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Dihydrogen Intermolecular Contacts in Group 13 Compounds: H···H or E···H (E = B, Al, Ga) Interactions?

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Electronic Supplementary Information

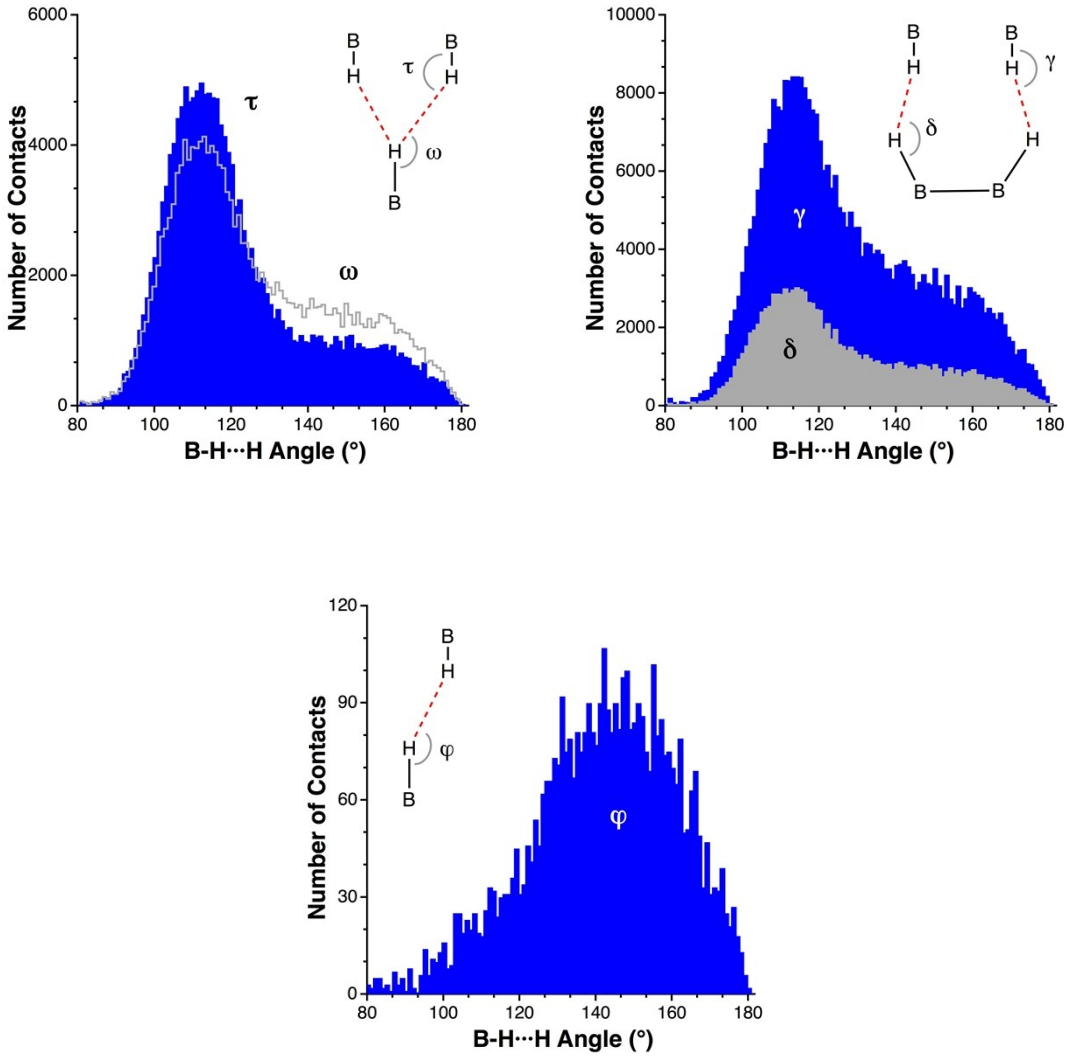

Fig. S1. Angular distribution of B-H···H-B intermolecular contacts at ≤ 3.5 Å with interaction topologies **2** – **4**.

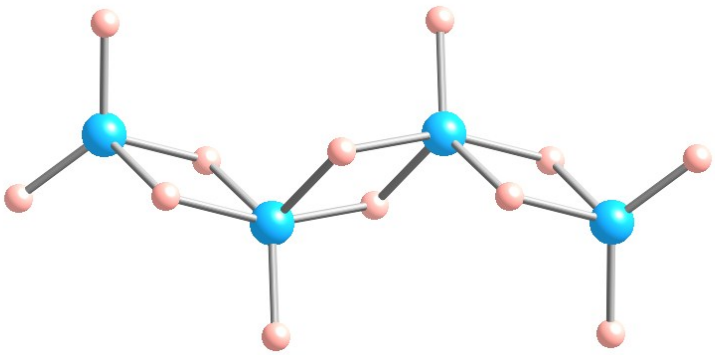

Fig. S2. Structure of Al_4H_{12}, a tetramer obtained from the geometry optimization of two close dialane molecules.

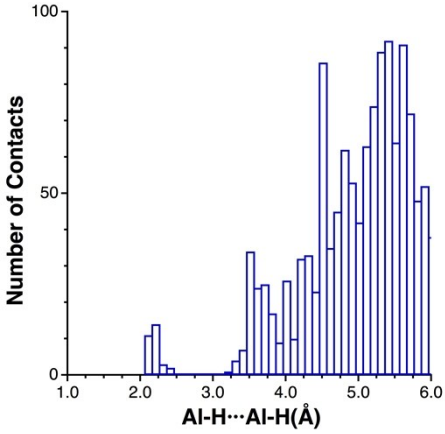

Fig. S3. Distribution of Al-H···Al-H short contacts in Å.

Table S1. Optimized Cartesian coordinates *x, y, z* of B_2H_6, Al_2H_6 and Ga_2H_6.

B_2H_6

B	0.212025	-0.805265	-0.273653
H	0.544330	-0.126297	0.794461
H	-0.544330	0.126297	-0.794461
H	1.171089	-0.942876	-0.953870
B	-0.212025	0.805265	0.273653
H	0.469877	1.717268	-0.050357
H	-0.469877	-1.717268	0.050357
H	-1.171089	0.942876	0.953870

Al_2H_6

Al	1.300464	-0.000010	-0.000418
Al	-1.300460	0.000006	0.000418
H	1.989910	1.407750	0.002410
H	-1.990078	-1.407669	-0.002415
H	1.989734	-1.407845	0.002119
H	-1.989591	1.407908	-0.002111
H	0.001694	0.000322	-1.139601
H	-0.001716	-0.000413	1.139606

Ga_2H_6

Ga	-4.812774	0.614117	-0.004137
Ga	-2.771140	-1.052745	0.010692
H	-4.435649	2.124959	0.149767
H	-3.152299	-2.562460	-0.142192

H	-1.368759	-0.379045	0.169982
H	-6.218070	-0.055058	-0.163203
H	-3.880923	-0.315922	1.174438
H	-3.707394	-0.122398	-1.167704

Table S2. Optimized Cartesian coordinates *x, y, z* of $(B_2H_6)_2$ and $(Ga_2H_6)_2$ with terminal-bridging interaction topology (**8b**).

$(B_2H_6)_2$

B	1.529000	-0.519000	-0.324000
B	2.807000	-0.326000	0.857000
B	-1.649000	1.042000	0.070000
B	-2.687000	-0.197000	-0.603000
H	1.317000	0.363000	-1.087000
H	3.018000	-1.208000	1.618000
H	0.902000	-1.524000	-0.334000
H	3.430000	0.680000	0.864000
H	1.531000	-0.034000	0.890000
H	2.802000	-0.812000	-0.360000
H	-1.044000	0.799000	1.059000
H	-3.296000	0.039000	-1.590000
H	-2.754000	-1.243000	-0.051000
H	-1.572000	2.091000	-0.472000
H	-2.910000	0.756000	0.267000
H	-1.427000	0.095000	-0.805000

$(Ga_2H_6)_2$

Ga	0.821000	-1.542000	0.474000
Ga	3.446000	-1.745000	0.541000
Ga	-0.821000	1.543000	-0.475000
Ga	-3.447000	1.744000	-0.540000
H	0.256000	-1.090000	-0.923000
H	4.039000	-2.211000	1.911000
H	0.049000	-1.962000	1.765000
H	4.170000	-1.337000	-0.785000
H	2.196000	-0.528000	0.875000
H	2.073000	-2.768000	0.143000
H	-0.255000	1.089000	0.921000
H	-4.041000	2.211000	-1.909000
H	-4.168000	1.333000	0.786000

H	-0.049000	1.966000	-1.765000
H	-2.074000	2.767000	-0.142000
H	-2.195000	0.528000	-0.877000

Table S3. Optimized Cartesian coordinates *x, y, z* of $(B_4H_{10})_2$ and $(B_5H_9)_2$ with ***b-f*** and ***b-s*** interaction topologies.

$(B_4H_{10})_2$ ***b-f***

B	2.459874	1.215171	0.854082
B	-1.694363	1.183040	-0.406950
B	1.835738	-0.506464	0.652769
B	-2.106895	-0.564066	-0.803392
B	3.126130	-1.105407	-0.517823
B	-2.676416	-1.068759	0.871429
B	2.120224	0.417128	-0.771206
B	-3.319697	0.393519	-0.043133
H	1.652565	2.007691	1.206887
H	-1.691258	1.921110	-1.335277
H	3.598953	1.356384	1.173001
H	-0.956505	1.390743	0.505588
H	2.671284	1.508988	-0.509506
H	-2.867075	1.508051	0.303202
H	1.184616	0.557340	-1.474845
H	-4.328067	0.491169	-0.645043
H	3.115137	-0.006908	-1.400860
H	-3.512134	0.034963	1.140358
H	2.802174	-2.031468	-1.183241
H	-3.402358	-2.005930	0.896669
H	4.269409	-0.979630	-0.208107
H	-1.943874	-0.873529	1.791180
H	2.679380	-1.421880	0.780871
H	-1.651160	-1.432195	-0.026023
H	0.733017	-0.902919	0.779950
H	-2.414196	-1.019898	-1.845801
H	2.234854	0.091100	1.676431
H	-1.010098	0.037253	-0.853886

B	0.223953	22.648365	3.494939
B	5.259620	23.001498	3.897111
B	-0.787544	22.381622	5.009319
B	4.049980	23.896108	4.957533
B	-1.943571	23.797772	4.787457
B	3.327165	24.969662	3.652526
B	-0.108711	23.944513	4.757801
B	5.130212	24.835278	3.999614
H	1.313667	22.180624	3.535846
H	6.182800	22.529703	4.472025
H	-0.335189	22.725463	2.445923
H	4.849151	22.468344	2.913675
H	0.421903	24.040497	3.627665
H	5.796735	24.117637	3.221194
H	0.606418	24.316323	5.618144
H	5.810091	25.582665	4.605821
H	-0.986789	24.789590	4.478448
H	4.528185	25.403771	3.059818
H	-2.462617	24.183172	5.780861
H	2.809607	25.959674	4.050940
H	-2.524926	23.885333	3.751432
H	2.905549	24.450052	2.665204
H	-2.030180	22.392197	4.863918
H	2.879583	23.953629	4.518231
H	-0.462216	21.856934	6.012934
H	4.101684	24.101483	6.116595
H	-0.615447	21.642931	4.013342
H	4.138887	22.677161	4.689685

$(B_5H_9)_2$ ***b-f***

B	6.875668	-18.152880	-8.844100
B	12.074446	-18.132051	-8.785261
B	5.737028	-17.748459	-7.659108
B	5.752094	-16.959666	-9.266085
B	5.752759	-19.355492	-8.447777
B	5.767825	-18.566697	-10.054763
B	10.928773	-17.728020	-7.602857
B	10.943808	-16.941259	-9.206625
B	10.944071	-19.331849	-8.389504
B	10.959100	-18.545085	-9.993277
H	8.050840	-18.147974	-8.830647
H	13.251292	-18.127375	-8.771939
H	5.853535	-17.369223	-6.548897
H	5.882541	-15.850317	-9.643307
H	5.883823	-20.463746	-8.067564
H	5.912841	-18.944830	-11.161991
H	11.041894	-17.348220	-6.491740
H	11.070882	-15.830998	-9.584509
H	11.071416	-20.441097	-8.008745
H	11.100396	-18.923874	-11.101512
H	4.844430	-16.965874	-8.280492
H	4.844927	-18.748100	-7.671758
H	4.867342	-17.574547	-10.062593
H	4.867844	-19.356784	-9.453867
H	10.031522	-16.951833	-8.225427
H	10.031720	-18.723080	-7.620000
H	10.053994	-17.557214	-9.996540
H	10.054189	-19.328457	-9.391117

$(B_5H_9)_2$ ***b-s***

B	14.299713	1.241997	-18.238019
B	19.225314	1.234334	-17.621449
B	15.056459	0.851681	-16.771274
B	15.431248	-0.020185	-18.285429
B	15.349828	2.409056	-17.596944
B	15.723488	1.536365	-19.108211
B	19.515203	0.769808	-19.224041
B	19.456276	2.490971	-18.733064
B	20.691227	0.438174	-17.916967
B	20.632294	2.157598	-17.426442
H	13.164377	1.290810	-18.544350
H	18.346420	0.991505	-16.875732
H	14.622508	0.539162	-15.719861
H	15.348115	-1.142723	-18.638998
H	15.191003	3.542664	-17.311070
H	15.919427	1.859912	-20.226546
H	18.901740	0.100563	-19.977157
H	18.788155	3.416240	-19.031233
H	21.163100	-0.539252	-17.457122
H	21.049643	2.773461	-16.512105
H	16.041543	0.002427	-17.092570
H	15.981212	1.802478	-16.582408
H	16.536471	0.511206	-18.821404
H	19.870326	1.894858	-19.859424
H	16.476260	2.307188	-18.312386
H	20.792565	0.368165	-19.251570
H	20.704926	2.926709	-18.521692
H	21.624158	1.399830	-17.913531

Table S4. Values of enthalpy, H, Gibbs free energy, G, in kcal mol^{-1}, and entropy, S, in cal $mol^{-1}K^{-1}$ of all calculated molecules characterized as minima.

	H (kcal mol^{-1})	G (kcal mol^{-1})	S (cal K^{-1} mol^{-1})
(B_2H_6) *t-b*	-66553.89	-66583.41	99.03
(Ga_2H_6) *t-b*	-4831862.52	-4831898.87	121.90
$(B_5H_9)_2$ *b-f*	-162075.73	-162103.76	94.02
$(B_4H_{10})_2$ *b-s*	-131673.82	-131706.73	110.39
$(B_4H_{10})_2$ *b-f*	-131673.46	-131707.59	114.49