0.962344	-2.613868	-1.087167
C	0.172785	-4.070037	-4.069577
H	0.932259	-3.820697	-4.828083
H	-0.812945	-4.106328	-4.562619
H	0.396372	-5.081701	-3.691611
C	4.512761	-0.400427	-2.115533
H	3.864600	0.398400	-2.507595
C	5.121097	0.103730	-0.793725
H	5.803719	-0.639861	-0.351454
H	4.342558	0.321892	-0.047158
H	5.699777	1.026215	-0.965297
C	5.604871	-0.662948	-3.174253
H	5.155881	-0.989734	-4.125636
H	6.296738	-1.453840	-2.839954
H	6.194304	0.249747	-3.363454
C	4.105141	-5.218184	-0.561365
H	5.060000	-4.893814	-0.110743
C	3.245673	-5.839650	0.556416
H	2.305821	-6.254187	0.156273
H	2.984367	-5.093292	1.321501
H	3.788805	-6.665342	1.045481
C	4.433229	-6.266509	-1.647367
H	4.957827	-7.132750	-1.209371
H	5.071625	-5.835294	-2.435009
H	3.510542	-6.634937	-2.125689
C	1.388672	4.070741	-2.252103
H	1.929631	3.150643	-2.522868
C	2.011617	4.603455	-0.951160
H	1.526274	5.534523	-0.616424
H	3.079271	4.823635	-1.104598
H	1.925034	3.871150	-0.135057
C	1.574208	5.070831	-3.412610

H	1.153130	4.667959	-4.347207
H	2.643282	5.287224	-3.576290
H	1.061531	6.022361	-3.194759
C	-3.308877	5.539403	-1.047807
H	-2.678181	6.365866	-0.674534
C	-4.228373	5.095788	0.104841
H	-3.642912	4.720958	0.957118
H	-4.909246	4.290613	-0.213410
H	-4.847761	5.940396	0.450787
C	-4.136822	6.083226	-2.232535
H	-3.481902	6.426523	-3.049359
H	-4.767645	6.929823	-1.912040
H	-4.799663	5.300942	-2.638049
C	-2.585256	0.894485	-2.999444
H	-1.754380	0.211142	-3.230158
C	-3.337077	1.180897	-4.317853
H	-2.684529	1.674870	-5.054829
H	-4.199998	1.842971	-4.134690
H	-3.716695	0.244213	-4.759479
C	-3.508525	0.171915	-2.003303
H	-3.863158	-0.776466	-2.436273
H	-4.396928	0.773818	-1.756048
H	-2.988415	-0.062028	-1.065647

Ga-P(Ar*)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	2.575262	-3.070058	7.343023
P	0.566436	-1.881820	8.267290
H	0.479469	-0.540789	3.683076
C	0.965559	-0.277058	4.623724
C	2.011179	0.594790	7.098399

C	0.389903	-0.746929	5.824391
C	2.125093	0.498245	4.627917
C	2.603179	0.948533	5.862396
C	0.974344	-0.414040	7.107704
H	2.600056	0.811753	3.694744
H	3.426374	1.666258	5.890690
C	-0.866718	-1.563223	5.640959
C	-3.266501	-3.013933	5.122180
C	-2.139682	-0.957668	5.873617
C	-0.813184	-2.860176	5.059717
C	-2.011069	-3.564852	4.834620
C	-3.305645	-1.697062	5.613539
H	-1.967078	-4.573039	4.411658
H	-4.274855	-1.232339	5.799645
C	2.398456	1.628746	8.143368
C	3.339838	4.023193	9.422254
C	1.700136	2.870314	7.994955
C	3.581092	1.612865	8.934437
C	4.006649	2.799426	9.569571
C	2.183399	4.025740	8.631659
H	4.918298	2.753381	10.171330
H	1.650362	4.970417	8.489557
C	-2.257167	0.512789	6.279204
H	-1.454059	0.729518	6.998812
C	-3.592475	0.886018	6.944137
H	-4.420810	0.883167	6.215631
H	-3.525714	1.901989	7.359951
H	-3.846455	0.206160	7.765034
C	-2.057567	1.407446	5.033037
H	-1.059191	1.286621	4.592695
H	-2.191449	2.469600	5.293967
H	-2.806230	1.148749	4.265503
C	0.493417	-3.490342	4.583776
H	1.323501	-2.858398	4.944441
C	0.727820	-4.916800	5.109348

H	-0.048489	-5.613999	4.756489
H	0.727605	-4.955557	6.208540
H	1.702327	-5.295921	4.761032
C	0.560408	-3.477921	3.040616
H	0.383769	-2.469317	2.638196
H	-0.209597	-4.143289	2.616268
H	1.546589	-3.825184	2.689481
C	-4.543312	-3.802107	4.860585
H	-4.238528	-4.816991	4.547800
C	-5.406413	-3.941130	6.130437
H	-5.749125	-2.956467	6.487335
H	-4.837098	-4.411144	6.946658
H	-6.300267	-4.555531	5.929020
C	-5.354387	-3.179419	3.704427
H	-4.739778	-3.095758	2.793664
H	-5.702274	-2.167206	3.969518
H	-6.242000	-3.792271	3.471834
C	0.497635	3.042562	7.062790
H	0.223610	2.060156	6.664674
C	0.862295	3.936623	5.858130
H	1.092591	4.965630	6.180342
H	0.020002	3.983006	5.148733
H	1.739838	3.543301	5.324032
C	-0.734640	3.594855	7.799207
H	-1.058744	2.915936	8.598193
H	-1.571674	3.720971	7.094642
H	-0.537877	4.581355	8.250137
C	3.865206	5.326854	10.012686
H	3.002401	6.013197	10.089294
C	4.887417	5.968433	9.046368
H	4.448874	6.114145	8.046359
H	5.770831	5.317384	8.935225
H	5.228046	6.947208	9.425394
C	4.472909	5.176844	11.419325
H	5.396348	4.575470	11.397872

H	3.770309	4.694337	12.116501
H	4.737210	6.166548	11.827176
C	4.472487	0.398504	9.175693
H	5.363198	0.793456	9.694996
C	4.998487	-0.289262	7.904184
H	5.758080	-1.042565	8.169604
H	5.460675	0.440561	7.220562
H	4.199696	-0.798227	7.346250
C	3.803239	-0.589222	10.141656
H	4.522838	-1.356097	10.458136
H	2.944247	-1.086345	9.669618
H	3.433424	-0.072791	11.040189
H	1.377831	-4.562295	12.333197
C	1.014048	-3.586436	12.006190
C	-0.076691	-1.169555	11.080957
C	1.096851	-3.274142	10.636354
C	0.435068	-2.710228	12.931514
C	-0.131522	-1.531692	12.446716
C	0.600084	-2.007538	10.144715
H	0.371816	-2.971934	13.990690
H	-0.685767	-0.877395	13.122062
C	1.583263	-4.431865	9.793502
C	2.409094	-6.869533	8.540761
C	2.944907	-4.865418	9.863505
C	0.626633	-5.266803	9.126539
C	1.068741	-6.446182	8.501125
C	3.326078	-6.068544	9.233589
H	0.340218	-7.078082	7.988633
H	4.368533	-6.386933	9.302570
C	-1.028061	-0.054889	10.742928
C	-3.120154	1.863846	10.565517
C	-2.359786	-0.463355	10.445167
C	-0.747059	1.320214	10.999428
C	-1.809482	2.240571	10.906360
C	-3.372501	0.506801	10.339597

H	-1.616666	3.291247	11.112846
H	-4.395804	0.190051	10.117341
C	3.998097	-4.121638	10.682680
H	3.561564	-3.161665	10.987252
C	5.286425	-3.845182	9.882735
H	5.807880	-4.779989	9.621859
H	5.984066	-3.235733	10.480141
H	5.078261	-3.309544	8.944125
C	4.345385	-4.905901	11.967918
H	3.451421	-5.107020	12.575597
H	5.057603	-4.332983	12.584821
H	4.810954	-5.874676	11.721952
C	-0.872388	-4.972510	9.194458
H	-0.992486	-3.883643	9.240320
C	-1.674799	-5.459440	7.976867
H	-1.682411	-6.560217	7.898082
H	-1.291989	-5.039695	7.038367
H	-2.721048	-5.134924	8.077647
C	-1.465691	-5.576440	10.487779
H	-0.975154	-5.176196	11.385687
H	-1.350335	-6.673637	10.488201
H	-2.541396	-5.345296	10.553233
C	2.837711	-8.168131	7.870387
H	1.934626	-8.612324	7.415709
C	3.855124	-7.905560	6.740614
H	4.789425	-7.480484	7.143028
H	3.452149	-7.192453	6.004361
H	4.108431	-8.843573	6.218586
C	3.392475	-9.178898	8.896087
H	3.634812	-10.136930	8.406301
H	2.660797	-9.372942	9.696659
H	4.314709	-8.800573	9.367111
C	-2.768527	-1.935793	10.395369
H	-1.859900	-2.542387	10.461558
C	-3.478849	-2.326181	9.091753

H	-4.400428	-1.743574	8.930484
H	-3.769362	-3.388163	9.123487
H	-2.823556	-2.177194	8.224577
C	-3.631399	-2.284552	11.627427
H	-3.109915	-2.023717	12.561623
H	-3.855543	-3.364191	11.647588
H	-4.589488	-1.738884	11.609603
C	-4.255789	2.879814	10.530585
H	-5.112611	2.389582	10.034475
C	-3.910002	4.147753	9.727791
H	-3.614182	3.901025	8.697369
H	-3.077577	4.701427	10.191117
H	-4.777842	4.826889	9.687214
C	-4.686635	3.238263	11.969873
H	-4.962551	2.332067	12.532661
H	-5.549253	3.926198	11.966227
H	-3.859013	3.729059	12.508869
C	0.653397	1.832387	11.381000
H	1.341688	1.507930	10.584105
C	1.194394	1.280421	12.723406
H	1.474670	0.223865	12.665964
H	0.443577	1.395595	13.523659
H	2.091218	1.851172	13.018314
C	0.726857	3.367278	11.472507
H	1.771759	3.667166	11.621082
H	0.144800	3.736531	12.334430
H	0.367453	3.867269	10.565401

(Tbt)2Ga-P

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	2.095842	1.712571	0.781728

P	-0.104353	2.148576	0.939595
C	2.842621	1.941580	-1.087194
C	4.184730	2.045503	-3.647127
C	3.471166	3.158247	-1.544760
C	2.779007	0.833186	-2.010743
C	3.428187	0.927169	-3.263011
C	4.183359	3.137342	-2.767373
H	3.348481	0.096138	-3.964527
H	4.719755	4.040431	-3.062934
C	2.676286	1.571317	2.694597
C	3.408891	2.739946	5.235113
C	3.986266	1.365147	3.255390
C	1.674050	2.110771	3.582795
C	2.058788	2.664004	4.833937
C	4.330625	2.039299	4.440672
H	1.288364	3.048145	5.505683
H	5.364267	1.968146	4.790764
C	2.007819	-0.472731	-1.760439
H	1.775349	-0.574176	-0.680843
C	3.380705	4.584036	-0.959789
H	3.810894	5.191450	-1.783102
C	4.887307	2.105874	-4.988390
H	4.762628	1.115204	-5.470408
C	4.996113	0.285808	2.852990
H	5.692744	0.278915	3.719000
C	0.137431	2.008626	3.352012
H	-0.191796	1.873646	4.407283
C	3.906796	3.363378	6.527474
H	5.001267	3.495194	6.404550
Si	2.925586	-2.114424	-2.229703
Si	0.277880	-0.489791	-2.632630
Si	3.977965	3.295433	-6.175077
Si	6.785231	2.320035	-4.912223
Si	1.653614	5.416815	-0.986219
Si	4.602424	5.229347	0.349107

Si	-1.069019	3.613458	3.462834
Si	-0.741848	0.221847	3.084677
Si	3.798072	2.056219	7.917382
Si	3.314069	5.118819	6.956869
Si	4.263998	-1.456503	3.133999
Si	6.348230	0.562704	1.546952
C	2.778740	-2.609336	-4.055793
H	3.227952	-1.875582	-4.743530
H	1.745522	-2.791764	-4.385432
H	3.335120	-3.554664	-4.188665
C	2.193838	-3.552712	-1.232207
H	3.000516	-4.217026	-0.880231
H	1.510706	-4.160048	-1.845289
H	1.636168	-3.217964	-0.345843
C	4.784383	-2.055095	-1.925366
H	5.268181	-1.248539	-2.495477
H	5.218948	-3.014934	-2.257000
H	5.041030	-1.920271	-0.867267
C	-0.554795	-2.183498	-2.477485
H	-0.081847	-2.977951	-3.072197
H	-1.595522	-2.082932	-2.832960
H	-0.599864	-2.526745	-1.431654
C	0.416672	-0.025962	-4.451567
H	0.682244	1.035544	-4.555155
H	-0.566730	-0.171129	-4.932512
H	1.154510	-0.612930	-5.014694
C	-0.979208	0.697254	-1.895909
H	-0.656471	1.748150	-1.934004
H	-1.223771	0.450312	-0.851078
H	-1.912320	0.625588	-2.484271
C	2.203917	2.698835	-6.372075
H	2.157301	1.631846	-6.644062
H	1.684882	3.271864	-7.159690
H	1.641168	2.830011	-5.434458
C	4.801563	3.275345	-7.874269

H	5.788057	3.766196	-7.874411
H	4.165871	3.810014	-8.601277
H	4.938454	2.246600	-8.247470
C	3.907902	5.073258	-5.548706
H	4.901992	5.499820	-5.347931
H	3.312263	5.147822	-4.625452
H	3.420386	5.707501	-6.309895
C	1.816245	7.111114	-1.818762
H	2.283989	7.865464	-1.168419
H	0.808793	7.481427	-2.078971
H	2.399309	7.060874	-2.754113
C	0.505090	4.417088	-2.088898
H	0.418742	3.376565	-1.750774
H	0.896251	4.397204	-3.120511
H	-0.504484	4.860762	-2.112030
C	0.935378	5.714847	0.720035
H	-0.093859	6.104771	0.654156
H	1.534809	6.447901	1.283452
H	0.896303	4.773991	1.283145
C	-0.076237	5.119807	3.982002
H	0.857667	5.231823	3.420851
H	0.168466	5.090671	5.053511
H	-0.690169	6.018163	3.801005
C	-2.254725	4.079949	2.072496
H	-2.917741	4.882004	2.450936
H	-2.884757	3.230332	1.770338
H	-1.731073	4.440397	1.178562
C	-2.221499	3.228818	4.928545
H	-1.668810	3.038352	5.865642
H	-2.892226	2.372388	4.755689
H	-2.865910	4.109420	5.101905
C	-2.520903	0.347722	2.454852
H	-3.166628	0.984174	3.079812
H	-2.951266	-0.670463	2.475084
H	-2.565217	0.717485	1.420989

C	-0.919064	-0.477372	4.846342
H	0.049393	-0.619939	5.352284
H	-1.414159	-1.464101	4.794919
H	-1.546834	0.165422	5.487705
C	0.176031	-1.080524	2.094843
H	1.253874	-1.030686	2.285126
H	0.008280	-0.944775	1.018811
H	-0.180691	-2.082609	2.394190
C	2.065743	1.326903	8.008103
H	1.997316	0.611450	8.845470
H	1.813131	0.788778	7.081167
H	1.301330	2.103885	8.167992
C	5.035276	0.683875	7.531903
H	6.068062	1.073439	7.520155
H	4.840073	0.223450	6.551885
H	4.988547	-0.110734	8.296419
C	4.275367	2.766894	9.599589
H	5.268655	3.244222	9.569989
H	4.323101	1.949964	10.340595
H	3.553785	3.510889	9.972082
C	4.578088	5.918356	8.114088
H	5.607953	5.760172	7.749487
H	4.526681	5.537044	9.144682
H	4.410609	7.008745	8.153717
C	3.259606	6.177390	5.403389
H	4.269969	6.282205	4.975120
H	2.888137	7.189369	5.640711
H	2.612401	5.747309	4.628272
C	1.627115	5.119791	7.802693
H	1.271682	6.154606	7.946328
H	1.672003	4.644518	8.796377
H	0.863484	4.587178	7.214297
C	4.549189	7.123558	0.335886
H	4.659632	7.540882	-0.678460
H	5.393158	7.501440	0.940093

H	3.626823	7.536936	0.773100
C	6.351798	4.780927	-0.198505
H	6.566124	5.215123	-1.190447
H	6.517005	3.697308	-0.267595
H	7.093618	5.189623	0.509247
C	4.288802	4.677511	2.110297
H	3.234891	4.799503	2.399795
H	4.548668	3.626238	2.282608
H	4.893980	5.285675	2.803708
C	7.476323	1.458923	-3.390295
H	8.578806	1.430429	-3.437839
H	7.113575	0.421067	-3.313642
H	7.187876	1.983421	-2.468074
C	7.341955	4.122996	-4.859485
H	8.437874	4.168290	-4.733110
H	6.891489	4.668709	-4.014732
H	7.093656	4.665648	-5.785705
C	7.535672	1.493453	-6.436021
H	8.632766	1.430914	-6.331486
H	7.320300	2.038925	-7.367081
H	7.156697	0.463765	-6.555422
C	2.976371	-1.363270	4.512230
H	3.466184	-1.175921	5.481279
H	2.439870	-2.324335	4.592334
H	2.239165	-0.567016	4.352219
C	5.610928	-2.612231	3.790353
H	6.264559	-3.011501	3.000724
H	5.137139	-3.470590	4.297960
H	6.250309	-2.105733	4.533461
C	3.528650	-2.236367	1.590280
H	4.305546	-2.744496	1.000160
H	3.045238	-1.498624	0.935694
H	2.770895	-2.992058	1.852263
C	5.777877	0.779522	-0.217705
H	6.562415	0.412314	-0.896008

H	5.563356	1.821038	-0.485457
H	4.868570	0.209669	-0.432855
C	7.355087	2.055413	2.111992
H	8.185238	2.250490	1.411400
H	7.795281	1.872599	3.107694
H	6.748866	2.970580	2.176612
C	7.528099	-0.914454	1.579101
H	8.408741	-0.673809	0.957992
H	7.075532	-1.829081	1.163788
H	7.890672	-1.146077	2.593349

Tbt-Ga-P-Tbt

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ga	0.764258	1.104367	0.398883
P	-0.602346	-0.050805	-0.842841
C	-2.401325	-0.107422	-0.516429
C	-5.130515	-0.395545	0.240665
C	-3.004291	-1.414696	-0.516299
C	-3.206337	1.059521	-0.284840
C	-4.542586	0.875486	0.116715
C	-4.354358	-1.514709	-0.123749
H	-5.145543	1.755943	0.350424
H	-4.807680	-2.507298	-0.086505
C	2.700292	0.756761	0.516099
C	5.077670	-0.825872	0.442430
C	3.205903	0.160527	1.722765
C	3.465360	0.672276	-0.701164
C	4.618678	-0.145397	-0.700804
C	4.369597	-0.631076	1.641884
H	5.194530	-0.222086	-1.625303
H	4.749860	-1.100027	2.554561

C	-2.690004	2.474964	-0.479606
H	-1.614242	2.405467	-0.726452
C	-2.319911	-2.714622	-0.963166
H	-3.124582	-3.471113	-0.852145
C	-6.556879	-0.530514	0.726110
H	-6.897249	0.484716	1.014180
C	2.652562	0.371007	3.139725
H	3.498716	0.054038	3.784229
C	3.235915	1.463590	-1.999781
H	4.201516	1.339201	-2.532099
C	6.338080	-1.660149	0.434024
H	6.485757	-2.027174	1.469669
Si	-2.737632	3.586349	1.071450
Si	-3.412205	3.273644	-2.063213
Si	-7.717461	-0.984300	-0.712000
Si	-6.710570	-1.515844	2.350014
Si	-2.017116	-2.894706	-2.860388
Si	-1.065087	-3.600887	0.181795
Si	2.115548	0.818335	-3.431139
Si	3.294232	3.357062	-1.807090
Si	7.897089	-0.603495	0.127213
Si	6.149395	-3.273514	-0.562659
Si	2.496954	2.180080	3.752673
Si	1.379753	-0.866955	3.869925
C	-4.246825	4.714497	1.185593
H	-5.194396	4.166155	1.067474
H	-4.225109	5.516236	0.430624
H	-4.261358	5.196333	2.178993
C	-1.221407	4.713994	1.080344
H	-1.263020	5.398490	1.945409
H	-1.154052	5.329498	0.169683
H	-0.280957	4.146942	1.157598
C	-2.728906	2.512252	2.616164
H	-3.710189	2.037352	2.770364
H	-2.491850	3.113407	3.510266

H	-1.988794	1.703447	2.535577
C	-2.359134	4.775424	-2.520386
H	-2.453464	5.597637	-1.792372
H	-2.675144	5.168138	-3.502808
H	-1.291179	4.513934	-2.598797
C	-5.215637	3.815623	-1.922177
H	-5.829001	3.060340	-1.407867
H	-5.631651	3.933401	-2.937937
H	-5.341757	4.774552	-1.398543
C	-3.348899	2.038059	-3.474088
H	-4.041045	1.203520	-3.282240
H	-2.345298	1.617802	-3.615697
H	-3.655904	2.522671	-4.417265
C	-7.557060	0.368162	-2.016098
H	-7.804266	1.360138	-1.601778
H	-8.236742	0.180586	-2.865411
H	-6.528099	0.418223	-2.407648
C	-9.505367	-1.040220	-0.110232
H	-9.700776	-1.911150	0.536318
H	-10.193606	-1.104555	-0.970591
H	-9.767606	-0.133302	0.459747
C	-7.282065	-2.631358	-1.517849
H	-7.282341	-3.466923	-0.801504
H	-6.289064	-2.592823	-1.991744
H	-8.018913	-2.865506	-2.305904
C	-3.479950	-3.893756	-3.520701
H	-3.528066	-4.891388	-3.050923
H	-3.398795	-4.042435	-4.611514
H	-4.436171	-3.381671	-3.321565
C	-2.009727	-1.253321	-3.766662
H	-1.247254	-0.560235	-3.385273
H	-2.986183	-0.757720	-3.673984
H	-1.811575	-1.421119	-4.839579
C	-0.465420	-3.860065	-3.354534
H	-0.591348	-4.940416	-3.186649

H	0.451511	-3.537660	-2.843100
H	-0.302907	-3.715277	-4.437371
C	1.808159	-1.023245	-3.238461
H	1.232557	-1.261274	-2.335147
H	2.764452	-1.569068	-3.191907
H	1.245661	-1.401333	-4.107252
C	0.533203	1.806057	-3.707525
H	-0.111076	1.818380	-2.818480
H	-0.044828	1.348219	-4.528068
H	0.753265	2.844206	-4.003924
C	3.106681	0.994627	-5.035060
H	4.104588	0.530017	-4.959000
H	3.240980	2.040741	-5.348801
H	2.563756	0.476633	-5.845515
C	3.561231	4.158390	-3.497640
H	4.423066	3.717229	-4.024808
H	3.776358	5.232025	-3.354654
H	2.685437	4.083381	-4.160354
C	4.809513	3.767507	-0.768092
H	4.817708	3.206066	0.175779
H	4.856494	4.843041	-0.527441
H	5.727622	3.506203	-1.321732
C	1.747419	4.131192	-1.058313
H	1.666302	3.947373	0.023856
H	0.825804	3.766088	-1.535509
H	1.774508	5.227310	-1.189784
C	8.295993	-0.383889	-1.703416
H	9.142920	0.314038	-1.821935
H	7.444099	0.034173	-2.263399
H	8.581647	-1.334624	-2.182186
C	7.639421	1.097449	0.896152
H	7.373228	1.016322	1.963560
H	6.832241	1.653219	0.394874
H	8.564138	1.696007	0.822888
C	9.365151	-1.421460	0.986343

H	9.122332	-1.673941	2.032872
H	10.227597	-0.733043	1.003936
H	9.687364	-2.347120	0.485836
C	7.733941	-4.290377	-0.420879
H	8.057304	-4.398171	0.627946
H	8.569008	-3.844224	-0.985207
H	7.567207	-5.304637	-0.823107
C	4.729041	-4.250132	0.197288
H	4.901458	-4.441369	1.270089
H	4.610457	-5.226904	-0.303035
H	3.777139	-3.703574	0.104039
C	5.765302	-2.982449	-2.383497
H	5.723076	-3.951829	-2.910166
H	6.524251	-2.363262	-2.885367
H	4.786943	-2.493848	-2.510110
C	-1.031993	-5.430498	-0.321149
H	-2.027202	-5.814738	-0.601486
H	-0.679424	-6.026962	0.539144
H	-0.343456	-5.630213	-1.155357
C	-1.804216	-3.563904	1.914657
H	-2.697219	-4.211247	1.953703
H	-2.113823	-2.552135	2.206687
H	-1.085217	-3.937076	2.663196
C	0.735718	-3.051497	0.189529
H	1.125683	-2.934298	-0.831530
H	0.886799	-2.094277	0.702469
H	1.340124	-3.827449	0.690593
C	-5.202777	-1.169347	3.426588
H	-5.317701	-1.648562	4.414782
H	-5.069265	-0.086952	3.590665
H	-4.278726	-1.551071	2.965213
C	-6.851639	-3.378063	2.083171
H	-6.861412	-3.897575	3.057082
H	-6.003379	-3.778454	1.504942
H	-7.780240	-3.648493	1.554562

C	-8.245319	-0.910019	3.269513
H	-8.261501	-1.309380	4.298274
H	-9.180667	-1.217397	2.776995
H	-8.251946	0.191256	3.342268
C	3.460680	3.336914	2.632493
H	4.493198	2.976776	2.496386
H	3.506243	4.346293	3.075582
H	3.008824	3.419632	1.635636
C	3.295690	2.275259	5.462505
H	2.707541	1.766058	6.240443
H	3.409274	3.330284	5.766278
H	4.303139	1.824407	5.453847
C	0.724660	2.804814	3.899161
H	0.153595	2.248618	4.658855
H	0.160611	2.737267	2.955814
H	0.726721	3.867851	4.196249
C	-0.402954	-0.645532	3.327492
H	-1.023137	-1.399962	3.839792
H	-0.564190	-0.759812	2.245546
H	-0.785326	0.340651	3.627249
C	1.995423	-2.614262	3.531855
H	1.227383	-3.354448	3.814239
H	2.896353	-2.822530	4.134301
H	2.253560	-2.775595	2.477155
C	1.379273	-0.669951	5.753029
H	0.808931	-1.506687	6.193928
H	0.901912	0.262607	6.093104
H	2.396409	-0.707227	6.176950

Ga-P(Tbt)2

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Ga	5.917200	-0.096588	0.627940
P	3.754879	0.866606	0.856788
C	3.291242	1.672040	-0.813481
C	2.552134	2.502302	-3.510231
C	3.526277	3.035151	-1.262657
C	2.857592	0.711843	-1.827001
C	2.468570	1.161363	-3.103671
C	3.095805	3.390482	-2.571785
H	2.133291	0.418214	-3.829363
H	3.264986	4.420266	-2.889173
C	3.185072	1.352879	2.579115
C	3.098594	2.930783	4.992629
C	4.130906	1.091195	3.666027
C	1.969332	2.056897	2.948971
C	2.024109	2.902475	4.087950
C	4.070677	1.933666	4.794376
H	1.139051	3.500093	4.309081
H	4.807106	1.776814	5.588848
C	2.943247	-0.808534	-1.691603
H	3.197470	-1.048671	-0.644415
C	4.337508	4.209288	-0.647864
H	4.820697	4.610690	-1.563682
C	2.209515	2.904173	-4.933383
H	1.725525	2.024995	-5.404789
C	5.087964	-0.128755	3.909673
H	5.025901	-0.138911	5.018542
C	0.512904	1.825189	2.453385
H	-0.038617	2.152750	3.361418
C	3.106889	3.761022	6.265505
H	4.085793	3.580410	6.755885
Si	4.415676	-1.526769	-2.707168
Si	1.319239	-1.786503	-1.980416
Si	0.901645	4.278083	-5.148379
Si	3.795111	3.136005	-5.981851
Si	3.411624	5.839365	-0.190909

Si	5.955945	4.014604	0.324699
Si	-0.435653	3.051121	1.344435
Si	-0.171351	0.029595	2.521218
Si	1.867950	3.042074	7.529659
Si	3.102808	5.649727	6.027506
Si	4.354294	-1.904215	3.823933
Si	7.037445	-0.075336	4.003257
C	4.034214	-1.891369	-4.523084
H	3.528490	-2.858219	-4.659766
H	4.986914	-1.935985	-5.077788
H	3.418514	-1.115366	-4.998942
C	4.959604	-3.147030	-1.902908
H	4.211141	-3.943556	-2.039510
H	5.130472	-3.032185	-0.820484
H	5.903663	-3.497033	-2.355294
C	5.887610	-0.338719	-2.746704
H	5.575124	0.716099	-2.769581
H	6.489562	-0.533668	-3.651128
H	6.561099	-0.479229	-1.883862
C	-0.135469	-0.739307	-1.421825
H	-1.003754	-1.375884	-1.184841
H	-0.431444	-0.045963	-2.225257
H	0.106304	-0.139602	-0.538132
C	1.421413	-3.408970	-1.013168
H	1.958932	-4.182088	-1.585838
H	0.406409	-3.796221	-0.817484
H	1.928161	-3.296863	-0.044345
C	0.905182	-2.273637	-3.762812
H	1.034475	-1.453978	-4.486313
H	-0.159620	-2.566581	-3.791861
H	1.489478	-3.134585	-4.119753
C	-0.382042	4.154344	-3.785722
H	-0.770365	3.127481	-3.689930
H	-1.233772	4.823349	-3.997949
H	0.040692	4.440786	-2.814507

C	0.011261	4.008777	-6.793119
H	0.631675	4.252902	-7.668247
H	-0.890611	4.644173	-6.835733
H	-0.321189	2.961612	-6.898299
C	1.636557	6.017422	-5.133245
H	2.266233	6.210144	-6.016915
H	2.248700	6.205357	-4.236989
H	0.824231	6.764951	-5.137939
C	4.268003	7.291792	-1.061525
H	5.196943	7.619785	-0.573935
H	3.580473	8.156202	-1.075241
H	4.507105	7.050997	-2.111975
C	1.665175	5.861465	-0.889846
H	1.125746	4.921809	-0.736852
H	1.691896	6.063594	-1.970900
H	1.090122	6.673415	-0.414765
C	3.403800	6.237326	1.652314
H	3.118798	5.383469	2.282061
H	2.691647	7.054618	1.856200
H	4.395024	6.577505	1.990144
C	0.086654	4.787893	1.835101
H	1.166767	4.949043	1.776694
H	-0.228704	4.983547	2.873102
H	-0.409969	5.533987	1.194578
C	-0.348880	2.757662	-0.502354
H	0.674351	2.657265	-0.890563
H	-0.841450	3.591235	-1.026326
H	-0.899369	1.843790	-0.768891
C	-2.270359	3.014498	1.844274
H	-2.407516	2.771931	2.912142
H	-2.875235	2.307512	1.259706
H	-2.694930	4.021097	1.685663
C	-1.858304	-0.187571	1.684497
H	-2.669942	0.287202	2.254641
H	-2.066259	-1.272583	1.662994

H	-1.908173	0.171463	0.647833
C	-0.533840	-0.315503	4.346669
H	0.302808	-0.045431	5.006957
H	-0.763303	-1.381955	4.514062
H	-1.412844	0.268389	4.671585
C	0.944442	-1.300714	1.809510
H	1.471839	-1.841459	2.602540
H	1.701303	-0.883091	1.133159
H	0.343079	-2.033074	1.252044
C	0.089090	3.552018	7.163691
H	-0.603356	3.030811	7.847145
H	-0.206561	3.293898	6.134516
H	-0.063509	4.635081	7.300990
C	1.991528	1.162408	7.479809
H	3.013608	0.825932	7.723256
H	1.740117	0.761803	6.487567
H	1.304875	0.712777	8.217892
C	2.321240	3.585313	9.282109
H	3.410902	3.534952	9.447814
H	1.844421	2.913606	10.016705
H	1.997405	4.611575	9.510739
C	3.096186	6.529941	7.699326
H	3.848859	6.117750	8.391163
H	2.115816	6.479868	8.199436
H	3.333692	7.597689	7.548711
C	4.703448	6.130100	5.157107
H	5.574603	5.897576	5.793553
H	4.725132	7.212126	4.940666
H	4.828582	5.591043	4.208000
C	1.624146	6.275376	5.046706
H	1.645323	7.378612	5.008081
H	0.668717	5.977590	5.506683
H	1.630042	5.908096	4.012402
C	6.908823	5.656637	0.254377
H	7.005545	6.060355	-0.766650

H	7.931167	5.455064	0.623344
H	6.485302	6.444239	0.896048
C	7.092915	2.831333	-0.619006
H	7.604637	3.386901	-1.425554
H	6.550994	2.002298	-1.098642
H	7.877314	2.402951	0.027942
C	5.749583	3.629848	2.141570
H	4.811233	4.044767	2.529678
H	5.704912	2.555229	2.332285
H	6.580771	4.056910	2.723981
C	4.714164	1.495452	-6.048517
H	5.616616	1.583298	-6.678285
H	4.084102	0.700599	-6.480618
H	5.029699	1.166579	-5.048061
C	4.951286	4.439642	-5.263781
H	5.814177	4.577606	-5.938900
H	5.342456	4.131796	-4.281018
H	4.462584	5.418607	-5.145720
C	3.366738	3.610210	-7.760487
H	4.280737	3.566727	-8.378393
H	2.956670	4.628640	-7.851706
H	2.636789	2.912363	-8.203249
C	2.755101	-1.853730	4.818920
H	2.999096	-1.763581	5.891675
H	2.161135	-2.774854	4.693585
H	2.124039	-0.998418	4.553859
C	5.431003	-3.126840	4.795340
H	6.442161	-3.282999	4.392277
H	4.914428	-4.103704	4.766121
H	5.523026	-2.847798	5.857004
C	4.140440	-2.680121	2.123968
H	5.120626	-2.928242	1.683105
H	3.603564	-2.030338	1.423482
H	3.575547	-3.623932	2.219472
C	7.995632	-1.305351	2.920408

H	7.432657	-2.221554	2.687457
H	8.914433	-1.606531	3.456024
H	8.300324	-0.860451	1.960258
C	7.794198	1.626481	3.748102
H	8.819167	1.609668	4.157412
H	7.230098	2.410125	4.275003
H	7.860259	1.908778	2.688176
C	7.472522	-0.529429	5.793856
H	8.539489	-0.303960	5.967819
H	7.325071	-1.596109	6.016470
H	6.888734	0.053569	6.526802
