Supplementary Information.

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Complete reference 43 citation **S2**

Table 1S. Computed Total energy, E^{o}_{0}, Hartree; Zero-point vibrational energy ZPVE, kcal mol^{-1}; Sum of electronic and thermal Enthalpies, H^{o}_{298}, Hartree; Standard entropy S^{o}_{298}, cal mol^{-1} K^{-1}. B3LYP/TZVP level of theory. **S3**

Table 2S. Relative energies E in kJ mol^{-1} (0K, without ZPE corrections) of the tetrameric species with respect to the cubane $[HMYH]_4$ structure. B3LYP/TZVP level of theory. Structures are minima on PES, if not noted otherwise. **S5**

Table 3S. Relative energies of C_2 *ring*-$[HMYH]_4$ isomers with respect to D_{2d} *ring*-$[HMYH]_4$ isomers. ΔE in kJ mol^{-1} (0K, without ZPE corrections). B3LYP/TZVP level of theory. Structures are minima on PES, if not noted otherwise. **S5**

Figure 1S. Optimized structures of alternative $[HMYH]_4$ ring isomers. B3LYP/TZVP level of theory. All distances in angstroms, all angles in degrees. **S6**

Table 4S. Optimized geometries of compounds. xyz coordinates in angstroms. B3LYP/TZVP level of theory. **S7**

Table 5S. Unscaled Harmonic vibrational frequencies (ω, cm^{-1}) scaled Harmonic vibrational frequencies (ν^{a}, cm^{-1}) and Infra-red Intensities (I, km mol^{-1}) of the studied compounds. B3LYP/TZVP level of theory. **S32**

[a)]Scaled according to equation $\nu = 0.9461\omega+22.1$ (Timoshkin, A.Y.; Bettinger, H.F.; Schaefer, H.F. *J. Am. Chem. Soc.* **1997**, *119*, 5668).

Complete reference 43 citation:

43 Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Gill, P.M.W.; Johnson, B.G.; Robb, M.A.; Cheeseman, J.R.; Keith, T.; Petersson, G.A.; Montgomery, J.A.; Raghavachari, K.; Al-Laham, M.A.; Zakrzewski, V.G.; Ortiz, J.V.; Foresman, J.B.; Cioslowski, J.; Stefanov, B.B.; Nanayakkara, A.; Challacombe, M.; Peng, C.Y.; Ayala, P.Y.; Chen, W.; Wong, M.W.; Andres, J.L.; Replogle, E.S.; Gomperts, R.; Martin, R.L.; Fox, D.J.; Binkley, J.S.; Defrees, D.J.; Baker, J.; Stewart, J.P.; Head-Gordon, M.; Gonzalez, C.; and Pople, J.A. GAUSSIAN 94 Revision C.3, Gaussian, Inc., Pittsburgh PA, **1995**.

Table 1S. Computed Total energy, E^o_0, Hartree; Zero-point vibrational energy ZPVE, kcal mol^{-1}; Sum of electronic and thermal Enthalpies, H^o_{298}, Hartree; Standard entropy S^o_{298}, cal mol^{-1} K^{-1}. B3LYP/TZVP level of theory.

Compound	Point group	E^o_0	ZPVE	H^o_{298}	S^o_{298}
tetrahedral $[BNH_2]_4$	C_1	-323.4335546	74.84021	-323.301318	105.448
tetrahedral $[BPH_2]_4$	S_4	-1469.6836787	54.09820	-1469.583061	116.040
tetrahedral $[BAsH_2]_4$	S_4	-9047.8409626	49.42124	-9047.746555	130.193
tetrahedral $[AlNH_2]_4$	C_1	-1193.8785034	63.95377	-1193.758700	134.185
tetrahedral $[AlPH_2]_4$	S_4	-2340.1797123	45.01759	-2340.088617	148.823
tetrahedral $[AlAsH_2]_4$	S_4	-9918.3603356	41.78444	-9918.274094	152.462
tetrahedral $[GaNH_2]_4$	C_1	-7923.6451165	61.22063	-7923.527400	152.095
tetrahedral $[GaPH_2]_4$	S_4	-9070.0184449	43.72991	-9069.928069	159.218
tetrahedral $[GaAsH_2]_4$	S_4	-16648.2041567	40.43339	-16648.118626	164.569
ring $[BNH_2]_4$	C_{2h}	-323.2845269	81.28079	-323.146726	79.794
ring $[BPH_2]_4$	C_{2h}	-1469.5315265	56.61778	-1469.429705	95.834
ring $[BAsH_2]_4$	C_1	-9047.7530473	50.08681	-9047.658734	120.730
ring $[AlNH_2]_4$	C_{2h}	-1193.8886042	69.07825	-1193.764961	108.844
ring $[AlPH_2]_4$	C_{2h}	-2340.1713119	47.64613	-2340.078446	124.419
ring $[AlAsH_2]_4$	C_{2h}	-9918.3313819	42.38325	-9918.244943	139.637
ring $[GaNH_2]_4$	C_{2h}	-7923.6919073	66.44242	-7923.570687	122.867
ring $[GaPH_2]_4$	C_{2h}	-9070.025245	44.97115	-9069.934254	142.768
ring $[GaAsH_2]_4$	C_{2h}	-16648.1945746	39.98248	-16648.109625	158.566
cubane-$[HBNH]_4$	T_d	-323.5523204	77.01991	-323.422979	69.489
cubane-$[HBPH]_4$	T_d	-1469.727954	57.69538	-1469.6257	85.628
cubane-$[HBAsH]_4$	T_d	-9047.864128	53.22610	-9047.767064	97.793
cubane-$[HAlNH]_4$	T_d	-1194.095101	60.44001	-1193.988531	84.933
cubane-$[HAlPH]_4$	T_d	-2340.300352	44.06115	-2340.214659	109.013
cubane-$[HAlAsH]_4$	T_d	-9918.470703	40.71593	-9918.388513	121.622
cubane-$[HGaNH]_4$	T_d	-7923.728886	58.24803	-7923.624188	96.043
cubane-$[HGaPH]_4$	T_d	-9070.062349	42.78200	-9069.97748	118.737
cubane-$[HGaAsH]_4$	T_d	-16648.24519	39.15462	-16648.16401	131.927
ladder-$[HBNH]_4$	C_i	-323.5679018	76.37401	-323.438167	81.081
ladder-$[HBPH]_4$	C_i	-1469.7366537	58.05583	-1469.632531	99.854
ladder-$[HBAsH]_4$	C_i	-9047.8851661	54.15233	-9047.785710	112.701
ladder-$[HAlNH]_4$	C_i	-1194.0201388	59.34744	-1193.913873	98.885

ladder-$[HAlPH]_4$	C_i	−2340.2642739	43.30424	−2340.178871	124.036
ladder-$[HAlAsH]_4$	C_i	−9918.4470995	40.98650	−9918.364192	134.881
ladder-$[HGaNH]_4$	C_i	−7923.6666924	57.00137	−7923.562546	111.019
ladder-$[HGaPH]_4$	C_i	−9070.0396398	42.59518	−9069.954452	132.892
ladder-$[HGaAsH]_4$	C_i	−16648.2338121	39.71357	−16648.151641	144.821
ring-$[HBNH]_4$	D_{4h}	−323.6544730	78.43051	−323.520823	81.756
ring-$[HBPH]_4$	D_{2d}	−1469.7670756	57.82434	−1469.662551	101.806
ring-$[HBAsH]_4$	D_{2d}	−9047.9030402	53.53098	−9047.803916	113.650
ring-$[HAlNH]_4$	D_{4h}	−1194.0056257	58.29089	−1193.899637	104.548
ring-$[HAlPH]_4$	D_{2d}	−2340.2574174	43.29236	−2340.171535	126.687
ring-$[HAlAsH]_4$	D_{2d}	−9918.4451382	40.13707	−9918.362858	138.921
ring-$[HGaNH]_4$	D_{4h}	−7923.6635510	56.56582	−7923.558887	117.922
ring-$[HGaPH]_4$	D_{2d}	−9070.0507918	42.34883	−9069.965491	136.119
ring-$[HGaAsH]_4$	D_{2d}	−16648.2478696	38.93728	−16648.166321	149.451
ring-$[HBPH]_4$	C_{4v} (TS)	−1469.7591064	57.91696	−1469.655136	98.069
ring-$[HBAsH]_4$	C_2	−9047.8924481	54.49984	−9047.791947	116.010
ring-$[HAlPH]_4$	C_2	−2340.2511458	43.35460	−2340.165095	130.850
ring-$[HAlAsH]_4$	C_2	−9918.4398323	41.16430	−9918.356237	141.190
ring-$[HGaPH]_4$	C_2	−9070.0428811	42.86386	−9069.956956	138.355
ring-$[HGaAsH]_4$	C_2	−16648.2411756	39.75243	−16648.158732	150.425
ring-$[H_2BN]_4$	D_{4h}	−323.2727186	69.40300	−323.152496	84.679
ring-$[H_2BP]_4$	D_{2d}	−1469.7020534	56.62994	−1469.597650	109.372
ring-$[H_2BAs]_4$	D_{2d}	−9047.8977404	53.63957	−9047.795958	124.965
ring-$[H_2AlN]_4$	D_2	−1193.5758957	47.32095	−1193.486074	111.325
ring-$[H_2GaN]_4$	D_2	−7923.3263501	46.37447	−7923.237093	122.616
bridged ring-$[H_2BN]_4$	C_2	−323.1694764	69.37219	−323.050542	80.585
bridged ring-$[H_2BP]_4$	D_{2h}	−1469.7657838	59.53591	−1469.659369	94.647
bridged ring-$[H_2BAs]_4$	D_{2h}	−9047.9616469	56.58574	−9047.858010	107.950
bridged ring-$[H_2AlN]_4$	C_2	−1193.5861472	47.87966	−1193.496991	101.252
bridged ring-$[H_2AlP]_4$	D_{2h}	−2340.1846157	40.83086	−2340.102953	119.885
bridged ring-$[H_2AlAs]_4$	D_{2h}	−9918.4127194	38.80566	−9918.332586	132.034
bridged ring-$[H_2GaN]_4$	C_2	−7923.3054514	46.67373	−7923.216842	113.827
bridged ring-$[H_2GaP]_4$	D_{2h}	−9069.9672654	40.49729	−9069.885241	130.013
bridged ring-$[H_2GaAs]_4$	D_{2h}	−16648.2023829	38.37626	−16648.121954	142.163

Table 2S. Relative energies ΔE, kJ mol^{-1} (0K, without ZPE correction) of the tetrameric species with respect to the cubane $[HMYH]_4$ structure. B3LYP/TZVP level of theory. Structures are minima on PES, if not noted otherwise.

M,Y	*tetrahedral*-$[MYH_2]_4$		*ring*-$[MYH_2]_4$		*cubane*-$[HMYH]_4$	*ladder*-$[HMYH]_4$	*ring*-$[HMYH]_4$		$[H_2MY]_4$		*bridged*-$[H_2MY]_4$	
Point group	S_4	C_1	C_{2h}	C_1	T_d	C_i	D_{4h}	D_{2d}	D_{4h}	D_2	D_{2h}	C_2
BN	311.8[a]	311.8	703.1		0.0	-40.9	-268.2		734.1			1005.2
BP	116.2		515.7		0.0	-22.8		-102.7		68.0[b]	-99.3	
BAs	60.8		589.7[a]	291.6	0.0	-55.2		-102.2		-88.2[b]	-256.0	
AlN	570.2[a]	568.7	542.2		0.0	196.8	234.9			1363.2		1336.3
AlP	316.7		338.8		0.0	94.7		112.7			303.9	
AlAs	289.8		365.8		0.0	62.0		67.1			152.2	
GaN	221.3[a]	219.9	97.1		0.0	163.3	171.5			1056.8	1133.9[a]	1111.7
GaP	115.3		97.4		0.0	59.6		30.3			249.6	
GaAs	107.7		132.9		0.0	29.9		-7.0			112.4	

[a] TS ; [b] D_{2d} point group.

Table 3S. Relative energies of C_2 *ring*-$[HMYH]_4$ isomers with respect to D_{2d} *ring*-$[HMYH]_4$ isomers. ΔE, kJ mol^{-1} (0K, without ZPE correction). B3LYP/TZVP level of theory. Structures are minima on PES, if not noted otherwise.

M,Y	ΔE
BN	-
BP	20.9[a]
BAs	27.8
AlN	-
AlP	16.5
AlAs	13.9
GaN	-
GaP	20.8
GaAs	17.6

[a] C_{4v} symmetric TS. Optimization in C_2 point group results in D_{2d} ring structure.

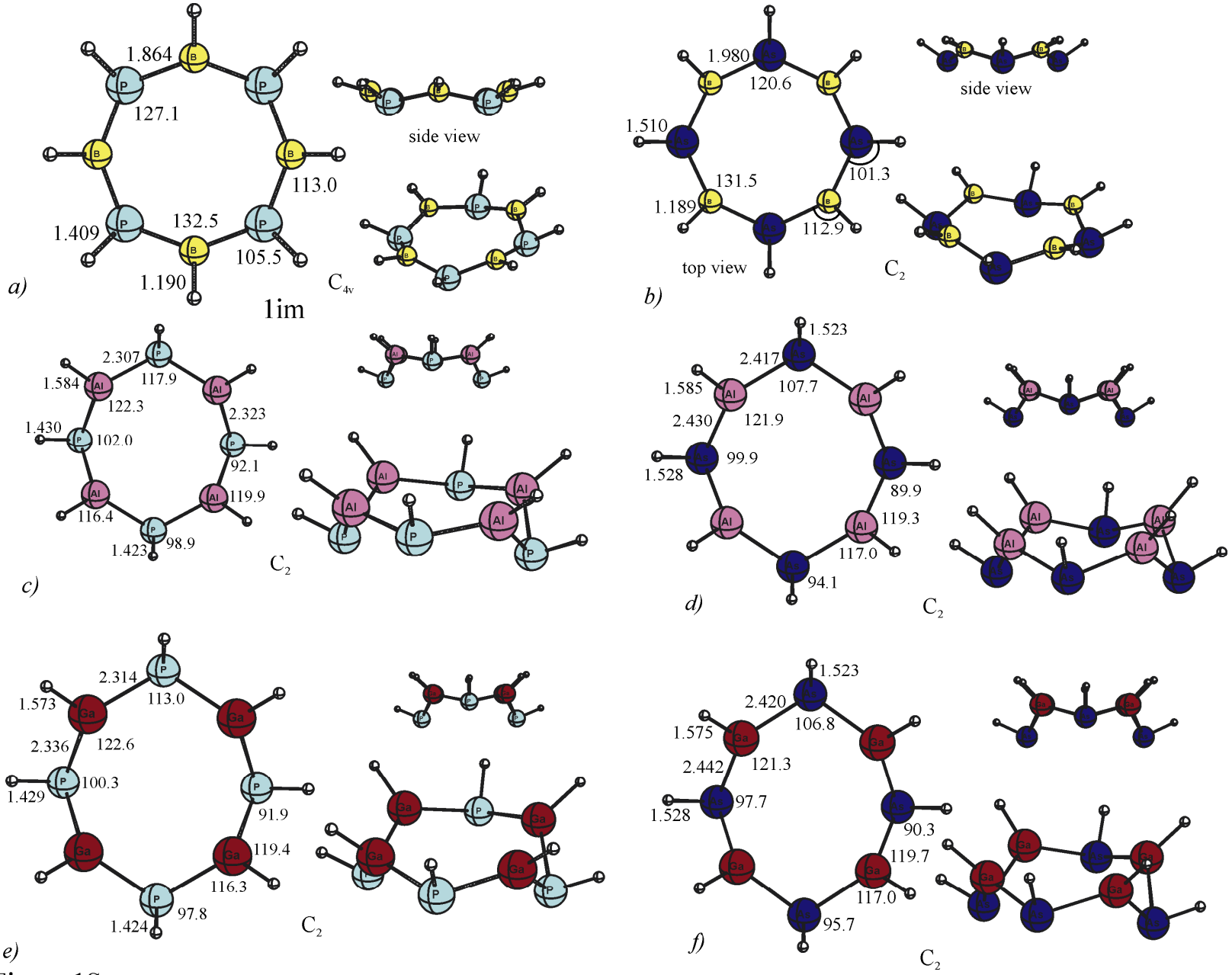
1.864
127.1
113.0
1.409
132.5
105.5
1.190
side view
C_{4v}
1im
a)
1.980
120.6
1.510
131.5
101.3
1.189
112.9
top view
side view
C_2
b)
2.307
1.584
117.9
122.3
2.323
1.430
102.0
92.1
119.9
116.4
1.423
98.9
C_2
c)
1.523
2.417
1.585
107.7
121.9
2.430
99.9
1.528
89.9
119.3
117.0
94.1
C_2
d)
2.314
113.0
1.573
122.6
2.336
100.3
1.429
91.9
119.4
116.3
97.8
1.424
C_2
e)
1.523
2.420
106.8
1.575
121.3
2.442
97.7
1.528
90.3
119.7
117.0
95.7
C_2
f)

Figure 1S

Table 4S. Optimized geometries of compounds. xyz coordinates in angstroms. B3LYP/TZVP level of theory.

$[MYH_2]_4$ structures.
Tetrahedral structures.

tetrahedral $[BNH_2]_4$ C_1

B	0.85533	0.14132	-0.57468
B	-0.84376	-0.16205	-0.586
B	0.14552	-0.8384	0.59743
B	-0.15742	0.8611	0.56186
N	2.0069	0.36058	-1.38013
N	0.3721	-1.96607	1.43411
N	-1.97928	-0.41368	-1.40505
N	-0.40086	2.01984	1.35034
H	2.57707	1.18726	-1.30081
H	2.17297	-0.15489	-2.22934
H	-0.12876	-2.09993	2.29775
H	1.20172	-2.53362	1.36685
H	-2.54592	-1.24098	-1.30798
H	-2.12096	0.06105	-2.2821
H	0.08911	2.19078	2.21366
H	-1.23558	2.57569	1.25401

tetrahedral $[BPH_2]_4$ S_4

B	0.0102213649	0.8437112572	0.5902150016
B	-0.0102213649	-0.8437112572	0.5902150016
B	-0.8437112572	0.0102213649	-0.5902150016
B	0.8437112572	-0.0102213649	-0.5902150016
P	-0.0606234151	2.451092362	1.6221832066
P	-2.451092362	-0.0606234151	-1.6221832066
P	0.0606234151	-2.451092362	1.6221832066
P	2.451092362	0.0606234151	-1.6221832066
H	1.3311958544	2.7564519163	1.6037201842
H	-0.0486538625	1.8369459027	2.9085843137
H	-1.8369459027	-0.0486538625	-2.9085843137
H	-2.7564519163	1.3311958544	-1.6037201842
H	-1.3311958544	-2.7564519163	1.6037201842
H	0.0486538625	-1.8369459027	2.9085843137
H	1.8369459027	0.0486538625	-2.9085843137
H	2.7564519163	-1.3311958544	-1.6037201842

tetrahedral $[BAsH_2]_4$ S_4

B	-0.0010088486	0.843123309	0.5907923695
B	0.0010088486	-0.843123309	0.5907923695
B	-0.843123309	-0.0010088486	-0.5907923695
B	0.843123309	0.0010088486	-0.5907923695
As	-0.098659203	2.543198916	1.6949657277
As	-2.543198916	-0.098659203	-1.6949657277
As	0.098659203	-2.543198916	1.6949657277
As	2.543198916	0.098659203	-1.6949657277

H	1.3897782997	2.8580161695	1.5898510103
H	0.0530925416	1.8258226833	3.0324413661
H	-1.8258226833	0.0530925416	-3.0324413661
H	-2.8580161695	1.3897782997	-1.5898510103
H	-1.3897782997	-2.8580161695	1.5898510103
H	-0.0530925416	-1.8258226833	3.0324413661
H	1.8258226833	-0.0530925416	-3.0324413661
H	2.8580161695	-1.3897782997	-1.5898510103

tetrahedral $[AlNH_2]_4$ C_1

Al	-0.0403333404	0.8722249142	1.3518782462
Al	-0.0605183725	0.8959059312	-1.3356187991
Al	1.3448815594	-0.8939686211	-0.0189181221
Al	-1.2301620916	-1.0441994327	-0.0017180599
N	-0.0998421068	2.0018070306	2.7568578651
N	2.9308878838	-1.7553841632	-0.0343859927
N	-0.1393897085	2.051062929	-2.7186700149
N	-2.7092238473	-2.0784213844	0.0019648988
H	-0.9445402411	2.3117705428	3.2166643245
H	0.7059650162	2.4127553217	3.2071109302
H	3.0454202669	-2.7589783125	-0.04299564
H	3.835283738	-1.3058474673	-0.0352728948
H	0.6601198895	2.4612274465	-3.1807104008
H	-0.9911127778	2.3790361616	-3.1522602975
H	-2.7095699331	-3.0883846213	0.008992813
H	-3.6588723193	-1.7345462452	-0.0049985737

tetrahedral $[AlPH_2]_4$ S_4

Al	-0.578644413	1.1733490133	-0.9212193145
Al	0.578644413	-1.1733490133	-0.9212193145
Al	1.1733490133	0.578644413	0.9212193145
Al	-1.1733490133	-0.578644413	0.9212193145
P	-1.3675071917	2.9942499596	-2.2342598903
P	2.9942499596	1.3675071917	2.2342598903
P	1.3675071917	-2.9942499596	-2.2342598903
P	-2.9942499596	-1.3675071917	2.2342598903
H	-2.7295054551	2.5718807091	-2.1393284848
H	-1.1404675791	2.3016734203	-3.4637979166
H	2.3016734203	1.1404675791	3.4637979166
H	2.5718807091	2.7295054551	2.1393284848
H	2.7295054551	-2.5718807091	-2.1393284848
H	1.1404675791	-2.3016734203	-3.4637979166
H	-2.3016734203	-1.1404675791	3.4637979166
H	-2.5718807091	-2.7295054551	2.1393284848

tetrahedral $[AlAsH_2]_4$ S_4

Al	-0.5870881303	1.1658321582	-0.9284075541
Al	0.5870881303	-1.1658321582	-0.9284075541
Al	1.1658321582	0.5870881303	0.9284075541

Al	-1.1658321582	-0.5870881303	0.9284075541
As	-1.4649757002	3.0523872252	-2.2949592424
As	3.0523872252	1.4649757002	2.2949592424
As	1.4649757002	-3.0523872252	-2.2949592424
As	-3.0523872252	-1.4649757002	2.2949592424
H	-2.7543918432	2.2808794649	-2.5732784935
H	-0.7842162006	2.4827314156	-3.5390655288
H	2.4827314156	0.7842162006	3.5390655288
H	2.2808794649	2.7543918432	2.5732784935
H	2.7543918432	-2.2808794649	-2.5732784935
H	0.7842162006	-2.4827314156	-3.5390655288
H	-2.4827314156	-0.7842162006	3.5390655288
H	-2.2808794649	-2.7543918432	2.5732784935

tetrahedral $[GaNH_2]_4$ C_1

Ga	-0.03877	-1.22322	1.07577
Ga	-1.31733	0.02052	-0.98554
Ga	0.10447	1.39011	0.79149
Ga	1.3459	-0.1198	-0.87296
N	-0.2695	-2.67597	2.21782
N	-0.00468	3.03277	1.67465
N	-2.87832	-0.1302	-1.99101
N	2.86429	-0.43897	-1.91062
H	-0.02639	-3.62567	1.97455
H	-0.82797	-2.64572	3.05885
H	0.76373	3.68955	1.67114
H	-0.57002	3.15382	2.50375
H	-3.70645	0.42706	-1.83581
H	-2.95416	-0.66934	-2.84178
H	3.46926	0.30684	-2.22513
H	2.94755	-1.24576	-2.51321

tetrahedral $[GaPH_2]_4$ S_4

Ga	-0.5828361315	1.1723864029	-0.9178498472
Ga	0.5828361315	-1.1723864029	-0.9178498472
Ga	1.1723864029	0.5828361315	0.9178498472
Ga	-1.1723864029	-0.5828361315	0.9178498472
P	-1.3630527811	3.0072755331	-2.2416654538
P	3.0072755331	1.3630527811	2.2416654538
P	1.3630527811	-3.0072755331	-2.2416654538
P	-3.0072755331	-1.3630527811	2.2416654538
H	-2.7287658585	2.6030984916	-2.1256968094
H	-1.1644805145	2.2970118034	-3.4657944123
H	2.2970118034	1.1644805145	3.4657944123
H	2.6030984916	2.7287658585	2.1256968094
H	2.7287658585	-2.6030984916	-2.1256968094
H	1.1644805145	-2.2970118034	-3.4657944123
H	-2.2970118034	-1.1644805145	3.4657944123
H	-2.6030984916	-2.7287658585	2.1256968094

tetrahedral $[GaAsH_2]_4$ S_4

Ga	0.	1.3066736891	0.927787652
Ga	0.	-1.3066736891	0.927787652
Ga	-1.3066736891	0.	-0.927787652
Ga	1.3066736891	0.	-0.927787652
As	-0.0772777606	3.3917527511	2.3072251514
As	-3.3917527511	-0.0772777606	-2.3072251514
As	0.0772777606	-3.3917527511	2.3072251514
As	3.3917527511	0.0772777606	-2.3072251514
H	1.4198933686	3.2908115942	2.5951779422
H	-0.4297502571	2.5741521161	3.549150982
H	-2.5741521161	-0.4297502571	-3.549150982
H	-3.2908115942	1.4198933686	-2.5951779422
H	-1.4198933686	-3.2908115942	2.5951779422
H	0.4297502571	-2.5741521161	3.549150982
H	2.5741521161	0.4297502571	-3.549150982
H	3.2908115942	-1.4198933686	-2.5951779422

$[MYH_2]_4$ structures.
Bridged ring structures.

ring $[BNH_2]_4$ C_{2h}

N	1.2734355596	-0.7796269365	-1.1202583894
B	1.4603453009	0.4531626916	0.
B	-1.4603374878	-0.4531193712	0.
B	-0.2270222751	0.8724188954	0.
B	0.2270300882	-0.872375575	0.
N	-1.2734277465	0.7796702569	1.1202583894
N	-1.2734277465	0.7796702569	-1.1202583894
N	1.2734355596	-0.7796269365	1.1202583894
H	1.0028104599	-0.4918082805	-2.0508202171
H	2.0230464449	-1.454836336	-1.1934589772
H	-1.0028026468	0.4918516009	-2.0508202171
H	-2.0230386318	1.4548796564	-1.1934589772
H	2.0230464449	-1.454836336	1.1934589772
H	1.0028104599	-0.4918082805	2.0508202171
H	-2.0230386318	1.4548796564	1.1934589772
H	-1.0028026468	0.4918516009	2.0508202171

ring $[BPH_2]_4$ C_{2h}

P	1.4383490084	-0.7999301637	-1.3268676523
B	1.6599900557	0.6556498041	0.
B	-1.6599822426	-0.6556064837	0.
B	-0.0468649829	1.0008617169	0.
B	0.046872796	-1.0008183965	0.
P	-1.4383411953	0.7999734841	1.3268676523
P	-1.4383411953	0.7999734841	-1.3268676523

P	1.4383490084	-0.7999301637	1.3268676523
H	1.0942724648	-0.4509749408	-2.6471290346
H	2.4007006896	-1.8172329131	-1.5195269549
H	-1.0942646517	0.4510182612	-2.6471290346
H	-2.4006928765	1.8172762335	-1.5195269549
H	2.4007006896	-1.8172329131	1.5195269549
H	1.0942724648	-0.4509749408	2.6471290346
H	-2.4006928765	1.8172762335	1.5195269549
H	-1.0942646517	0.4510182612	2.6471290346

ring $[BAsH_2]_4$ C_1

As	2.1717461604	-1.6075144615	-1.8565252656
B	0.8611507894	0.8702873281	0.1573032573
B	-0.5449130055	-0.1531503877	-0.2395776881
B	-0.4830539484	1.6858299293	0.4574547311
B	1.1043122783	-0.5855323873	-0.4186192335
As	-1.6529819024	0.3915136787	1.4655699599
As	-1.3282040349	1.3663394136	-1.3655085291
As	1.9889879184	-0.9454493819	1.5458929649
H	1.238895002	-1.2405143092	-3.0119264361
H	1.4888716138	-2.9625646283	-1.6667947391
H	-0.5513980501	1.8127936967	-2.5596762209
H	-2.7745627465	1.6466161842	-1.6674441183
H	0.7960918082	-1.346154536	2.4134411322
H	2.1054179782	0.4228670008	2.2167615042
H	-3.1252079503	0.6440270304	1.7325263679
H	-1.0950893856	0.0009524037	2.7955622082

ring $[AlNH_2]_4$ C_{2h}

N	1.8143668545	-1.0456225759	-1.2948421657
Al	2.460928009	0.5546891463	0.
Al	-2.4609201959	-0.5546458259	0.
Al	-0.3766599192	1.2628990386	0.
Al	0.3766677323	-1.2628557182	0.
N	-1.8143590414	1.0456658963	1.2948421657
N	-1.8143590414	1.0456658963	-1.2948421657
N	1.8143668545	-1.0456225759	1.2948421657
H	1.5914022702	-0.8082709006	-2.2571555801
H	2.5517256005	-1.7437881473	-1.3410214805
H	-1.5913944571	0.808314221	-2.2571555801
H	-2.5517177874	1.7438314677	-1.3410214805
H	2.5517256005	-1.7437881473	1.3410214805
H	1.5914022702	-0.8082709006	2.2571555801
H	-2.5517177874	1.7438314677	1.3410214805
H	-1.5913944571	0.808314221	2.2571555801

ring $[AlPH_2]_4$ C_{2h}

P	-0.0000025585	2.1687347923	1.5677385116
Al	2.0432476006	1.8321699125	0.
Al	-2.0432433735	-1.8321598214	0.
Al	1.1368585921	-0.7572265093	0.
Al	-1.1368468209	0.7572187478	0.
P	-0.0000025585	-2.1687354574	-1.5677362243
P	-0.0000025585	-2.1687354574	1.5677362243
P	-0.0000025585	2.1687347923	-1.5677385116
H	0.0476496578	1.678702516	2.8952710024
H	-0.4573119356	3.4867259722	1.8221529733
H	-0.0476579932	-1.6787028568	2.8952685298
H	0.4572930379	-3.486730798	1.8221542428
H	-0.4573119356	3.4867259722	-1.8221529733
H	0.0476496578	1.678702516	-2.8952710024
H	0.4572930379	-3.486730798	-1.8221542428
H	-0.0476579932	-1.6787028568	-2.8952685298

ring $[AlAsH_2]_4$ C_{2h}

As	1.9664420144	-1.0504795723	-1.6421639348
Al	2.6373078656	1.0218882963	0.
Al	-2.6372999314	-1.0218441724	0.
Al	-0.1123930261	1.3695027311	0.
Al	0.1124009603	-1.3694586072	0.
As	-1.9664340802	1.0505236962	1.6421639348
As	-1.9664340802	1.0505236962	-1.6421639348
As	1.9664420144	-1.0504795723	1.6421639348
H	1.5024521958	-0.7978646165	-3.0577378222
H	2.9391040935	-2.1756531573	-1.9245829501
H	-1.5024442617	0.7979087404	-3.0577378222
H	-2.9390961594	2.1756972812	-1.9245829501
H	2.9391040935	-2.1756531573	1.9245829501
H	1.5024521958	-0.7978646165	3.0577378222
H	-2.9390961594	2.1756972812	1.9245829501
H	-1.5024442617	0.7979087404	3.0577378222

ring $[GaNH_2]_4$ C_{2h}

N	1.8957198386	-1.0639473439	-1.3260909382
Ga	2.6264317541	0.6265627296	0.
Ga	-2.6264240924	-0.6265201	0.
Ga	-0.378659312	1.254800968	0.
Ga	0.3786669737	-1.2547583384	0.
N	-1.8957121769	1.0639899736	1.3260909382
N	-1.8957121769	1.0639899736	-1.3260909382
N	1.8957198386	-1.0639473439	1.3260909382
H	1.6721477279	-0.8738636127	-2.2983951888
H	2.6035404158	-1.7937308168	-1.3265068796
H	-1.6721400663	0.8739062424	-2.2983951888

H -2.6035327541 1.7937734464 -1.3265068796
H 2.6035404158 -1.7937308168 1.3265068796
H 1.6721477279 -0.8738636127 2.2983951888
H -2.6035327541 1.7937734464 1.3265068796
H -1.6721400663 0.8739062424 2.2983951888

ring $[GaPH_2]_4$ C_{2h}
P 2.010083156 -1.0606929816 -1.6000472112
Ga 2.6287247027 1.0798314459 0.
Ga -2.6287180781 -1.0797888555 0.
Ga -0.2040635619 1.3209138138 0.
Ga 0.2040718906 -1.3208728335 0.
P -2.0100751194 1.0607377855 1.6000475096
P -2.0100751194 1.0607377855 -1.6000475096
P 2.010083156 -1.0606929816 1.6000472112
H 1.5746493111 -0.9741680427 -2.9457617332
H 2.9157113048 -2.1454812293 -1.7194371746
H -1.5746417987 0.9742164061 -2.9457624497
H -2.9157003818 2.1455290773 -1.7194331844
H 2.9157113048 -2.1454812293 1.7194371746
H 1.5746493111 -0.9741680427 2.9457617332
H -2.9157003818 2.1455290773 1.7194331844
H -1.5746417987 0.9742164061 2.9457624497

ring $[GaAsH_2]_4$ C_{2h}
As 2.0793313711 -1.0596768079 -1.6850903002
Ga 2.641020106 1.1962260741 0.
Ga -2.6410121718 -1.1961819502 0.
Ga -0.2213324298 1.3209692863 0.
Ga 0.221340364 -1.3209251624 0.
As -2.0793234369 1.0597209318 1.6850903002
As -2.0793234369 1.0597209318 -1.6850903002
As 2.0793313711 -1.0596768079 1.6850903002
H 1.5592951645 -1.0236770312 -3.1056945501
H 2.9960996166 -2.2576661234 -1.8234273309
H -1.5592872303 1.0237211551 -3.1056945501
H -2.9960916824 2.2577102473 -1.8234273309
H 2.9960996166 -2.2576661234 1.8234273309
H 1.5592951645 -1.0236770312 3.1056945501
H -2.9960916824 2.2577102473 1.8234273309
H -1.5592872303 1.0237211551 3.1056945501

$[HMYH]_4$ structures.
Cubane structures.

cubane-$[HBNH]_4$ T_d

N	-0.8127114709	-0.8127114709	-0.8127114709
B	0.7811652327	0.7811652327	0.7811652327
N	0.8127114709	0.8127114709	-0.8127114709
B	-0.7811652327	-0.7811652327	0.7811652327
H	-1.3948570414	-1.3948570414	-1.3948570414
H	1.470430403	1.470430403	1.470430403
H	1.3948570414	1.3948570414	-1.3948570414
H	-1.470430403	-1.470430403	1.470430403
B	-0.7811652327	0.7811652327	-0.7811652327
N	0.8127114709	-0.8127114709	0.8127114709
B	0.7811652327	-0.7811652327	-0.7811652327
N	-0.8127114709	0.8127114709	0.8127114709
H	1.3948570414	-1.3948570414	1.3948570414
H	-1.470430403	1.470430403	-1.470430403
H	-1.3948570414	1.3948570414	1.3948570414
H	1.470430403	-1.470430403	-1.470430403

cubane-$[HBPH]_4$ T_d

P	0.	-0.0000000096	1.7377245999
B	0.	0.0000000098	-1.7739130641
P	0.	1.6383424678	-0.5792415242
B	0.	-1.6724612791	0.5913043454
H	0.	-0.0000000175	3.1587800175
H	0.	0.0000000164	-2.9622270169
H	0.	2.9781263667	-1.052926656
H	0.	-2.7928144202	0.9874089902
B	1.4483939517	0.8362306346	0.5913043593
P	-1.4188461944	-0.8191712291	-0.5792415378
B	-1.4483939517	0.8362306346	0.5913043593
P	1.4188461944	-0.8191712291	-0.5792415378
H	-2.5791330842	-1.4890631746	-1.0529266808
H	2.4186482312	1.3964072019	0.9874090134
H	2.5791330842	-1.4890631746	-1.0529266808
H	-2.4186482312	1.3964072019	0.9874090134

cubane-$[HBAsH]_4$ T_d

As	-1.0612993604	-1.0612993604	-1.0612993604
B	1.0766605849	1.0766605849	1.0766605849
As	1.0612993604	1.0612993604	-1.0612993604
B	-1.0766605849	-1.0766605849	1.0766605849
H	-1.9361696471	-1.9361696471	-1.9361696471
H	1.7616654084	1.7616654084	1.7616654084
H	1.9361696471	1.9361696471	-1.9361696471
H	-1.7616654084	-1.7616654084	1.7616654084

B	-1.0766605849	1.0766605849	-1.0766605849
As	1.0612993604	-1.0612993604	1.0612993604
B	1.0766605849	-1.0766605849	-1.0766605849
As	-1.0612993604	1.0612993604	1.0612993604
H	1.9361696471	-1.9361696471	1.9361696471
H	-1.7616654084	1.7616654084	-1.7616654084
H	-1.9361696471	1.9361696471	1.9361696471
H	1.7616654084	-1.7616654084	-1.7616654084

cubane-$[HAlNH]_4$ T_d

N	0.	-0.0000000092	1.6674769801
Al	0.	0.0000000094	-1.6921308119
N	0.	1.5721123765	-0.5558256513
Al	0.	-1.5953562321	0.5640435951
H	0.	-0.0000000148	2.6777239988
H	0.	0.0000000181	-3.2720458773
H	0.	2.5245824019	-0.8925746523
H	0.	-3.0849144436	1.090681942
Al	1.3816190224	0.7976781114	0.5640436084
N	-1.361489253	-0.7860561837	-0.5558256644
Al	-1.3816190224	0.7976781114	0.5640436084
N	1.361489253	-0.7860561837	-0.5558256644
H	-2.1863524897	-1.2622911935	-0.8925746733
H	2.6716142714	1.5424572127	1.0906819676
H	2.1863524897	-1.2622911935	-0.8925746733
H	-2.6716142714	1.5424572127	1.0906819676

cubane-$[HAlPH]_4$ T_d

P	-1.2059793654	-1.2059793654	-1.2059793654
Al	1.2312709743	1.2312709743	1.2312709743
P	1.2059793654	1.2059793654	-1.2059793654
Al	-1.2312709743	-1.2312709743	1.2312709743
H	-2.0221037434	-2.0221037434	-2.0221037434
H	2.1429810808	2.1429810808	2.1429810808
H	2.0221037434	2.0221037434	-2.0221037434
H	-2.1429810808	-2.1429810808	2.1429810808
Al	-1.2312709743	1.2312709743	-1.2312709743
P	1.2059793654	-1.2059793654	1.2059793654
Al	1.2312709743	-1.2312709743	-1.2312709743
P	-1.2059793654	1.2059793654	1.2059793654
H	2.0221037434	-2.0221037434	2.0221037434
H	-2.1429810808	2.1429810808	-2.1429810808
H	-2.0221037434	2.0221037434	2.0221037434
H	2.1429810808	-2.1429810808	-2.1429810808

cubane-$[HAlAsH]_4$ T_d

As	-1.2488734078	-1.2488734078	-1.2488734078
Al	1.2856725323	1.2856725323	1.2856725323
As	1.2488734078	1.2488734078	-1.2488734078

Al	-1.2856725323	-1.2856725323	1.2856725323
H	-2.1171939314	-2.1171939314	-2.1171939314
H	2.197347239	2.197347239	2.197347239
H	2.1171939314	2.1171939314	-2.1171939314
H	-2.197347239	-2.197347239	2.197347239
Al	-1.2856725323	1.2856725323	-1.2856725323
As	1.2488734078	-1.2488734078	1.2488734078
Al	1.2856725323	-1.2856725323	-1.2856725323
As	-1.2488734078	1.2488734078	1.2488734078
H	2.1171939314	-2.1171939314	2.1171939314
H	-2.197347239	2.197347239	-2.197347239
H	-2.1171939314	2.1171939314	2.1171939314
H	2.197347239	-2.197347239	-2.197347239

cubane-$[HGaNH]_4$ T_d

N	0.	-0.0000000094	1.6986359778
Ga	0.	0.0000000098	-1.7710709791
N	0.	1.6014893613	-0.5662119837
Ga	0.	-1.6697817356	0.5903569838
H	0.	-0.000000015	2.7105493246
H	0.	0.0000000184	-3.3289942238
H	0.	2.5555304159	-0.9035164274
H	0.	-3.1386058597	1.1096647239
Ga	1.446073399	0.8348908629	0.5903569976
N	-1.3869304681	-0.800744676	-0.566211997
Ga	-1.446073399	0.8348908629	0.5903569976
N	1.3869304681	-0.800744676	-0.566211997
H	-2.213154256	-1.2777652004	-0.9035164486
H	2.7181124016	1.5693029206	1.1096647499
H	2.213154256	-1.2777652004	-0.9035164486
H	-2.7181124016	1.5693029206	1.1096647499

cubane-$[HGaPH]_4$ T_d

P	-1.1985618254	-1.1985618254	-1.1985618254
Ga	1.2489288539	1.2489288539	1.2489288539
P	1.1985618254	1.1985618254	-1.1985618254
Ga	-1.2489288539	-1.2489288539	1.2489288539
H	-2.0166082168	-2.0166082168	-2.0166082168
H	2.1498640857	2.1498640857	2.1498640857
H	2.0166082168	2.0166082168	-2.0166082168
H	-2.1498640857	-2.1498640857	2.1498640857
Ga	-1.2489288539	1.2489288539	-1.2489288539
P	1.1985618254	-1.1985618254	1.1985618254
Ga	1.2489288539	-1.2489288539	-1.2489288539
P	-1.1985618254	1.1985618254	1.1985618254
H	2.0166082168	-2.0166082168	2.0166082168
H	-2.1498640857	2.1498640857	-2.1498640857
H	-2.0166082168	2.0166082168	2.0166082168
H	2.1498640857	-2.1498640857	-2.1498640857

cubane-$[HGaAsH]_4$ T_d

As	1.2415177799	-1.2415177799	-1.2415177799
Ga	-1.299079171	1.299079171	1.299079171
As	-1.2415177799	1.2415177799	-1.2415177799
Ga	1.299079171	-1.299079171	1.299079171
H	2.1129145427	-2.1129145427	-2.1129145427
H	-2.2006791706	2.2006791706	2.2006791706
H	-2.1129145427	2.1129145427	-2.1129145427
H	2.2006791706	-2.2006791706	2.2006791706
Ga	-1.299079171	-1.299079171	-1.299079171
As	1.2415177799	1.2415177799	1.2415177799
Ga	1.299079171	1.299079171	-1.299079171
As	-1.2415177799	-1.2415177799	1.2415177799
H	2.1129145427	2.1129145427	2.1129145427
H	-2.2006791706	-2.2006791706	-2.2006791706
H	-2.1129145427	-2.1129145427	2.1129145427
H	2.2006791706	2.2006791706	-2.2006791706

$[HMYH]_4$ structures.
Ladder structures.

ladder-$[HBNH]_4$ C_i

N	0.6876952663	-0.1290456359	-1.9775010845
B	0.6942166668	0.5956021589	-0.6353324576
B	-0.6978967307	-0.159431617	-2.0008066378
N	-0.9372408932	0.3812155152	-0.6033623524
H	1.3973441594	-0.3693514663	-2.6463296935
H	-1.5000885939	-0.4548607482	-2.8282166845
N	0.9372408932	-0.3812155152	0.6033623524
B	-0.6942166668	-0.5956021589	0.6353324576
H	-1.6075050325	1.1239592998	-0.451975674
H	1.1533429335	1.6994274314	-0.5456624166
N	-0.6876952663	0.1290456359	1.9775010845
B	0.6978967307	0.159431617	2.0008066378
H	-1.1533429335	-1.6994274314	0.5456624166
H	1.6075050325	-1.1239592998	0.451975674
H	1.5000885939	0.4548607482	2.8282166845
H	-1.3973441594	0.3693514663	2.6463296935

ladder-$[HBPH]_4$ C_i

P	0.7987608569	-0.6381148446	-2.6477485321
B	0.5083340774	0.7682986276	-1.1801142927
B	-0.9404652236	-0.107282403	-2.2054048279
P	-1.3636354305	-0.0008197804	-0.4052906258
H	0.867955024	0.195769948	-3.8044643457
H	-1.655311764	0.5725933171	-2.8663156917
P	1.3636354305	0.0008197804	0.4052906258
B	-0.5083340774	-0.7682986276	1.1801142927

H	-2.3796308928	0.9482483456	-0.162289237
H	0.6541615889	1.9300245205	-1.3661667129
P	-0.7987608569	0.6381148446	2.6477485321
B	0.9404652236	0.107282403	2.2054048279
H	-0.6541615889	-1.9300245205	1.3661667129
H	2.3796308928	-0.9482483456	0.162289237
H	1.655311764	-0.5725933171	2.8663156917
H	-0.867955024	-0.195769948	3.8044643457

ladder-$[HBAsH]_4$ C_i

As	0.8781360437	-0.7266499861	-2.7932098581
B	0.4600830399	0.7637841567	-1.2612353199
B	-0.9068425238	-0.037379112	-2.2977279655
As	-1.5106719966	-0.1213321425	-0.4174285756
H	0.9345446969	0.1825434088	-4.0185580752
H	-1.6239690868	0.6492372125	-2.9450732244
As	1.5106719966	0.1213321425	0.4174285756
B	-0.4600830399	-0.7637841567	1.2612353199
H	-2.3686051671	1.0863559889	-0.1352207618
H	0.5260818813	1.9386471293	-1.4074977047
As	-0.8781360437	0.7266499861	2.7932098581
B	0.9068425238	0.037379112	2.2977279655
H	-0.5260818813	-1.9386471293	1.4074977047
H	2.3686051671	-1.0863559889	0.1352207618
H	1.6239690868	-0.6492372125	2.9450732244
H	-0.9345446969	-0.1825434088	4.0185580752

ladder-$[HAlNH]_4$ C_i

N	1.054451566	-0.452606767	-2.3007787178
Al	1.1688352202	0.3945369138	-0.6561857403
Al	-0.6395743598	0.0054718303	-2.565668691
N	-0.7953529492	0.7512548535	-0.8567007748
H	1.7368846875	-0.9368183525	-2.8602558993
H	-1.696194492	-0.0556111885	-3.7293084429
N	0.7953529492	-0.7512548535	0.8567007748
Al	-1.1688352202	-0.3945369138	0.6561857403
H	-1.2091594911	1.6728694876	-0.7600561787
H	2.1679878385	1.5871097098	-0.3287959172
N	-1.054451566	0.452606767	2.3007787178
Al	0.6395743598	-0.0054718303	2.565668691
H	-2.1679878385	-1.5871097098	0.3287959172
H	1.2091594911	-1.6728694876	0.7600561787
H	1.696194492	0.0556111885	3.7293084429
H	-1.7368846875	0.9368183525	2.8602558993

ladder-$[HAlPH]_4$ C_i

P	1.1395610109	-0.4803934222	-2.992587124
Al	0.9015081093	0.9998469576	-1.1111192554
Al	-1.1383862847	-0.1252746327	-3.0463867067

P	-1.5009483662	0.3935186695	-0.7912416738
H	1.4149795935	0.4475047281	-4.0447797823
H	-2.2104243569	0.0634956142	-4.1930561488
P	1.5009483662	-0.3935186695	0.7912416738
Al	-0.9015081093	-0.9998469576	1.1111192554
H	-2.5295906383	1.3335161638	-0.545031465
H	1.3514477763	2.5163624991	-1.0992066052
P	-1.1395610109	0.4803934222	2.992587124
Al	1.1383862847	0.1252746327	3.0463867067
H	-1.3514477763	-2.5163624991	1.0992066052
H	2.5295906383	-1.3335161638	0.545031465
H	2.2104243569	-0.0634956142	4.1930561488
H	-1.4149795935	-0.4475047281	4.0447797823

ladder-$[HAlAsH]_4$ C_i

As	1.2294038486	-0.5288077441	-3.1389867136
Al	0.9426458303	1.0304407079	-1.1905103976
Al	-1.1570986054	-0.1473577605	-3.1478911448
As	-1.5467473415	0.3980522388	-0.8085481673
H	1.4067264383	0.5364512427	-4.2220100899
H	-2.2255245501	0.0978983126	-4.2901922488
As	1.5467473415	-0.3980522388	0.8085481673
Al	-0.9426458303	-1.0304407079	1.1905103976
H	-2.6390463203	1.4142261767	-0.5903758693
H	1.4021479164	2.5440279994	-1.1679407179
As	-1.2294038486	0.5288077441	3.1389867136
Al	1.1570986054	0.1473577605	3.1478911448
H	-1.4021479164	-2.5440279994	1.1679407179
H	2.6390463203	-1.4142261767	0.5903758693
H	2.2255245501	-0.0978983126	4.2901922488
H	-1.4067264383	-0.5364512427	4.2220100899

ladder-$[HGaNH]_4$ C_i

N	1.0687322759	-0.4552364981	-2.3293261321
Ga	1.2334372921	0.4478521861	-0.64604474
Ga	-0.6641964076	0.0064032023	-2.6498463424
N	-0.7905900374	0.7771904529	-0.8773984094
H	1.7439875655	-0.9193417341	-2.9162525732
H	-1.722319285	-0.0912182047	-3.7767071863
N	0.7905900374	-0.7771904529	0.8773984094
Ga	-1.2334372921	-0.4478521861	0.64604474
H	-1.2205459692	1.6912246091	-0.7811940253
H	2.2546754652	1.5952688353	-0.3350287682
N	-1.0687322759	0.4552364981	2.3293261321
Ga	0.6641964076	-0.0064032023	2.6498463424
H	-2.2546754652	-1.5952688353	0.3350287682
H	1.2205459692	-1.6912246091	0.7811940253
H	1.722319285	0.0912182047	3.7767071863
H	-1.7439875655	0.9193417341	2.9162525732

ladder-$[HGaPH]_4$ C_i

P	1.1493863372	-0.4602409765	-2.9910941145
Ga	0.9572675229	1.0414003837	-1.1091245628
Ga	-1.1551988683	-0.1511733265	-3.0475481112
P	-1.460530803	0.4233866456	-0.7843776045
H	1.3982165618	0.4694961184	-4.0485678805
H	-2.2345358562	0.0136282963	-4.1712540953
P	1.460530803	-0.4233866456	0.7843776045
Ga	-0.9572675229	-1.0414003837	1.1091245628
H	-2.5395007904	1.3144204784	-0.5544955399
H	1.428182556	2.5322545062	-1.0575992014
P	-1.1493863372	0.4602409765	2.9910941145
Ga	1.1551988683	0.1511733265	3.0475481112
H	-1.428182556	-2.5322545062	1.0575992014
H	2.5395007904	-1.3144204784	0.5544955399
H	2.2345358562	-0.0136282963	4.1712540953
H	-1.3982165618	-0.4694961184	4.0485678805

ladder-$[HGaAsH]_4$ C_i

As	1.2305013616	-0.4975321356	-3.1369114875
Ga	0.9987434763	1.0698630112	-1.1839493286
Ga	-1.18495093	-0.1731553623	-3.1564387768
As	-1.5027446522	0.4367624482	-0.8081461951
H	1.4039828107	0.5686363389	-4.219961576
H	-2.2657387728	0.0166089265	-4.2808585765
As	1.5027446522	-0.4367624482	0.8081461951
Ga	-0.9987434763	-1.0698630112	1.1839493286
H	-2.6432549318	1.4077972945	-0.5945290048
H	1.4817942273	2.5581041456	-1.112370415
As	-1.2305013616	0.4975321356	3.1369114875
Ga	1.18495093	0.1731553623	3.1564387768
H	-1.4817942273	-2.5581041456	1.112370415
H	2.6432549318	-1.4077972945	0.5945290048
H	2.2657387728	-0.0166089265	4.2808585765
H	-1.4039828107	-0.5686363389	4.219961576

$[HMYH]_4$ structures.
Ring structures.

ring-$[HBNH]_4$ D_{4h}

N	-1.8293126017	0.	0.
B	-1.3482700007	0.	-1.3482700007
H	-2.1953849131	0.	-2.1953849131
N	0.	0.	-1.8293126017
H	-2.8404423285	0.	0.
B	-1.3482700007	0.	1.3482700007
H	-2.1953849131	0.	2.1953849131
N	0.	0.	1.8293126017

B 1.3482700007 0. 1.3482700007
H 0. 0. 2.8404423285
H 0. 0. -2.8404423285
B 1.3482700007 0. -1.3482700007
H 2.1953849131 0. 2.1953849131
H 2.1953849131 0. -2.1953849131
N 1.8293126017 0. 0.
H 2.8404423285 0. 0.

ring-$[HBPH]_4$ D_{2d}
P -1.9940666322 0.0575071829 0.913574276
B -1.5380596534 1.6294066842 0.
H -2.3544925616 2.4943284282 0.
H -3.4024321969 0.0981232459 1.0277104154
B -1.6294066842 -1.5380596534 0.
H -2.4943284282 -2.3544925616 0.
B 1.5380596534 -1.6294066842 0.
B 1.6294066842 1.5380596534 0.
H 2.3544925616 -2.4943284282 0.
H 2.4943284282 2.3544925616 0.
P 1.9940666322 -0.0575071829 0.913574276
H 3.4024321969 -0.0981232459 1.0277104154
P -0.0575071829 -1.9940666322 -0.913574276
P 0.0575071829 1.9940666322 -0.913574276
H -0.0981232459 -3.4024321969 -1.0277104154
H 0.0981232459 3.4024321969 -1.0277104154

ring-$[HBAsH]_4$ D_{2d}
As -1.9863164474 0.0572836742 1.0878781694
B -1.5788540004 1.6726238517 0.
H -2.3945847945 2.5368017823 0.
H -3.49724725 0.1008576314 1.1560954187
B -1.6726238517 -1.5788540004 0.
H -2.5368017823 -2.3945847945 0.
B 1.5788540004 -1.6726238517 0.
B 1.6726238517 1.5788540004 0.
H 2.3945847945 -2.5368017823 0.
H 2.5368017823 2.3945847945 0.
As 1.9863164474 -0.0572836742 1.0878781694
H 3.49724725 -0.1008576314 1.1560954187
As -0.0572836742 -1.9863164474 -1.0878781694
As 0.0572836742 1.9863164474 -1.0878781694
H -0.1008576314 -3.49724725 -1.1560954187
H 0.1008576314 3.49724725 -1.1560954187

ring-$[HAlNH]_4$ D_{4h}
N -2.2633254405 0. 0.
Al -1.7117904214 0. -1.7117904214
H -2.8318108027 0. -2.8318108027

N	0.	0.	-2.2633254405
H	-3.2828174999	0.	0.
Al	-1.7117904214	0.	1.7117904214
H	-2.8318108027	0.	2.8318108027
N	0.	0.	2.2633254405
Al	1.7117904214	0.	1.7117904214
H	0.	0.	3.2828174999
H	0.	0.	-3.2828174999
Al	1.7117904214	0.	-1.7117904214
H	2.8318108027	0.	2.8318108027
H	2.8318108027	0.	-2.8318108027
N	2.2633254405	0.	0.
H	3.2828174999	0.	0.

ring-$[HAlPH]_4$ D_{2d}

P	-2.0986187404	0.0605223767	1.3683919107
Al	-1.7967162352	1.9034251609	0.
H	-2.8833773414	3.0546242487	0.
H	-3.5196600742	0.1015039982	1.4619927176
Al	-1.9034251609	-1.7967162352	0.
H	-3.0546242487	-2.8833773414	0.
Al	1.7967162352	-1.9034251609	0.
Al	1.9034251609	1.7967162352	0.
H	2.8833773414	-3.0546242487	0.
H	3.0546242487	2.8833773414	0.
P	2.0986187404	-0.0605223767	1.3683919107
H	3.5196600742	-0.1015039982	1.4619927176
P	-0.0605223767	-2.0986187404	-1.3683919107
P	0.0605223767	2.0986187404	-1.3683919107
H	-0.1015039982	-3.5196600742	-1.4619927176
H	0.1015039982	3.5196600742	-1.4619927176

ring-$[HAlAsH]_4$ D_{2d}

As	0.	2.080557712	1.5224290459
Al	1.8722266912	1.8722266912	0.
H	2.9928059312	2.9928059312	0.
H	0.	3.6034608243	1.5679386759
Al	-1.8722266912	1.8722266912	0.
H	-2.9928059312	2.9928059312	0.
Al	-1.8722266912	-1.8722266912	0.
Al	1.8722266912	-1.8722266912	0.
H	-2.9928059312	-2.9928059312	0.
H	2.9928059312	-2.9928059312	0.
As	0.	-2.080557712	1.5224290459
H	0.	-3.6034608243	1.5679386759
As	-2.080557712	0.	-1.5224290459
As	2.080557712	0.	-1.5224290459
H	-3.6034608243	0.	-1.5679386759
H	3.6034608243	0.	-1.5679386759

ring-$[HGaNH]_4$ D_{4h}

N	-2.3252751415	0.	0.
Ga	-1.7561363231	0.	-1.7561363231
H	-2.8643057159	0.	-2.8643057159
N	0.	0.	-2.3252751415
H	-3.3412533527	0.	0.
Ga	-1.7561363231	0.	1.7561363231
H	-2.8643057159	0.	2.8643057159
N	0.	0.	2.3252751415
Ga	1.7561363231	0.	1.7561363231
H	0.	0.	3.3412533527
H	0.	0.	-3.3412533527
Ga	1.7561363231	0.	-1.7561363231
H	2.8643057159	0.	2.8643057159
H	2.8643057159	0.	-2.8643057159
N	2.3252751415	0.	0.
H	3.3412533527	0.	0.

ring-$[HGaPH]_4$ D_{2d}

P	0.	2.059273268	1.4106305042
Ga	1.8297718088	1.8297718088	0.
H	2.9404149066	2.9404149066	0.
H	0.	3.4811203116	1.4996964284
Ga	-1.8297718088	1.8297718088	0.
H	-2.9404149066	2.9404149066	0.
Ga	-1.8297718088	-1.8297718088	0.
Ga	1.8297718088	-1.8297718088	0.
H	-2.9404149066	-2.9404149066	0.
H	2.9404149066	-2.9404149066	0.
P	0.	-2.059273268	1.4106305042
H	0.	-3.4811203116	1.4996964284
P	-2.059273268	0.	-1.4106305042
P	2.059273268	0.	-1.4106305042
H	-3.4811203116	0.	-1.4996964284
H	3.4811203116	0.	-1.4996964284

ring-$[HGaAsH]_4$ D_{2d}

As	0.	2.0587597675	1.5483501486
Ga	1.8600702988	1.8600702988	0.
H	2.9732217668	2.9732217668	0.
H	0.	3.5823979449	1.5922899781
Ga	-1.8600702988	1.8600702988	0.
H	-2.9732217668	2.9732217668	0.
Ga	-1.8600702988	-1.8600702988	0.
Ga	1.8600702988	-1.8600702988	0.
H	-2.9732217668	-2.9732217668	0.
H	2.9732217668	-2.9732217668	0.
As	0.	-2.0587597675	1.5483501486

H 0. -3.5823979449 1.5922899781
As -2.0587597675 0. -1.5483501486
As 2.0587597675 0. -1.5483501486
H -3.5823979449 0. -1.5922899781
H 3.5823979449 0. -1.5922899781

[HMYH]$_4$ structures.
Alternative ring structures

ring-[HBPH]$_4$ C_{4v} (TS)
P 1.7058192677 1.7058192677 0.0501884599
B 2.3595614574 0. 0.4179610012
H 3.5070284247 0. 0.7340226766
H 2.5955960353 2.5955960353 0.6848278623
B 0. 2.3595614574 0.4179610012
H 0. 3.5070284247 0.7340226766
B -2.3595614574 0. 0.4179610012
B 0. -2.3595614574 0.4179610012
H -3.5070284247 0. 0.7340226766
H 0. -3.5070284247 0.7340226766
P -1.7058192677 -1.7058192677 0.0501884599
H -2.5955960353 -2.5955960353 0.6848278623
P -1.7058192677 1.7058192677 0.0501884599
P 1.7058192677 -1.7058192677 0.0501884599
H -2.5955960353 2.5955960353 0.6848278623
H 2.5955960353 -2.5955960353 0.6848278623

ring-[HBAsH]$_4$ C_2
As 1.80581 1.80579 −0.11064
B 2.4325 0.00009 0.40797
H 3.54234 0.00019 0.83548
H 2.68211 2.68195 0.75146
B 0.00017 2.4325 0.40809
H 0.00029 3.54229 0.83572
B −2.4325 −0.00009 0.40797
B −0.00017 −2.4325 0.40809
H −3.54234 −0.00019 0.83548
H −0.00029 −3.54229 0.83572
As −1.80581 −1.80579 −0.11064
H −2.68211 −2.68195 0.75146
As −1.80581 1.8059 −0.10925
As 1.80581 −1.8059 −0.10925
H −2.68167 2.68177 0.75355
H 2.68167 −2.68177 0.75355

ring-[HAlPH]$_4$ C_2
P -2.9471544975 0.0850334255 0.0505242318
Al -1.7474572655 2.0272908052 0.3803702308
H -2.4110747106 3.1122931491 1.3242300018
H -3.7352640228 0.1077639371 1.2353959444
Al -1.8614496685 -1.9231757581 0.3803434955
H -2.5865501702 -2.9681223096 1.324168393

Al	1.7474572655	-2.0272908052	0.3803702308
Al	1.8614496685	1.9231757581	0.3803434955
H	2.4110747106	-3.1122931491	1.3242300018
H	2.5865501702	2.9681223096	1.324168393
P	2.9471544975	-0.0850334255	0.0505242318
H	3.7352640228	-0.1077639371	1.2353959444
P	-0.0750069211	-2.5998447856	-0.9416118426
P	0.0750069211	2.5998447856	-0.9416118426
H	-0.113243758	-3.9250375623	-0.4067586187
H	0.113243758	3.9250375623	-0.4067586187

ring-$[HAlAsH]_4$ C_2

As	-3.1216891256	0.0900744444	-0.0042923827
Al	-1.8036395484	2.004835357	0.6571496635
H	-2.4191486243	2.9543294302	1.7675953785
H	-3.9882952244	0.1150883736	1.2483117311
Al	-1.9162121579	-1.897471913	0.6571855449
H	-2.5854001185	-2.8098597007	1.7676884314
Al	1.8036395484	-2.004835357	0.6571496635
Al	1.9162121579	1.897471913	0.6571855449
H	2.4191486243	-2.9543294302	1.7675953785
H	2.5854001185	2.8098597007	1.7676884314
As	3.1216891256	-0.0900744444	-0.0042923827
H	3.9882952244	-0.1150883736	1.2483117311
As	-0.0804112279	-2.7865885727	-0.6632021162
As	0.0804112279	2.7865885727	-0.6632021162
H	-0.117577738	-4.0745851642	0.1573652136
H	0.117577738	4.0745851642	0.1573652136

ring-$[HGaPH]_4$ C_2

P	-3.0071708685	0.0867673564	-0.1433601221
Ga	-1.7369537284	1.9804940376	0.2512139246
H	-2.3525326696	3.039804956	1.2369535248
H	-3.7656881619	0.1086393279	1.0613161179
Ga	-1.8482856668	-1.8770764185	0.2511643923
H	-2.5239754434	-2.8991608226	1.2368359718
Ga	1.7369537284	-1.9804940376	0.2512139246
Ga	1.8482856668	1.8770764185	0.2511643923
H	2.3525326696	-3.039804956	1.2369535248
H	2.5239754434	2.8991608226	1.2368359718
P	3.0071708685	-0.0867673564	-0.1433601221
H	3.7656881619	-0.1086393279	1.0613161179
P	-0.0744996344	-2.5822930992	-1.0947356633
P	0.0744996344	2.5822930992	-1.0947356633
H	-0.1124370432	-3.8971870534	-0.5373966581
H	0.1124370432	3.8971870534	-0.5373966581

ring-$[HGaAsH]_4$ C_2

As	-3.1800500175	0.0917525832	-0.0520081591

Ga	-1.7825463243	1.9955600725	0.4777842011
H	-2.338313702	3.0172494706	1.5395710582
H	-3.9669700118	0.1144540995	1.2513298057
Ga	-1.8946522503	-1.8894767672	0.4777688678
H	-2.5084186361	-2.8774352146	1.5395347085
Ga	1.7825463243	-1.9955600725	0.4777842011
Ga	1.8946522503	1.8894767672	0.4777688678
H	2.338313702	-3.0172494706	1.5395710582
H	2.5084186361	2.8774352146	1.5395347085
As	3.1800500175	-0.0917525832	-0.0520081591
H	3.9669700118	-0.1144540995	1.2513298057
As	-0.0762982435	-2.6444831145	-0.9673976307
As	0.0762982435	2.6444831145	-0.9673976307
H	-0.1161163826	-4.0246268969	-0.3121896429
H	0.1161163826	4.0246268969	-0.3121896429

$[H_2MY]_4$ structures.
Unbridgrd Ring structures.

ring-$[H_2BN]_4$ D_{4h}

B	-1.6902155778	1.6902155778	0.
N	-0.7124095613	0.7124095613	0.
N	0.7124095613	-0.7124095613	0.
N	-0.7124095613	-0.7124095613	0.
N	0.7124095613	0.7124095613	0.
B	-1.6902155778	-1.6902155778	0.
B	1.6902155778	-1.6902155778	0.
B	1.6902155778	1.6902155778	0.
H	-2.8179941233	1.3280088001	0.
H	-1.3280088001	2.8179941233	0.
H	2.8179941233	-1.3280088001	0.
H	1.3280088001	-2.8179941233	0.
H	1.3280088001	2.8179941233	0.
H	2.8179941233	1.3280088001	0.
H	-2.8179941233	-1.3280088001	0.
H	-1.3280088001	-2.8179941233	0.

ring-$[H_2BP]_4$ D_{2d}

B	-2.4163462392	0.	1.6789041291
P	-1.5936758542	0.	-0.0016601002
P	1.5936758542	0.	-0.0016601002
P	0.	1.5936758542	0.0016601002
P	0.	-1.5936758542	0.0016601002
B	0.	2.4163462392	-1.6789041291
B	2.4163462392	0.	1.6789041291
B	0.	-2.4163462392	-1.6789041291
H	-2.7492207752	1.0379104079	2.1561610809
H	-2.7492207752	-1.0379104079	2.1561610809
H	2.7492207752	-1.0379104079	2.1561610809

H 2.7492207752 1.0379104079 2.1561610809
H -1.0379104079 -2.7492207752 -2.1561610809
H 1.0379104079 -2.7492207752 -2.1561610809
H 1.0379104079 2.7492207752 -2.1561610809
H -1.0379104079 2.7492207752 -2.1561610809

ring-$[H_2BAs]_4$ D_{2d}
B -2.5712980264 0. 1.6910930555
As -1.7573561937 0. -0.1363988936
As 1.7573561937 0. -0.1363988936
As 0. 1.7573561937 0.1363988936
As 0. -1.7573561937 0.1363988936
B 0. 2.5712980264 -1.6910930555
B 2.5712980264 0. 1.6910930555
B 0. -2.5712980264 -1.6910930555
H -2.8731777147 1.0355693922 2.1948789799
H -2.8731777147 -1.0355693922 2.1948789799
H 2.8731777147 -1.0355693922 2.1948789799
H 2.8731777147 1.0355693922 2.1948789799
H -1.0355693922 -2.8731777147 -2.1948789799
H 1.0355693922 -2.8731777147 -2.1948789799
H 1.0355693922 2.8731777147 -2.1948789799
H -1.0355693922 2.8731777147 -2.1948789799

ring-$[H_2AlN]_4$ D_2
Al -1.8615092442 1.8614975677 0.8962210812
N -0.7099501081 0.7099501827 0.0964596696
N 0.7099501081 -0.7099501827 0.0964596696
N 0.7099501081 0.7099501827 -0.0964596696
N -0.7099501081 -0.7099501827 -0.0964596696
Al 1.8615092442 1.8614975677 -0.8962210812
Al 1.8615092442 -1.8614975677 0.8962210812
Al -1.8615092442 -1.8614975677 -0.8962210812
H -1.2995483666 3.3164206406 1.1123120399
H -3.3164238725 1.299515208 1.1123130696
H 1.2995483666 -3.3164206406 1.1123120399
H 3.3164238725 -1.299515208 1.1123130696
H -3.3164238725 -1.2995152079 -1.1123130696
H -1.2995483667 -3.3164206405 -1.1123120399
H 1.2995483667 3.3164206405 -1.1123120399
H 3.3164238725 1.2995152079 -1.1123130696

ring-$[H_2GaN]_4$ D_2
Ga 0.0000006955 2.6459290206 0.9664053307
N -0.0000000279 1.0000642527 0.0622367248
N 0.0000000279 -1.0000642527 0.0622367248
N 1.0000642527 0.0000000172 -0.0622367249
N -1.0000642527 -0.0000000172 -0.0622367249
Ga 2.6459290206 0.0000008147 -0.9664053307

Ga	-0.0000006955	-2.6459290206	0.9664053307
Ga	-2.6459290206	-0.0000008147	-0.9664053307
H	1.4269147222	3.2464352737	1.1155116131
H	-1.4269120141	3.2464390005	1.1155088729
H	-1.4269147222	-3.2464352737	1.1155116131
H	1.4269120141	-3.2464390005	1.1155088729
H	-3.2464390648	1.4269118678	-1.1155088729
H	-3.2464352094	-1.4269148685	-1.1155116131
H	3.2464352094	1.4269148685	-1.1155116131
H	3.2464390648	-1.4269118678	-1.1155088729

$[H_2MY]_4$ structures.
Bridged Ring structures.

bridged ring-$[H_2BN]_4$ C_2

B	0.403185904	1.8368924116	-0.1776753231
N	-0.4047868321	0.6629799807	-0.7757748292
N	0.3269782789	-0.7044815464	0.775321125
N	0.4047868321	-0.6629799807	-0.7757748292
N	-0.3269782789	0.7044815464	0.775321125
B	-0.403185904	-1.8368924116	-0.1776753231
B	1.7521881909	-0.6837536478	0.1777317317
B	-1.7521881909	0.6837536478	0.1777317317
H	1.5680667038	1.8689041249	-0.3072182575
H	-0.2342780219	2.8305990808	-0.1054626723
H	2.4253988789	0.2674411438	0.3078544449
H	2.2254013436	-1.7654189975	0.1056028247
H	-2.2254013436	1.7654189975	0.1056028247
H	-2.4253988789	-0.2674411438	0.3078544449
H	0.2342780219	-2.8305990808	-0.1054626723
H	-1.5680667038	-1.8689041249	-0.3072182575

bridged ring-$[H_2BP]_4$ D_{2h}

B	-1.3458157205	-1.1797136565	1.4930059936
P	-1.6247708764	0.0007719321	-0.0917824392
P	1.6237883372	0.0002415163	0.0604476358
P	0.0227151996	1.6243814715	-0.0967234021
P	-0.0236977389	-1.6233680231	0.0653885986
B	1.3448331812	1.1807271049	-1.5243407971
B	1.2038210885	1.3329720076	1.4853593974
B	-1.2048036278	-1.3319585592	-1.5166942008
H	-0.9603038291	-0.7017136068	2.5053187447
H	-2.1949020971	-2.0183351832	1.4765313306
H	0.723328667	0.9575184931	2.5002693754
H	2.054690094	2.1696689039	1.4637864112
H	-2.0556726333	-2.1686554555	-1.4951212147
H	-0.7243112063	-0.9565050447	-2.5316041788
H	2.1939195578	2.0193486316	-1.5078661341
H	0.9593212898	0.7027270552	-2.5366535482

bridged ring-$[H_2BAs]_4$ D_{2h}

B	-1.4189867327	-1.2436745775	1.5774404693
As	-1.7808788839	0.0030068067	-0.0992095463
As	1.7798963446	-0.0019933583	0.0678747428
As	0.0227360717	1.7804824951	-0.1046187541
As	-0.023718611	-1.7794690467	0.0732839506
B	1.4180041935	1.2446880259	-1.6087752727
B	1.2690996157	1.405454117	1.5693786501
B	-1.270082155	-1.4044406686	-1.6007134535
H	-1.0056796888	-0.7404507416	2.5672610788
H	-2.2698095881	-2.0800657172	1.6017028931
H	0.7629121533	1.0025094131	2.5619569085
H	2.1178877798	2.2440420284	1.5885437835
H	-2.1188703191	-2.24302858	-1.6198785869
H	-0.7638946926	-1.0014959648	-2.593291712
H	2.2688270489	2.0810791656	-1.6330376965
H	1.0046971496	0.74146419	-2.5985958822

bridged ring-$[H_2AlN]_4$ C_2

Al	-0.5013185826	2.1860438314	0.37234278
N	0.5013185826	0.565368848	0.7772718125
N	-0.2696677831	-0.7059554289	-0.7777323538
N	-0.5013185826	-0.565368848	0.7772718125
N	0.2696677831	0.7059554289	-0.7777323538
Al	0.5013185826	-2.1860438314	0.37234278
Al	-2.1700766586	-0.5654157917	-0.3721696189
Al	2.1700766586	0.5654157917	-0.3721696189
H	-1.927281547	2.1720973906	1.0282810612
H	0.3628928361	3.4496889687	0.0197917313
H	-2.8155076062	0.7073705367	-1.025698163
H	-2.8917411815	-1.9159160517	-0.0214019361
H	2.8917411815	1.9159160517	-0.0214019361
H	2.8155076062	-0.7073705367	-1.025698163
H	-0.3628928361	-3.4496889687	0.0197917313
H	1.927281547	-2.1720973906	1.0282810612

bridged ring-$[H_2AlP]_4$ D_{2h}

Al	-1.56942	-1.36122	1.89508
P	-1.664	0.04966	-0.0961
P	1.66302	-0.04865	0.06475
P	-0.02563	1.6643	-0.101
P	0.02465	-1.66329	0.06968
Al	1.56841	1.36226	-1.92641
Al	1.38981	1.5551	1.8862
Al	-1.39076	-1.55411	-1.91753
H	-1.06292	-0.73179	3.23946
H	-2.6727	-2.46983	1.67849
H	0.75718	1.06186	3.23401

H	2.5137	2.64145	1.66292
H	-2.51467	-2.64044	-1.69426
H	-0.75811	-1.06088	-3.26533
H	2.6717	2.47085	-1.70981
H	1.0619	0.73285	-3.2708

bridged ring-$[H_2AlAs]_4$ D_{2h}

Al	-1.6183664226	-1.4019066824	1.9734709978
As	-1.8295228714	0.0556517587	-0.1041521383
As	1.8285405109	-0.0546380561	0.0728173098
As	-0.0292195281	1.8298750054	-0.1095517748
As	0.0282371676	-1.8288613028	0.0782169463
Al	1.6173840621	1.402920385	-2.0048058263
Al	1.431419291	1.6036983067	1.9643237981
Al	-1.4324016516	-1.6026846042	-1.9956586266
H	-1.0829340422	-0.7460760987	3.2961536311
H	-2.7325217517	-2.5145425509	1.8257289641
H	0.7718762602	1.081864492	3.2905905123
H	2.5597339947	2.701046926	1.8098559407
H	-2.5607163552	-2.7000332234	-1.8411907691
H	-0.7728586208	-1.0808507894	-3.3219253408
H	2.7315393911	2.5155562535	-1.8570637926
H	1.0819516817	0.7470898013	-3.3274884596

bridged ring-$[H_2GaN]_4$ C_2

Ga	1.4125517791	0.9141702958	-1.6823594901
N	0.5086914685	-0.5903610499	-0.7394751454
N	-0.6669350515	0.4030597812	0.7394370328
N	0.6669350515	-0.4030597812	0.7394370328
N	-0.5086914685	0.5903610499	-0.7394751454
Ga	-0.6669350515	-1.5444741931	1.6823710966
Ga	0.6669350515	1.5444741931	1.6823710966
Ga	-1.4125517791	-0.9141702958	-1.6823594901
H	2.5955175707	1.5007273669	-0.8757834596
H	1.0162716333	1.0097893403	-3.1789041961
H	1.0481672424	2.8085369966	0.8755086751
H	0.82680224	1.1701594469	3.179085969
H	-1.0162716333	-1.0097893403	-3.1789041961
H	-2.5955175707	-1.5007273669	-0.8757834596
H	-0.82680224	-1.1701594469	3.179085969
H	-1.0481672424	-2.8085369966	0.8755086751

bridged ring-$[H_2GaP]_4$ D_{2h}

Ga	-1.568031013	-1.3586446663	1.9078352341
P	-1.6665940763	0.0534495059	-0.0964072263
P	1.6656122633	-0.052435034	0.0650723612
P	-0.0293777048	1.6669559136	-0.1013174669
P	0.0283958918	-1.6659414416	0.0699826018
Ga	1.5670492	1.3596591383	-1.9391700992

Ga	1.3872211893	1.5538099413	1.8989720198
Ga	-1.3882030023	-1.5527954693	-1.9303068849
H	-1.0314783378	-0.7043302248	3.2034127834
H	-2.6550894818	-2.4524398518	1.6788047605
H	0.7290975621	1.030749234	3.1981325703
H	2.4960496948	2.6241011681	1.6633557744
H	-2.4970315078	-2.6230866962	-1.6946906396
H	-0.7300793751	-1.029734762	-3.2294674354
H	2.6541076688	2.4534543238	-1.7101396256
H	1.0304965248	0.7053446968	-3.2347476485

bridged ring-$[H_2GaAs]_4$ D_{2h}

Ga	-1.6166866107	-1.3997569239	1.9786257563
As	-1.8333372833	0.0591535352	-0.1045080103
As	1.8323551664	-0.058139486	0.0731731477
As	-0.0326718701	1.8337392326	-0.1099086776
As	0.0316897533	-1.8327251834	0.078573815
Ga	1.6157044939	1.4007709731	-2.0099606188
Ga	1.4292561127	1.6020702633	1.9694901761
Ga	-1.4302382295	-1.601056214	-2.0008250387
H	-1.0526326926	-0.7203488988	3.2533660325
H	-2.7165481035	-2.4988866582	1.8248762898
H	0.7455765757	1.051816227	3.2479727318
H	2.5438359708	2.6853092912	1.8090990199
H	-2.5448180876	-2.6842952419	-1.8404338825
H	-0.7465586925	-1.0508021778	-3.2793075944
H	2.7155659867	2.4999007075	-1.8562111524
H	1.0516505758	0.721362948	-3.2847008951

Table 5S. Unscaled Harmonic vibrational frequencies (ω, cm^{-1}) scaled Harmonic vibrational frequencies (ν^a, cm^{-1}) and Infra-red Intensities (I, km mol^{-1}) of the studied compounds. B3LYP/TZVP level of theory.

[a)]Scaled according to equation $\nu = 0.9461\omega+22.1$ (Timoshkin, A.Y.; Bettinger, H.F.; Schaefer, H.F. *J. Am. Chem. Soc.* **1997**, *119*, 5668).

ω	ν^a	I	ω	ν^a	I	ω	ν^a	I
tetrahedral $[BNH_2]_4$								
18.7	39.8	48.34	115.9	131.7	43.84	117.6	133.3	43.53
152.9	166.8	0.00	163.6	176.9	0.02	205.8	216.8	5.33
206.8	217.7	5.22	215.5	226.0	0.60	284.9	291.6	323.86
293.5	299.8	398.32	295.9	302.1	70.79	316.2	321.3	118.51
333.2	337.4	0.47	463.0	460.1	0.26	464.0	461.1	8.61
464.4	461.5	9.58	538.8	531.9	0.00	572.4	563.7	0.00
621.6	610.2	2.46	635.1	623.0	19.77	652.6	639.5	1.74
652.7	639.6	1.78	946.2	917.3	0.97	946.5	917.6	0.88
967.7	937.6	20.99	979.2	948.5	0.01	1250.8	1205.5	324.93
1265.1	1219.0	465.92	1265.4	1219.3	465.19	1491.8	1433.5	0.00
1609.5	1544.8	163.30	1611.0	1546.3	116.17	1611.0	1546.3	114.63
1620.4	1555.1	0.04	3579.8	3408.9	41.52	3580.0	3409.1	43.63
3580.5	3409.6	37.72	3581.7	3410.7	8.45	3669.4	3493.8	26.97
3669.7	3494.0	22.45	3669.8	3494.1	30.07	3671.0	3495.2	27.02
tetrahedral $[BPH_2]_4$								
74.6	92.6	3.23	76.3	94.3	0.00	80.4	98.2	1.59
83.0	100.6	4.85	83.0	100.6	4.85	103.1	119.7	5.36
103.1	119.7	5.36	113.2	129.2	9.96	120.3	135.9	0.00
305.6	311.3	0.00	317.2	322.2	2.86	317.2	322.2	2.86
326.6	331.1	0.00	413.9	413.7	0.07	432.2	431.0	1.06
432.2	431.0	1.06	563.4	555.2	0.00	599.5	589.3	13.45
657.6	644.3	0.00	660.4	646.9	1.48	660.4	646.9	1.48
689.8	674.7	31.39	751.4	733.0	11.26	751.4	733.0	11.26
779.7	759.7	7.63	803.5	782.3	0.00	966.5	936.5	371.75
966.5	936.5	371.75	981.9	951.1	336.54	1085.7	1049.3	15.80
1085.7	1049.3	15.80	1089.6	1052.9	0.00	1095.1	1058.2	26.08
1268.0	1221.8	0.00	2368.9	2263.3	21.89	2368.9	2263.3	21.89
2370.6	2264.9	0.00	2371.0	2265.3	73.77	2380.9	2274.7	43.50
2380.9	2274.7	43.50	2381.3	2275.0	0.00	2381.8	2275.6	62.74
tetrahedral $[BAsH_2]_4$								
46.6	66.2	0.00	46.9	66.4	0.26	53.7	72.9	0.84
56.4	75.5	0.79	56.4	75.5	0.79	76.8	94.7	1.95
76.8	94.7	1.95	82.0	99.7	2.90	90.0	107.2	0.00
189.2	201.1	0.00	293.8	300.1	0.48	293.8	300.1	0.48
304.0	309.7	0.00	326.4	330.9	0.24	354.5	357.4	1.17
354.5	357.4	1.17	552.0	544.3	0.00	571.5	562.8	12.50
619.3	608.0	21.37	619.3	608.0	21.37	633.0	621.0	0.00
658.6	645.2	7.81	681.6	667.0	5.63	681.6	667.0	5.63
740.3	722.5	9.37	754.4	735.8	0.00	931.0	902.9	359.14
931.0	902.9	359.14	943.4	914.6	369.43	978.0	947.4	3.47
978.0	947.4	3.47	979.7	949.0	0.00	985.7	954.7	9.69
1234.8	1190.4	0.00	2166.2	2071.6	32.95	2166.2	2071.6	32.95
2168.3	2073.5	0.00	2169.4	2074.6	147.42	2181.0	2085.6	95.10
2181.0	2085.6	95.10	2181.2	2085.8	0.00	2182.3	2086.7	88.79

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
tetrahedral $[AlNH_2]_4$								
27.4	48.0	2.73	39.6	59.6	2.34	72.5	90.7	0.01
77.1	95.0	0.03	81.4	99.1	0.01	94.7	111.7	0.10
101.0	117.6	0.08	104.0	120.5	1.10	136.3	151.1	0.03
139.5	154.1	0.01	143.9	158.3	0.31	147.3	161.4	0.02
258.3	266.5	5.86	273.5	280.8	14.51	276.8	284.0	1.90
278.7	285.8	0.96	286.8	293.4	0.04	287.3	293.9	0.64
319.0	323.9	2.99	322.1	326.8	107.67	339.4	343.2	358.08
347.0	350.4	208.64	603.8	593.3	3.20	617.0	605.8	11.34
617.9	606.7	0.92	635.4	623.2	14.82	756.0	737.4	253.40
758.2	739.4	252.26	759.8	741.0	253.49	803.9	782.7	0.17
1563.6	1501.4	63.53	1563.6	1501.4	62.46	1564.1	1501.9	31.75
1566.0	1503.7	43.35	3549.9	3380.7	9.08	3550.0	3380.8	12.09
3554.3	3384.8	11.12	3554.9	3385.4	10.61	3638.8	3464.8	4.12
3638.9	3464.8	29.21	3643.1	3468.9	15.85	3643.6	3469.3	15.91
tetrahedral $[AlPH_2]_4$								
37.2	57.3	0.00	38.9	58.9	4.77	38.9	58.9	4.77
41.6	61.5	5.89	47.5	67.1	2.31	51.8	71.1	0.57
51.8	71.1	0.57	52.8	72.0	0.00	54.4	73.5	1.20
106.7	123.1	0.00	109.2	125.4	0.32	109.2	125.4	0.32
194.1	205.7	0.00	215.3	225.8	0.04	219.0	229.3	0.16
219.0	229.3	0.16	252.1	260.6	0.00	256.0	264.3	0.03
427.9	426.9	105.40	428.5	427.5	116.53	428.5	427.5	116.53
506.0	500.9	0.00	519.0	513.1	11.55	519.0	513.1	11.55
528.0	521.6	0.00	529.5	523.1	15.24	566.8	558.4	36.61
566.8	558.4	36.61	576.6	567.6	0.00	583.2	573.9	39.82
1091.3	1054.5	12.22	1091.3	1054.5	12.22	1092.1	1055.4	0.00
1093.1	1056.3	34.84	2350.4	2245.8	28.01	2350.4	2245.8	28.01
2350.7	2246.1	0.00	2351.0	2246.4	65.82	2361.1	2255.9	44.01
2361.1	2255.9	44.01	2361.3	2256.2	0.00	2361.4	2256.2	57.73
tetrahedral $[AlAsH_2]_4$								
23.6	44.5	0.01	31.3	51.7	0.34	31.3	51.7	0.34
32.8	53.2	0.00	43.2	62.9	0.46	92.4	109.5	0.00
101.4	118.0	0.06	101.4	118.0	0.06	125.4	140.7	0.00
126.2	141.5	0.47	126.8	142.1	0.75	126.8	142.1	0.75
128.6	143.7	0.00	174.2	186.9	0.34	175.6	188.2	0.04
175.6	188.2	0.04	244.9	253.8	0.15	254.7	263.0	0.00
386.3	387.5	92.49	386.3	387.5	92.49	390.7	391.7	112.48
465.3	462.3	0.00	467.5	464.4	39.79	467.5	464.4	39.79
479.0	475.3	0.73	485.7	481.6	0.00	540.7	533.7	29.78
540.7	533.7	29.78	556.1	548.2	0.00	560.2	552.1	14.90
992.7	961.3	5.62	992.7	961.3	5.62	992.7	961.3	0.00
993.8	962.3	44.24	2163.4	2068.9	0.00	2163.7	2069.2	91.96
2163.7	2069.2	91.96	2164.2	2069.7	41.55	2189.6	2093.7	40.96
2189.6	2093.7	40.96	2190.3	2094.3	0.00	2190.4	2094.5	160.39

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
tetrahedral $[GaNH_2]_4$								
27.6	48.2	9.10	42.3	62.1	2.24	49.9	69.3	0.68
55.6	74.7	5.66	60.3	79.1	19.52	62.8	81.5	4.70
65.0	83.6	0.89	78.6	96.5	4.37	83.9	101.4	3.67
100.6	117.3	3.49	129.4	144.5	8.01	137.0	151.7	59.36
142.4	156.8	8.03	147.4	161.5	76.77	165.8	179.0	67.47
184.2	196.4	19.56	192.7	204.4	10.59	196.4	207.9	18.21
198.3	209.7	32.53	206.0	217.0	8.39	212.2	222.9	194.17
240.5	249.7	218.75	617.0	605.8	154.35	619.9	608.5	233.90
621.9	610.5	235.54	626.2	614.5	69.42	634.7	622.6	0.97
652.2	639.2	2.49	658.8	645.4	13.19	681.2	666.6	12.64
1545.5	1484.3	16.84	1546.8	1485.5	16.85	1549.5	1488.1	13.80
1550.7	1489.2	22.35	3534.7	3366.2	5.38	3538.4	3369.8	5.78
3542.8	3373.9	6.53	3543.4	3374.5	7.16	3638.7	3464.6	11.57
3643.3	3469.0	12.17	3649.8	3475.2	12.98	3650.1	3475.5	16.18
tetrahedral $[GaPH_2]_4$								
42.2	62.0	0.00	43.4	63.2	1.89	43.4	63.2	1.89
43.8	63.5	0.12	46.1	65.8	0.20	47.5	67.0	0.97
47.5	67.0	0.97	52.3	71.6	0.00	56.3	75.4	7.55
65.2	83.7	0.00	67.6	86.1	1.91	67.6	86.1	1.91
149.9	163.9	0.66	152.5	166.3	1.84	152.5	166.3	1.84
152.6	166.5	0.00	156.2	169.9	0.24	159.7	173.2	0.00
312.3	317.6	65.50	312.3	317.6	65.50	312.8	318.0	66.66
359.7	362.4	0.00	536.8	530.0	0.00	539.9	532.9	9.24
539.9	532.9	9.24	553.1	545.4	1.03	578.6	569.5	33.20
578.6	569.5	33.20	588.2	578.6	0.00	595.9	585.8	29.42
1094.0	1057.1	13.17	1094.0	1057.1	13.17	1094.7	1057.8	0.00
1095.8	1058.9	37.52	2351.3	2246.7	33.26	2351.3	2246.7	33.26
2351.6	2246.9	0.00	2351.9	2247.3	66.79	2362.4	2257.2	47.40
2362.4	2257.2	47.40	2362.6	2257.4	0.00	2362.8	2257.5	66.65
tetrahedral $[GaAsH_2]_4$								
23.0	43.9	0.01	26.7	47.3	0.15	26.7	47.3	0.15
31.4	51.8	0.00	37.4	57.5	0.26	47.5	67.1	0.00
54.9	74.1	0.02	54.9	74.1	0.02	111.4	127.5	0.00
123.6	139.0	0.51	125.3	140.7	0.79	125.3	140.7	0.79
134.5	149.4	0.00	136.1	150.9	0.06	136.2	151.0	0.54
136.2	151.0	0.54	150.4	164.4	0.08	154.8	168.5	0.00
249.5	258.2	45.63	249.5	258.2	45.63	250.3	259.0	52.85
312.1	317.4	0.00	473.3	469.9	0.00	479.4	475.7	29.20
479.4	475.7	29.20	492.5	488.0	6.53	551.8	544.2	28.90
551.8	544.2	28.90	568.9	560.3	0.00	571.9	563.2	6.15
996.0	964.5	0.00	996.1	964.5	6.14	996.1	964.5	6.14
997.0	965.4	46.22	2165.3	2070.7	0.00	2165.6	2071.0	99.13
2165.6	2071.0	99.13	2166.0	2071.4	46.99	2191.9	2095.8	44.06
2191.9	2095.8	44.06	2192.5	2096.4	0.00	2192.7	2096.6	170.79

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring $[BNH_2]_4$								
208.6	219.4	11.17	235.8	245.2	5.67	375.0	376.9	423.35
377.1	378.9	0.00	440.0	438.4	0.00	446.1	444.2	16.90
461.3	458.5	0.00	507.3	502.0	6.05	520.5	514.5	0.00
534.0	527.3	0.00	591.9	582.1	58.67	660.9	647.4	0.00
681.1	666.5	63.90	756.3	737.6	0.00	771.0	751.5	0.08
787.5	767.1	0.00	849.6	825.9	20.42	853.1	829.2	91.98
857.9	833.8	0.00	862.1	837.8	0.00	862.9	838.5	0.00
871.3	846.5	1.39	916.2	888.9	46.91	937.2	908.8	0.00
968.1	938.0	0.00	977.1	946.5	12.05	1003.1	971.1	0.00
1028.4	995.0	25.79	1152.3	1112.2	141.65	1165.0	1124.3	0.00
1625.9	1560.3	0.00	1657.0	1589.8	152.05	1658.9	1591.6	89.16
1692.3	1623.2	0.00	3526.4	3358.4	100.92	3530.6	3362.4	0.00
3535.2	3366.7	0.00	3538.2	3369.6	40.51	3603.2	3431.1	66.16
3605.6	3433.4	0.00	3610.7	3438.2	0.00	3614.4	3441.7	20.11
ring $[BPH_2]_4$								
137.5	152.2	1.03	202.0	213.2	0.20	204.1	215.2	236.94
214.8	225.3	0.00	241.6	250.7	0.00	256.1	264.4	10.94
290.0	296.5	0.00	327.7	332.1	0.00	354.7	357.6	115.54
439.2	437.6	0.00	476.7	473.1	0.00	491.9	487.5	0.00
506.1	500.9	0.14	524.8	518.6	0.00	532.5	525.9	0.00
540.1	533.1	0.55	556.5	548.6	0.00	575.5	566.6	0.74
609.2	598.4	0.91	612.1	601.2	18.49	634.0	622.0	0.00
670.3	656.3	0.00	675.7	661.3	22.97	686.8	671.8	0.00
717.7	701.1	23.42	721.5	704.7	0.00	746.1	727.9	0.00
755.1	736.5	1.17	878.8	853.5	0.00	901.6	875.1	79.92
1086.9	1050.4	0.00	1108.3	1070.7	52.26	1110.9	1073.1	102.71
1141.5	1102.1	0.00	2433.3	2324.3	0.00	2434.7	2325.6	44.25
2436.5	2327.2	123.26	2439.2	2329.8	0.00	2475.3	2364.0	15.40
2475.9	2364.6	0.00	2490.4	2378.2	0.00	2491.7	2379.5	54.29
ring $[BAsH_2]_4$								
22.9	43.8	4.69	68.5	86.9	0.43	81.9	99.6	4.83
98.9	115.7	0.18	121.8	137.3	0.90	144.4	158.7	0.09
154.1	167.9	1.70	180.4	192.7	3.71	190.6	202.5	3.34
266.4	274.1	2.42	313.8	319.0	36.06	348.8	352.1	12.65
394.4	395.2	9.78	423.6	422.9	4.25	437.2	435.7	15.00
464.7	461.7	2.12	481.0	477.2	2.86	516.8	511.0	2.05
543.7	536.5	14.48	584.0	574.7	8.03	600.6	590.3	16.47
612.1	601.2	11.62	674.2	660.0	20.49	675.8	661.5	3.18
685.7	670.8	12.55	712.3	696.0	7.49	727.1	710.0	12.83
757.5	738.7	22.01	939.3	910.7	68.02	966.6	936.6	35.30
969.4	939.3	18.61	991.4	960.1	30.62	1012.7	980.2	33.11
1226.5	1182.5	23.49	2146.4	2052.8	156.38	2151.1	2057.2	31.96
2156.2	2062.1	179.84	2157.8	2063.6	87.12	2165.1	2070.5	155.00
2234.6	2136.2	126.86	2314.6	2212.0	12.30	2321.3	2218.3	4.82

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring $[AlNH_2]_4$								
31.7	52.1	0.92	60.4	79.2	8.75	96.3	113.2	4.82
116.8	132.6	0.00	190.7	202.6	0.00	211.4	222.1	0.00
230.7	240.4	1.72	271.3	278.8	13.75	280.2	287.2	0.00
284.8	291.5	0.00	292.8	299.1	7.95	310.1	315.4	0.00
347.2	350.6	0.00	355.9	358.8	21.09	536.8	530.0	0.00
544.9	537.6	1.21	555.6	547.8	40.77	564.0	555.7	0.00
586.7	577.1	90.62	593.9	584.0	0.00	674.2	660.0	0.00
680.5	665.9	38.88	683.3	668.6	0.00	683.3	668.6	4.83
743.8	725.8	40.34	749.9	731.6	11.69	753.8	735.3	0.00
762.0	743.0	0.00	790.1	769.6	0.00	794.7	774.0	166.83
1585.1	1521.8	0.00	1589.4	1525.9	125.68	1610.0	1545.4	71.28
1615.5	1550.5	0.00	3479.2	3313.7	0.00	3479.3	3313.8	22.68
3481.4	3315.9	0.00	3482.5	3316.9	15.19	3553.2	3383.8	0.00
3553.5	3384.1	50.37	3556.7	3387.1	0.00	3557.2	3387.6	8.20
ring $[AlPH_2]_4$								
51.1	70.4	0.33	70.7	89.0	0.22	93.7	110.8	0.00
100.4	117.1	3.27	126.4	141.6	0.00	137.9	152.6	1.58
167.5	180.6	0.00	183.7	195.9	0.00	194.6	206.2	0.14
214.2	224.7	9.97	224.3	234.3	0.00	229.5	239.2	0.00
236.5	245.8	6.51	253.0	261.5	0.00	337.1	341.0	2.30
345.9	349.3	0.00	367.1	369.4	10.02	372.3	374.4	0.00
376.6	378.4	4.00	386.8	388.0	0.00	413.7	413.5	48.99
416.9	416.6	0.00	450.6	448.5	0.00	451.1	448.9	1.26
540.2	533.2	0.34	546.6	539.2	8.15	552.7	545.0	0.00
553.1	545.4	0.00	608.1	597.4	28.94	613.7	602.8	0.00
1075.4	1039.6	0.00	1082.5	1046.3	97.35	1097.4	1060.3	92.40
1106.9	1069.4	0.00	2402.0	2294.6	0.00	2402.3	2294.9	72.66
2404.6	2297.1	180.09	2406.0	2298.4	0.00	2432.7	2323.7	7.49
2433.6	2324.5	0.00	2434.0	2324.9	0.00	2435.5	2326.3	61.74
ring $[AlAsH_2]_4$								
33.0	53.4	0.17	48.8	68.3	0.03	64.0	82.6	0.00
74.2	92.3	0.46	92.0	109.1	0.00	108.7	124.9	1.46
117.2	133.0	0.00	149.9	163.9	0.00	157.6	171.2	9.63
168.7	181.7	0.00	170.5	183.4	1.58	186.9	198.9	8.70
199.9	211.3	0.00	235.0	244.4	0.00	270.1	277.7	0.00
272.7	280.1	2.72	294.4	300.6	7.10	303.9	309.6	0.00
306.3	311.9	0.33	314.2	319.4	0.00	336.6	340.6	31.34
347.1	350.5	0.00	357.1	359.9	1.19	358.7	361.4	0.00
468.2	465.1	1.61	479.1	475.4	0.00	481.1	477.2	0.30
502.2	497.3	0.00	546.5	539.2	24.39	555.5	547.7	0.00
967.5	937.5	0.00	973.9	943.5	135.80	985.8	954.8	112.06
993.6	962.2	0.00	2196.6	2100.3	0.00	2197.1	2100.8	179.03
2201.1	2104.6	377.42	2203.5	2106.8	0.00	2229.9	2131.8	0.00
2231.7	2133.5	27.87	2232.9	2134.7	136.56	2233.6	2135.3	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring $[GaNH_2]_4$								
27.5	48.1	0.01	39.6	59.6	3.37	57.2	76.2	0.00
81.7	99.4	1.39	132.7	147.6	0.00	157.7	171.3	0.00
182.2	194.5	0.00	186.1	198.2	1.52	208.8	219.7	19.76
214.8	225.4	0.00	215.7	226.1	24.50	217.8	228.2	0.00
257.4	265.6	35.32	262.7	270.7	0.00	437.0	435.5	0.00
447.4	445.4	59.78	490.0	485.7	150.82	497.1	492.4	10.93
497.4	492.7	0.00	499.1	494.3	0.00	606.7	596.1	0.00
613.0	602.1	18.88	646.2	633.5	0.64	657.0	643.7	0.00
687.5	672.5	75.29	710.7	694.5	0.65	713.1	696.8	0.00
716.0	699.5	0.00	769.8	750.4	157.60	772.2	752.7	0.00
1563.2	1501.0	0.00	1568.1	1505.6	91.38	1590.3	1526.7	62.07
1595.9	1532.0	0.00	3474.5	3309.3	7.81	3474.7	3309.5	0.00
3476.1	3310.8	0.00	3476.7	3311.4	2.93	3563.2	3393.2	22.57
3563.2	3393.2	0.00	3564.4	3394.4	0.00	3564.7	3394.6	6.31
ring $[GaPH_2]_4$								
33.2	53.5	0.05	46.4	66.0	1.84	49.0	68.4	0.15
76.1	94.1	0.00	91.3	108.5	0.00	101.9	118.5	0.00
118.8	134.5	3.81	120.0	135.6	0.00	126.4	141.7	13.66
132.6	147.6	0.00	139.0	153.6	11.02	151.1	165.1	0.00
151.2	165.1	1.98	154.1	167.9	0.00	270.1	277.6	0.00
276.8	284.0	15.73	289.3	295.8	37.13	289.9	296.3	0.00
298.4	304.4	4.57	301.9	307.8	0.00	340.3	344.0	0.00
346.3	349.7	13.81	378.7	380.3	4.80	390.9	391.9	0.00
450.7	448.5	0.04	477.2	473.6	0.50	492.2	487.8	0.00
511.5	506.0	0.00	576.9	568.0	27.76	592.5	582.7	0.00
1071.3	1035.6	0.00	1076.8	1040.8	107.91	1090.7	1054.1	91.82
1095.4	1058.4	0.00	2405.2	2297.7	0.00	2406.4	2298.8	105.01
2407.6	2299.9	132.25	2408.7	2301.0	0.00	2429.7	2320.8	0.00
2430.0	2321.1	44.48	2430.5	2321.6	0.00	2431.0	2322.0	45.52
ring $[GaAsH_2]_4$								
22.7	43.6	0.00	34.5	54.7	0.21	42.0	61.8	3.07
54.5	73.7	0.00	65.3	83.9	0.00	73.9	92.0	0.00
79.1	96.9	9.56	83.4	101.0	1.80	89.6	106.8	0.00
91.4	108.6	0.00	107.3	123.6	5.27	130.7	145.8	0.00
135.0	149.8	10.74	139.2	153.8	0.00	197.1	208.6	0.00
205.2	216.2	11.02	216.7	227.1	13.28	224.8	234.8	0.00
233.5	243.0	1.52	233.8	243.3	0.00	258.6	266.8	0.00
260.8	268.8	11.68	299.3	305.2	2.75	326.2	330.7	0.00
384.6	386.0	8.20	428.0	427.0	0.00	431.3	430.1	0.77
466.6	463.5	0.00	530.5	524.0	18.99	544.3	537.0	0.00
961.6	931.9	0.00	967.9	937.8	144.27	977.0	946.5	113.51
981.5	950.7	0.00	2195.0	2098.7	0.00	2197.2	2100.9	231.97
2199.3	2102.9	273.48	2201.0	2104.5	0.00	2222.2	2124.5	0.00
2224.3	2126.5	94.26	2225.3	2127.5	99.73	2226.2	2128.3	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
cubane-[HBNH]$_4$								
501.0	496.1	0.00	501.0	496.1	0.00	564.3	556.0	13.32
564.3	556.0	13.32	564.3	556.0	13.32	643.8	631.2	0.00
643.8	631.2	0.00	643.8	631.2	0.00	702.8	687.1	0.00
702.8	687.1	0.00	720.9	704.2	10.03	720.9	704.2	10.03
720.9	704.2	10.03	817.0	795.0	1.03	817.0	795.0	1.03
817.0	795.0	1.03	860.0	835.7	0.00	860.0	835.7	0.00
860.0	835.7	0.00	899.0	872.7	0.00	899.0	872.7	0.00
914.7	887.5	0.00	967.3	937.2	0.00	1038.9	1005.0	0.00
1038.9	1005.0	0.00	1038.9	1005.0	0.00	1075.1	1039.2	0.00
1075.1	1039.2	0.00	1122.7	1084.3	392.42	1122.7	1084.3	392.42
1122.7	1084.3	392.42	1162.4	1121.8	88.66	1162.4	1121.8	88.66
1162.4	1121.8	88.66	2598.0	2480.1	301.42	2598.0	2480.1	301.42
2598.0	2480.1	301.42	2613.7	2494.9	0.00	3608.4	3436.0	0.00
3610.9	3438.3	25.81	3610.9	3438.3	25.81	3610.9	3438.3	25.81
cubane-[HBPH]$_4$								
301.6	307.4	0.18	301.6	307.4	0.18	301.6	307.4	0.18
304.1	309.9	0.00	304.1	309.9	0.00	447.9	445.9	0.00
456.2	453.7	0.00	456.2	453.7	0.00	456.2	453.7	0.00
493.2	488.7	3.18	493.2	488.7	3.18	493.2	488.7	3.18
516.2	510.5	0.00	516.2	510.5	0.00	522.7	516.6	0.55
522.7	516.6	0.55	522.7	516.6	0.55	575.4	566.5	0.00
575.4	566.5	0.00	575.4	566.5	0.00	672.0	657.9	0.00
672.0	657.9	0.00	680.0	665.5	0.00	807.2	785.8	7.70
807.2	785.8	7.70	807.2	785.8	7.70	809.3	787.8	0.00
809.3	787.8	0.00	809.6	788.1	0.00	809.6	788.1	0.00
809.6	788.1	0.00	885.4	859.8	27.18	885.4	859.8	27.18
885.4	859.8	27.18	2375.3	2269.3	95.62	2375.3	2269.3	95.62
2375.3	2269.3	95.62	2376.8	2270.8	0.00	2642.2	2521.9	127.59
2642.2	2521.9	127.59	2642.2	2521.9	127.59	2644.3	2523.9	0.00
cubane-[HBAsH]$_4$								
196.3	207.8	0.00	196.3	207.8	0.00	199.8	211.1	0.23
199.8	211.1	0.23	199.8	211.1	0.23	282.5	289.4	0.00
391.8	392.7	0.00	391.8	392.7	0.00	391.8	392.7	0.00
429.6	428.6	5.23	429.6	428.6	5.23	429.6	428.6	5.23
448.0	445.9	0.00	448.0	445.9	0.00	468.5	465.4	0.13
468.5	465.4	0.13	468.5	465.4	0.13	477.4	473.8	0.00
477.4	473.8	0.00	477.4	473.8	0.00	589.1	579.5	0.00
589.1	579.5	0.00	629.4	617.6	0.00	719.8	703.1	25.05
719.8	703.1	25.05	719.8	703.1	25.05	777.7	757.9	0.00
777.7	757.9	0.00	778.8	758.9	0.00	778.8	758.9	0.00
778.8	758.9	0.00	854.1	830.2	24.52	854.1	830.2	24.52
854.1	830.2	24.52	2174.8	2079.7	180.73	2174.8	2079.7	180.73
2174.8	2079.7	180.73	2179.6	2084.2	0.00	2658.3	2537.1	123.77
2658.3	2537.1	123.77	2658.3	2537.1	123.77	2660.0	2538.7	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
cubane-[HAlNH]$_4$								
297.2	303.3	0.00	297.2	303.3	0.00	344.2	347.7	0.51
344.2	347.7	0.51	344.2	347.7	0.51	451.2	449.0	0.00
451.2	449.0	0.00	451.2	449.0	0.00	457.7	455.1	0.00
457.7	455.1	0.00	499.5	494.6	23.02	499.5	494.6	23.02
499.5	494.6	23.02	511.7	506.2	0.00	536.7	529.9	0.00
536.7	529.9	0.00	536.7	529.9	0.00	598.6	588.5	0.00
598.6	588.5	0.00	624.9	613.3	84.37	624.9	613.3	84.37
624.9	613.3	84.37	727.8	710.7	0.00	738.2	720.5	392.80
738.2	720.5	392.80	738.2	720.5	392.80	783.1	763.0	0.00
783.1	763.0	0.00	783.1	763.0	0.00	843.4	820.0	0.00
843.4	820.0	0.00	854.3	830.3	469.68	854.3	830.3	469.68
854.3	830.3	469.68	1934.1	1852.0	364.29	1934.1	1852.0	364.29
1934.1	1852.0	364.29	1946.2	1863.4	0.00	3598.5	3426.7	0.00
3600.7	3428.7	23.93	3600.7	3428.7	23.93	3600.7	3428.7	23.93
cubane-[HAlPH]$_4$								
143.0	157.4	0.18	143.0	157.4	0.18	143.0	157.4	0.18
149.1	163.2	0.00	149.1	163.2	0.00	296.7	302.8	0.00
297.9	303.9	0.00	297.9	303.9	0.00	297.9	303.9	0.00
312.4	317.6	0.00	312.4	317.6	0.00	340.1	343.9	4.45
340.1	343.9	4.45	340.1	343.9	4.45	371.1	373.2	21.62
371.1	373.2	21.62	371.1	373.2	21.62	374.7	376.6	0.00
389.1	390.2	0.00	389.1	390.2	0.00	389.1	390.2	0.00
484.9	480.9	0.00	484.9	480.9	0.00	498.4	493.7	0.00
498.4	493.7	0.00	498.4	493.7	0.00	554.5	546.7	0.00
554.5	546.7	0.00	564.1	555.8	223.97	564.1	555.8	223.97
564.1	555.8	223.97	620.5	609.2	107.17	620.5	609.2	107.17
620.5	609.2	107.17	1931.8	1849.8	337.27	1931.8	1849.8	337.27
1931.8	1849.8	337.27	1937.4	1855.1	0.00	2435.2	2326.0	0.00
2435.8	2326.6	29.77	2435.8	2326.6	29.77	2435.8	2326.6	29.77
cubane-[HAlAsH]$_4$								
107.5	123.8	0.35	107.5	123.8	0.35	107.5	123.8	0.35
107.9	124.1	0.00	107.9	124.1	0.00	204.2	215.3	0.00
243.5	252.5	0.00	243.5	252.5	0.00	243.5	252.5	0.00
246.7	255.5	0.00	246.7	255.5	0.00	277.3	284.5	4.38
277.3	284.5	4.38	277.3	284.5	4.38	302.7	308.5	17.87
302.7	308.5	17.87	302.7	308.5	17.87	314.0	319.2	0.00
339.3	343.1	0.00	339.3	343.1	0.00	339.3	343.1	0.00
467.8	464.7	0.00	467.8	464.7	0.00	474.5	471.0	0.00
474.5	471.0	0.00	474.5	471.0	0.00	504.8	499.7	0.00
504.8	499.7	0.00	527.1	520.8	94.47	527.1	520.8	94.47
527.1	520.8	94.47	591.5	581.7	183.66	591.5	581.7	183.66
591.5	581.7	183.66	1931.4	1849.4	342.60	1931.4	1849.4	342.60
1931.4	1849.4	342.60	1936.4	1854.2	0.00	2246.7	2147.7	91.77
2246.7	2147.7	91.77	2246.7	2147.7	91.77	2248.0	2148.9	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
cubane-[HGaNH]$_4$								
181.8	194.1	0.00	181.8	194.1	0.00	217.9	228.3	0.09
217.9	228.3	0.09	217.9	228.3	0.09	313.0	318.2	0.00
362.3	364.9	0.00	362.3	364.9	0.00	362.3	364.9	0.00
400.9	401.4	0.00	400.9	401.4	0.00	474.0	470.6	7.76
474.0	470.6	7.76	474.0	470.6	7.76	542.4	535.2	0.00
542.4	535.2	0.00	542.4	535.2	0.00	566.0	557.6	81.33
566.0	557.6	81.33	566.0	557.6	81.33	592.3	582.4	0.00
592.3	582.4	0.00	633.8	621.7	275.23	633.8	621.7	275.23
633.8	621.7	275.23	682.7	668.0	0.00	816.8	794.8	0.00
816.8	794.8	0.00	816.8	794.8	0.00	863.2	838.8	0.00
863.2	838.8	0.00	879.1	853.8	214.26	879.1	853.8	214.26
879.1	853.8	214.26	1971.9	1887.7	331.83	1971.9	1887.7	331.83
1971.9	1887.7	331.83	1983.1	1898.3	0.00	3572.9	3402.5	0.00
3574.9	3404.3	9.55	3574.9	3404.3	9.55	3574.9	3404.3	9.55
cubane-[HGaPH]$_4$								
104.1	120.6	0.00	104.1	120.6	0.00	123.8	139.2	0.37
123.8	139.2	0.37	123.8	139.2	0.37	205.5	216.5	0.00
223.5	233.6	0.00	223.5	233.6	0.00	223.5	233.6	0.00
272.2	279.6	0.00	272.2	279.6	0.00	281.2	288.1	20.05
281.2	288.1	20.05	281.2	288.1	20.05	312.9	318.1	8.99
312.9	318.1	8.99	312.9	318.1	8.99	347.0	350.4	0.00
419.1	418.6	0.00	419.1	418.6	0.00	419.1	418.6	0.00
487.1	483.0	0.00	487.1	483.0	0.00	488.1	483.9	0.00
488.1	483.9	0.00	488.1	483.9	0.00	546.2	538.8	139.44
546.2	538.8	139.44	546.2	538.8	139.44	557.2	549.2	0.00
557.2	549.2	0.00	617.6	606.4	21.91	617.6	606.4	21.91
617.6	606.4	21.91	1958.7	1875.2	336.64	1958.7	1875.2	336.64
1958.7	1875.2	336.64	1966.1	1882.2	0.00	2413.4	2305.4	48.20
2413.4	2305.4	48.20	2413.4	2305.4	48.20	2413.7	2305.7	0.00
cubane-[HGaAsH]$_4$								
84.5	102.0	0.00	84.5	102.0	0.00	104.6	121.1	0.55
104.6	121.1	0.55	104.6	121.1	0.55	167.2	180.3	0.00
167.2	180.3	0.00	167.2	180.3	0.00	184.0	196.2	0.00
189.2	201.1	0.00	189.2	201.1	0.00	206.5	217.4	7.86
206.5	217.4	7.86	206.5	217.4	7.86	225.9	235.8	0.00
225.9	235.8	8.35	225.9	235.8	8.35	225.9	235.8	8.35
339.0	342.8	0.00	339.0	342.8	0.00	339.0	342.8	0.00
463.1	460.3	0.00	463.1	460.3	0.00	464.9	462.0	0.00
464.9	462.0	0.00	464.9	462.0	0.00	498.2	493.4	0.00
498.2	493.4	0.00	523.1	517.0	67.19	523.1	517.0	67.19
523.1	517.0	67.19	575.2	566.3	82.91	575.2	566.3	82.91
575.2	566.3	82.91	1952.4	1869.3	344.61	1952.4	1869.3	344.61
1952.4	1869.3	344.61	1959.3	1875.8	0.00	2217.7	2120.3	117.27
2217.7	2120.3	117.27	2217.7	2120.3	117.27	2220.3	2122.7	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ladder-[HBNH]$_4$								
163.7	177.0	3.32	202.5	213.6	2.42	260.6	268.6	0.00
331.3	335.5	2.03	370.9	373.0	0.00	513.6	508.0	0.00
582.2	572.9	195.20	586.8	577.3	0.00	598.3	588.2	36.17
660.6	647.1	0.00	738.6	720.9	0.00	760.4	741.5	13.49
803.3	782.1	31.65	806.5	785.1	0.00	858.7	834.5	0.00
873.7	848.7	0.00	878.3	853.1	100.33	894.3	868.2	48.97
918.9	891.4	0.00	923.4	895.7	14.09	930.7	902.6	0.00
944.7	915.9	41.61	1003.5	971.5	135.45	1019.5	986.7	0.00
1043.0	1008.9	21.54	1058.0	1023.1	0.00	1084.7	1048.3	0.00
1130.8	1092.0	220.89	1150.7	1110.8	0.00	1178.7	1137.3	41.31
1214.8	1171.4	0.00	1230.1	1185.9	640.50	1398.2	1344.9	274.75
1401.5	1348.0	0.00	2555.7	2440.0	403.61	2559.6	2443.8	0.00
2653.2	2532.3	368.13	2656.3	2535.2	0.00	3567.5	3397.3	0.00
3568.6	3398.4	37.39	3673.9	3498.0	75.03	3674.2	3498.3	0.00
ladder-[HBPH]$_4$								
54.2	73.4	0.85	132.2	147.2	3.74	157.6	171.2	0.00
182.8	195.1	1.51	201.9	213.1	0.00	282.5	289.4	0.00
300.3	306.2	0.00	305.8	311.4	3.19	341.3	345.0	2.33
368.9	371.1	0.00	468.6	465.4	4.64	480.2	476.5	0.00
531.1	524.6	4.04	557.9	549.9	0.00	593.7	583.8	0.00
616.3	605.2	10.55	659.6	646.2	4.30	683.3	668.5	0.00
713.7	697.3	0.20	736.8	719.2	0.00	757.4	738.6	0.00
770.1	750.7	5.28	775.0	755.3	8.23	781.2	761.1	0.00
800.7	779.7	6.52	805.4	784.1	0.00	834.6	811.7	11.35
840.8	817.5	0.00	876.6	851.5	0.00	905.9	879.2	75.76
938.6	910.1	0.00	945.3	916.4	25.03	997.9	966.2	175.54
998.9	967.2	0.00	2349.5	2245.0	157.32	2350.3	2245.7	0.00
2447.0	2337.2	0.00	2448.0	2338.2	29.07	2650.9	2530.1	83.96
2650.9	2530.1	0.00	2658.1	2536.9	129.82	2659.0	2537.8	0.00
ladder-[HBAsH]$_4$								
33.0	53.3	0.28	92.1	109.2	0.00	93.7	110.7	0.61
122.6	138.1	0.00	163.8	177.1	4.72	172.9	185.7	0.00
201.3	212.5	0.77	233.8	243.3	0.00	298.8	304.8	7.73
319.0	323.9	0.00	395.5	396.3	4.11	423.6	422.8	0.00
478.9	475.2	0.00	482.5	478.6	28.63	495.5	490.8	0.00
522.8	516.7	8.30	606.8	596.2	16.17	634.7	622.5	0.88
641.0	628.6	0.00	664.6	650.9	0.00	672.5	658.4	0.00
709.2	693.0	5.43	726.2	709.2	9.35	733.5	716.1	0.00
743.7	725.7	0.00	758.9	740.1	6.55	784.8	764.6	0.00
798.4	777.4	59.43	805.8	784.5	33.36	811.0	789.4	0.00
901.8	875.3	0.00	919.5	892.0	130.52	940.1	911.5	120.56
953.9	924.6	0.00	2185.7	2090.0	241.47	2186.5	2090.7	0.00
2262.1	2162.2	0.00	2262.9	2163.0	57.09	2654.0	2533.0	76.39
2654.6	2533.6	0.00	2669.2	2547.4	103.92	2669.4	2547.7	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ladder-[HAlNH]$_4$								
87.5	104.8	4.06	95.9	112.8	0.12	167.7	180.8	0.00
197.1	208.5	1.20	203.2	214.3	0.00	325.9	330.5	0.00
387.7	388.9	0.00	420.1	419.6	7.30	422.9	422.2	0.00
445.5	443.6	54.13	459.7	457.0	41.86	467.7	464.5	0.00
515.7	510.0	69.41	525.1	518.9	0.00	538.5	531.6	389.10
545.8	538.5	0.00	560.1	552.0	0.00	567.3	558.8	68.06
635.0	622.9	0.00	640.2	627.7	21.56	644.3	631.6	0.00
689.8	674.7	110.30	696.6	681.1	0.00	714.4	698.0	421.68
727.8	710.7	0.00	752.9	734.4	472.16	777.0	757.2	91.39
804.1	782.8	0.00	839.7	816.5	0.00	850.3	826.6	349.53
900.1	873.7	0.00	910.0	883.0	431.36	944.8	916.0	403.39
946.6	917.7	0.00	1893.6	1813.6	518.93	1896.0	1815.9	0.00
1965.9	1882.0	451.90	1968.7	1884.7	0.00	3540.2	3371.5	0.00
3540.8	3372.0	30.37	3650.9	3476.3	39.54	3651.1	3476.4	0.00
ladder-[HAlPH]$_4$								
42.9	62.7	0.95	50.8	70.2	0.99	64.4	83.0	0.00
96.8	113.7	1.70	102.9	119.4	0.00	147.5	161.7	0.00
194.4	206.0	0.00	200.1	211.4	37.37	253.8	262.2	0.00
267.2	274.9	12.48	313.6	318.8	2.09	333.1	337.2	0.00
348.1	351.4	0.00	366.2	368.6	40.89	384.5	385.8	0.00
388.8	389.9	142.97	417.2	416.8	0.00	421.7	421.0	69.17
422.0	421.4	0.00	430.9	429.8	37.50	443.2	441.4	0.00
471.8	468.5	24.48	483.0	479.1	18.52	491.8	487.4	0.00
504.6	499.5	49.98	517.4	511.6	0.00	553.0	545.3	0.00
558.6	550.6	168.80	604.9	594.4	0.00	609.0	598.3	635.01
611.2	600.4	0.00	635.2	623.1	125.87	658.6	645.2	18.90
681.3	666.7	0.00	1915.8	1834.7	430.30	1915.9	1834.7	0.00
1923.8	1842.2	578.41	1926.8	1845.1	0.00	2345.2	2240.9	93.95
2345.3	2241.0	0.00	2424.2	2315.6	0.00	2424.4	2315.8	26.03
ladder-[HAlAsH]$_4$								
31.1	51.5	0.41	49.3	68.8	0.62	54.8	74.0	0.00
69.9	88.3	0.73	73.2	91.3	0.00	106.2	122.5	0.00
147.2	161.3	0.00	148.8	162.9	11.37	215.9	226.4	0.00
227.3	237.2	8.21	263.3	271.2	4.41	273.1	280.5	0.00
290.0	296.5	0.00	305.8	311.5	21.09	323.3	328.0	97.69
323.6	328.2	0.00	339.9	343.7	0.00	349.7	353.0	18.22
385.1	386.5	0.00	392.4	393.4	88.87	459.8	457.1	0.00
472.1	468.8	29.72	482.9	479.0	0.00	487.0	482.8	18.96
506.7	501.5	0.00	509.3	504.0	13.09	540.1	533.1	0.00
545.9	538.6	166.00	594.1	584.2	673.35	599.6	589.4	0.00
603.4	593.0	0.00	624.6	613.0	65.31	639.1	626.8	50.91
662.6	649.0	0.00	1912.3	1831.3	0.00	1913.2	1832.2	637.68
1914.6	1833.5	397.85	1918.3	1837.0	0.00	2192.8	2096.7	179.67
2192.9	2096.8	0.00	2264.2	2164.2	0.00	2264.7	2164.7	96.68

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ladder-[HGaNH]$_4$								
54.3	73.5	0.95	71.9	90.1	0.70	110.3	126.5	0.00
150.5	164.5	6.52	155.4	169.2	0.00	207.9	218.8	0.00
268.0	275.7	0.00	284.7	291.4	5.02	319.8	324.6	0.00
362.8	365.4	31.79	417.0	416.7	16.06	435.1	433.8	0.00
436.8	435.4	0.00	438.3	436.8	312.32	473.2	469.8	16.32
493.4	488.9	0.00	519.3	513.4	0.00	535.8	529.0	35.35
564.8	556.5	0.00	571.9	563.2	179.48	605.3	594.7	0.00
614.0	603.0	450.59	633.3	621.3	0.00	642.4	629.9	149.13
651.6	638.5	0.00	663.7	650.0	114.89	738.9	721.2	67.31
742.1	724.2	0.00	807.9	786.4	134.27	813.0	791.3	0.00
943.4	914.6	0.00	946.8	917.9	100.97	968.2	938.1	219.79
973.0	942.7	0.00	1941.5	1858.9	464.35	1943.9	1861.2	0.00
2017.0	1930.4	410.77	2019.6	1932.8	0.00	3538.1	3369.5	0.00
3538.8	3370.2	17.71	3629.5	3455.9	27.82	3629.6	3456.1	0.00
ladder-[HGaPH]$_4$								
40.0	59.9	0.64	44.7	64.4	0.32	58.1	77.1	0.00
79.9	97.7	1.32	86.3	103.7	0.00	107.7	124.0	0.00
149.7	163.8	12.58	157.3	170.9	0.00	178.8	191.3	0.00
202.4	213.6	12.20	249.9	258.5	14.12	268.0	275.7	0.00
291.9	298.2	59.77	294.3	300.6	0.00	337.5	341.4	0.00
350.0	353.3	25.80	356.7	359.6	0.00	364.9	367.4	96.71
439.2	437.6	0.00	442.1	440.3	48.92	477.7	474.0	0.00
501.0	496.1	0.00	502.1	497.1	19.99	514.8	509.1	20.60
520.8	514.8	20.28	531.0	524.5	0.00	544.2	537.0	122.13
553.3	545.6	0.00	596.8	586.8	393.46	603.0	592.6	0.00
631.9	619.9	0.00	638.3	626.0	32.27	669.1	655.1	14.40
683.1	668.4	0.00	1955.7	1872.4	0.00	1956.4	1873.0	638.26
1958.4	1874.9	423.19	1963.0	1879.3	0.00	2341.9	2237.7	107.82
2342.0	2237.8	0.00	2406.0	2298.4	46.77	2406.0	2298.4	0.00
ladder-[HGaAsH]$_4$								
30.6	51.0	0.19	41.5	61.3	0.28	50.5	69.9	0.00
60.3	79.2	0.32	62.7	81.4	0.00	85.6	103.1	0.00
121.9	137.4	10.31	133.1	148.0	0.00	136.9	151.6	0.00
155.7	169.4	6.13	187.6	199.6	6.18	194.4	206.0	0.00
213.0	223.7	0.00	217.4	227.8	17.32	245.2	254.0	0.00
248.7	257.4	19.19	250.6	259.2	0.00	261.0	269.1	49.39
409.1	409.2	0.00	436.3	434.9	20.13	440.4	438.8	0.00
444.1	442.3	46.72	478.0	474.3	0.00	499.4	494.6	46.21
513.7	508.1	67.85	519.8	513.9	0.00	524.4	518.2	92.34
527.7	521.4	0.00	587.4	577.9	424.48	604.4	593.9	0.00
608.8	598.1	30.67	611.3	600.5	0.00	643.8	631.2	36.24
644.1	631.5	0.00	1936.5	1854.2	757.59	1936.6	1854.3	0.00
1940.3	1857.8	364.08	1943.8	1861.1	0.00	2192.1	2096.1	192.76
2192.2	2096.1	0.00	2224.5	2126.7	133.29	2224.7	2126.9	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring-[HBNH]$_4$			D_{4h}					
65.2	83.7	0.00	138.7	153.3	0.00	238.4	247.6	0.00
299.0	305.0	0.00	299.0	305.0	0.00	333.7	337.8	0.00
353.5	356.5	22.04	651.9	638.9	0.31	651.9	638.9	0.31
670.2	656.2	0.00	695.2	679.8	39.54	712.0	695.7	0.00
712.0	695.7	0.00	749.7	731.4	0.00	855.1	831.1	0.45
855.1	831.1	0.45	902.6	876.1	0.00	933.4	905.1	0.00
943.0	914.3	0.00	943.0	914.3	0.00	957.7	928.2	320.92
1061.4	1026.3	0.00	1143.3	1103.7	0.00	1179.7	1138.2	0.00
1195.2	1152.9	0.59	1195.2	1152.9	0.59	1294.8	1247.1	0.00
1396.9	1343.7	0.00	1416.8	1362.5	0.00	1429.3	1374.4	110.74
1429.3	1374.4	110.74	1507.8	1448.6	1118.53	1507.8	1448.6	1118.53
1532.3	1471.8	0.00	2573.8	2457.2	0.00	2577.1	2460.3	441.98
2577.1	2460.3	441.98	2587.0	2469.6	0.00	3574.1	3403.6	0.00
3574.3	3403.8	54.05	3574.3	3403.8	54.05	3575.2	3404.6	0.00
ring-[HBPH]$_4$			D_{2d}					
59.2	78.1	0.00	97.2	114.1	0.43	130.5	145.6	0.00
159.2	172.8	0.00	164.9	178.1	1.24	164.9	178.1	1.24
192.7	204.4	6.58	264.7	272.5	0.11	264.7	272.5	0.11
310.1	315.5	0.00	483.6	479.6	73.97	509.6	504.2	0.00
523.1	517.0	71.82	523.1	517.0	71.82	548.9	541.4	0.53
548.9	541.4	0.53	604.0	593.6	0.00	655.7	642.5	0.00
705.7	689.8	11.72	707.5	691.5	0.00	745.8	727.7	7.63
745.8	727.7	7.63	802.1	781.0	2.32	820.2	798.1	32.37
820.2	798.1	32.37	830.2	807.6	0.00	860.1	835.8	0.00
908.1	881.2	6.24	908.1	881.2	6.24	928.1	900.2	0.00
955.9	926.5	0.00	1053.1	1018.4	170.37	1053.1	1018.4	170.37
1084.7	1048.4	22.13	2435.8	2326.6	0.00	2436.1	2326.9	65.25
2436.1	2326.9	65.25	2437.9	2328.6	22.05	2641.8	2521.5	0.00
2642.0	2521.7	152.84	2642.0	2521.7	152.84	2643.3	2522.9	0.00
ring-[HBAsH]$_4$			D_{2d}					
45.9	65.5	0.00	62.1	80.8	0.01	107.3	123.6	0.00
110.9	127.0	0.00	145.7	159.9	0.18	145.7	159.9	0.18
170.0	183.0	0.03	170.0	183.0	0.03	187.2	199.2	0.00
187.5	199.5	0.42	432.5	431.3	46.96	448.7	446.6	25.13
448.7	446.6	25.13	463.7	460.8	0.00	475.0	471.5	0.00
493.4	488.9	23.51	493.4	488.9	23.51	617.4	606.2	0.00
647.6	634.8	0.00	668.4	654.4	1.57	714.4	698.0	10.74
714.4	698.0	10.74	728.1	711.0	8.32	728.1	711.0	8.32
743.1	725.2	0.00	753.1	734.6	0.00	756.5	737.8	3.43
801.9	780.8	38.12	801.9	780.8	38.12	805.1	783.8	0.00
906.9	880.1	0.00	991.0	959.6	151.83	991.0	959.6	151.83
1022.4	989.4	20.31	2214.1	2116.9	169.41	2214.1	2116.9	169.41
2215.0	2117.7	0.00	2216.5	2119.1	46.79	2651.4	2530.6	0.00
2651.5	2530.7	149.20	2651.5	2530.7	149.20	2652.5	2531.7	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring-[HAlNH]$_4$			D_{4h}					
42.4	62.3	0.00	57.0	76.0	0.00	115.8	131.7	0.00
135.4	150.2	0.00	147.8	161.9	0.00	147.8	161.9	0.00
181.7	194.0	1.50	324.1	328.7	21.10	324.1	328.7	21.10
404.2	404.5	0.00	439.6	438.0	86.93	448.2	446.2	0.00
448.2	446.2	0.00	491.1	486.8	0.00	502.8	497.8	10.72
502.8	497.8	10.72	506.5	501.3	0.00	520.7	514.7	0.00
582.0	572.7	0.00	582.0	572.7	0.00	584.7	575.3	0.00
615.6	604.5	617.21	625.7	614.1	0.00	712.1	695.8	395.33
712.1	695.8	395.33	801.0	779.9	0.00	867.8	843.1	0.00
936.0	907.6	0.00	950.8	921.7	551.54	950.8	921.7	551.54
1085.5	1049.1	0.00	1114.9	1076.9	368.34	1114.9	1076.9	368.34
1138.8	1099.5	0.00	1922.5	1841.0	0.00	1926.1	1844.4	493.46
1926.1	1844.4	493.46	1934.4	1852.2	0.00	3486.9	3321.1	0.00
3487.7	3321.8	24.36	3487.7	3321.8	24.36	3488.6	3322.7	0.00
ring-[HAlPH]$_4$			D_{2d}					
37.8	57.9	0.00	55.2	74.3	0.00	60.2	79.0	0.06
76.9	94.9	0.00	81.2	98.9	0.42	81.2	98.9	0.42
104.1	120.6	3.15	129.8	144.9	10.80	129.8	144.9	10.80
183.2	195.4	0.00	326.6	331.1	0.00	352.6	355.7	9.79
352.6	355.7	9.79	379.2	380.9	0.87	400.8	401.3	0.00
405.1	405.3	95.59	405.1	405.3	95.59	406.0	406.2	0.00
440.4	438.8	18.50	462.4	459.6	0.00	475.2	471.7	47.73
475.2	471.7	47.73	491.2	486.9	4.36	491.2	486.9	4.36
496.8	492.1	101.29	538.2	531.3	0.00	558.5	550.5	0.00
618.4	607.1	320.58	618.4	607.1	320.58	668.7	654.8	185.94
671.2	657.1	0.00	700.2	684.6	0.00	709.3	693.2	83.38
709.3	693.2	83.38	1920.8	1839.3	0.00	1922.1	1840.6	480.75
1922.1	1840.6	480.75	1926.4	1844.7	0.00	2374.4	2268.6	66.74
2374.4	2268.6	66.74	2375.0	2269.1	0.00	2376.0	2270.0	15.31
ring-[HAlAsH]$_4$			D_{2d}					
34.1	54.4	0.00	39.9	59.9	0.00	40.9	60.8	0.01
59.0	77.9	0.00	69.1	87.4	0.98	69.1	87.4	0.98
90.3	107.5	2.91	90.3	107.5	2.91	94.7	111.7	4.48
124.4	139.8	0.00	264.0	271.9	0.00	274.9	282.2	23.19
274.9	282.2	23.19	292.5	298.9	0.00	344.8	348.3	2.33
374.2	376.1	85.25	374.2	376.1	85.25	376.7	378.5	0.00
385.8	387.1	0.00	396.0	396.8	10.87	402.5	402.9	0.74
402.5	402.9	0.74	470.5	467.3	4.73	470.5	467.3	4.73
483.3	479.4	47.46	521.0	515.0	0.00	534.7	528.0	0.00
584.5	575.1	133.99	584.5	575.1	133.99	603.5	593.1	0.00
620.7	609.3	0.00	647.6	634.8	208.51	651.0	638.0	239.85
651.0	638.0	239.85	1912.2	1831.2	0.00	1913.4	1832.4	498.42
1913.4	1832.4	498.42	1917.5	1836.2	0.00	2179.2	2083.8	150.75
2179.2	2083.8	150.75	2181.6	2086.1	0.00	2181.9	2086.4	28.14

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring-[HGaNH]$_4$			D_{4h}					
19.2	40.2	0.00	32.0	52.4	0.00	82.1	99.8	0.00
112.1	128.2	0.00	115.0	130.9	0.00	115.0	130.9	0.00
134.9	149.7	10.99	230.1	239.8	6.16	230.1	239.8	6.16
247.1	255.9	0.00	392.2	393.2	75.28	413.4	413.2	0.00
413.4	413.2	0.00	431.9	430.7	6.71	431.9	430.7	6.71
453.0	450.6	0.00	460.6	457.8	0.00	474.3	470.8	0.00
521.6	515.6	0.00	547.7	540.3	0.00	559.4	551.3	0.00
559.4	551.3	0.00	590.5	580.8	350.74	648.8	635.9	472.63
648.8	635.9	472.63	687.0	672.0	0.00	833.7	810.9	0.00
845.9	822.4	0.00	861.9	837.5	383.54	861.9	837.5	383.54
1159.4	1119.0	0.00	1183.8	1142.1	118.00	1183.8	1142.1	118.00
1206.6	1163.6	0.00	1945.1	1862.4	0.00	1949.5	1866.5	467.67
1949.5	1866.5	467.67	1958.2	1874.7	0.00	3518.7	3351.1	0.00
3519.5	3351.9	22.43	3519.5	3351.9	22.43	3520.4	3352.7	0.00
ring-[HGaPH]$_4$			D_{2d}					
24.0	44.8	0.00	54.5	73.7	0.00	55.0	74.1	0.00
55.9	74.9	0.22	64.8	83.4	0.18	64.8	83.4	0.18
87.5	104.9	1.87	111.7	127.7	5.26	111.7	127.7	5.26
152.6	166.5	0.00	282.9	289.8	0.00	293.8	300.1	0.00
293.8	300.1	0.00	322.8	327.5	7.42	339.0	342.8	0.00
353.9	356.9	0.00	382.7	384.1	141.28	382.7	384.1	141.28
383.6	385.0	0.00	396.4	397.1	0.00	396.4	397.1	0.00
399.9	400.5	6.31	516.7	511.0	16.24	516.7	511.0	16.24
518.8	512.9	57.29	531.4	524.8	0.00	589.1	579.5	160.57
589.1	579.5	160.57	595.9	585.9	0.00	616.7	605.5	96.89
696.4	681.0	0.00	722.1	705.2	0.00	728.2	711.0	50.37
728.2	711.0	50.37	1940.1	1857.7	0.00	1941.6	1859.1	515.95
1941.6	1859.1	515.95	1946.8	1863.9	0.00	2372.9	2267.1	74.26
2372.9	2267.1	74.26	2373.6	2267.8	0.00	2374.4	2268.5	17.79
ring-[HGaAsH]$_4$			D_{2d}					
18.2	39.3	0.00	41.3	61.2	0.00	41.3	61.2	0.08
45.9	65.5	0.00	50.3	69.7	0.20	50.3	69.7	0.20
67.7	86.1	1.81	78.6	96.5	1.87	78.6	96.5	1.87
113.8	129.8	0.00	197.3	208.8	0.00	211.1	221.8	4.17
211.1	221.8	4.17	233.3	242.8	0.00	258.7	266.9	0.00
260.9	269.0	4.11	281.9	288.8	50.29	281.9	288.8	50.29
353.1	356.2	0.00	371.5	373.6	14.42	371.5	373.6	14.42
373.4	375.3	3.85	488.6	484.4	3.47	488.6	484.4	3.47
494.4	489.9	20.20	509.4	504.0	0.00	558.1	550.1	0.00
564.1	555.8	153.21	564.1	555.8	153.21	599.1	588.9	139.41
619.5	608.2	0.00	641.0	628.5	0.00	654.2	641.0	109.00
654.2	641.0	109.00	1922.1	1840.6	0.00	1923.5	1841.9	542.87
1923.5	1841.9	542.87	1928.5	1846.7	0.00	2176.6	2081.4	159.56
2176.6	2081.4	159.56	2179.4	2084.1	0.00	2179.5	2084.1	29.48

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring-[HBPH]$_4$			C_{4v} (TS)			Optimization in C_2 point group converges to D_{2d}		
-12.2	10.5	0.00	111.9	128.0	0.00	128.1	143.3	0.00
145.9	160.1	6.73	145.9	160.1	6.73	172.5	185.3	0.00
199.7	211.0	1.66	284.8	291.6	0.65	284.8	291.6	0.65
294.7	300.9	2.09	391.2	392.2	0.00	464.2	461.3	0.02
504.1	499.0	54.07	504.1	499.0	54.07	531.0	524.5	2.41
531.0	524.5	2.41	602.4	592.0	0.00	622.2	610.7	4.71
707.8	691.7	22.08	707.8	691.7	22.08	710.5	694.3	9.46
769.9	750.5	0.00	815.0	793.2	0.00	837.2	814.2	0.00
856.0	832.0	0.00	859.4	835.2	46.20	859.4	835.2	46.20
922.3	894.7	0.71	922.3	894.7	0.71	973.7	943.3	0.00
977.0	946.4	0.00	1082.3	1046.1	242.30	1082.3	1046.1	242.30
1095.9	1058.9	0.00	2469.1	2358.1	44.81	2469.1	2358.1	44.81
2469.1	2358.2	0.00	2469.4	2358.4	1.71	2634.4	2514.5	0.00
2634.5	2514.6	137.83	2634.5	2514.6	137.83	2635.8	2515.9	14.81
ring-[HBAsH]$_4$			C_2					
20.8	41.8	0.00	66.5	85.0	0.00	108.4	124.7	0.00
136.2	150.9	0.00	148.2	162.3	1.95	148.2	162.3	1.95
171.0	183.9	0.14	175.6	188.2	0.70	175.6	188.2	0.71
204.5	215.6	0.30	420.1	419.6	0.37	450.0	447.8	0.27
450.0	447.9	0.27	453.7	451.4	0.00	456.8	454.3	0.00
534.8	528.1	42.10	535.1	528.4	42.15	619.6	608.3	0.31
664.1	650.4	20.28	664.3	650.6	20.25	712.2	695.9	0.00
716.2	699.7	0.77	721.3	704.5	0.00	753.8	735.3	0.00
781.5	761.4	22.14	781.5	761.5	22.19	801.8	780.7	0.00
843.3	819.9	24.18	843.3	820.0	24.20	890.3	864.4	0.00
935.2	906.9	0.00	1027.1	993.8	231.92	1027.1	993.9	232.03
1035.3	1001.6	0.00	2269.0	2168.8	0.01	2269.8	2169.5	125.40
2269.8	2169.6	125.29	2271.6	2171.3	21.25	2642.1	2521.8	130.86
2642.1	2521.8	130.88	2642.3	2521.9	0.00	2643.1	2522.7	26.43
ring-[HAlPH]$_4$			C_2					
21.2	42.2	0.20	43.2	63.0	0.00	49.2	68.6	0.17
71.1	89.4	0.29	75.3	93.4	0.70	90.2	107.4	0.00
90.7	107.9	2.37	120.9	136.4	4.13	148.3	162.4	1.12
153.9	167.7	7.49	311.7	317.0	2.48	333.0	337.1	2.56
352.1	355.2	18.47	382.7	384.2	4.69	398.5	399.1	0.00
407.0	407.1	0.00	422.7	422.0	44.55	429.7	428.6	4.96
430.5	429.4	0.20	465.2	462.2	147.37	468.3	465.1	19.38
471.0	467.7	0.00	483.6	479.6	0.91	498.3	493.6	81.33
534.4	527.7	108.74	558.6	550.6	0.00	578.4	569.3	29.11
635.1	623.0	405.01	640.2	627.8	372.77	670.1	656.1	0.00
674.5	660.2	34.51	713.9	697.5	177.25	728.4	711.3	126.54
732.7	715.3	0.00	1915.7	1834.5	0.00	1916.7	1835.5	239.46
1918.4	1837.1	435.31	1922.6	1841.1	222.17	2354.9	2250.1	59.02
2355.4	2250.6	2.13	2379.3	2273.1	33.57	2379.5	2273.3	21.29

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring-[HAlAsH]$_4$			C_2					
20.0	41.0	0.01	33.7	53.9	0.03	41.8	61.6	0.00
60.9	79.7	0.76	61.0	79.8	1.12	77.7	95.6	0.58
79.0	96.8	0.00	94.2	111.2	0.25	105.2	121.7	0.00
108.8	125.0	6.19	254.5	262.9	6.01	268.3	275.9	7.08
272.5	279.9	16.13	297.5	303.6	0.00	369.6	371.8	0.00
377.0	378.8	0.00	377.3	379.1	0.24	381.3	382.9	3.93
396.3	397.1	2.89	397.2	397.8	92.54	402.8	403.2	93.76
428.0	427.1	36.88	508.5	503.2	0.20	538.2	531.3	52.81
538.3	531.4	49.13	556.6	548.7	0.00	598.9	588.7	3.39
627.8	616.1	262.06	629.8	617.9	294.14	639.7	627.4	0.00
657.9	644.5	16.52	686.2	671.3	296.12	701.1	685.4	0.00
706.5	690.6	234.55	1907.2	1826.5	0.00	1908.3	1827.5	223.27
1909.5	1828.7	364.53	1913.9	1832.8	305.28	2200.7	2104.2	105.90
2201.4	2104.9	13.61	2229.8	2131.7	73.03	2230.2	2132.1	51.65
ring-[HGaPH]$_4$			C_2					
25.5	46.2	0.13	32.5	52.8	0.00	48.0	67.5	0.07
61.2	80.0	0.57	63.0	81.7	0.00	66.7	85.2	0.97
75.8	93.9	0.52	102.0	118.6	2.81	122.8	138.3	0.81
136.4	151.2	4.53	260.8	268.8	0.25	280.0	287.0	0.10
300.4	306.3	0.39	342.3	345.9	0.00	342.7	346.3	1.50
362.8	365.4	55.79	370.5	372.6	0.00	398.3	398.9	88.18
401.1	401.6	0.00	411.6	411.5	72.74	429.3	428.3	63.32
434.2	432.9	19.42	513.9	508.3	0.01	526.4	520.1	23.71
573.8	564.9	67.54	585.7	576.2	0.00	612.5	601.6	17.37
639.9	627.5	261.51	657.2	643.9	165.16	672.6	658.4	15.74
703.8	687.9	0.00	738.1	720.4	91.81	751.6	733.2	95.53
753.0	734.5	0.00	1927.1	1845.3	0.00	1928.3	1846.5	247.38
1929.3	1847.4	447.58	1934.6	1852.4	251.80	2357.1	2252.1	63.65
2357.7	2252.7	2.44	2376.7	2270.7	37.24	2376.9	2270.8	26.62
ring-[HGaAsH]$_4$			C_2					
14.9	36.2	0.01	33.6	53.9	0.08	37.0	57.1	0.00
51.9	71.2	0.00	54.0	73.2	0.61	58.2	77.2	0.55
69.4	87.7	0.05	76.1	94.1	0.38	85.0	102.6	0.04
91.2	108.4	2.84	193.8	205.4	0.67	203.4	214.6	1.65
215.1	225.6	3.97	234.5	243.9	0.00	264.9	272.7	0.00
269.5	277.0	1.07	274.7	282.0	50.26	291.5	297.8	57.94
413.5	413.3	0.00	416.4	416.1	10.69	430.0	429.0	13.83
440.9	439.2	14.16	496.7	492.0	1.38	502.8	497.8	2.11
539.8	532.8	9.49	544.3	537.0	0.00	570.9	562.3	3.86
577.8	568.8	11.29	606.9	596.3	0.00	634.0	621.9	160.75
660.1	646.6	22.49	661.0	647.5	433.34	678.1	663.7	0.00
701.5	685.8	221.60	1920.9	1839.5	0.00	1921.8	1840.3	222.23
1923.2	1841.6	432.10	1927.9	1846.1	301.87	2155.0	2061.0	129.27
2156.2	2062.1	7.61	2204.3	2107.5	77.31	2204.7	2107.9	63.08

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring-[H_2BN]$_4$			D_{4h}					
57.0	76.0	0.00	171.9	184.8	1.34	249.9	258.6	0.00
249.9	258.6	0.00	283.9	290.7	3.88	283.9	290.7	3.88
284.5	291.3	0.00	444.6	442.7	0.00	471.8	468.4	0.00
549.2	541.7	0.00	561.8	553.6	0.00	600.6	590.3	0.00
600.6	590.3	0.00	655.4	642.2	0.00	691.3	676.2	0.00
746.2	728.1	0.39	746.2	728.1	0.39	825.2	802.8	0.00
933.2	905.0	0.00	938.0	909.5	0.00	938.0	909.5	0.00
944.9	916.0	82.24	986.6	955.6	0.00	1025.1	992.0	14.88
1025.1	992.0	14.88	1117.2	1079.1	0.00	1172.3	1131.2	0.00
1191.1	1149.0	33.09	1191.1	1149.0	33.09	1206.7	1163.8	0.00
1430.0	1375.0	34.42	1430.0	1375.0	34.42	1516.2	1456.6	0.00
1523.6	1463.6	0.00	2633.2	2513.4	0.00	2638.0	2517.9	101.10
2638.0	2517.9	101.10	2645.1	2524.6	0.00	2731.5	2606.4	0.00
2738.2	2612.7	109.40	2738.2	2612.7	109.40	2743.2	2617.4	0.00
ring-[H_2BP]$_4$			D_{2d}					
52.0	71.3	0.00	94.2	111.2	0.38	109.9	126.1	4.77
109.9	126.1	4.77	145.7	159.9	0.00	166.1	179.3	0.00
174.4	187.1	0.35	174.4	187.1	0.35	193.5	205.2	0.00
234.9	244.3	12.46	330.6	334.9	0.00	337.9	341.7	11.49
337.9	341.7	11.49	344.5	348.0	0.00	394.4	395.2	0.00
430.1	429.1	0.01	430.1	429.1	0.01	444.9	443.0	0.00
672.9	658.7	0.00	693.2	677.9	19.38	693.2	677.9	19.38
701.5	685.8	0.00	705.4	689.5	0.03	705.4	689.5	0.03
712.2	695.9	26.21	727.8	710.6	0.00	913.3	886.1	9.50
913.3	886.1	9.50	913.5	886.4	3.94	923.3	895.6	0.00
1165.0	1124.3	110.94	1166.2	1125.5	49.90	1166.2	1125.5	49.90
1172.3	1131.3	0.00	2595.7	2477.9	206.50	2595.8	2478.0	103.93
2595.8	2478.0	103.93	2599.0	2481.0	0.00	2693.6	2570.5	0.00
2694.4	2571.3	96.28	2694.4	2571.3	96.28	2694.5	2571.3	0.00
ring-[H_2BAs]$_4$			D_{2d}					
29.3	49.8	0.00	93.4	110.4	0.00	100.0	116.7	1.24
100.0	116.7	1.24	111.5	127.6	0.00	119.8	135.5	2.24
119.8	135.5	2.24	122.2	137.7	0.00	134.8	149.7	1.80
135.9	150.7	0.00	222.4	232.5	4.60	222.4	232.5	4.60
231.6	241.2	0.00	234.5	243.9	0.00	243.0	252.0	0.00
291.2	297.6	0.00	318.0	323.0	7.31	318.0	323.0	7.31
566.4	558.0	24.68	566.4	558.0	24.68	572.9	564.1	0.00
574.1	565.2	17.35	653.3	640.2	0.00	675.1	660.8	0.33
675.1	660.8	0.33	691.4	676.3	0.00	903.8	877.2	1.13
905.7	878.9	10.66	905.7	878.9	10.66	917.0	889.6	0.00
1161.2	1120.7	142.38	1161.6	1121.1	67.01	1161.6	1121.1	67.01
1166.3	1125.5	0.00	2588.7	2471.3	240.84	2588.8	2471.4	127.12
2588.8	2471.4	127.12	2591.8	2474.2	0.00	2689.0	2566.2	0.00
2689.7	2566.8	96.90	2689.7	2566.8	96.90	2689.8	2566.9	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
ring-[H_2AlN]$_4$			D_2					
34.5	54.7	0.00	83.0	100.6	2.42	95.2	112.2	0.00
112.6	128.7	0.21	112.6	128.7	0.21	163.0	176.3	2.82
163.0	176.3	2.82	255.4	263.7	0.00	256.0	264.3	0.00
283.9	290.7	0.00	304.8	310.5	1.68	304.8	310.5	1.68
386.5	387.8	0.00	429.1	428.1	17.17	450.5	448.3	13.61
450.5	448.3	13.61	504.1	499.0	0.00	517.7	511.9	67.72
517.7	511.9	67.72	520.5	514.6	262.05	523.3	517.2	0.00
557.3	549.4	0.00	580.1	571.0	0.00	627.7	616.0	133.59
627.7	616.0	133.59	719.8	703.1	113.72	730.6	713.4	537.60
730.6	713.4	537.61	748.4	730.2	0.00	1041.5	1007.4	0.00
1078.1	1042.1	0.15	1078.1	1042.1	0.15	1186.0	1144.1	23.08
1207.7	1164.7	0.00	1950.2	1867.1	98.94	1952.0	1868.9	142.15
1952.0	1868.9	142.16	1958.3	1874.9	0.00	1971.1	1887.0	0.00
1977.2	1892.8	394.65	1977.2	1892.8	394.63	1981.0	1896.3	0.00
ring-[H_2GaN]$_4$			D_2					
20.1	41.1	0.00	53.2	72.4	1.20	62.1	80.9	0.00
78.8	96.6	0.06	78.8	96.6	0.06	156.0	169.7	5.56
156.0	169.7	5.56	237.3	246.6	0.00	260.6	268.7	0.00
272.2	279.6	0.00	287.8	294.4	0.00	292.5	298.8	0.96
292.5	298.8	0.96	309.8	315.2	16.58	402.3	402.7	3.22
402.3	402.7	3.22	482.4	478.5	62.36	482.4	478.5	62.36
485.8	481.7	0.00	487.3	483.1	0.00	487.3	483.1	4.98
554.1	546.3	0.00	578.1	569.0	285.91	578.1	569.0	285.91
590.6	580.9	0.00	684.9	670.0	95.13	688.2	673.2	229.40
688.2	673.2	229.40	692.1	676.9	0.00	1055.7	1020.9	6.72
1055.7	1020.9	6.72	1086.1	1049.6	0.00	1152.0	1112.0	0.00
1170.8	1129.8	15.09	1994.3	1908.9	97.05	1995.5	1910.1	143.53
1995.5	1910.1	143.53	1999.6	1913.9	0.00	2018.3	1931.6	0.00
2023.5	1936.6	316.26	2023.5	1936.6	316.26	2027.0	1939.9	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
bridged ring-$[H_2BN]_4$			C_2					
97.4	114.2	0.00	292.9	299.2	4.12	312.0	317.3	24.89
373.2	375.2	7.11	431.3	430.2	0.90	446.4	444.4	2.30
485.3	481.2	9.12	512.4	506.9	0.00	576.9	567.9	10.11
581.2	572.0	0.21	634.2	622.1	0.00	674.2	659.9	0.58
697.3	681.8	0.00	709.6	693.4	4.71	762.5	743.5	0.01
767.6	748.4	1.19	816.2	794.3	2.65	868.2	843.5	0.00
868.6	843.9	4.89	890.1	864.2	10.42	901.1	874.6	18.43
961.0	931.3	83.93	972.7	942.4	0.00	993.3	961.8	0.00
994.6	963.1	14.59	1006.5	974.4	9.93	1009.5	977.2	17.66
1031.4	997.9	57.98	1039.7	1005.7	0.07	1066.8	1031.4	2.00
1185.8	1144.0	0.23	1218.4	1174.8	49.47	1244.1	1199.2	84.75
1275.0	1228.4	0.00	2649.4	2528.7	0.93	2657.9	2536.7	47.82
2670.1	2548.3	164.63	2682.3	2559.8	0.00	2773.2	2645.9	4.52
2778.9	2651.2	61.03	2807.2	2678.0	130.60	2810.2	2680.9	0.00
bridged ring-$[H_2BP]_4$			D_{2h}					
92.4	109.5	0.00	154.2	168.0	0.00	226.4	236.3	2.70
244.2	253.1	15.29	244.2	253.1	0.00	277.9	285.0	0.00
294.4	300.6	0.40	337.2	341.2	0.00	354.6	357.6	0.00
394.1	395.0	0.00	397.7	398.3	0.00	413.6	413.4	13.91
454.9	452.4	15.96	474.3	470.9	0.00	580.6	571.4	2.10
598.2	588.1	0.00	610.4	599.6	4.65	626.4	614.7	0.00
643.8	631.2	0.00	657.1	643.8	5.04	691.5	676.3	0.00
697.7	682.2	0.00	734.5	717.0	0.00	735.3	717.8	71.88
777.8	758.0	0.00	782.4	762.4	0.19	820.8	798.6	0.00
837.6	814.6	0.00	884.8	859.2	0.00	923.0	895.4	13.45
1117.0	1078.9	0.00	1132.9	1093.9	58.72	1138.6	1099.3	83.63
1158.5	1118.2	0.00	2573.5	2456.9	0.00	2577.2	2460.3	82.71
2582.4	2465.3	120.45	2585.9	2468.6	0.00	2698.1	2574.8	16.43
2698.4	2575.1	0.00	2710.3	2586.3	97.78	2711.3	2587.3	0.00
bridged ring-$[H_2BAs]_4$			D_{2h}					
64.1	82.7	0.00	93.2	110.3	0.00	176.5	189.1	1.77
186.9	199.0	0.00	188.3	200.2	16.24	209.0	219.8	0.44
211.2	221.9	0.00	247.3	256.1	0.00	274.0	281.3	0.00
287.7	294.3	5.13	290.2	296.6	0.00	292.7	299.1	0.00
293.0	299.3	0.00	312.1	317.3	4.22	497.6	492.9	5.19
506.9	501.7	0.00	524.3	518.1	7.15	543.9	536.6	0.00
615.1	604.1	1.32	617.1	605.9	0.00	651.4	638.4	0.00
654.7	641.5	0.00	680.6	666.0	0.00	703.8	688.0	68.42
729.4	712.2	0.00	731.5	714.1	0.49	785.7	765.5	0.00
811.0	789.4	0.00	877.8	852.6	0.00	912.9	885.8	13.68
1109.2	1071.5	0.00	1122.4	1084.0	110.25	1127.0	1088.3	75.29
1144.4	1104.8	0.00	2572.4	2455.8	0.00	2575.2	2458.5	119.59
2578.8	2461.9	128.22	2581.9	2464.9	0.00	2695.5	2572.3	18.62
2695.7	2572.5	0.00	2704.3	2580.7	90.49	2705.8	2582.0	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
bridged ring-$[H_2AlN]_4$			C_2					
105.8	122.2	0.00	106.4	122.7	2.97	172.9	185.7	0.00
210.7	221.4	2.28	216.4	226.9	0.27	245.7	254.6	11.05
267.8	275.5	62.87	310.5	315.8	0.52	311.2	316.5	27.74
345.1	348.6	2.97	372.2	374.2	0.00	381.4	382.9	0.29
409.4	409.4	0.00	414.4	414.1	31.73	479.6	475.8	52.20
502.2	497.2	325.17	518.1	512.2	1.84	556.0	548.2	0.03
610.1	599.4	46.27	614.9	603.9	0.00	619.8	608.5	10.02
637.4	625.1	508.02	661.2	647.7	482.22	693.4	678.1	26.22
710.2	694.0	0.05	727.8	710.6	146.46	733.2	715.8	64.36
747.7	729.5	328.03	766.8	747.6	582.34	775.5	755.8	0.00
794.9	774.2	5.89	818.2	796.2	0.00	820.3	798.2	4.53
970.1	939.9	0.00	1969.3	1885.2	30.04	1972.7	1888.5	89.55
1973.0	1888.8	93.47	1982.5	1897.7	45.16	1983.7	1898.8	42.94
1991.7	1906.4	206.31	1993.8	1908.4	603.30	1998.4	1912.8	0.01
bridged ring-$[H_2AlP]_4$			D_{2h}					
26.5	47.2	0.00	109.6	125.8	0.00	113.2	129.2	3.90
139.7	154.3	1.95	148.5	162.6	0.00	157.5	171.1	0.00
194.8	206.4	4.30	206.0	217.0	0.00	238.3	247.6	0.00
252.4	260.9	0.00	273.3	280.7	0.00	276.1	283.3	4.84
318.4	323.4	0.00	350.6	353.8	3.47	357.7	360.5	0.00
357.7	360.6	0.00	362.6	365.1	3.59	370.0	372.2	0.65
397.1	397.8	0.00	405.2	405.5	0.00	415.9	415.6	22.92
438.7	437.2	0.00	441.7	440.0	106.09	447.9	445.9	7.25
454.7	452.3	0.00	504.6	499.5	0.00	521.6	515.6	0.00
525.6	519.4	0.00	547.6	540.2	0.00	600.6	590.3	364.39
686.2	671.3	0.00	698.6	683.1	647.61	712.0	695.7	996.92
750.4	732.1	0.00	1938.2	1855.8	0.00	1939.3	1856.9	48.54
1946.1	1863.3	423.68	1948.8	1865.9	0.00	1985.8	1900.8	0.00
1987.5	1902.5	90.94	2006.8	1920.7	341.22	2007.6	1921.5	0.00
bridged ring-$[H_2AlAs]_4$			D_{2h}					
25.1	45.8	0.00	84.1	101.7	0.00	88.2	105.5	3.36
91.7	108.9	0.00	126.2	141.5	1.45	141.2	155.6	0.00
158.2	171.8	0.62	168.4	181.5	0.00	176.4	189.0	0.00
195.4	207.0	0.00	198.3	209.7	0.69	206.8	217.7	0.00
222.7	232.8	0.00	239.9	249.0	3.11	300.7	306.6	0.00
301.3	307.1	20.18	303.2	308.9	15.27	317.3	322.3	0.00
345.3	348.8	0.00	355.7	358.6	0.00	369.1	371.3	0.00
369.4	371.6	0.00	385.4	386.8	2.93	396.2	396.9	0.02
413.7	413.5	48.13	480.3	476.5	0.00	500.8	495.9	0.00
506.7	501.5	0.00	542.8	535.7	0.00	595.9	585.9	335.22
691.8	676.7	0.00	702.6	686.8	637.90	714.1	697.7	1076.64
748.7	730.5	0.00	1927.1	1845.3	0.00	1928.1	1846.3	73.77
1934.1	1851.9	474.82	1936.7	1854.4	0.00	1978.7	1894.2	0.00
1980.0	1895.4	77.27	1998.0	1912.4	341.75	1998.6	1913.0	0.00

ω	ν [a]	I	ω	ν [a]	I	ω	ν [a]	I
bridged ring-$[H_2GaN]_4$			C_2					
50.4	69.8	0.00	94.6	111.6	0.75	115.9	131.7	0.00
144.3	158.6	3.56	150.8	164.8	25.27	176.0	188.6	7.97
191.8	203.5	27.79	194.1	205.8	1.86	222.5	232.6	0.01
293.3	299.6	1.00	336.4	340.4	5.27	341.3	345.0	0.12
410.7	410.7	0.41	432.1	430.9	29.54	432.2	431.0	0.01
474.1	470.7	6.48	483.3	479.4	181.54	534.4	527.7	295.36
538.6	531.6	0.17	569.2	560.6	0.01	603.3	592.9	205.17
608.7	598.0	3.31	616.2	605.1	66.85	659.9	646.5	37.19
694.1	678.8	7.99	695.4	680.0	1.32	697.2	681.7	225.10
720.2	703.5	278.00	722.9	706.0	40.78	736.3	718.7	0.77
783.6	763.5	0.06	827.9	805.4	3.05	829.3	806.7	5.28
968.9	938.8	0.00	2023.9	1936.9	3.62	2025.0	1937.9	62.00
2028.5	1941.3	75.19	2034.5	1946.9	34.24	2036.4	1948.7	68.65
2047.1	1958.8	377.39	2049.1	1960.8	199.31	2054.6	1965.9	10.76
bridged ring-$[H_2GaP]_4$			D_{2h}					
16.9	38.0	0.00	91.7	108.9	1.12	92.1	109.2	2.04
96.7	113.6	0.00	103.1	119.6	0.00	148.6	162.7	0.00
155.8	169.5	5.91	170.2	183.1	0.00	175.6	188.2	0.00
176.0	188.7	0.00	201.2	212.5	8.76	227.8	237.6	0.00
301.4	307.2	0.00	303.2	308.9	49.89	350.1	353.3	0.00
353.7	356.7	4.25	363.4	366.0	7.53	370.8	372.9	0.00
419.5	419.0	0.00	419.7	419.2	0.00	421.2	420.6	0.00
421.3	420.6	7.10	427.0	426.1	40.65	433.6	432.3	0.00
458.7	456.1	7.42	503.1	498.1	0.00	529.6	523.2	0.00
531.1	524.6	0.00	554.2	546.5	0.00	594.3	584.4	138.67
662.8	649.1	0.00	681.6	667.0	366.71	684.2	669.4	596.17
724.6	707.7	0.00	1995.2	1909.8	0.00	1996.2	1910.7	49.76
2001.4	1915.6	378.31	2004.1	1918.2	0.00	2030.0	1942.7	0.00
2033.7	1946.2	112.86	2050.6	1962.2	262.60	2052.1	1963.6	0.00
bridged ring-$[H_2GaAs]_4$			D_{2h}					
17.7	38.9	0.00	68.4	86.8	1.63	80.4	98.1	0.00
81.7	99.4	0.74	84.9	102.4	0.00	91.3	108.5	0.00
121.4	137.0	1.32	123.0	138.5	0.00	130.1	145.2	0.00
157.4	171.0	0.00	160.6	174.1	0.00	162.0	175.3	5.27
214.6	225.1	0.00	226.7	236.5	30.92	229.8	239.5	3.46
232.7	242.3	0.00	238.7	247.9	6.18	265.5	273.3	0.00
361.4	364.0	0.00	379.1	380.7	0.00	379.2	380.9	0.00
395.1	395.9	0.00	398.2	398.8	0.24	409.4	409.4	17.12
417.5	417.1	0.02	469.2	466.0	0.00	506.4	501.2	0.00
515.7	510.0	0.00	552.7	545.0	0.00	591.5	581.7	140.14
661.1	647.6	0.00	681.0	666.4	681.59	681.7	667.0	378.27
719.7	703.0	0.00	1979.1	1894.6	0.00	1980.2	1895.6	74.67
1984.8	1899.9	433.37	1987.5	1902.4	0.00	2016.6	1930.0	0.00
2019.4	1932.6	103.15	2035.3	1947.7	262.42	2036.2	1948.6	0.00