Supporting Information for

Oligomeric Rods of Alkyl- and Hydridogallium Imides

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Table S1. Computed heavy-atom bond lengths and angles for $H_3[HGaNH]_{3n}H_3$ at B3LYP/MB for n = 1-9. Computed structures have C_{3v} symmetry; redundant bond lengths and angles are not reported.

	Ga-N	Ga-N (conn.)	Ga-N-Ga	N-Ga-N	H···H
n = 1					
	1.994	-	124.605	106.785	-
n = 2					
	2.008	1.936	112.853	99.799	2.408
	1.994		118.317	101.600	
n = 3					
	2.000	1.944	113.345	98.807	2.464
	1.996	1.941	113.443	100.041	2.506
	1.993		118.322	101.717	

n = 4					
	1.998	1.947	113.384	98.927	2.508
	1.988	1.950	113.800	99.289	2.570
	1.993	1.944	113.599	100.264	2.531
	1.993		118.310	101.598	
n = 5					
	1.998	1.950	113.405	98.963	2.513
	1.986	1.954	113.873	99.459	2.614
	1.985	1.954	114.051	99.617	2.581
	1.992	1.947	113.806	100.426	2.539
	1.993		118.541	101.648	
n = 6					
	1.997	1.951	113.355	98.974	2.522
	1.985	1.956	113.821	99.543	2.624
	1.983	1.958	114.073	99.802	2.629
	1.983	1.957	114.189	99.764	2.594
	1.991	1.948	113.849	100.508	2.552
	1.993		118.567	101.631	
n = 7					
	1.997	1.953	113.402	98.996	2.522
	1.984	1.958	113.859	99.606	2.629
	1.981	1.961	114.316	99.914	2.634
	1.981	1.961	114.327	99.972	2.637
	1.982	1.959	114.348	99.867	2.602
	1.989	1.949	113.989	100.502	2.565
	1.993		118.536	101.403	

n = 8

1.997	1.953	113.352	98.996	2.529
1.983	1.959	113.819	99.633	2.636
1.980	1.963	114.102	99.966	2.643
1.980	1.964	114.305	100.074	2.648
1.980	1.963	114.397	100.062	2.648
1.981	1.960	114.365	99.919	2.607
1.989	1.950	113.949	100.620	2.563
1.992		118.688	101.603	

n = 9

1.997	1.954	113.393	99.009	2.528
1.983	1.961	113.853	99.667	2.638
1.980	1.964	114.154	100.015	2.646
1.979	1.966	114.366	100.146	2.652
1.978	1.966	114.469	100.184	2.654
1.979	1.964	114.514	100.135	2.652
1.981	1.961	114.459	99.965	2.611
1.989	1.951	114.034	100.603	2.576
1.993		118.658	101.586	

Table S2. Computed heavy-atom bond lengths and angles for $H_3[HGaNH]_{3n}H_3$ at B3LYP/CEP for n = 1-4. Computed structures have C_{3v} symmetry; redundant bond lengths and angles are not reported.

	Ga-N	Ga-N (conn.)	Ga-N-Ga	N-Ga-N	H···H
n = 1					
	2.020	-	120.902	104.933	-
n = 2					
	2.017	1.929	114.077	101.688	2.172
	2.012		117.345	102.201	
n = 3					
	2.015	1.934	114.315	101.322	2.231
	2.004	1.928	113.646	101.916	2.396
	2.016		117.549	101.705	
n = 4					
	2.013	1.937	114.242	101.379	2.271
	2.001	1.935	113.794	101.590	2.436
	2.006	1.934	113.861	102.004	2.414
	2.016		117.681	101.597	

Table S3. Computed heavy-atom bond lengths and angles for $H_3[HGeCH]_{3n}H_3$ at B3LYP/MB for n = 1-9. Computed structures have C_{3v} symmetry; redundant bond lengths and angles are not reported.

	Ge-C	Ge-C (conn.)	Ge-C-Ge	C-Ge-C	H···H
n = 1					
	2.035	-	113.417	111.691	-
n = 2					
	2.039	2.050	109.460	107.108	2.756
	2.038		110.410	107.361	
n = 3					
	2.037	2.056	109.619	106.546	2.755
	2.041	2.050	108.941	106.414	2.774
	2.036		110.118	107.492	
n = 4					
	2.037	2.055	109.655	106.587	2.771
	2.038	2.056	109.212	105.897	2.764
	2.039	2.050	108.767	106.388	2.774
	2.037		110.072	107.407	
n = 5					
	2.038	2.055	109.649	106.583	2.773
	2.039	2.055	109.214	105.884	2.782
	2.038	2.055	108.907	105.904	2.773
	2.039	2.050	108.720	106.380	2.771

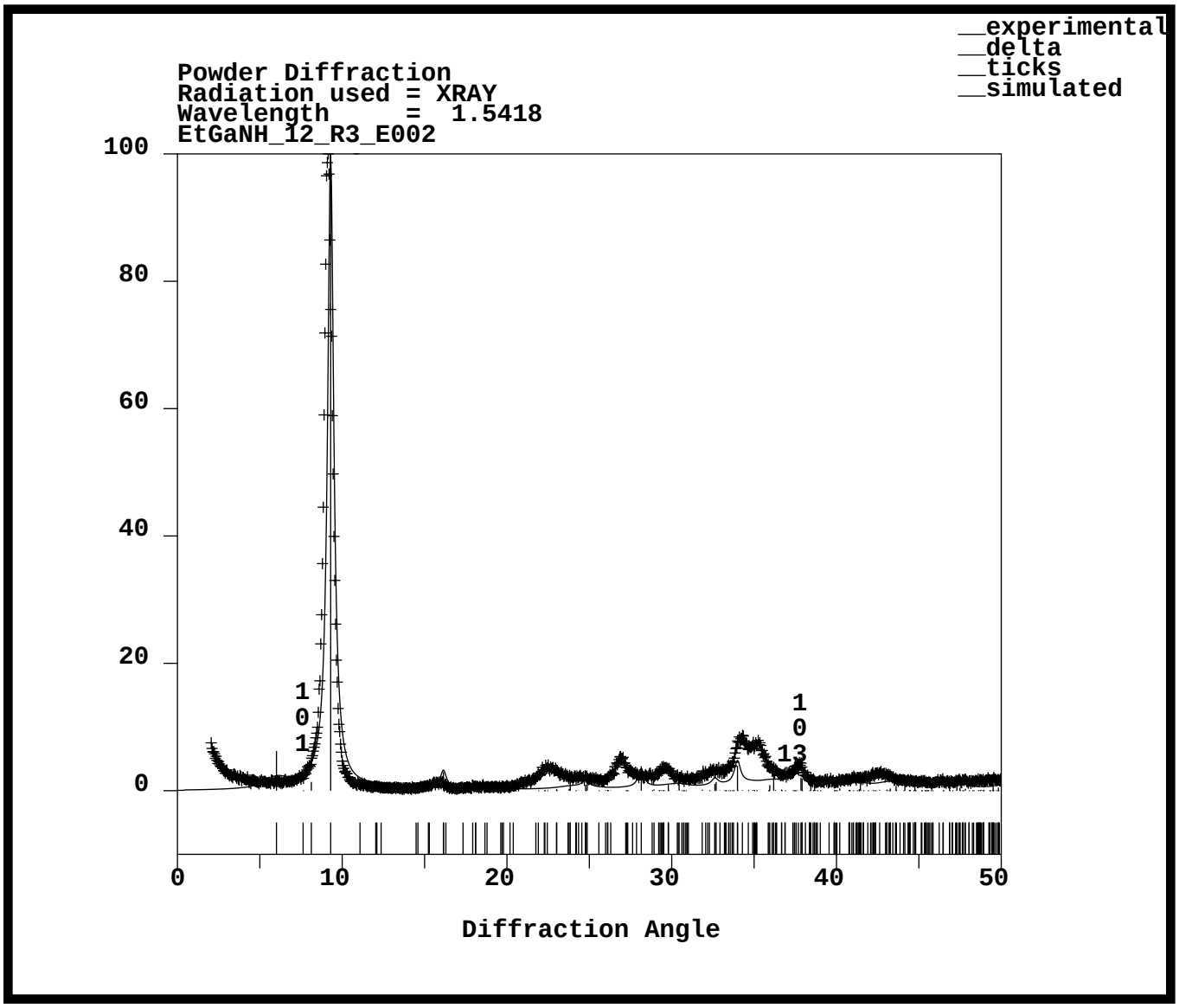
2.037		110.052	107.456	
n = 6				
2.037	2.055	109.661	106.580	2.771
2.039	2.055	109.248	105.881	2.779
2.038	2.054	108.970	105.888	2.787
2.038	2.055	108.926	105.882	2.769
2.039	2.050	108.743	106.356	2.773
2.037		110.045	107.366	
n = 7				
2.037	2.055	109.665	106.576	2.772
2.039	2.055	109.227	105.872	2.781
2.038	2.054	108.940	105.883	2.789
2.038	2.054	108.922	105.872	2.788
2.038	2.055	108.884	105.872	2.771
2.040	2.050	108.709	106.349	2.769
2.037		110.025	107.458	
n = 8				
2.037	2.054	109.671	106.575	2.770
2.039	2.054	109.254	105.868	2.778
2.038	2.054	108.976	105.874	2.785
2.038	2.054	108.958	105.863	2.785
2.038	2.054	108.942	105.853	2.785
2.038	2.054	108.904	105.857	2.769
2.039	2.049	108.730	106.341	2.773
2.037		110.032	107.354	
n = 9				

2.038	2.055	109.659	106.574	2.772
2.039	2.055	109.232	105.864	2.780
2.038	2.054	108.948	105.871	2.788
2.038	2.054	108.931	105.857	2.787
2.038	2.054	108.917	105.849	2.787
2.038	2.054	108.904	105.847	2.787
2.038	2.055	108.871	105.850	2.770
2.040	2.050	108.689	106.353	2.775
2.037		110.038	107.337	

Table S4. Computed heavy-atom bond lengths and angles for $H_3[HGeCH]_{3n}H_3$ at B3LYP/CEP for n = 1-4. Computed structures have C_{3v} symmetry; redundant bond lengths and angles are not reported.

	Ge-C	Ge-C (conn.)	Ge-C-Ge	C-Ge-C	H···H
n = 1					
	1.975	-	113.993	110.993	-
n = 2					
	1.985	2.002	109.613	107.046	2.695
	1.982		111.123	106.417	
n = 3					
	1.983	2.004	109.831	106.673	2.667
	1.991	2.000	109.148	106.042	2.715
	1.981		110.746	106.512	
n = 4					
	1.983	2.003	109.890	106.708	2.678
	1.986	2.000	109.390	105.674	2.686
	1.991	1.999	108.818	106.060	2.720
	1.981		110.716	106.525	

Graph S1 (next page). Experimental (+) and calculated (line) X-ray powder diffraction patterns for $[EtGaNH]_n$. The experimental pattern is the same as shown in Figure 1 of the main text. The calculated pattern was based on the structure as modeled using Cerius2. Space group = *R3*; *a* = 19.019 Å, *c* = 32.641 Å; each $H_3\{[EtGaNH]_3\}_{12}H_3$ formula unit lies on a 3-fold axis thus Z = 3; coherence length along a = 200Å and c = 30Å. The latter was chosen to represent the disorder resulting from the presence of differing length rods.


__experimental
__delta
__ticks
__simulated
Powder Diffraction
Radiation used = XRAY
Wavelength = 1.5418
EtGaNH_12_R3_E002
100
80
60
40
20
0
1
0
1
1
0
13
0
10
20
30
40
50
Diffraction Angle