

Supplementary Materials

Table 1S.

Geometric parameters of HMYH compounds (singlet states, B3LYP/TZVP level of theory).
Bond distances in angstroms, bond angles in degrees, dissociation energy E^{diss} in kJ mol^{-1} .^a

M,Y	R(H-M)	R(M-Y)	R(Y-H)	$\angle\text{HMY}$	$\angle\text{MYH}$	E^{diss}
CC	1.063	1.198	1.063	180.0	180.0	972.9
BN	1.167	1.235	0.992	180.0	180.0	779.1
BP	1.175	1.697	1.541	177.2	52.7	466.8
BAs	1.176	1.799	1.693	179.5	46.6	425.0
AlN	1.555	1.637	1.001	166.8	157.9	335.6
AlP	1.581	2.152	1.449	179.3	80.2	223.7
AlAs	1.583	2.242	1.560	174.6	73.4	206.3
GaN	1.531	1.705	1.015	161.2	123.6	270.0
GaP	1.558	2.149	1.442	177.8	85.0	202.5
GaAs	1.564	2.245	1.544	179.8	81.6	185.2

^aDissociation energy for the reaction $\text{HMYH} = \text{HM} + \text{YH}$

Table 2S. Geometric parameters of T_d symmetric $[\text{HMYH}]_4$ tetramers predicted at B3LYP/TZVP. Bond distances are in angstroms, bond angles are in degrees.

M,Y	R(M-Y)	R(H-M)	R(Y-H)	$\angle\text{YMY}$	$\angle\text{MYM}$
CC	1.570	1.088	1.088	90.0	90.0
BN	1.595	1.194	1.008	92.2	87.7
BP	2.028	1.188	1.421	88.8	91.2
BAs	2.138	1.186	1.515	89.2	90.8
AlN	1.940	1.580	1.010	89.2	90.8
AlP	2.438	1.759	1.414	88.8	91.2
AlAs	2.535	1.579	1.504	88.3	91.7
GaN	2.004	1.558	1.012	87.6	92.4
GaP	2.449	1.560	1.417	87.6	92.3
GaAs	2.542	1.562	1.509	87.4	92.6

Table 3S. Bonding pattern, computed (B3LYP/TZVP) and predicted according to mean bond energies relative energies of isomers I-VI, and mixtures of [HMYH]₃ trimers.

Isomer	Number of the MY bonds									E ^{rel}	E ^{rel}	E ^{rel}
	B-N	Al-N	Ga-N	B-P	Al-P	Ga-P	B-As	Al-As	Ga-As	TZV	TZVP	estim
B-N,Al-P,Ga-As	2	0	0	0	2	0	0	0	2	0	0.0	0.0
B-N,Al-As,Ga-P	2	0	0	0	0	2	0	2	0	8.5	6.0	6.0
I	1	1	0	1	0	1	0	1	1	79.1	73.3	53.9
II	1	1	0	0	1	1	1	0	1	84.4	86.5	72.3
III	1	0	1	1	1	0	0	1	1	110.0	112.7	96.5
B-P,Al-N,Ga-As	0	2	0	2	0	0	0	0	2	111.4	101.9	101.9
IV	1	0	1	0	1	1	1	1	0	119.1	128.4	117.8
B-As, Al-N, Ga-P	0	2	0	0	0	2	2	0	0	137.6	144.6	144.6
V	0	1	1	1	1	0	1	0	1	168.7	172.7	165.8
VI	0	1	1	1	0	1	1	1	0	171.5	176.1	194.7
B-P, Al-As, Ga-N	0	0	2	2	0	0	0	2	0	186.5	192.9	192.9
B-As, Al-P, Ga-N	0	0	2	0	2	0	2	0	0	204.2	229.7	229.7

Table 4S. Cartesian coordinates (Angstroms) for optimized structures of [BAIGaNPAs]₂H₁₂ species.

Compound	Atom	X	Y	Z	Compound	Atom	X	Y	Z
I+I via ALN	As	-0.165775	2.683725	0.515210	I+I via BN	N	.018051	1.170627	2.593979
	N	1.323529	-0.267899	2.069885		P	2.346549	-.447524	1.131607
	P	1.587153	-0.158227	-1.118621		As	-0.18051	1.748952	-1.048790
	B	1.686447	-1.028621	0.744933		Ga	1.828647	.048411	-1.173772
	Ga	0.165775	1.712166	-1.735169		Al	-.810601	2.307658	1.259706
	Al	0.310005	1.318854	2.457160		B	1.086276	.016215	2.670964
	H	2.121770	-0.338893	2.694355		H	3.693193	-.402524	1.557070
	H	2.886228	-0.130223	-1.685794		H	.022406	2.901623	-2.020153
	Al	-0.310005	-1.318854	2.457160		Al	.810601	-2.307658	1.259706
	H	-1.018260	3.900775	0.760276		H	.069483	1.705534	3.456934
	H	2.761066	-1.552060	0.784992		H	2.961718	.131609	-2.247134
	H	0.394731	2.521993	-3.048617		H	-1.063261	3.801183	1.716764
	H	0.560282	1.901755	3.905448		H	1.749716	.026786	3.670600
	B	-1.686447	1.028621	0.744933		B	-1.086276	-.016215	2.670964
	Ga	-0.165775	-1.712166	-1.735169		Ga	-1.828647	-.048411	-1.173772
	P	-1.587153	0.158227	-1.118621		P	-2.346549	.447524	1.131607
	As	0.165775	-2.683725	0.515210		As	.018051	-1.748952	-1.048790
	N	-1.323529	0.267899	2.069885		N	-.018051	-1.170627	2.593979
	H	-2.761066	1.552060	0.784992		H	-1.749716	-.026786	3.670600
	H	-0.394731	-2.521993	-3.048617		H	-2.961718	-.131609	-2.247134
H	1.018260	-3.900775	0.760276	H	-.022406	-2.901623	-2.020153		
H	-2.886228	0.130223	-1.685794	H	-3.693193	.402524	1.557070		
H	-2.121770	0.338893	2.694355	H	-.069483	-1.705534	3.456934		
H	-0.560282	-1.901755	3.905448	H	1.063261	-3.801183	1.716764		
I+I via BP	Al	-0.649062	-1.236171	1.610524	I+I rotated	P	1.899690	2.065153	0.261543
	B	0.685178	2.013119	-1.266459		N	-1.083356	1.945779	1.372888
	B	-0.684808	2.013085	1.266742		As	0.656590	-1.375508	1.238944
	Al	0.648766	-1.236040	-1.610456		Al	-1.270393	0.094876	1.934028
	Ga	2.731203	0.526025	-0.122364		Ga	2.584126	-0.232837	0.102872
	Ga	-2.731088	0.526404	0.122097		B	-0.002616	2.767300	0.595606
	As	1.678375	-1.538904	0.676592		H	-1.412163	2.502709	2.157717
	P	-1.283536	2.219344	-0.665514		H	0.906703	-2.517220	2.192577
	N	-1.259444	0.603840	1.666581		Al	-2.133009	1.959582	-0.309462
	N	1.259564	0.603844	-1.666622		H	2.847054	3.113547	0.348232
	P	1.284004	2.219004	0.665818		H	-1.893167	-0.040788	3.382938
	As	-1.678664	-1.538807	-0.676527		H	4.053753	-0.747805	0.195669
	H	-1.055937	-2.058448	2.900624		H	0.067228	3.912974	0.945264
	H	0.968062	2.885799	-2.035955		B	0.915682	1.946674	-1.510363
	H	-0.967422	2.885662	2.036445		Ga	-0.456669	-1.754639	-1.013697
	H	1.055477	-2.058509	-2.900492		P	1.091324	-0.071908	-1.833984
	H	4.223832	0.697369	-0.542936		As	-2.463560	-0.470731	-0.242661
	H	-4.223663	0.698140	0.542731		N	-0.428827	2.571097	-0.961638
	H	2.477046	-2.764234	1.016339		H	1.375373	2.504840	-2.464240
	H	-1.814118	3.492113	-0.983729		H	-0.597103	-3.121375	-1.758323
H	-1.656500	0.705883	2.599369	H	-3.869336	-0.984558	-0.365138		
H	1.656595	0.705868	-2.599444	H	1.496805	-0.307130	-3.171908		
H	1.814672	3.491784	0.983837	H	-0.560953	3.461860	-1.433387		
H	-2.477889	-2.763507	-1.017228	H	-3.336339	2.965951	-0.508887		
III+III open C _i	As	-1.174586	-1.370484	-2.698540	I+I C _i	As	-1.215397	-0.269952	-2.335978
	P	1.817691	-1.272248	-0.311893		P	1.889187	-1.261605	-0.524208
	N	-0.689693	-1.640073	1.125452		N	-0.881133	-1.542429	1.064240
	B	0.530210	-2.262130	0.686048		B	0.687801	-1.524333	1.133034
	Ga	-2.114894	-1.035452	-0.475062		Al	-2.240400	-1.005049	-0.204101
	Al	0.832935	-0.048944	-2.191651		Ga	1.200133	-0.038792	-2.434425
	H	2.945876	-2.085013	-0.546690		H	2.833825	-2.297483	-0.697285
	H	-1.250693	-2.320934	1.634891		H	-1.173265	-2.451410	1.419094
	Ga	2.114894	1.035452	0.475062		Al	2.240400	1.005049	0.204101
	H	-2.016022	-0.210402	-3.234786		H	-2.112293	0.289990	-3.407513
	H	0.748967	-3.411475	0.918363		H	1.145204	-2.481932	1.687417
	H	-3.433110	-1.642694	0.124738		H	-3.546894	-1.893161	-0.122530

H	1.926200	0.271046	-3.295477	H	2.098316	0.248072	-3.676992		
B	-0.530210	2.262130	-0.686048	B	-0.687801	1.524333	-1.133034		
Al	-0.832935	0.048944	2.191651	Ga	-1.200133	0.038792	2.434425		
P	-1.817691	1.272248	0.311893	P	-1.889187	1.261605	0.524208		
As	1.174586	1.370484	2.698540	As	1.215397	0.269952	2.335978		
N	0.689693	1.640073	-1.125452	N	0.881133	1.542429	-1.064240		
H	-0.748967	3.411475	-0.918363	H	-1.145204	2.481932	-1.687417		
H	-1.926200	-0.271046	3.295477	H	-2.098316	-0.248072	3.676992		
H	2.016022	0.210402	3.234786	H	2.112293	-0.289990	3.407513		
H	-2.945876	2.085013	0.546690	H	-2.833825	2.297483	0.697285		
H	1.250693	2.320934	-1.634891	H	1.173265	2.451410	-1.419094		
H	3.433110	1.642694	-0.124738	H	3.546894	1.893161	0.122530		
II+II C _i	H	-2.123311	-1.401883	-2.999034	IV+IV C _i	P	-1.182794	-0.137031	-2.244464
As	-1.301981	-0.689200	-1.959739	As	1.894707	-1.371935	-0.571627		
N	-0.599986	-1.656337	1.133203	N	-0.893200	-1.543904	1.174724		
P	2.278594	-0.665614	-0.808495	B	0.678064	-1.593730	1.252162		
Al	1.336002	-1.683973	1.155560	Ga	-2.248366	-0.969785	-0.258997		
Ga	0.924977	0.110390	-2.579578	Al	1.162441	0.046107	-2.440852		
B	-1.729842	-1.195664	0.150140	H	3.020546	-2.360325	-0.697559		
Ga	-0.924977	-0.110390	2.579578	H	-1.238944	-2.456893	1.459194		
H	1.923919	-2.998737	1.811076	Ga	2.248366	0.969785	0.258997		
H	-2.658745	-1.948602	0.094648	H	-2.101797	0.205775	-3.264192		
H	-0.870687	-2.580998	1.464849	H	1.093162	-2.574473	1.798327		
H	3.689437	-0.709116	-0.909597	H	-3.467774	-1.951804	-0.259471		
H	1.396385	0.553546	-4.000000	H	1.998910	0.243702	-3.766041		
B	1.729842	1.195664	-0.150140	B	-0.678064	1.593730	-1.252162		
Al	-1.336002	1.683973	-1.155560	Al	-1.162441	-0.046107	2.440852		
N	0.599986	1.656337	-1.133203	As	-1.894707	1.371935	0.571627		
P	-2.278594	0.665614	0.808495	P	1.182794	0.137031	2.244464		
As	1.301981	0.689200	1.959739	N	0.893200	1.543904	-1.174724		
H	2.658745	1.948602	-0.094648	H	-1.093162	2.574473	-1.798327		
H	-1.396385	-0.553546	4.000000	H	-1.998910	-0.243702	3.766041		
H	-1.923919	2.998737	-1.811076	H	2.101797	-0.205775	3.264192		
H	0.870687	2.580998	-1.464849	H	-3.020546	2.360325	0.697559		
H	-3.689437	0.709116	0.909597	H	1.238944	2.456893	-1.459194		
H	2.123311	1.401883	2.999034	H	3.467774	1.951804	0.259471		
V+V C _i	H	-2.045114	1.201354	-3.205442	VI+VI C _i	H	-2.033138	1.082553	-3.216214
As	-1.260545	0.452336	-2.162832	As	-1.225092	0.493678	-2.091783		
N	2.006289	0.809548	-0.374411	N	2.006264	0.779553	-0.426405		
P	-1.085550	1.772790	1.131933	P	-1.121721	1.807285	1.195567		
Al	1.329244	1.837298	1.114524	Ga	1.287438	1.838174	1.165624		
B	-2.103555	0.683166	-0.214132	B	-2.114236	0.709461	-0.169896		
Ga	1.221297	0.392616	-2.221803	Al	1.273222	0.400376	-2.182678		
B	2.103555	-0.683166	0.214132	B	2.114236	-0.709461	0.169896		
H	2.103610	3.159480	1.509650	H	2.118903	3.113369	1.527983		
H	2.104837	0.878918	-3.417797	H	2.087374	0.912184	-3.439617		
H	2.949810	1.143053	-0.568093	H	2.948098	1.148201	-0.552452		
H	-1.771107	2.940001	1.540718	H	-1.797219	3.009798	1.503938		
H	-3.221262	1.097333	-0.327926	H	-3.233376	1.120415	-0.280561		
Ga	-1.221297	-0.392616	2.221803	Al	-1.273222	-0.400376	2.182678		
Al	-1.329244	-1.837298	-1.114524	Ga	-1.287438	-1.838174	-1.165624		
N	-2.006289	-0.809548	0.374411	N	-2.006264	-0.779553	0.426405		
P	1.085550	-1.772790	-1.131933	P	1.121721	-1.807285	-1.195567		
As	1.260545	-0.452336	2.162832	As	1.225092	-0.493678	2.091783		
H	-2.104837	-0.878918	3.417797	H	-2.087374	-0.912184	3.439617		
H	3.221262	-1.097333	0.327926	H	3.233376	-1.120415	0.280561		
H	-2.103610	-3.159480	-1.509650	H	-2.118903	-3.113369	-1.527983		
H	-2.949810	-1.143053	0.568093	H	-2.948098	-1.148201	0.552452		
H	1.771107	-2.940001	-1.540718	H	1.797219	-3.009798	-1.503938		
H	2.045114	-1.201354	3.205442	H	2.033138	-1.082553	3.216214		

Table 5S. Calculated harmonic vibrational frequencies ω , cm^{-1} and IR intensities, I , km mol^{-1} for the $[\text{BAlGaNPAs}]_6\text{H}_6$ and $[\text{BAlGaNPAs}]_2\text{H}_{12}$ isomers.

	ω , cm^{-1}	I , km mol^{-1}	ω , cm^{-1}	I , km mol^{-1}	ω , cm^{-1}	I , km mol^{-1}
I	72.0	0.16	88.5	0.20	108.5	1.69
B-N-Al-As-Ga-P	172.0	1.79	230.4	0.72	245.7	9.77
	328.8	10.38	343.9	16.77	365.4	26.54
	416.9	22.00	449.7	24.66	484.5	23.24
	538.9	46.18	565.5	15.19	580.5	8.45
	615.6	51.79	640.0	47.98	656.1	58.19
	729.2	193.10	816.6	30.03	877.8	40.45
	1058.3	47.94	1256.1	159.40	1311.8	225.43
	1932.1	414.82	1936.1	101.47	2169.6	72.53
	2402.5	39.80	2578.9	174.57	3513.9	21.70
	II	74.8	0.04	90.8	0.36	106.9
B-N-Al-P-Ga-As	166.4	1.74	223.3	0.67	253.7	4.80
	329.0	24.66	339.2	11.18	407.9	17.47
	416.6	23.42	443.8	36.42	475.5	32.62
	510.7	9.75	551.6	47.16	574.2	18.38
	619.2	59.56	639.4	51.82	683.4	22.76
	722.4	188.49	737.6	27.35	872.3	43.27
	1052.2	63.52	1249.3	160.01	1316.8	230.99
	1931.8	330.65	1939.4	180.61	2193.0	78.92
2377.4	37.25	2584.4	169.10	3503.7	19.77	
III	73.6	0.23	86.4	0.06	116.1	1.89
B-N-Ga-As-Al-P	146.3	2.07	228.4	1.35	254.3	4.68
	323.2	15.85	363.9	12.52	409.2	27.48
	421.6	24.65	442.1	24.85	474.9	25.72
	507.7	3.04	564.5	38.41	567.3	52.62
	620.9	77.03	633.1	45.67	636.1	67.64
	683.4	129.08	814.3	28.52	868.1	36.70
	1054.7	40.45	1256.9	135.16	1314.9	242.41
	1918.4	271.44	1950.4	236.38	2173.8	72.47
2405.8	38.49	2577.3	177.09	3535.6	23.08	
IV	77.9	0.17	89.2	0.29	115.8	1.85
B-N-Ga-P-Al-As	135.5	1.86	221.4	0.75	330.3	2.66
	339.1	14.73	345.4	5.45	405.6	21.29
	421.1	53.49	440.6	20.71	465.9	26.73
	473.7	10.89	558.1	19.65	577.5	51.71
	601.4	13.06	623.5	158.25	668.0	120.52
	691.3	18.49	736.5	18.97	864.4	39.31
	1049.5	56.45	1251.2	139.72	1320.5	241.14
	1916.2	265.73	1960.6	228.73	2193.0	78.37
	2379.8	38.68	2581.8	170.40	3526.0	20.69
V	61.7	0.13	117.5	1.45	132.2	0.86
B-P-Al-N-Ga-As	150.5	0.57	180.3	0.40	248.2	2.56
	265.2	5.49	395.8	9.72	409.3	30.37
	447.7	22.70	481.3	16.54	511.0	1.35
	524.4	30.02	559.3	37.28	575.0	141.04

	587.3	23.95	683.1	141.40	688.9	176.15
	742.2	13.56	752.3	19.83	835.2	9.05
	840.9	83.27	991.7	167.74	1062.4	92.79
	1939.0	300.10	1947.8	231.35	2180.4	82.82
	2387.5	44.27	2634.1	85.89	3544.5	18.51
VI	64.5	0.10	113.1	1.27	132.6	0.94
B-P-Ga-N-Al-As	154.6	0.37	187.1	0.94	252.7	1.97
	327.7	4.09	338.2	15.20	416.8	46.49
	442.2	3.39	478.6	15.57	511.8	13.30
	517.8	10.46	561.5	37.18	576.0	143.43
	591.6	17.81	684.0	120.78	687.9	194.07
	739.0	19.80	754.3	14.43	832.8	45.98
	843.2	50.35	992.7	168.05	1067.1	90.09
	1929.4	288.18	1961.4	235.33	2185.2	80.09
	2392.5	45.05	2633.4	86.11	3543.4	18.12
I+I via AlN	46.1	6.1	55.5	0.0	98.6	0.0
	115.3	1.2	126.4	0.1	140.3	0.2
	154.1	1.7	191.0	2.4	205.8	2.4
	208.0	8.8	213.9	7.9	262.6	0.1
	272.7	9.9	287.9	3.4	303.3	22.8
	314.8	12.8	323.7	0.1	335.0	16.5
	355.9	8.8	388.3	1.2	388.9	2.8
	430.0	0.8	442.1	6.1	443.2	7.6
	484.2	5.2	486.9	0.2	494.0	14.7
	498.3	4.7	503.5	13.1	512.1	0.6
	516.0	4.0	522.2	46.2	547.8	56.1
	550.5	56.7	554.5	70.3	556.3	2.3
	589.0	0.2	591.7	91.4	602.1	21.1
	621.8	92.1	647.6	22.7	667.5	246.2
	719.7	48.6	763.5	8.8	827.4	24.0
	830.6	7.0	865.8	45.8	891.8	58.6
	899.5	237.3	903.6	191.9	1021.0	25.0
	1033.4	231.4	1185.4	39.7	1197.6	4.6
	1928.5	92.9	1935.5	516.1	1963.2	167.1
	1966.8	270.7	2239.4	162.2	2239.9	7.6
	2405.3	19.3	2406.3	59.7	2562.8	206.1
	2563.6	2.0	3511.2	15.1	3513.3	32.5
I+I via BN	83.6	0.1	91.1	0.3	114.5	0.0
	120.5	0.9	131.3	0.0	136.9	0.4
	150.8	0.0	180.8	0.3	193.6	7.3
	214.2	6.6	218.3	0.1	255.9	6.9
	271.4	1.4	276.3	0.8	289.0	17.9
	314.0	19.2	314.1	11.2	320.4	6.3
	334.6	9.6	341.2	0.0	349.8	6.3
	432.4	0.3	436.4	1.5	449.6	0.1
	454.9	2.4	475.1	0.0	489.2	15.6
	491.1	1.1	498.6	55.6	500.9	0.8
	525.3	51.7	526.0	2.1	529.4	49.2
	547.1	5.2	552.3	66.0	569.0	151.3
	591.2	4.5	596.2	53.7	643.1	244.4
	658.2	0.0	707.4	14.1	710.8	8.2

	727.6	133.6	762.9	3.5	883.3	176.5
	897.0	0.0	926.4	19.8	953.2	127.5
	1029.7	197.3	1043.0	123.4	1092.6	22.9
	1106.9	40.9	1184.6	5.8	1193.9	47.7
	1923.9	527.3	1925.3	84.1	1951.3	272.5
	1954.1	195.6	2229.0	88.4	2229.1	50.6
	2439.7	48.1	2439.9	4.0	2533.4	98.9
	2541.0	252.8	3496.5	41.8	3496.7	9.4
I+I via BP	56.4	0.8	61.4	1.3	109.8	1.4
	115.2	0.1	129.4	0.2	142.1	0.7
	167.3	1.1	189.3	3.0	202.1	4.9
	218.4	0.5	222.7	4.4	248.9	0.7
	273.2	12.0	273.3	10.1	284.6	25.5
	292.8	2.5	294.9	10.2	309.7	7.6
	314.9	5.9	359.4	5.7	377.5	7.1
	382.8	3.8	406.4	7.0	430.5	0.1
	433.1	1.5	464.0	7.9	473.2	1.0
	481.0	2.9	491.1	0.6	495.8	21.3
	500.5	1.6	509.4	19.4	511.1	40.1
	545.8	32.3	552.7	13.5	566.1	7.6
	566.5	15.6	590.5	204.3	603.7	50.9
	621.1	195.6	639.6	261.3	688.4	11.6
	741.9	21.4	777.1	9.1	837.7	9.1
	845.3	26.1	868.7	116.2	876.2	30.9
	891.7	121.2	937.0	124.8	1019.6	150.3
	1022.7	28.8	1197.1	3.8	1199.1	20.9
	1918.9	396.3	1921.4	132.6	1963.4	522.3
	1965.9	2.4	2260.2	44.6	2260.5	66.3
	2425.6	23.2	2426.8	41.1	2556.1	153.9
	2556.8	144.6	3474.3	15.9	3474.5	21.0
I+I rotated	70.1	0.2	86.6	0.1	114.2	0.7
	117.4	0.9	128.8	0.3	135.2	0.2
	184.7	2.3	193.2	2.1	200.7	2.2
	212.5	2.9	215.8	5.4	253.2	5.7
	255.4	14.0	275.2	4.4	288.3	8.5
	296.8	11.4	302.5	13.3	309.8	4.2
	323.6	9.1	368.7	5.2	403.7	5.5
	423.6	2.0	433.3	5.3	445.6	0.6
	477.2	7.3	487.0	4.7	490.1	6.1
	490.7	7.6	499.5	20.8	502.9	19.7
	515.2	25.9	524.4	10.8	542.9	8.2
	543.5	38.1	569.8	26.6	570.2	141.2
	589.4	72.9	603.8	69.8	622.5	17.3
	630.9	70.6	670.3	245.7	712.8	20.0
	742.5	11.5	771.0	22.0	839.0	39.2
	868.8	74.2	881.6	78.4	899.9	73.7
	951.4	100.3	1000.7	53.0	1032.9	246.1
	1105.2	57.5	1180.8	18.4	1209.9	19.9
	1920.7	270.7	1931.6	334.1	1952.7	219.8
	1964.2	234.5	2226.7	68.3	2259.0	65.3
	2409.1	33.9	2420.5	42.9	2536.6	172.6
	2561.0	141.1	3498.5	26.9	3503.1	24.5

III+III open C_i	65.6	1.1	85.1	0.0	89.6	0.1	
	97.9	0.0	103.3	2.1	111.5	0.0	
	142.9	0.3	146.0	0.0	173.7	2.6	
	178.2	0.0	195.7	0.0	220.9	0.0	
	226.9	18.6	245.5	7.7	252.9	0.0	
	258.1	9.4	272.1	0.0	310.3	45.6	
	311.7	0.0	316.9	25.0	333.5	0.0	
	341.2	29.3	394.1	48.3	421.6	0.0	
	445.1	26.1	452.9	0.0	476.5	0.0	
	481.2	20.8	517.5	0.0	521.4	0.0	
	531.5	20.1	544.6	0.0	547.9	33.7	
	553.1	46.9	573.2	0.0	590.7	312.5	
	601.3	0.0	609.5	160.7	635.1	45.2	
	643.2	0.0	652.3	302.7	658.8	0.0	
	784.5	0.0	785.3	5.2	803.7	0.0	
	808.9	48.6	983.3	75.4	984.1	0.0	
	1028.0	19.9	1029.0	0.0	1194.4	0.0	
	1229.1	390.4	1261.5	71.3	1263.2	0.0	
	1909.5	0.0	1909.7	431.0	1934.4	508.9	
	1935.5	0.0	2133.9	0.0	2134.3	153.6	
	2464.5	24.8	2464.7	0.0	2614.5	273.6	
	2615.2	0.0	3479.3	55.3	3479.4	0.0	
	I+I C_i	47.0	7.1	59.8	0.0	98.9	0.6
		109.8	0.0	123.5	0.0	141.3	5.0
		169.0	0.0	173.1	1.4	191.3	0.0
		221.8	6.8	233.5	0.0	253.4	11.2
258.3		0.0	285.1	24.2	307.0	17.9	
308.7		0.0	336.5	29.2	349.7	0.0	
359.2		0.0	365.0	13.3	377.8	9.6	
388.0		0.0	393.5	0.0	395.6	4.7	
457.7		0.0	462.9	6.6	476.3	0.0	
487.3		0.0	492.8	11.6	505.2	9.3	
505.6		0.0	511.4	28.1	529.1	0.0	
529.2		98.9	547.4	0.0	552.1	34.8	
569.5		248.3	583.0	0.0	606.7	0.0	
607.7		10.6	630.4	0.0	641.9	372.7	
726.3		0.0	739.1	40.7	845.6	17.8	
847.2		0.0	870.8	0.0	891.5	270.6	
898.4		0.0	905.9	243.3	1026.8	0.0	
1033.7		213.8	1200.8	0.0	1201.3	21.7	
1925.7		538.9	1926.9	0.0	1965.8	514.1	
1968.0		0.0	2241.8	157.2	2242.3	0.0	
2440.7		50.5	2441.0	0.0	2551.9	225.1	
2552.4		0.0	3476.5	34.7	3476.5	0.0	
II+II C_i		79.7	0.4	93.8	0.0	111.4	3.3
		127.3	0.0	141.8	0.0	156.7	0.0
		159.5	5.8	170.5	0.0	172.6	9.0
		221.0	6.1	222.0	0.0	234.2	5.6
	264.1	0.0	273.2	7.2	286.0	0.0	
	293.7	15.7	311.4	11.9	329.1	0.0	
	345.4	0.0	350.7	8.7	373.8	0.0	
	378.6	36.3	402.2	0.0	422.3	10.0	

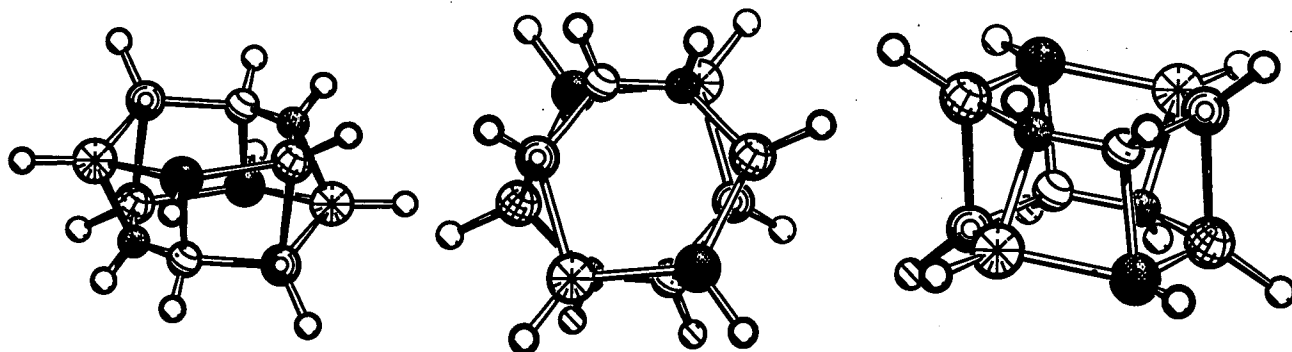
	424.1	18.4	457.6	0.0	467.9	0.0
	481.2	2.5	486.5	0.0	504.9	27.6
	512.8	0.0	520.4	51.7	536.5	68.7
	542.6	0.0	553.6	0.0	563.1	210.0
	591.7	0.0	595.2	19.8	610.9	0.0
	641.7	10.7	647.1	425.5	660.1	0.0
	700.3	0.0	711.7	40.5	835.4	22.9
	838.8	0.0	865.3	0.0	889.2	335.0
	907.2	0.0	912.3	189.9	1020.0	0.0
	1026.0	194.5	1203.3	0.0	1203.9	21.4
	1925.0	567.2	1926.2	0.0	1983.2	538.5
	1985.8	0.0	2239.2	139.2	2240.1	0.0
	2426.2	62.6	2426.7	0.0	2555.7	237.6
	2556.2	0.0	3471.5	35.4	3471.5	0.0
IV+IV C _i	77.3	0.2	88.8	0.0	109.1	3.4
	115.8	0.0	128.0	0.0	156.7	2.1
	167.3	0.0	171.1	7.4	184.8	0.0
	196.1	0.0	209.0	5.6	223.9	13.0
	270.6	0.0	275.7	3.0	307.6	21.1
	311.0	0.0	316.8	0.0	325.8	20.3
	341.6	7.9	356.8	0.0	364.8	0.0
	383.5	30.0	423.0	8.6	432.8	0.0
	459.2	13.1	463.1	0.0	480.0	0.0
	487.7	0.0	490.1	43.1	494.2	3.2
	505.1	0.0	516.3	77.1	538.5	48.5
	540.9	0.0	557.6	0.0	566.6	132.8
	569.3	0.0	603.9	176.3	604.0	0.0
	617.0	338.8	644.3	5.6	669.4	0.0
	702.9	0.0	714.0	54.1	831.2	0.0
	849.8	206.2	883.6	106.6	883.8	0.0
	911.3	0.0	917.8	229.9	1009.5	0.0
	1015.9	193.0	1182.4	0.0	1182.7	14.3
	1933.6	512.2	1934.7	0.0	1946.0	567.5
	1948.0	0.0	2252.7	126.8	2253.5	0.0
	2427.6	61.9	2428.0	0.0	2557.0	247.1
	2557.5	0.0	3497.0	0.0	3497.1	37.4
V+V C _i	79.2	0.1	90.8	0.0	121.7	0.0
	141.5	1.4	147.2	0.0	155.4	2.6
	177.4	5.1	184.7	0.0	197.4	0.0
	212.5	8.3	216.0	0.0	250.0	5.5
	250.6	0.0	265.9	4.7	281.2	14.5
	281.5	0.0	312.7	8.4	328.0	0.0
	339.1	12.9	354.7	0.0	387.9	8.1
	411.1	0.0	418.3	14.7	424.5	0.0
	460.8	9.1	466.6	0.0	486.3	15.9
	489.5	0.0	504.2	0.0	512.6	53.6
	521.7	0.0	526.2	72.1	531.2	0.0
	565.3	118.7	574.8	0.0	582.6	0.0
	588.8	81.3	612.7	174.1	615.5	0.0
	639.4	213.4	685.1	115.5	687.6	0.0
	743.3	0.0	746.6	79.9	778.4	0.0
	780.6	90.9	910.7	0.0	928.8	312.7

	958.3	96.1	960.0	0.0	979.8	104.3
	983.0	0.0	1119.8	0.0	1120.2	21.2
	1925.1	597.2	1926.5	0.0	1967.1	550.7
	1969.0	0.0	2233.6	149.7	2234.0	0.0
	2434.7	52.6	2435.0	0.0	2554.1	216.5
	2554.7	0.0	3466.9	35.2	3467.0	0.0
VI+VI C_i	78.1	0.2	85.5	0.0	125.2	0.0
	128.9	2.3	156.2	0.0	159.8	0.9
	165.4	0.0	190.5	0.0	204.5	7.2
	214.0	3.2	223.1	0.0	230.3	7.2
	264.3	0.0	269.7	3.1	289.2	0.0
	290.0	25.0	314.9	0.7	327.4	0.0
	332.5	8.3	363.1	0.0	370.6	12.5
	389.3	0.0	430.3	1.1	433.4	0.0
	462.9	4.1	470.7	0.0	484.8	26.0
	486.3	0.0	501.9	0.0	508.9	56.0
	518.9	0.0	529.3	0.0	529.6	88.8
	563.2	92.8	571.7	0.0	586.6	0.0
	588.2	126.9	610.9	0.0	612.4	197.3
	644.9	124.2	683.4	139.3	689.4	0.0
	733.4	0.0	734.0	109.1	777.7	0.0
	779.6	84.9	911.4	0.0	928.1	280.6
	958.9	153.3	961.3	0.0	980.7	81.4
	981.9	0.0	1117.5	0.0	1118.1	18.8
	1922.0	603.7	1923.2	0.0	1948.9	545.0
	1950.9	0.0	2245.0	141.1	2245.6	0.0
	2436.7	53.5	2437.0	0.0	2555.1	218.5
	2555.7	0.0	3469.0	35.1	3469.1	0.0

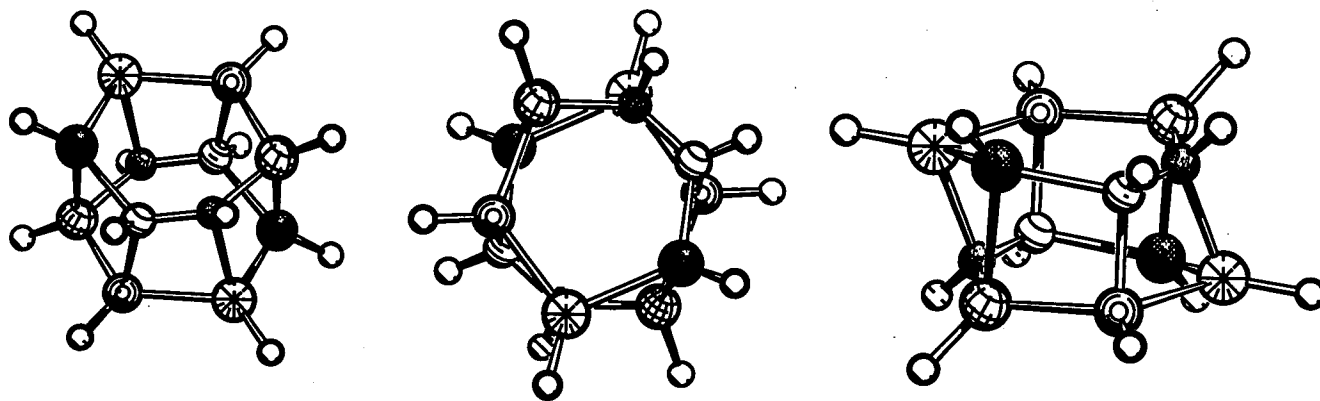
Table 6S. Total energies E^{tot} (0K, without ZPE correction), Hartree for all species considered in the present work. B3LYP/TZVP level of theory.

Compound	E^{tot}	Compound	E^{tot}
H ₂	-1.1795711	HBNH	-80.8391733
BH	-25.2989284	HBPH	-367.378167
AlH	-243.00189	HBAsh	-2261.922934
GaH	-1925.472486	HAlNH	-298.3732133
NH	-55.2435073	HAIPH	-584.9885213
PH	-341.9014328	HAlAsH	-2479.542584
AsH	-2236.462113	HGaNH	-1980.81885
CH	-38.4958576	HGaPH	-2267.451038
C ₂ H ₂	-77.3622700	HGaAsH	-4162.00515
C ₂ H ₆	-79.8619986	C ₆ H ₆	-232.3279992
H ₃ BNH ₃	-83.2546462	C ₈ H ₈	-309.5508324
H ₃ BPH ₃	-369.8248871	C ₁₂ H ₁₂	-464.4278076
H ₃ BAsH ₃	-2264.355497	[HBNH] ₃	-242.761912
H ₃ AlNH ₃	-300.8541204	[HBPH] ₃	-1102.331941
H ₃ AlPH ₃	-587.4155713	[HBAsh] ₃	-6785.930995
H ₃ AlAsH ₃	-2481.951465	[HAlNH] ₃	-895.5081018
H ₃ GaNH ₃	-1983.294311	[HAIPH] ₃	-1755.19454
H ₃ GaPH ₃	-2269.862604	[HAlAsH] ₃	-7438.835622
H ₃ GaAsH ₃	-4164.3992643	[HGaNh] ₃	-5942.756505
[HBNH] ₄	-323.5523204	[HGAPH] ₃	-6802.540169
[HBPH] ₄	-1469.727954	[HGAsH] ₃	-12486.18807
[HBAsh] ₄	-9047.864128	[HBNH] ₆	-485.4123262
[HAlNH] ₄	-1194.095101	[HBPH] ₆	-2204.6768260
[HAIPH] ₄	-2340.300352	[HBAsh] ₆	-13571.8774690
[HAlAsH] ₄	-9918.470703	[HAlNH] ₆	-1791.1965066
[HGaNh] ₄	-7923.728886	[HAIPH] ₆	-3510.4993407
[HGAPH] ₄	-9070.062349	[HAlAsH] ₆	-14877.7546955
[HGAsH] ₄	-16648.24519	[HGaNh] ₆	-11885.6394580
I	-4828.0202371	[HGAPH] ₆	-13605.1418248
II	-4828.0152253	[HGAsH] ₆	-24972.4163274
III	-4828.0052531	I+I via BN	-9656.0738348
IV	-4827.9992600	I+I rotated	-9656.0684180
V	-4827.9823866	I+I via AlN	-9656.0500534
VI	-4827.9810839	I+I via BP	-9656.0292339
		I+I C _i	-9656.0169347
		II+II C _i	-9656.020331
		IV+IV C _i	-9656.018652
		V+V C _i	-9656.032309
		VI+VI C _i	-9656.0316847
		III+III open C _i	-9656.0931804

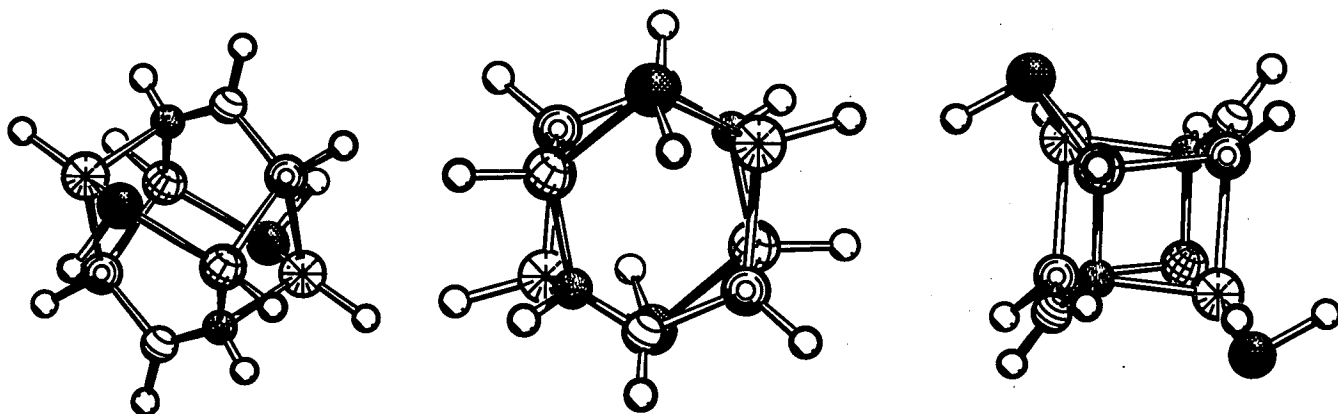
Structures of the $[\text{BaIGaNPAs}]_2\text{H}_{12}$ isomers



I+I (C_i)

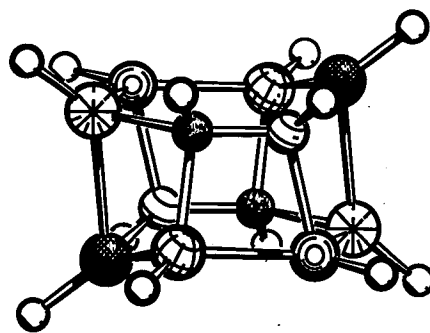
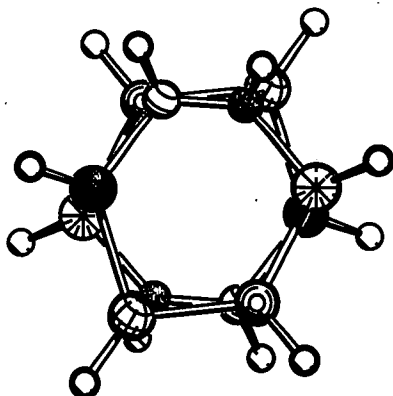
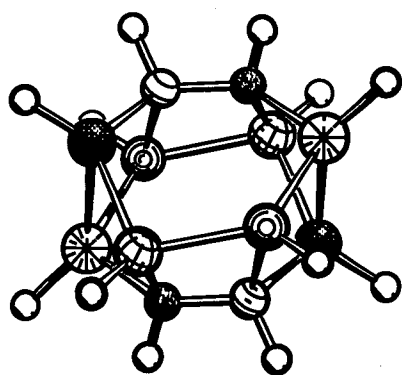


II+II (C_i)

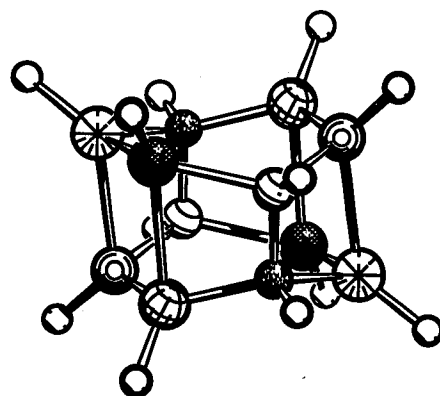
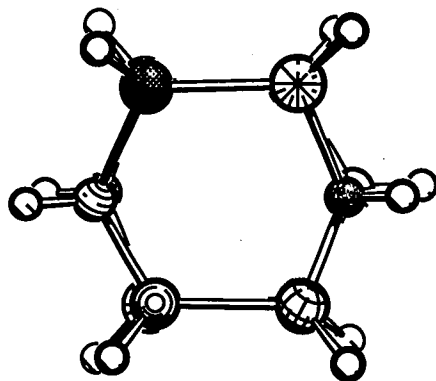
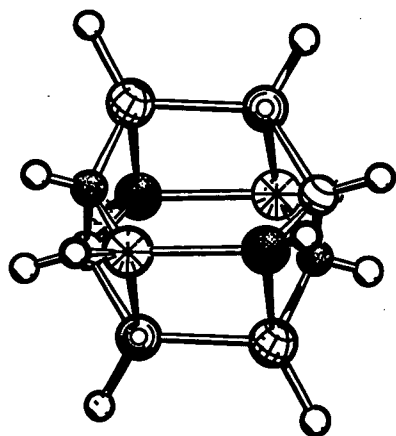


III+III open (C_i)

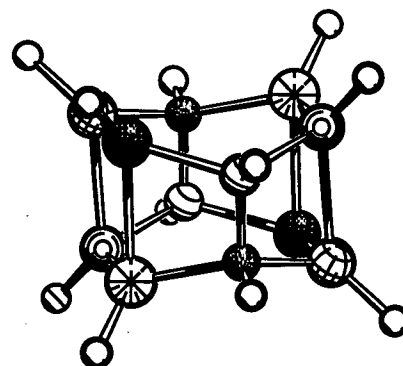
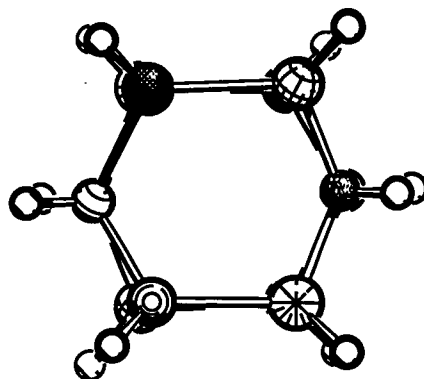
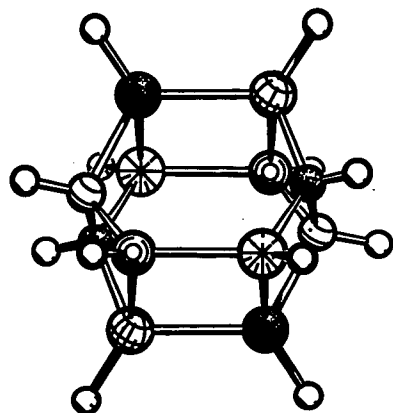
Structures of the $[\text{BaIGaNPAs}]_2\text{H}_{12}$ isomers



IV+IV (C_i)

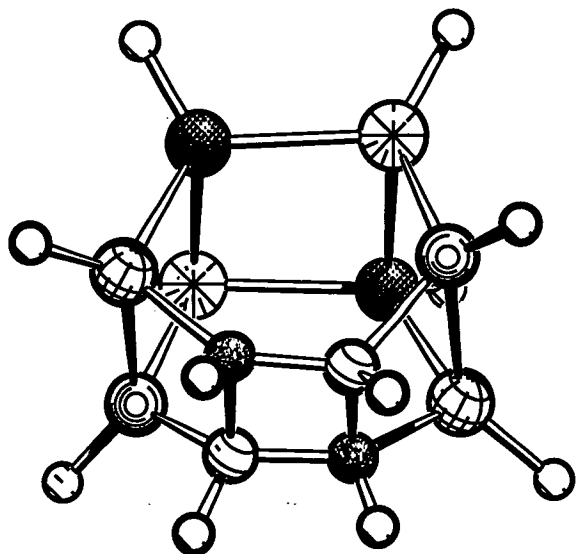


V+V (C_i)

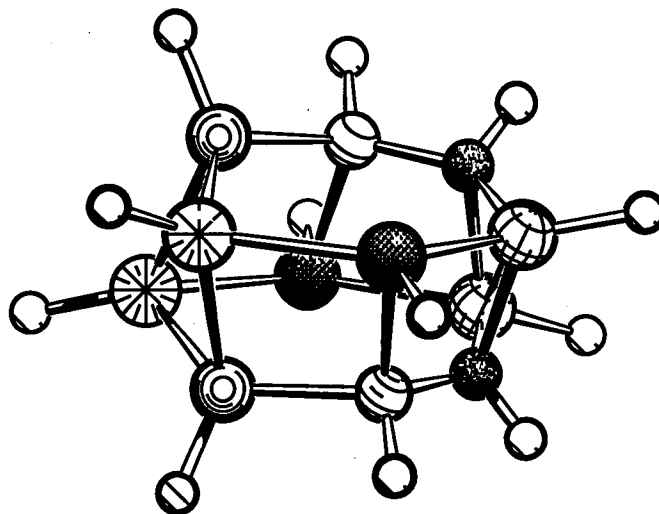


VI+VI (C_i)

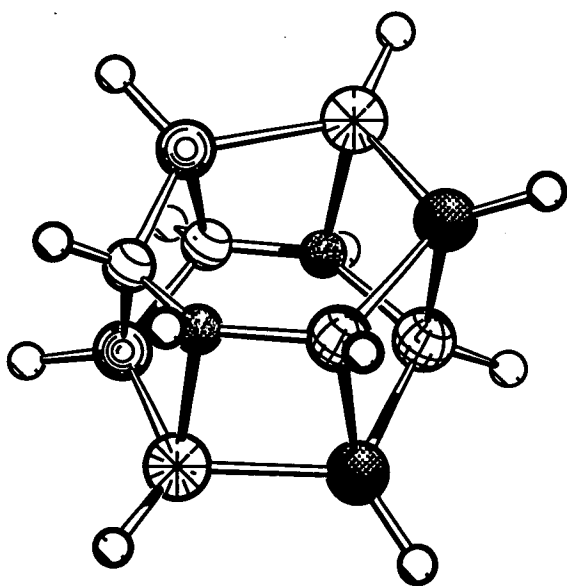
Structures of the $[\text{BAlGaNPAs}]_2\text{H}_{12}$ isomers



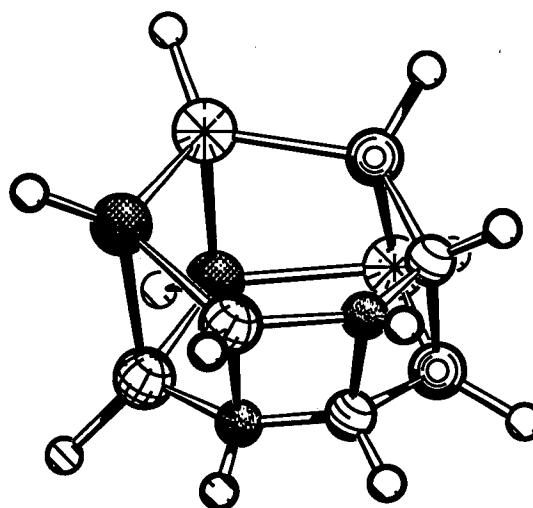
I+I via BN



I+I via AlN



I+I via BP



I+I 'rotated'