Real Space Indicators for Chemical bonding. Experimental and Theoretical Electron Density Studies of Four Deltahedral Boranes

Supplementary material

Details of data processing

For the data set of **4**, the SMART/SAINT package was used for integration [1], whereas the synchrotron data sets of the three other compounds were integrated with XDS [2], for which an oblique incidence correction was done with a program available at HASYLAB [3]. Merging was performed with SORTAV [4] for all data sets. The X-ray structures were solved by direct methods followed by a spherical refinement using SHELXL [5]. Residuals were analyzed using the Pixelstats program as implemented in WinGX [6]

Details of wavefunction analysis

Three programs were used to analyze the resulting wavefunction files of Gaussian03, models *gas*:

Bond topological parameters including the kinetic and total energy density over rho ratios, G/$\rho(\mathbf{r}_{bcp})$ and H/$\rho(\mathbf{r}_{bcp})$, respectively, and integrated properties like atomic charges and volumes (Q and V), the delocalization index, δ(x,y), [7], [8] and the integrated amount of electrons within the zero flux surface, $\oint_{x \cap y}$, were obtained with the program AIM2000 [9].

Theoretical structure factors (pseudo periodic calculations) were obtained with the program Tonto [10]. Subsequent multipole refinements were performed with XD2006 [11] using the same local coordinate systems and symmetry restrictions as in the experimental cases, but the chemical constraints of the H atoms were retained for refinements of the isolated molecules.

Finally, DGRID-4.4 [12] was applied to obtain atomic properties and the ELI-D of the above listed models. For all models, a grid size of 0.075 au was applied.

References

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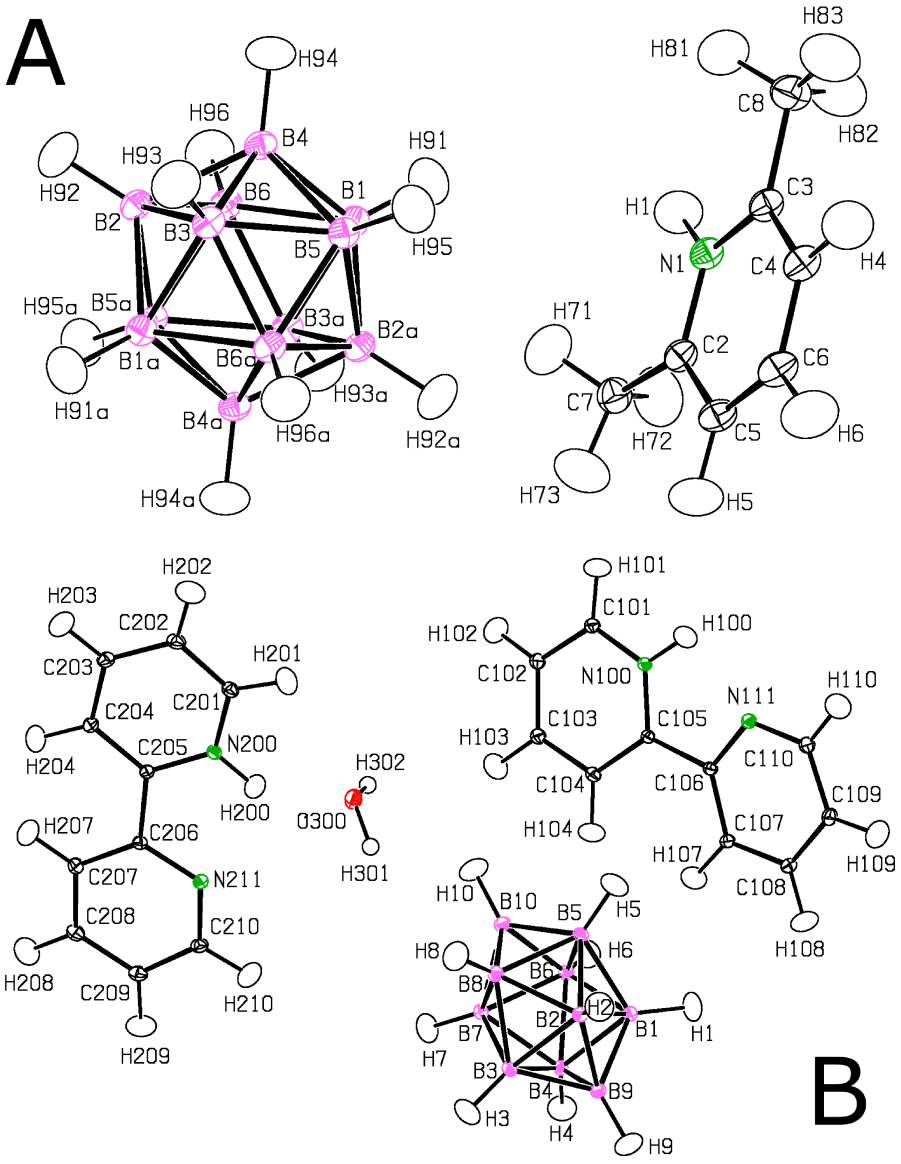

Figure S1: ORTEP plots of compounds **1** and **2** obtained by high resolution X-ray diffraction at low temperatures. In **1**, a center of inversion lies at the center of the $B_{12}H_{12}^{2-}$ cage.

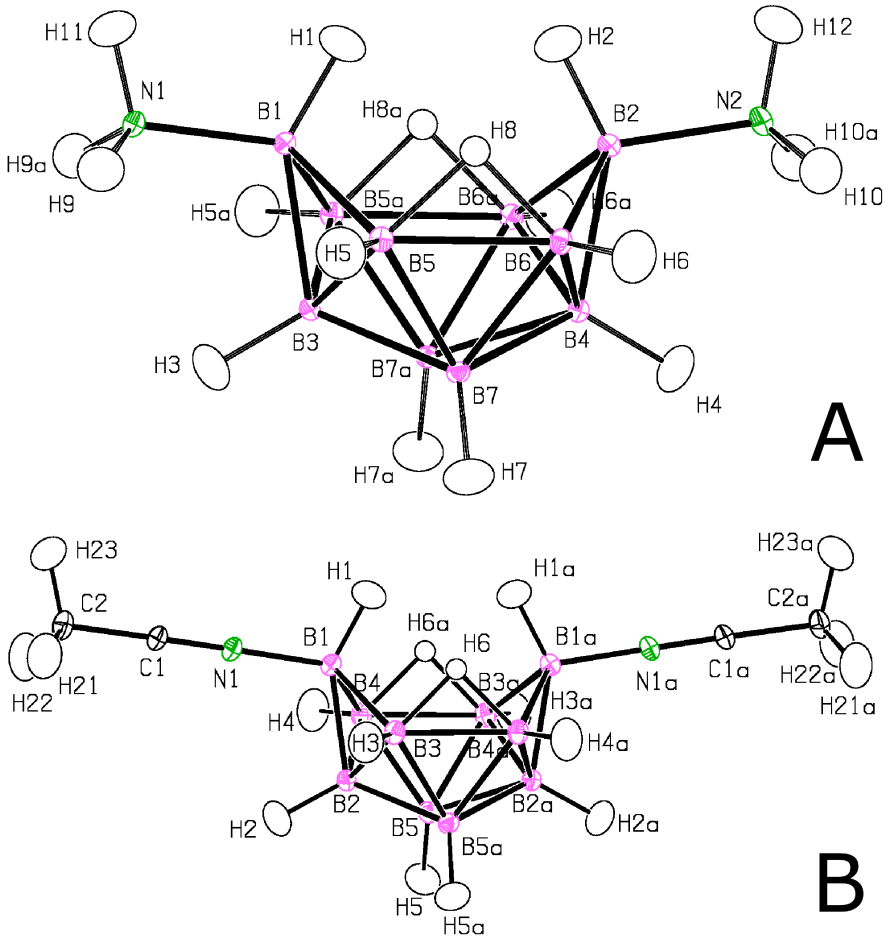

Figure S2: ORTEP plots of compounds **3** and **4** obtained by high resolution X-ray diffraction at low temperatures. In **3**, a mirror plane lies along the long molecular axis, resulting in special positions for the N atoms, four B atoms and six H atoms; in **4**, the molecule is constructed by a twofold axis which goes through the B(5)-B(5)a axis and the center of the cage.

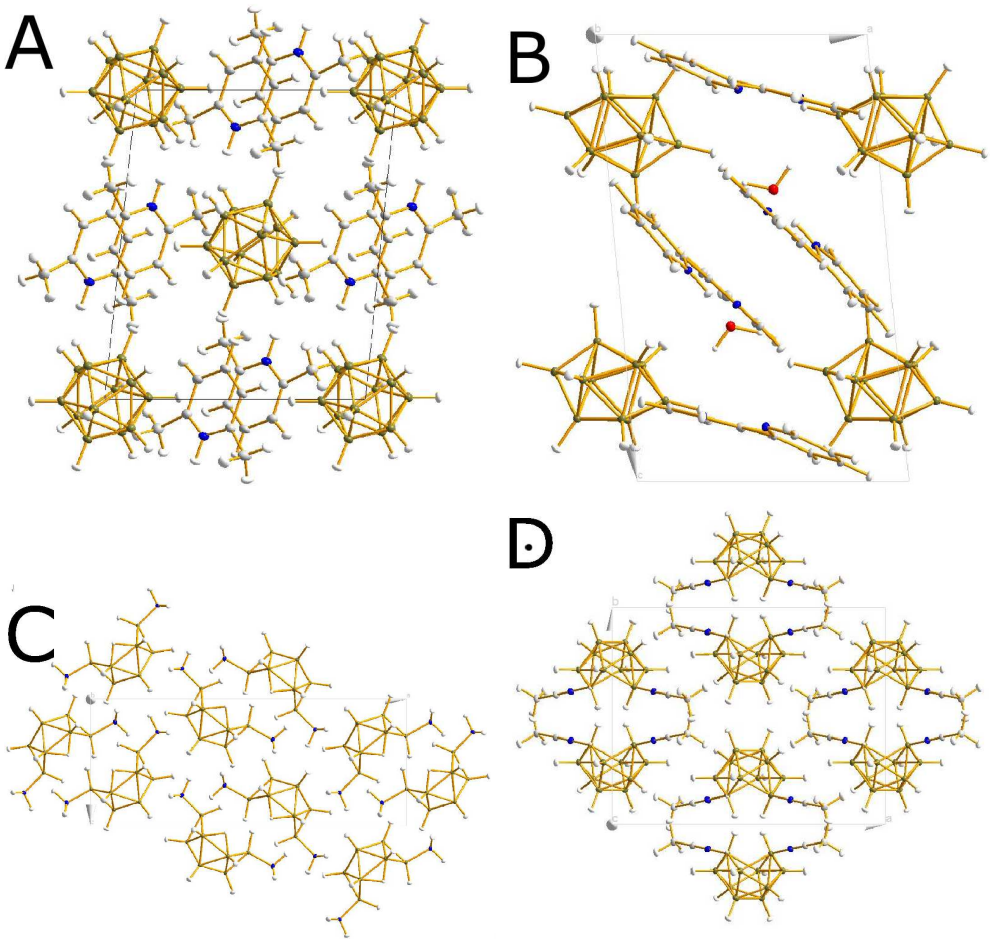

Figure S3: (A) Crystal packing diagram of **1** along the b-axis; (B) Crystal packing diagram of **2** along the b-axis; (C) Crystal packing diagram of **3** along the b-axis; (D) Crystal packing diagram of **4** along the c-axis.

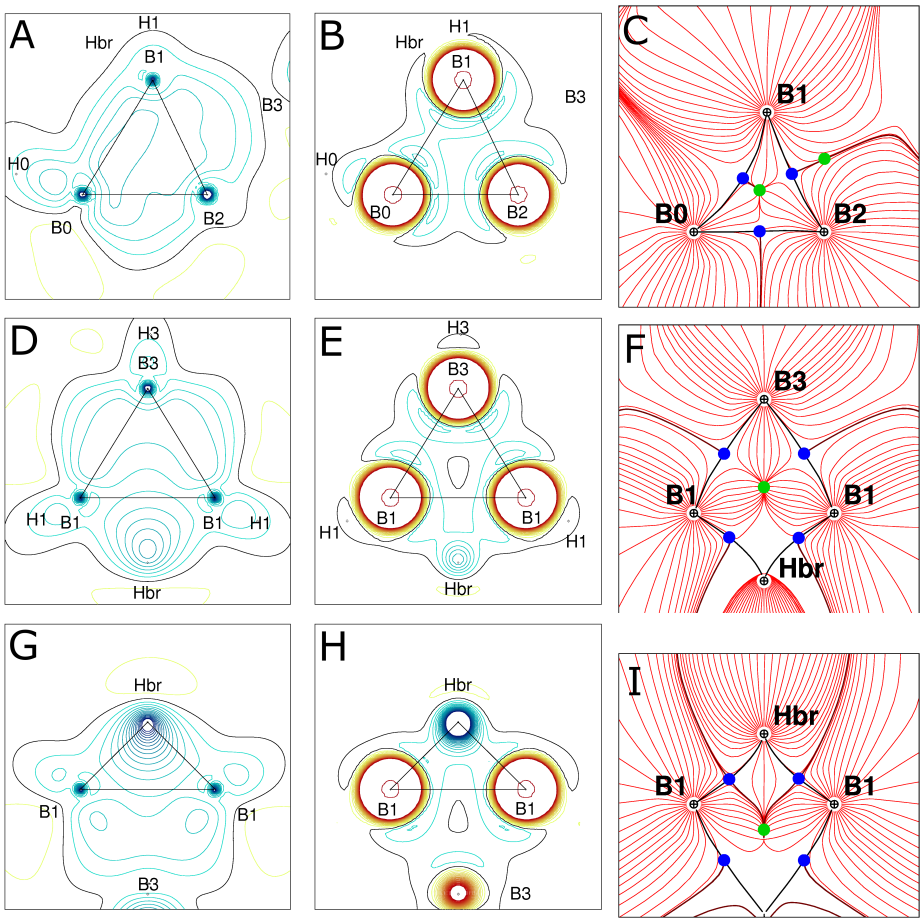

Figure S4: (A)-(C) Static deformation density, Laplacian and gradient vector field maps of the B0-B1-B2 ring in **3**; (D)-(F) corresponding maps of the B1-B3-B1 ring; (G)-(I) corresponding maps of the B1-H_{bridge}-B1 ring. Contour lines are 0.05 eÅ^{-3} for the deformation densities and 2.5 eÅ^{-5} for the Laplacians.

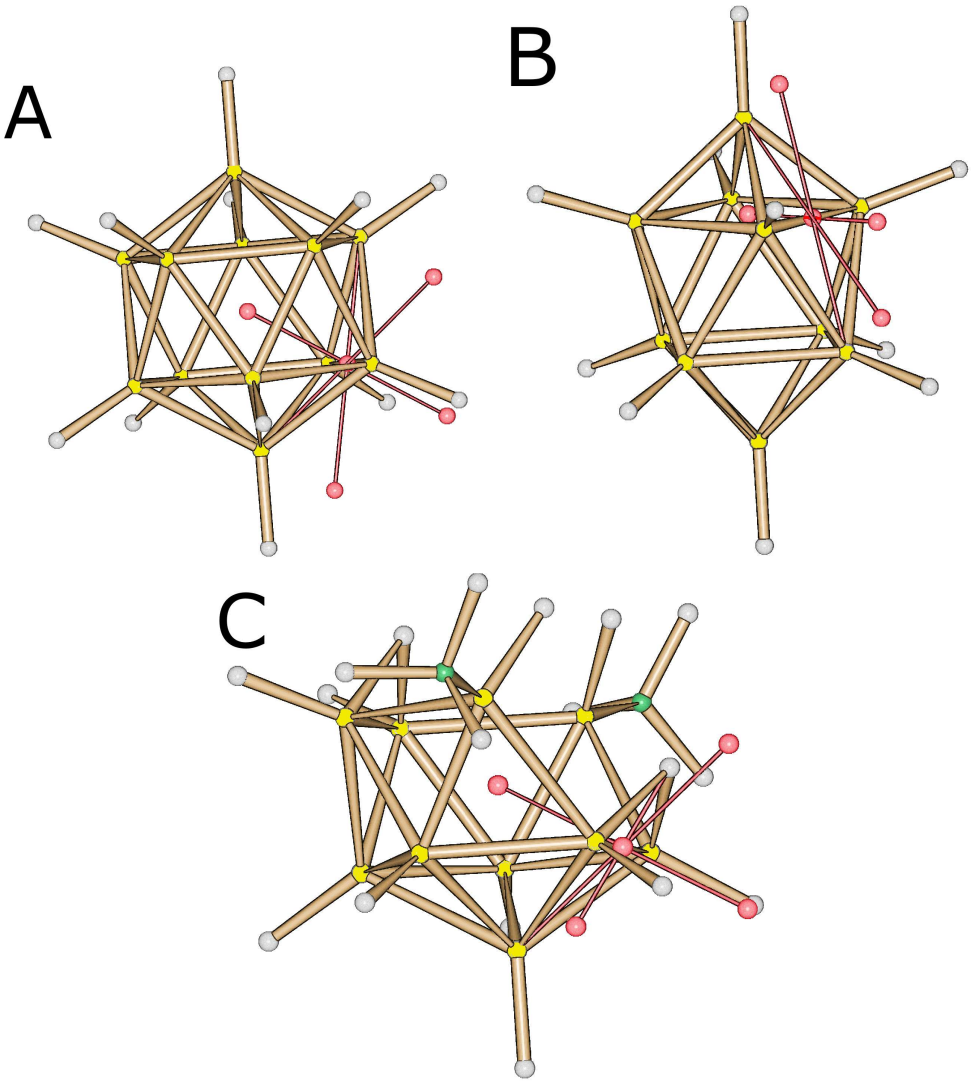

Figure S5: (A)-(C) Representations of the experimental geometries of compounds **1**-**3** including the lines (given in red) which were chosen for evaluation of ED, gradient of the ED and Laplacian, see next page. N atoms are blue coloured, B atoms are yellow, H atoms are white.

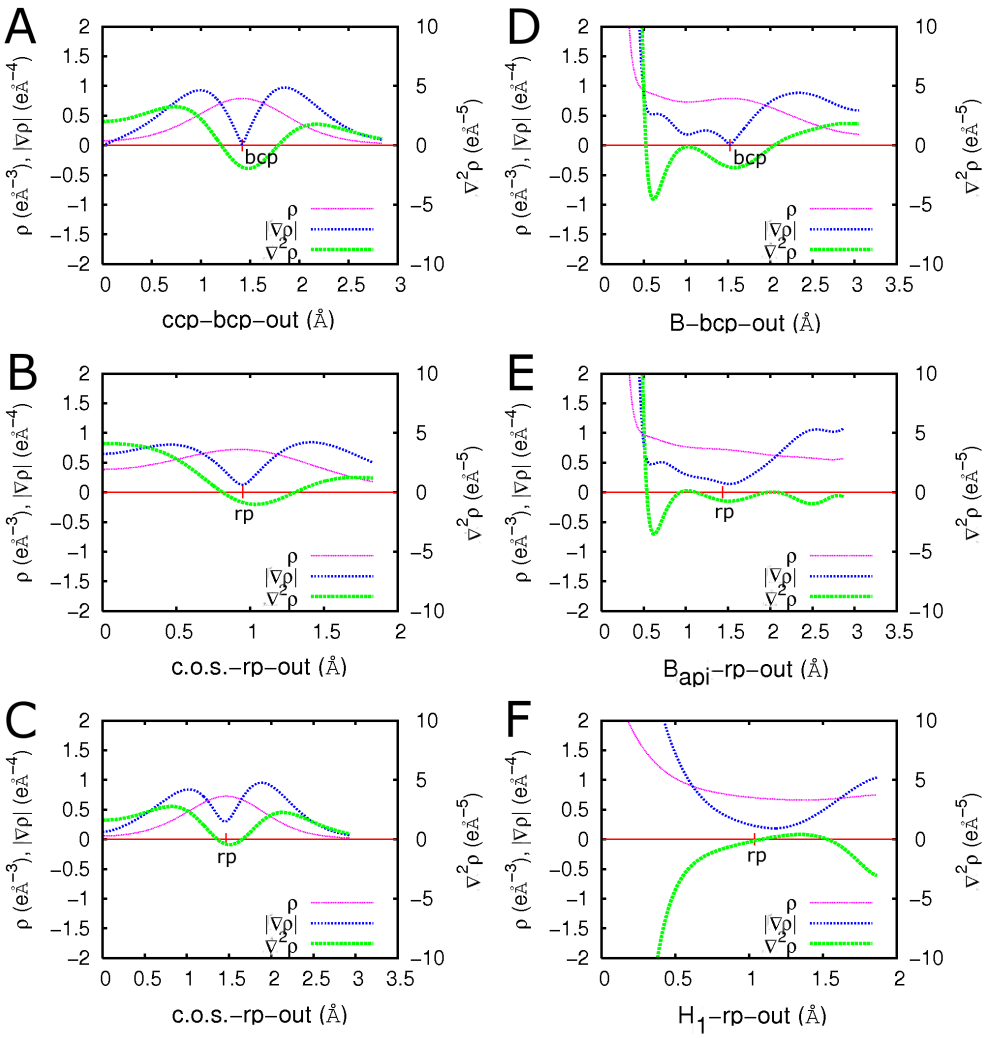

Figure S6: (A)-(C) Experimental ED, gradient of the ED, and Laplacian of lines perpendicular to the B-B axis in **1**-**3** starting at the cage critical point ′ccp′ (A) or at the center of a square ′c.o.s.′ spanned by four identical B atoms (B) and (C); (D)-(F) corresponding plots across B-B-B (B-H-B) planes. (D) B-B-B, (E) B_{cen}-B_{api}-B_{cen}, (E) B_1-H_{bridge}-B_1. ′bcp′ is bond critical point, ′out′ means a point outside the molecules which is the endpoint of the lines.

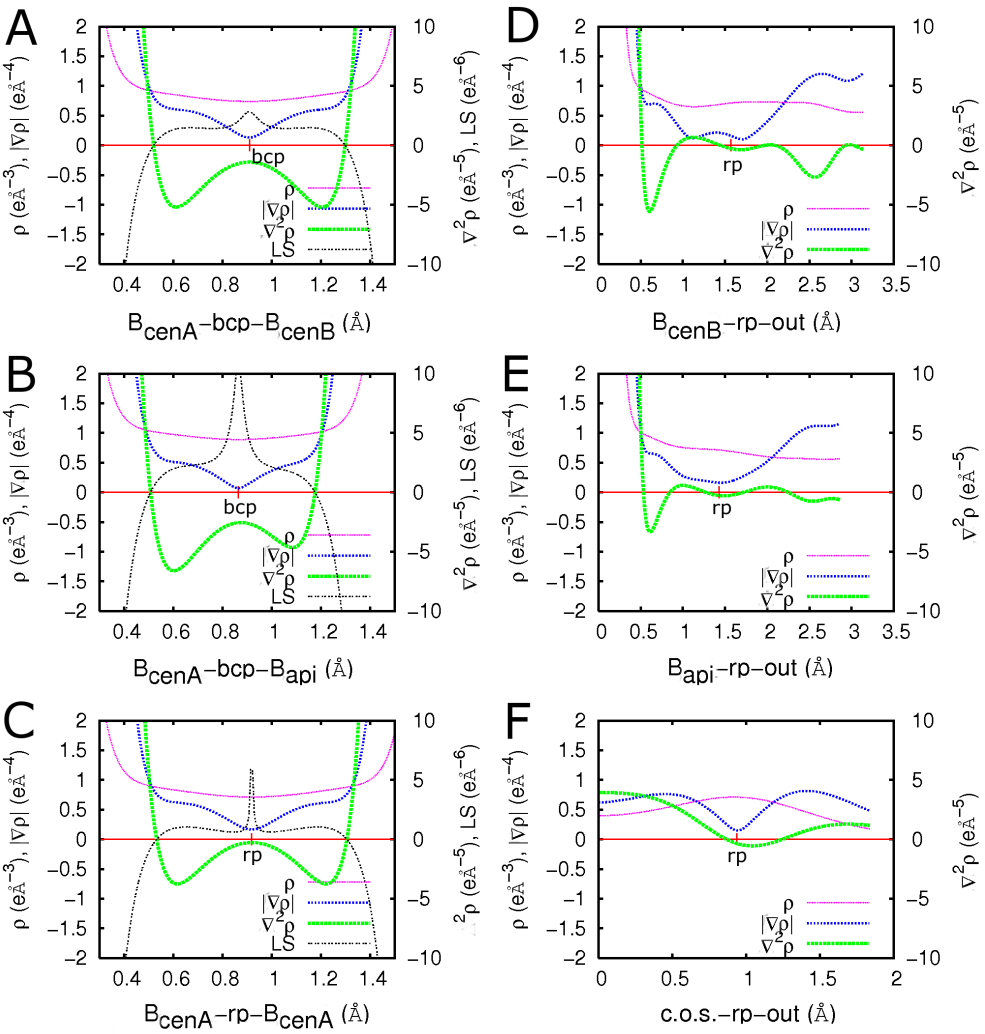

Figure S7: (A)-(C) Theoretical ED, gradient of the ED, Laplacian and Local Source (LS) along the B_{cenA}-B_{cenB} axis, the B_{cenA}-B_{api}, and the B_{cenA}-B_{cenA} axis in **2**; (D)-(F) corresponding plots (without LS) across axes which are perpendicular to B_{cenA}-B_{cenA}: (D) starting at B_{cenB} going across the B_{cenA}-B_{cenB}-B_{cenA} plane, (E) starting at B_{api} going across the B_{cen}-B_{api}-B_{cen} plane, (F) starting at the center of a square ′c.o.s.′ spanned by four identical B_{cenA} atoms.

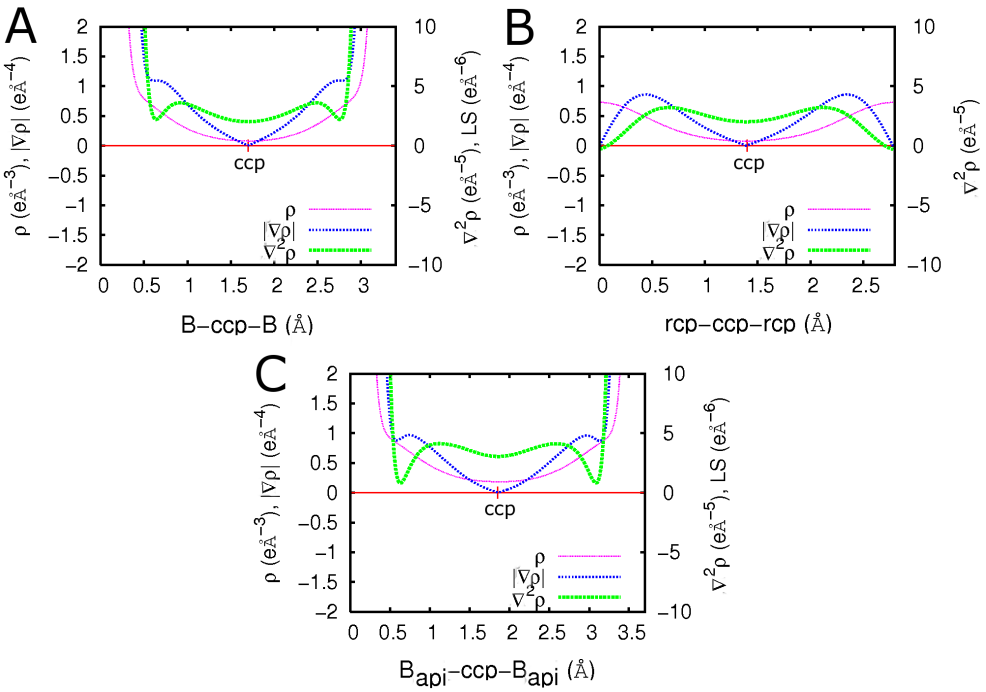

Figure S8: (A) Experimental ED, gradient of the ED, and Laplacian connecting two opposite B atoms in **1**. This axis crosses the cage critical point (ccp) at the center of the molecule; (B) corresponding properties along a line which connects two opposite ring critical points (rcp) in **1** also crossing the ccp; (C) corresponding properties along a line connecting the two opposite apical B atoms in **2.**

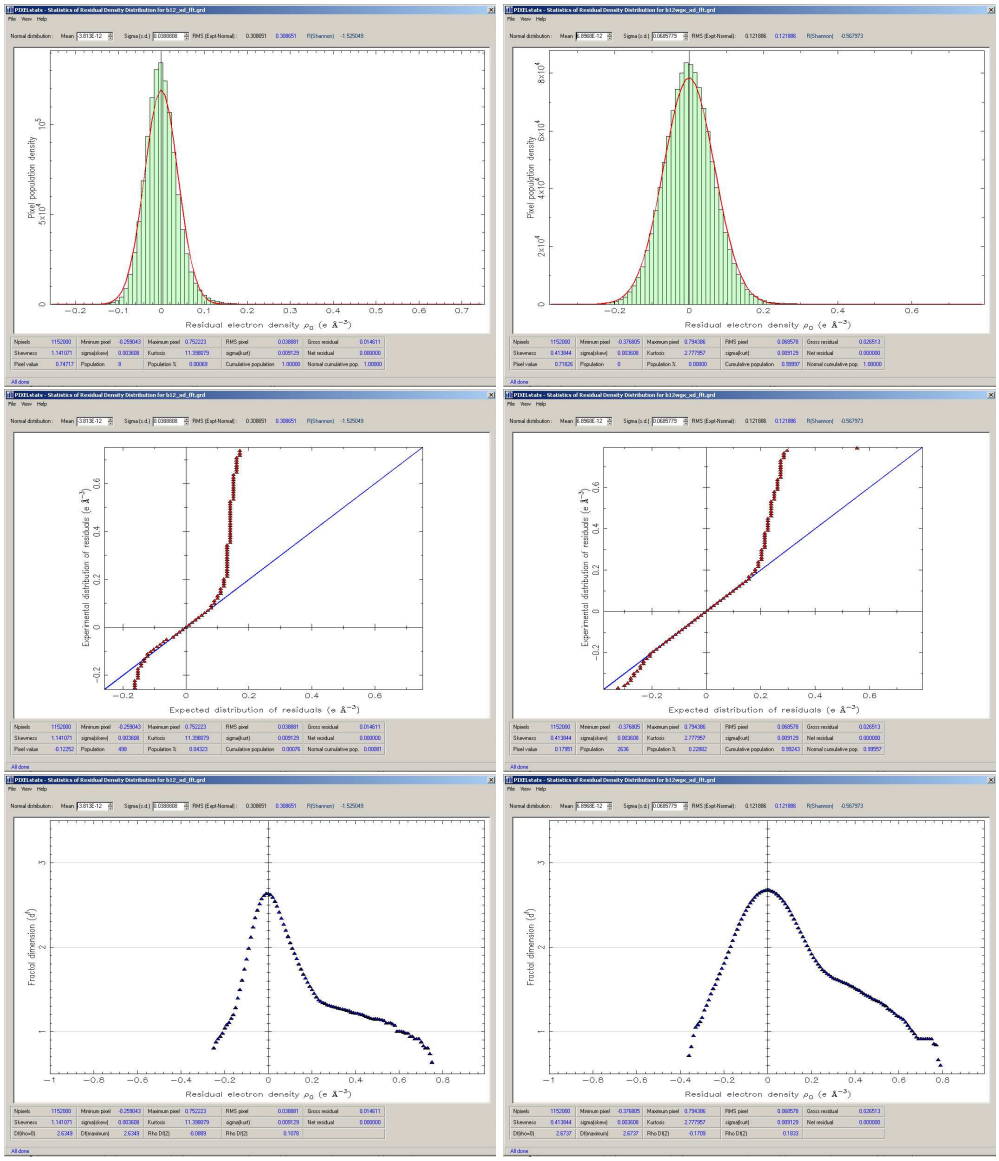

Figure S9: Probability distribution histogram, normal probability plot, and fractal dimension plot for the residual density in **1**. The left side refers to the model which were used in this study, the right side refers to a new data reduction with sortav as implemented in WinGX [6].

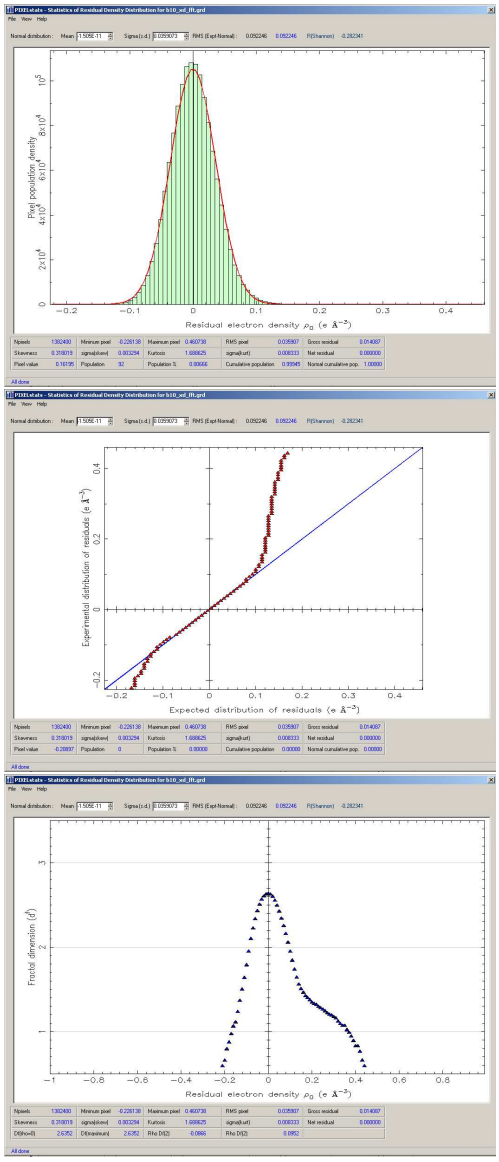

Figure S10: Probability distribution histogram, normal probability plot, and fractal dimension plot for the residual density in **2**.

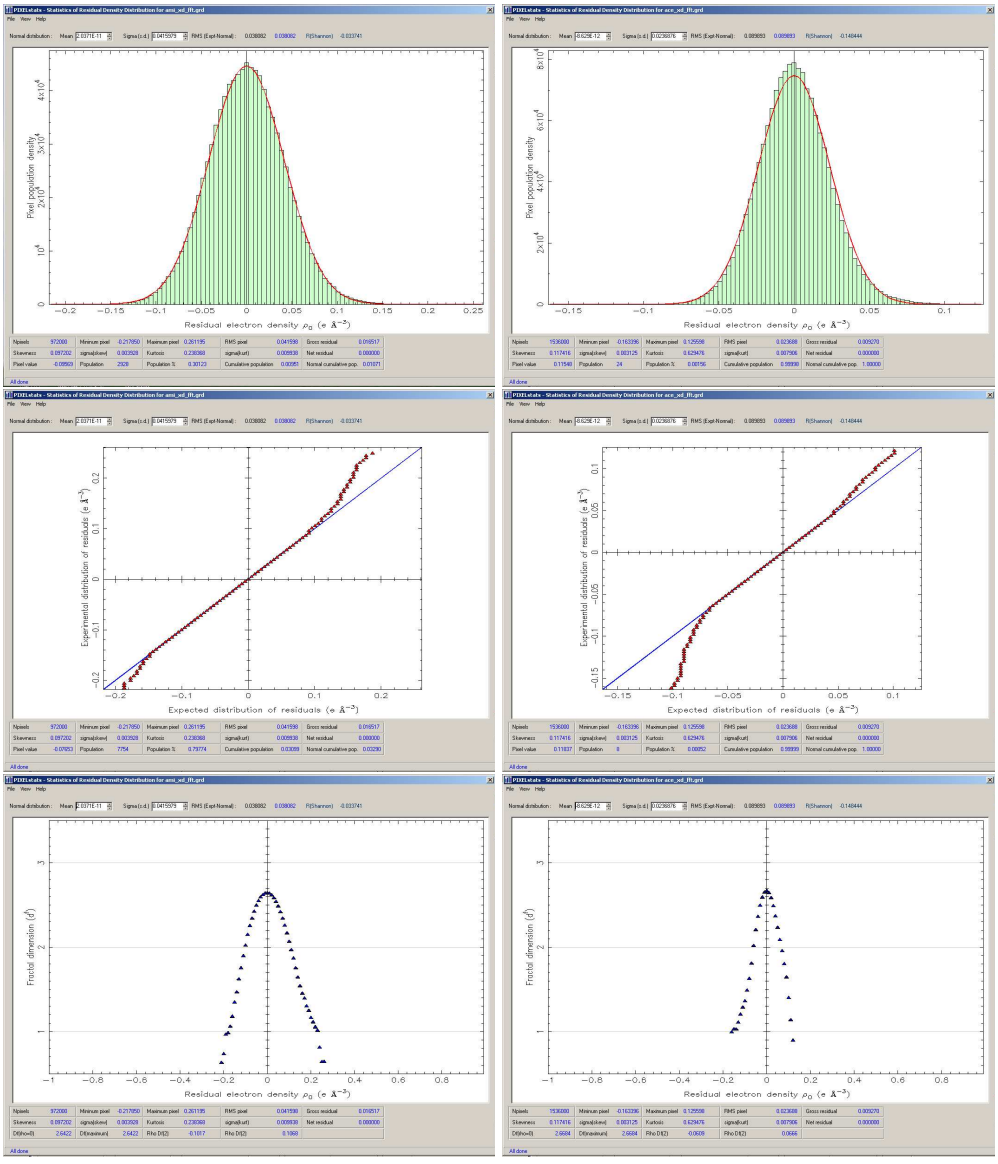

Figure S11: Probability distribution histogram, normal probability plot, and fractal dimension plot for the residual density in **3** (left side) and **4** (right side).

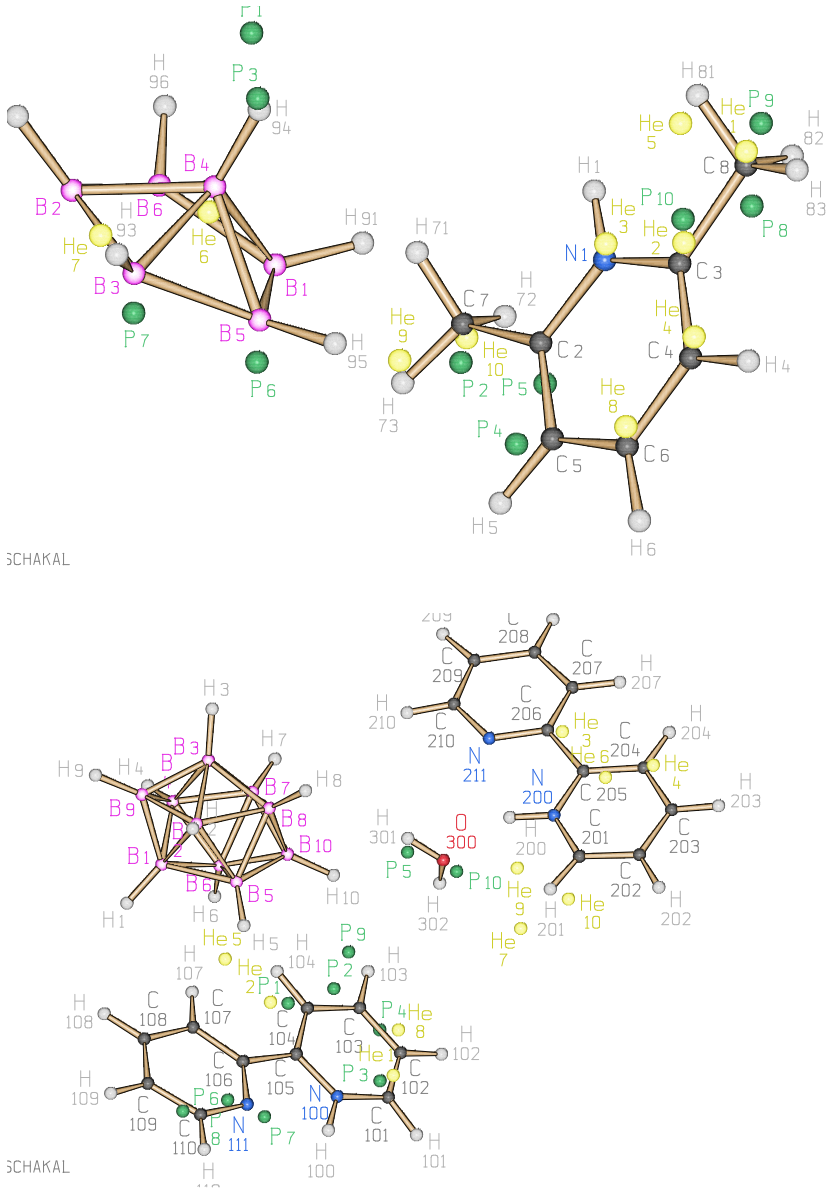

Figure S12: Schakal representations of the 10 largest residual density peaks (labeled P) and holes (labeled He) for **1** and **2**. One finds the major part of residual density close to the organic cations (especially for **2**) which reveals a proper modelling of the borane cages. These residuals may in part be due to disorder at the cations which, however, was to weak to be modelled.

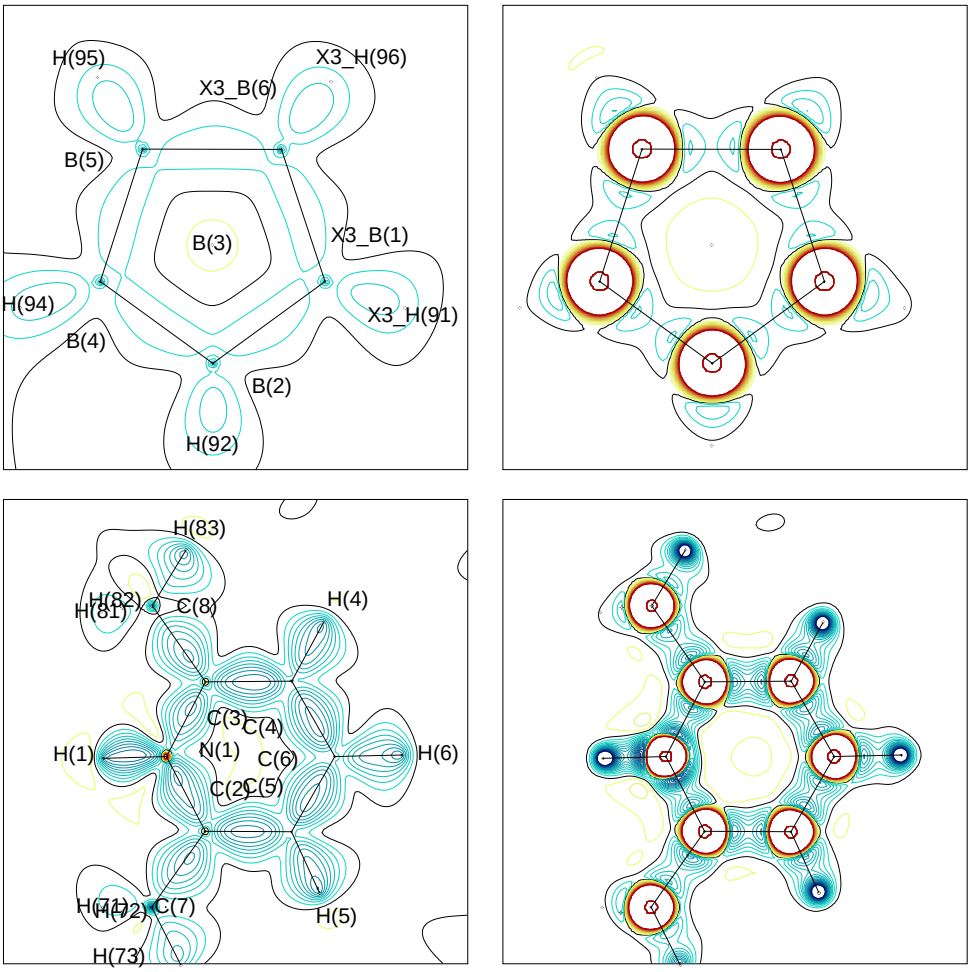

Figure S13: Static deformation densities (sdd) and Laplacian distribution (L) in the planes of a five-membered ring of the borane cage and the aromatic five-membered ring of the lutidinium. For sdd: Contour lines are 0.05 eÅ^{-3}; blue lines refer to positive values, black is zero, yellow is negative. For L: Contour lines are 2.5 eÅ^{-5}; blue lines refer to negative values, black is zero, yellow/red is positive.

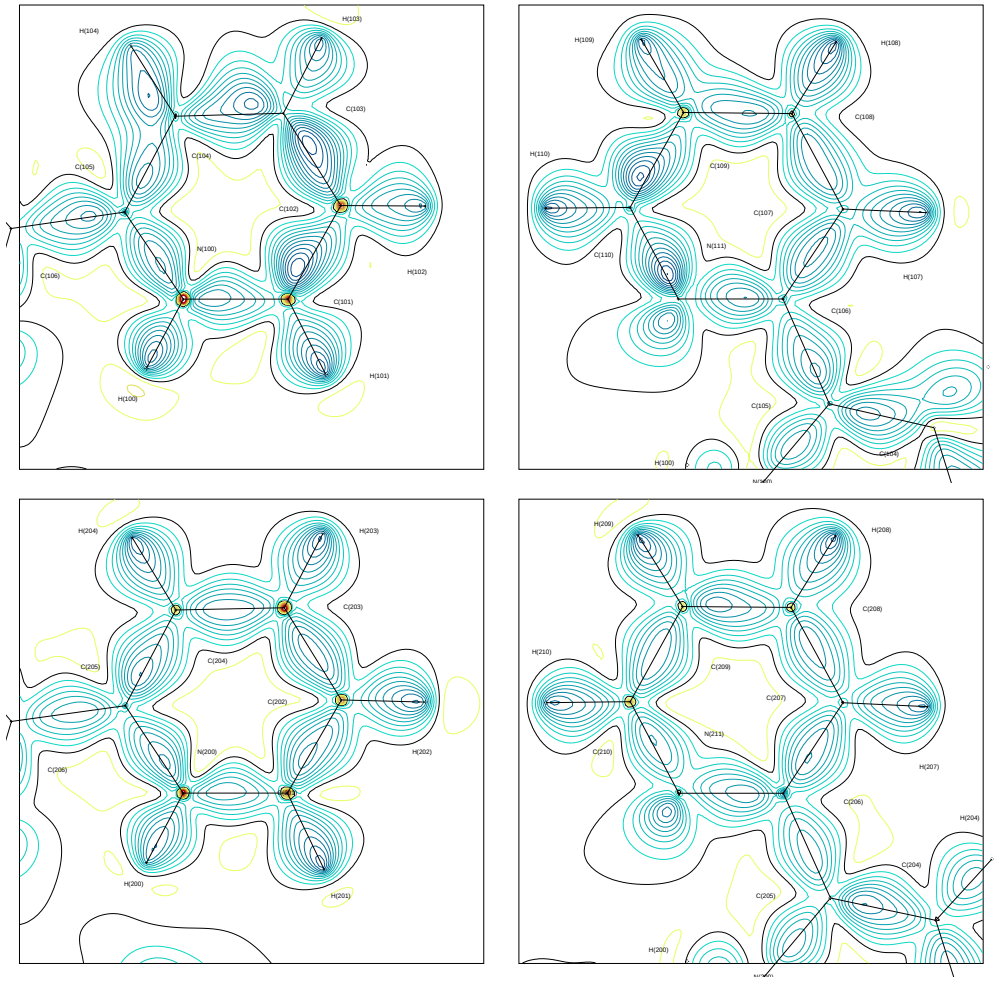

Figure S14: Static deformation densities in the planes of the two five-membered rings of each 2,2′-bipyridyn-1-ium molecule. Contour lines are 0.05 eÅ^{-3}; blue lines refer to positive values, black is zero, yellow is negative.

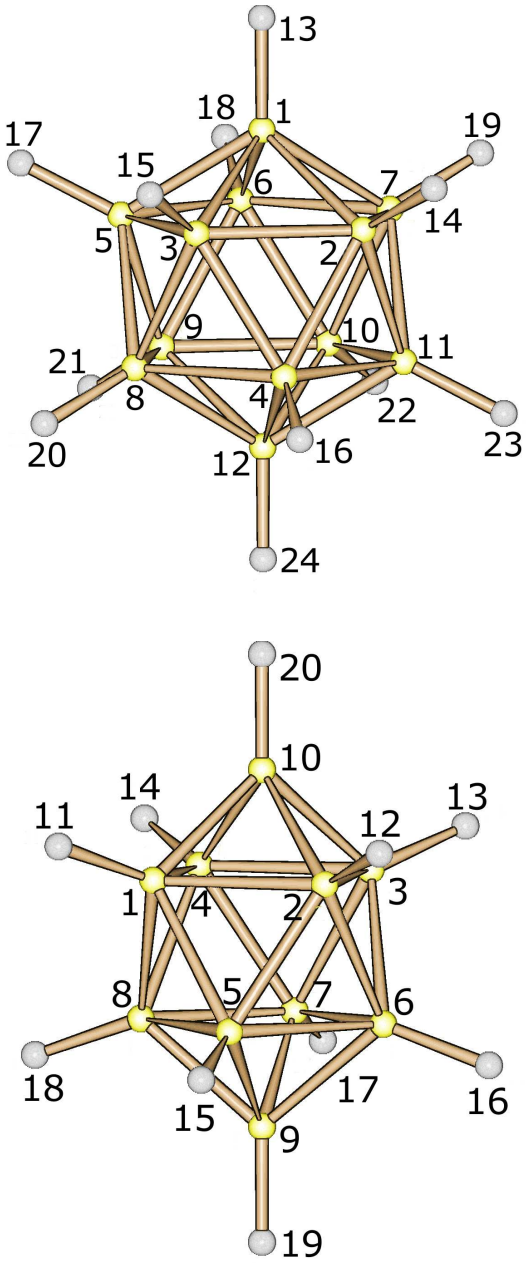

Figure S15: Labeling scheme of **1** and **2**, model *gas*.

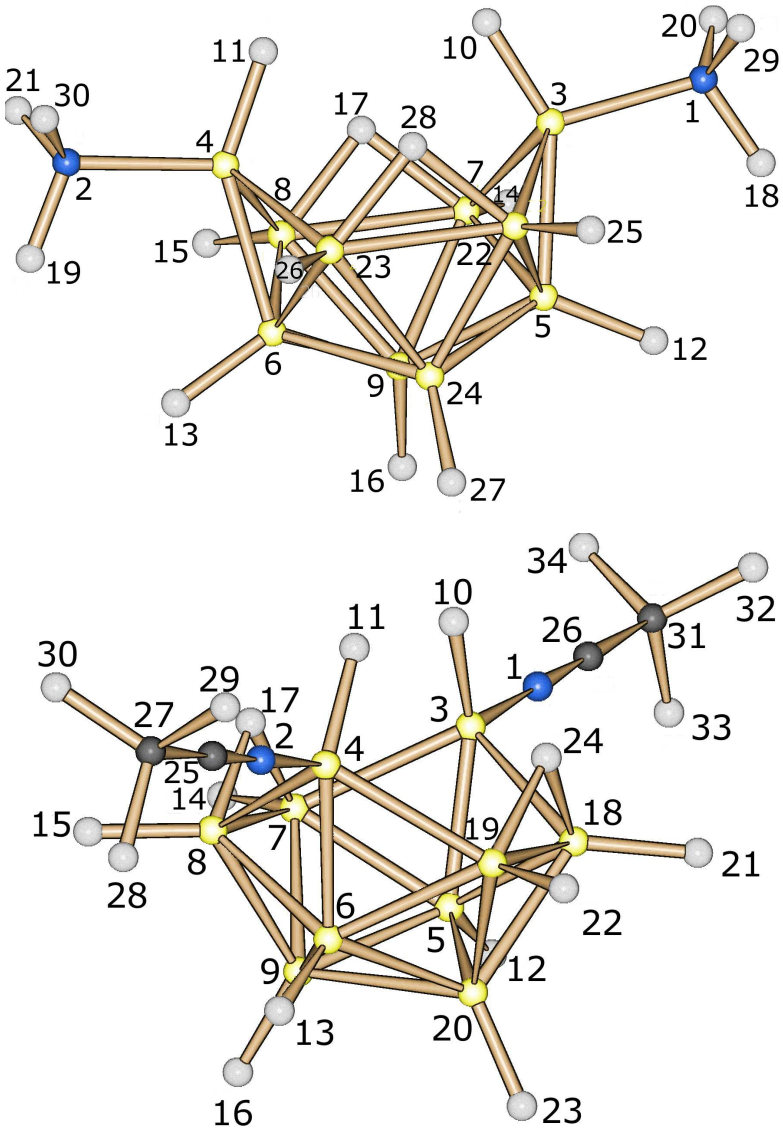

Figure S16: Labeling scheme of **3** and **4**, model *gas*.

Table S1: Averaged geometrical bond descriptors of the *closo*-boranes, model *exp*

1	Min. [Å, °]	Median [Å, °]	Mean [Å, °]	Max. [Å, °]	sd [Å, °]	av
B-B	1.780	1.785	1.785	1.791	0.003	2
B-B-B (acute)	59.7	60.0	60.0	60.3	0.1	30
B-B-B (braod)	107.6	108.0	108.0	108.4	0.2	30
B-B-H	117.8	121.8	121.7	125.9	1.9	30
2	Min. [Å, °]	Median [Å, °]	Mean [Å, °]	Max. [Å, °]	sd [Å, °]	av
B_{cen}-B_{api}	1.697	1.701	1.701	1.706	0.003	8
B_{cenA}-B_{cenB}	1.803	1.812	1.813	1.822	0.006	8
B_{cenA}-B_{cenA}	1.822	1.837	1.835	1.841	0.006	8
B_{cenA}-B_{cenA}-B_{cenB} (acute)	59.0	59.6	59.6	60.0	0.3	16
B_{cenA}-B_{cenB}-B_{cenA}	60.5	60.9	60.8	61.1	0.2	8
B_{cenA}-B_{cenA}-B_{api}	57.1	57.4	57.4	57.8	0.2	16
B_{cenA}-B_{api}-B_{cenB} (acute)	64.7	65.3	65.3	65.5	0.3	8
B_{cenA}-B_{cenA}-B_{cenB} (braod)	101.8	102.1	102.1	102.3	0.1	16
B_{cenA}-B_{cenB}-B_{api}	111.9	112.4	112.4	113.0	0.3	16
B_{cenA}-B_{cenA}-B_{cenA}	89.4	90.0	90.0	90.5	0.3	8
B_{cenA}-B_{api}-B_{cenA} (braod)	99.3	99.4	99.4	99.6	0.1	4
B_{cenA}-B_{cenA}-H	130.4	131.7	132.0	134.2	1.1	16
B_{cenA}-B_{cenB}-H	115.8	117.8	117.8	119.8	1.0	16
B_{api}-B_{cen}-H	119.8	120.7	121.0	122.8	1.0	8
B_{cen}-B_{api}-H	128.4	130.4	130.3	132.1	1.2	8

Table S2: Geometrical bond descriptors of the *arachno*-boranes 1: bond lengths, model *exp*

3	R_{xy} [Å]	**4**	R_{xy} [Å]	type
N(1)-B(1)	1.589	N(1)-B(1)	1.526	N-B
N(2)-B(2)	1.597			
B(1)-B(3)	1.734	B(1)-B(2)	1.749	B0-B2
B(2)-B(4)	1.729			
B(1)-B(5)	1.861	B(1)-B(3)	1.863	B0-B1
B(2)-B(6)	1.860	B(1)-B(4)	1.867	
B(3)-B(5)	1.758	B(2)-B(3)	1.762	B1-B2
B(4)-B(6)	1.751	B(2)-B(4)	1.764	
B(3)-B(7)	1.759	B(2)-B(5)	1.764	B2-B3
B(4)-B(7)	1.763	B(2)-B(5)a	1.765	
B(5)-B(6)	1.869	B(3)-B(4)a	1.872	B1-B1
B(5)-B(7)	1.778	B(3)-B(5)a	1.783	B1-B3
B(6)-B(7)	1.775	B(4)-B(5)	1.786	
B(7)-B(7)a	1.826	B(5)-B(5)a	1.825	B3-B3

Table S3: Geometrical bond descriptors of the *arachno*-boranes 2: bond angles, model *exp*

3	∠ [°]	**4**	∠ [°]	**3**	∠ [°]	**4**	∠ [°]
N(1)-B(1)-B(3)	106.66(4)	N(1) -B(1)-B(2)	107.54(1)	N(1)-B(1)-H(1)	112.38	N(1)-B(1)-H(1)	108.86
N(2)-B(2)-B(4)	108.59(4)			N(2)-B(2)-H(2)	108.89		
N(1)-B(1)-B(5)	117.50(2)	N(1) -B(1)-B(3)	116.54(1)	B(3)-B(1)-H(1)	140.96	B(2)-B(1)-H(1)	143.56
N(2)-B(2)-B(6)	117.94(2)	N(1) -B(1)-B(4)	117.96(1)	B(4)-B(2)-H(2)	142.53		
B(3)-B(1)-B(5)	58.44(2)	B(2)-B(1)-B(3)	58.29(1)	B(5)-B(1)-H(1)	101.63	B(3)-B(1)-H(1)	102.67
B(4)-B(2)-B(6)	58.25(2)	B(2)-B(1)-B(4)	58.30(1)	B(6)-B(2)-H(2)	102.97	B(4)-B(1)-H(1)	104.67
B(5)-B(1)-B(5)a	103.92(3)	B(3)-B(1)-B(4)	104.49(1)	B(1)-B(3)-H(3)	110.86	B(1)-B(2)-H(2)	110.06
				B(2)-B(4)-H(4)	110.65		
B(1)-B(3)-B(5)	64.40(2)	B(1)-B(2)-B(3)	64.10(1)	B(5)-B(6)-H(8)	44.95	H(6)-B(3)-B(4)a	44.82
B(2)-B(4)-B(6)	64.62(2)	B(1)-B(2)-B(4)	64.22(1)	B(6)-B(5)-H(8)	44.95	B(3)a-B(4)-H(6)a	44.83
B(1)-B(3)-B(7)	116.67(3)	B(1)-B(2)-B(5)	115.82(1)	B(5)-B(3)-H(3)	118.40	B(3)-B(2)-H(2)	117.78
B(2)-B(4)-B(7)	116.39(3)	B(1)-B(2)-B(5)a	115.65(1)	B(6)-B(4)-H(4)	117.82	B(4)-B(2)-H(2)	117.20
B(5)-B(3)-B(5)a	112.92(3)	B(3)-B(2)-B(4)	113.53(1)	B(1)-B(5)-H(8)	91.55	B(1)-B(3)-H(6)	86.50
				B(2)-B(6)-H(8)	90.32	B(1)-B(4)-H(6)a	86.89
B(5)-B(3)-B(7)a	112.11(3)	B(3)-B(2)-B(5)	112.16(1)	B(7)-B(3)-H(3)	121.32	B(5)-B(2)-H(2)	122.71
B(6)-B(4)-B(7)a	112.22(3)	B(4)-B(2)-B(5)a	112.10(1)	B(7)-B(4)-H(4)	121.81		
B(5)-B(3)-B(7)	60.72(2)	B(3)-B(2)-B(5)a	60.75(1)	B(1)-B(5)-H(5)	119.53	B(1)-B(3)-H(3)	120.20
B(6)-B(4)-B(7)	60.66(2)	B(4)-B(2)-B(5)	60.80(1)	B(2)-B(6)-H(6)	120.73	B(1)-B(4)-H(4)	121.72
B(1)-B(5)-B(3)	57.16(3)	B(1)-B(3)-B(2)	57.62(1)	B(3)-B(5)-H(5)	124.12	B(2)-B(3)-H(3)	124.27
B(2)-B(6)-B(4)	57.13(2)	B(1)-B(4)-B(2)	57.48(1)	B(4)-B(6)-H(6)	124.84	B(2)-B(4)-H(4)	127.40
B(1)-B(5)-B(6)	114.44(3)	B(1)-B(3)-B(4)a	112.77(1)	B(3)-B(5)-H(8)	125.96	B(2)-B(3)-H(6)	121.66
B(2)-B(6)-B(5)	113.28(3)	B(1)-B(4)-B(3)a	112.99(1)	B(4)-B(6)-H(8)	125.56	B(2)-B(4)-H(6)a	121.77
B(1)-B(5)-B(7)	109.56(3)	B(1)-B(3)-B(5)a	109.31(1)	B(6)-B(5)-H(5)	120.29	H(3)-B(3)-B(4)a	120.62
B(2)-B(6)-B(7)	109.47(3)	B(1)-B(4)-B(5)	109.10(1)	B(5)-B(6)-H(6)	119.79	H(4)-B(4)-B(3)a	117.85
B(3)-B(5)-B(6)	105.27(3)	B(2)-B(3)-B(4)a	105.34(1)	B(7)-B(5)-H(5)	119.63	H(3)-B(3)-B(5)a	120.11
B(4)-B(6)-B(5)	105.35(3)	B(2)-B(4)-B(3)a	105.24(1)	B(7)-B(6)-H(6)	119.44	B(5)-B(4)-H(4)	120.66
B(3)-B(5)-B(7)	59.66(3)	B(2)-B(3)-B(5)a	59.72(1)	B(7)-B(5)-H(8)	101.82	H(6)-B(3)-B(5)a	100.74
B(4)-B(6)-B(7)	60.02(2)	B(2)-B(4)-B(5)	59.59(1)	B(7)-B(6)-H(8)	101.96	B(5)-B(4)-H(6)a	100.63
B(6)-B(5)-B(7)	58.19(2)	B(4)a-B(3)-B(5)a	58.42(1)	H(5)-B(5)-H(8)	109.35	H(4)-B(4)-H(6)a	110.11
B(5)-B(6)-B(7)	58.34(2)	B(5) -B(4)-B(3)a	58.29(1)	H(6)-B(6)-H(8)	108.98		
B(3)-B(7)-B(4)	105.03(3)	B(2)-B(5)-B(2)a	105.13(1)	B(3)-B(7)-H(7)	123.51	B(2)-B(5)-H(5)	123.02
				B(4)-B(7)-H(7)	121.01	H(5)-B(5)-B(2)a	120.65
B(3)-B(7)-B(5)	59.62(2)	B(2)-B(5)-B(4)	59.61(1)				
B(4)-B(7)-B(6)	59.32(2)	B(2)a-B(5)-B(3)a	59.54(1)	B(5)-B(7)-H(7)	123.20	B(4)-B(5)-H(5)	123.88
				B(6)-B(7)-H(7)	121.16	H(5)-B(5)-B(3)a	122.16
B(3)-B(7)-B(6)	109.35(3)	B(2)-B(5)-B(3)a	109.16(1)				
B(4)-B(7)-B(5)	108.80(3)	B(4)-B(5)-B(2)a	108.98(1)	H(7)-B(7)-B(7)a	119.72	H(5)-B(5)-B(5)a	118.46
B(5)-B(7)-B(6)	63.47(2)	B(4)-B(5)-B(3)a	63.29(1)				
B(7)-B(3)-B(7)a	62.55(3)	B(5)-B(2)-B(5)a	62.27(1)				
B(7)-B(4)-B(7)a	62.38(2)						
B(3)-B(7)-B(7)a	58.72(2)	B(2)-B(5)-B(5)a	58.88(1)				
B(4)-B(7)-B(7)a	58.81(2)	B(2)a-B(5)-B(5)a	58.84(1)				
B(5)-B(7)-B(7)a	108.10(3)	B(4)-B(5)-B(5)a	108.36(1)				
B(6)-B(7)-B(7)a	108.20(2)	B(3)a-B(5)-B(5)a	108.37(1)				

Table S4: Topological bond descriptors 1: B-B bonds of **1**

model	example	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	λ_3	ϵ	Rxy [Å]	Rbp [Å]	Δ_{bcp} [Å]
exp	B(1) -B(4)	0.79(1)	-2.0(1)	0.890	0.893	2.77	2.67	1.782(7)	1.783	0.021
	B(1) -B(5)	0.79(1)	-1.8(1)	0.892	0.892	2.83	3.11	1.784(7)	1.786	0.029
	B(1) -B(6)	0.79(1)	-1.8(1)	0.891	0.897	2.86	3.13	1.786(6)	1.789	0.028
	B(1) -B(2)a	0.80(1)	-2.0(1)	0.889	0.895	2.76	2.59	1.783(6)	1.786	0.020
	B(1) -B(3)a	0.80(1)	-2.0(1)	0.890	0.898	2.78	2.64	1.788(7)	1.790	0.020
	B(2) -B(3)	0.79(1)	-1.8(1)	0.891	0.892	2.88	2.97	1.782(6)	1.785	0.030
	B(2) -B(4)	0.79(1)	-2.0(1)	0.895	0.893	2.79	2.61	1.787(6)	1.790	0.031
	B(2) -B(6)	0.79(1)	-1.8(1)	0.895	0.895	2.88	3.15	1.789(7)	1.791	0.026
	B(2) -B(5)a	0.80(1)	-2.0(1)	0.894	0.891	2.78	2.56	1.785(7)	1.788	0.019
	B(3) -B(4)	0.80(1)	-2.1(1)	0.893	0.889	2.78	2.53	1.781(6)	1.783	0.030
	B(3) -B(5)	0.78(1)	-1.7(1)	0.899	0.893	2.86	3.25	1.791(6)	1.793	0.027
	B(3) -B(6)a	0.80(1)	-2.1(1)	0.891	0.891	2.78	2.51	1.782(6)	1.784	0.019
	B(4) -B(5)	0.80(1)	-1.9(1)	0.895	0.890	2.80	2.93	1.785(6)	1.787	0.024
	B(4) -B(6)	0.80(1)	-1.9(1)	0.893	0.894	2.83	2.89	1.786(7)	1.788	0.023
	B(5) -B(6)a	0.80(1)	-2.0(1)	0.890	0.894	2.77	2.53	1.783(6)	1.785	0.019
cry	B(1) -B(4)	0.80	-2.2	0.891	0.892	2.46	2.73	1.782	1.784	0.016
	B(1) -B(5)	0.79	-2.0	0.891	0.893	2.47	3.06	1.784	1.786	0.019
	B(1) -B(6)	0.79	-2.0	0.893	0.894	2.48	3.11	1.786	1.789	0.018
	B(1) -B(2)a	0.79	-2.1	0.891	0.893	2.49	3.04	1.783	1.785	0.018
	B(1) -B(3)a	0.79	-2.0	0.893	0.896	2.50	3.09	1.788	1.790	0.018
	B(2) -B(3)	0.79	-2.0	0.891	0.892	2.47	3.05	1.782	1.784	0.019
	B(2) -B(4)	0.79	-2.1	0.894	0.893	2.49	2.93	1.787	1.788	0.023
	B(2) -B(6)	0.79	-2.0	0.894	0.895	2.49	3.10	1.789	1.790	0.018
	B(2) -B(5)a	0.79	-2.0	0.891	0.895	2.51	3.01	1.785	1.787	0.018
	B(3) -B(4)	0.80	-2.1	0.891	0.890	2.47	2.87	1.781	1.782	0.022
	B(3) -B(5)	0.79	-1.9	0.895	0.896	2.50	3.17	1.791	1.792	0.019
	B(3) -B(6)a	0.79	-2.1	0.891	0.892	2.49	3.00	1.782	1.784	0.019
	B(4) -B(5)	0.79	-2.1	0.890	0.895	2.48	2.93	1.785	1.786	0.019
	B(4) -B(6)	0.79	-2.0	0.891	0.895	2.49	2.89	1.786	1.788	0.016
	B(5) -B(6)a	0.79	-2.1	0.893	0.890	2.50	2.97	1.783	1.785	0.018
gas	B B	0.78	-1.6	0.892	0.892	3.06	2.40	1.783	1.784	0.023

Table S5: Topological bond descriptors 2: B-B bonds of **2**

model	example	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	λ_3	ϵ	Rxy [Å]	Rbp [Å]	Δ_{bcp} [Å]
exp	B(1) -B(9)	0.89(1)	-3.1(1)	0.875	0.831	2.28	1.39	1.706(1)	1.708	0.020
	B(2) -B(9)	0.89(1)	-3.2(1)	0.871	0.830	2.25	1.33	1.700(1)	1.703	0.018
	B(3) -B(9)	0.89(1)	-3.1(1)	0.868	0.837	2.25	1.33	1.704(1)	1.707	0.016
	B(4) -B(9)	0.90(1)	-3.2(1)	0.873	0.827	2.24	1.35	1.699(1)	1.701	0.018
	B(5) -B(10)	0.89(1)	-3.1(1)	0.876	0.829	2.24	1.37	1.704(1)	1.707	0.019
	B(6) -B(10)	0.89(1)	-3.2(1)	0.875	0.827	2.23	1.35	1.701(1)	1.704	0.018
	B(7) -B(10)	0.90(1)	-3.2(1)	0.875	0.823	2.21	1.36	1.697(1)	1.700	0.018
	B(8) -B(10)	0.89(1)	-3.2(1)	0.872	0.828	2.20	1.36	1.700(1)	1.702	0.017
cry	B(1) -B(9)	0.89	-3.2	0.877	0.829	2.40	1.08	1.706	1.707	0.004
	B(2) -B(9)	0.89	-3.3	0.874	0.826	2.38	1.04	1.700	1.702	0.001
	B(3) -B(9)	0.89	-3.2	0.874	0.830	2.40	1.04	1.704	1.706	0.001
	B(4) -B(9)	0.89	-3.3	0.876	0.823	2.38	1.06	1.699	1.700	0.000
	B(5) -B(10)	0.89	-3.2	0.873	0.831	2.40	1.06	1.704	1.706	0.003
	B(6) -B(10)	0.89	-3.2	0.874	0.827	2.39	1.04	1.701	1.703	0.001
	B(7) -B(10)	0.89	-3.3	0.874	0.823	2.36	1.04	1.697	1.699	0.001
	B(8) -B(10)	0.89	-3.3	0.877	0.823	2.38	1.05	1.700	1.702	0.000
gas	B -B	0.89	-2.5	0.865	0.835	3.07	1.17	1.699	1.700	0.018
exp	B(1) -B(5)	0.76(1)	-1.9(1)	0.912	0.908	2.68	1.75	1.818(1)	1.833	0.036
	B(1) -B(6)	0.77(1)	-1.9(1)	0.907	0.906	2.66	1.75	1.812(1)	1.826	0.037
	B(2) -B(5)	0.77(1)	-1.9(1)	0.908	0.907	2.66	1.73	1.813(1)	1.827	0.035
	B(2) -B(8)	0.77(1)	-2.0(1)	0.908	0.904	2.63	1.70	1.811(1)	1.825	0.034
	B(3) -B(7)	0.77(1)	-2.0(1)	0.898	0.906	2.60	1.65	1.803(1)	1.827	0.034
	B(3) -B(8)	0.76(1)	-1.9(1)	0.908	0.910	2.61	1.76	1.816(1)	1.832	0.032
	B(4) -B(6)	0.77(1)	-2.0(1)	0.905	0.904	2.64	1.71	1.807(1)	1.820	0.037
	B(4) -B(7)	0.76(1)	-1.8(1)	0.912	0.911	2.70	1.78	1.822(1)	1.836	0.034
cry	B(1) -B(5)	0.74	-1.9	0.908	0.911	2.72	1.85	1.818	1.830	0.011
	B(1) -B(6)	0.74	-2.0	0.905	0.908	2.69	1.88	1.812	1.824	0.014
	B(2) -B(5)	0.74	-1.9	0.906	0.908	2.71	1.82	1.813	1.825	0.012
	B(2) -B(8)	0.74	-2.0	0.907	0.903	2.70	1.81	1.811	1.822	0.013
	B(3) -B(7)	0.75	-2.1	0.903	0.900	2.67	1.76	1.803	1.814	0.013
	B(3) -B(8)	0.74	-1.9	0.909	0.908	2.71	1.83	1.816	1.828	0.012
	B(4) -B(6)	0.75	-2.0	0.904	0.903	2.69	1.79	1.807	1.818	0.015
	B(4) -B(7)	0.73	-1.8	0.911	0.911	2.74	1.92	1.822	1.834	0.012
gas	B -B	0.74	-1.3	0.910	0.910	3.17	1.53	1.818	1.831	0.040

Table S6: Topological bond descriptors 3: B-B bonds of **3** and **4**

model	example	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	λ_3	ϵ	Rxy [Å]	Rbp [Å]	Δ_{bcp} [Å]
3-*exp*	B(1) -B(3)	0.83(1)	-1.3(1)	0.918	0.818	3.14	10.12	1.734(1)	1.741	0.043
	B(2) -B(4)	0.83(1)	-1.4(1)	0.915	0.816	3.12	10.51	1.729(1)	1.737	0.043
4-*exp*	B(1) -B(2)	0.86(1)	-2.5(1)	0.880	0.871	3.06	2.26	1.749(1)	1.754	0.049
3-*cry*	B(1) -B(3)	0.83	-2.6	0.897	0.840	2.30	3.42	1.734	1.739	0.056
	B(2) -B(4)	0.84	-2.7	0.893	0.839	2.29	3.47	1.729	1.734	0.056
4-*cry*	B(1) -B(2)	0.80	-2.2	0.921	0.831	2.44	3.73	1.749	1.753	0.047
3-*gas*	B(3) -B(5)	0.82	-1.9	0.889	0.847	2.97	3.21	1.733	1.738	0.051
3-*exp*	B(1) -B(5)	0.80(1)	-2.6(1)	0.957	0.942	2.59	2.39	1.861(1)	1.918	0.187
	B(2) -B(6)	0.81(1)	-2.6(1)	0.957	0.943	2.57	2.55	1.860(1)	1.920	0.192
4-*exp*	B(1) -B(3)	0.79(1)	-2.0(1)	0.955	0.939	3.19	1.97	1.863(1)	1.907	0.172
	B(1) -B(4)	0.78(1)	-1.9(1)	0.962	0.939	3.15	2.06	1.867(1)	1.915	0.178
3-*cry*	B(1) -B(5)	0.80	-2.6	0.932	0.957	2.62	1.92	1.861	1.903	0.162
	B(2) -B(6)	0.80	-2.6	0.931	0.958	2.60	2.04	1.860	1.905	0.166
4-*cry*	B(1) -B(3)	0.78	-2.7	0.952	0.940	2.71	1.86	1.863	1.905	0.164
	B(1) -B(4)	0.77	-2.3	0.955	0.943	2.71	1.93	1.867	1.913	0.170
3-*gas*	B(3) -B(7)	0.77	-1.9	0.951	0.930	3.16	1.63	1.853	1.890	0.159
3-*exp*	B(3) -B(5)	0.85(1)	-2.5(1)	0.902	0.859	2.83	3.28	1.758(1)	1.765	0.054
	B(4) -B(6)	0.86(1)	-2.6(1)	0.899	0.856	2.80	3.24	1.751(1)	1.759	0.060
4-*exp*	B(2) -B(3)	0.82(1)	-1.2(1)	0.850	0.919	3.42	4.61	1.762(1)	1.777	0.079
	B(2) -B(4)	0.82(1)	-1.2(1)	0.856	0.916	3.42	4.67	1.764(1)	1.781	0.082
3-*cry*	B(3) -B(5)	0.80	-1.8	0.841	0.920	2.55	6.34	1.758	1.767	0.054
	B(4) -B(6)	0.81	-1.9	0.838	0.917	2.52	6.12	1.751	1.761	0.058
4-*cry*	B(2) -B(3)	0.81	-2.0	0.878	0.887	2.59	4.41	1.762	1.771	0.052
	B(2) -B(4)	0.80	-2.0	0.881	0.886	2.60	4.41	1.764	1.774	0.049
3-*gas*	B(5) -B(7)	0.80	-1.4	0.880	0.874	3.12	3.96	1.751	1.758	0.044
3-*exp*	B(3) -B(7)	0.84(1)	-2.5(1)	0.870	0.890	2.92	2.09	1.759(1)	1.765	0.027
	B(4) -B(7)	0.84(2)	-2.5(1)	0.872	0.893	2.93	2.15	1.763(1)	1.770	0.028
4-*exp*	B(2) -B(5)	0.84(1)	-1.9(1)	0.923	0.843	3.07	2.31	1.764(1)	1.767	0.037
	B(2) -B(5)a	0.84(1)	-1.9(1)	0.922	0.844	3.07	2.33	1.765(1)	1.769	0.039
3-*cry*	B(3) -B(7)	0.82	-2.5	0.905	0.858	2.49	2.52	1.759	1.771	0.061
	B(4) -B(7)	0.82	-2.4	0.908	0.862	2.51	2.58	1.763	1.778	0.068
4-*cry*	B(2) -B(5)	0.82	-2.4	0.902	0.865	2.51	2.77	1.764	1.770	0.049
	B(2) -B(5)a	0.82	-2.4	0.902	0.866	2.50	2.79	1.765	1.771	0.051
3-*gas*	B(5) -B(9)	0.82	-2.0	0.906	0.846	3.02	2.05	1.750	1.756	0.043
3-*exp*	B(5) -B(7)	0.83(1)	-1.9(1)	0.895	0.893	3.20	1.73	1.778(1)	1.795	0.092
	B(6) -B(7)	0.83(2)	-1.9(1)	0.894	0.891	3.19	1.72	1.775(1)	1.793	0.095
4-*exp*	B(3) -B(5)a	0.84(1)	-2.1(1)	0.930	0.857	3.20	1.87	1.783(1)	1.793	0.060
	B(4) -B(5)	0.84(1)	-2.1(1)	0.928	0.862	3.19	1.91	1.786(1)	1.795	0.058
3-*cry*	B(5) -B(7)	0.83	-2.6	0.898	0.885	2.55	1.84	1.778	1.787	0.071
	B(6) -B(7)	0.83	-2.6	0.898	0.883	2.54	1.83	1.775	1.786	0.074
4-*cry*	B(3) -B(5)a	0.82	-2.5	0.906	0.882	2.54	1.93	1.783	1.792	0.070
	B(4) -B(5)	0.82	-2.4	0.907	0.884	2.55	1.95	1.786	1.794	0.068
3-*gas*	B(7) -B(9)	0.80	-1.8	0.903	0.884	3.11	1.61	1.781	1.790	0.071
3-*exp*	B(7) -B(7)a	0.73(2)	-0.5(1)	0.913	0.913	3.07	9.50	1.826(1)	1.828	0.011
4-*exp*	B(5) -B(5)a	0.78(1)	-1.4(1)	0.915	0.915	3.10	3.00	1.825(1)	1.833	0.075
3-*cry*	B(7) -B(7)a	0.75	-1.5	0.914	0.914	2.55	3.90	1.826	1.828	0.021
4-*cry*	B(5) -B(5)a	0.76	-1.4	0.913	0.913	2.57	4.34	1.825	1.828	0.040
3-*gas*	B(9) -B(24)	0.73	-0.9	0.917	0.917	2.90	3.77	1.833	1.836	0.043

Table S7: Topological bond descriptors 4: B-H bonds of **1** and **2**

model	example	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	λ_3	ϵ	Rxy [Å]	Rbp [Å]	Δ_{bcp} [Å]
1-*exp*	B(1) -H(91)	1.17(2)	-8.3(1)	0.524	0.666	7.60	0.01	1.190	1.190	0.012
	B(2) -H(92)	1.20(2)	-9.0(1)	0.524	0.666	7.64	0.01	1.190	1.190	0.005
	B(3) -H(93)	1.19(2)	-10.3(1)	0.534	0.657	5.92	0.01	1.190	1.190	0.016
	B(4) -H(94)	1.19(2)	-7.0(1)	0.515	0.675	9.78	0.01	1.190	1.190	0.012
	B(5) -H(95)	1.19(2)	-8.3(1)	0.522	0.669	8.03	0.00	1.190	1.190	0.016
	B(6) -H(96)	1.22(2)	-8.3(1)	0.518	0.672	8.69	0.01	1.190	1.190	0.010
1-*cry*	B(1) -H(91)	1.14	-3.0	0.504	0.686	12.64	0.01	1.190	1.190	0.007
	B(2) -H(92)	1.15	-3.0	0.503	0.687	12.83	0.01	1.190	1.190	0.013
	B(3) -H(93)	1.14	-3.4	0.505	0.685	12.23	0.00	1.190	1.190	0.015
	B(4) -H(94)	1.13	-3.1	0.505	0.685	12.32	0.01	1.190	1.190	0.007
	B(5) -H(95)	1.14	-3.6	0.505	0.686	12.17	0.01	1.190	1.190	0.020
	B(6) -H(96)	1.15	-3.0	0.503	0.687	12.86	0.01	1.190	1.190	0.004
1-*gas*	B H	1.16	-6.4	0.517	0.683	9.23	0.00	1.200	1.200	0.000
2-*exp*	B(9) -H(9)	1.19(3)	-6.5(1)	0.512	0.678	10.24	0.00	1.190	1.190	0.002
	B(10)-H(10)	1.15(4)	-6.5(1)	0.516	0.674	9.31	0.00	1.190	1.190	0.009
2-*cry*	B(9) -H(209)	1.15	-11.6	0.563	0.627	3.13	0.01	1.190	1.190	0.003
	B(10)-H(210)	1.14	-12.0	0.578	0.612	2.53	0.01	1.190	1.190	0.010
2-*gas*	B -H	1.14	-7.5	0.528	0.672	7.66	0.00	1.200	1.200	0.000
2-*exp*	B(1) -H(1)	1.18(3)	-5.8(1)	0.507	0.683	11.09	0.11	1.190	1.190	0.013
	B(2) -H(2)	1.16(3)	-5.7(1)	0.510	0.681	10.58	0.12	1.190	1.190	0.016
	B(3) -H(3)	1.15(3)	-2.9(1)	0.501	0.689	12.97	0.12	1.190	1.190	0.010
	B(4) -H(4)	1.18(3)	-6.0(1)	0.508	0.682	10.83	0.11	1.190	1.190	0.010
	B(5) -H(5)	1.16(3)	-5.3(1)	0.508	0.683	10.94	0.12	1.190	1.190	0.020
	B(6) -H(6)	1.17(3)	-5.4(1)	0.507	0.683	11.06	0.11	1.190	1.190	0.007
	B(7) -H(7)	1.18(3)	-5.6(1)	0.507	0.683	11.16	0.11	1.190	1.190	0.010
	B(8) -H(8)	1.15(3)	-5.0(1)	0.508	0.682	10.87	0.12	1.190	1.190	0.011
2-*cry*	B(1) -H(110)	1.12	-12.8	0.585	0.606	2.09	0.05	1.190	1.195	0.023
	B(2) -H(200)	1.15	-12.0	0.553	0.637	3.57	0.06	1.190	1.191	0.008
	B(3) -H(201)	1.13	-12.5	0.567	0.623	2.71	0.05	1.190	1.191	0.012
	B(4) -H(202)	1.16	-12.0	0.547	0.644	4.17	0.03	1.190	1.190	0.004
	B(5) -H(203)	1.13	-12.3	0.566	0.625	2.85	0.03	1.190	1.191	0.017
	B(6) -H(204)	1.13	-12.2	0.563	0.627	2.98	0.05	1.190	1.191	0.001
	B(7) -H(207)	1.14	-12.4	0.559	0.631	3.04	0.03	1.190	1.190	0.006
	B(8) -H(208)	1.13	-12.4	0.566	0.625	2.98	0.03	1.190	1.191	0.006
2-*gas*	B -H	1.14	-5.5	0.516	0.688	9.51	0.14	1.204	1.204	0.002

Table S8: Topological bond descriptors 5: B-H bonds of **3** and **4**

model	example	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	λ_3	ϵ	Rxy [Å]	Rbp [Å]	Δ_{bcp} [Å]
3-*exp*	B(1) -H(1)	1.29(1)	-15.8(1)	0.578	0.612	1.82	0.20	1.190	1.190	0.004
	B(2) -H(2)	1.29(1)	-15.8(1)	0.578	0.612	1.83	0.20	1.190	1.190	0.013
4-*exp*	B(1) -H(1)	1.29(1)	-6.7(1)	0.510	0.680	10.53	0.14	1.190	1.190	0.006
3-*cry*	B(1) -H(1)	1.20	-6.1	0.511	0.679	10.24	0.20	1.190	1.191	0.014
	B(2) -H(2)	1.20	-5.6	0.509	0.681	10.80	0.20	1.190	1.190	0.007
4-*cry*	B(1) -H(1)	1.19	-4.8	0.508	0.682	11.37	0.15	1.190	1.190	0.009
3-*gas*	B(3) -H(10)	1.22	-8.1	0.520	0.669	8.64	0.25	1.189	1.189	0.008
3-*exp*	B(3) -H(3)	1.25(1)	-12.9(1)	0.555	0.636	3.29	0.01	1.190	1.190	0.013
	B(4) -H(4)	1.25(1)	-12.9(1)	0.555	0.636	3.29	0.01	1.190	1.190	0.012
4-*exp*	B(2) -H(2)	1.21(1)	-5.7(1)	0.515	0.675	9.75	0.03	1.190	1.190	0.005
3-*cry*	B(3) -H(3)	1.16	-3.7	0.504	0.686	12.52	0.03	1.190	1.190	0.006
	B(4) -H(4)	1.17	-3.2	0.501	0.689	13.38	0.03	1.190	1.190	0.006
4-*cry*	B(2) -H(2)	1.18	-3.9	0.504	0.686	12.41	0.01	1.190	1.190	0.006
3-*gas*	B(5) -H(12)	1.19	-6.2	0.512	0.684	9.83	0.01	1.195	1.196	0.024
3-*exp*	B(5) -H(5)	1.23(2)	-8.5(1)	0.521	0.669	7.93	0.15	1.190	1.190	0.007
	B(6) -H(6)	1.23(2)	-8.5(1)	0.522	0.669	7.86	0.15	1.190	1.190	0.015
4-*exp*	B(3) -H(3)	1.31(1)	-14.9(1)	0.559	0.632	2.44	0.18	1.190	1.190	0.007
	B(4) -H(4)	1.27(1)	-14.9(1)	0.606	0.585	1.58	0.16	1.190	1.191	0.019
3-*cry*	B(5) -H(5)	1.19	-6.3	0.511	0.679	10.09	0.08	1.190	1.190	0.006
	B(6) -H(6)	1.20	-6.3	0.510	0.680	10.31	0.08	1.190	1.190	0.003
4-*cry*	B(3) -H(3)	1.18	-4.7	0.507	0.683	11.75	0.10	1.190	1.190	0.012
	B(4) -H(4)	1.18	-4.8	0.508	0.682	11.57	0.10	1.190	1.190	0.002
3-*gas*	B(7) -H(14)	1.21	-8.4	0.523	0.667	8.34	0.10	1.190	1.190	0.008
3-*exp*	B(7) -H(7)	1.23(3)	-11.2(1)	0.542	0.648	4.88	0.01	1.190	1.190	0.006
4-*exp*	B(5) -H(5)	1.27(1)	-10.0(1)	0.534	0.656	7.12	0.14	1.190	1.190	0.011
3-*cry*	B(7) -H(7)	1.17	-5.2	0.510	0.680	11.01	0.00	1.190	1.190	0.006
4-*cry*	B(5) -H(5)	1.16	-3.4	0.504	0.686	12.57	0.01	1.190	1.190	0.006
3-*gas*	B(9) -H(16)	1.23	-8.4	0.521	0.663	8.72	0.01	1.184	1.184	0.002
3-*exp*	B(5) -H(8)	0.91(1)	-5.6(1)	0.624	0.714	1.97	0.86	1.320	1.345	0.110
	B(6) -H(8)	0.91(1)	-5.5(1)	0.626	0.712	1.99	0.85	1.320	1.345	0.110
4-*exp*	B(3) -H(6)	0.93(1)	-5.3(1)	0.616	0.714	3.68	0.49	1.320	1.343	0.082
	B(4) -H(6)a	0.92(1)	-5.4(1)	0.621	0.709	3.52	0.51	1.320	1.343	0.084
3-*cry*	B(5) -H(8)	0.84	-0.3	0.540	0.799	5.85	1.39	1.320	1.350	0.110
	B(6) -H(8)	0.83	-0.7	0.544	0.797	5.32	1.48	1.320	1.354	0.116
4-*cry*	B(3) -H(6)	0.83	-1.5	0.555	0.796	4.48	1.48	1.320	1.358	0.140
	B(4) -H(6)a	0.83	-1.5	0.555	0.795	4.46	1.45	1.320	1.358	0.140
3-*gas*	B(7) -H(17)	0.85	-2.4	0.566	0.767	4.17	1.03	1.317	1.346	0.101

Table S9: Topological bond descriptors 6: remaining bonds of **3** and **4**

model	example	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	λ_3	ϵ	Rxy [Å]
3-*exp*	N(1) -B(1)	1.02	1.9	1.095	0.495	16.19	0.18	1.589(1)
	N(2) -B(2)	1.01	1.3	1.101	0.497	15.44	0.19	1.597(1)
4-*exp*	N(1) -B(1)	1.08(1)	3.1(1)	1.031	0.495	17.90	0.07	1.526(1)
3-*cry*	N(1) -B(1)	0.89	6.3	1.093	0.497	17.17	0.05	1.589
	N(2) -B(2)	0.88	5.8	1.099	0.499	16.37	0.06	1.597
4-*cry*	N(1) -B(1)	0.93	9.0	1.036	0.490	20.72	0.00	1.526
3-*gas*	N(2) -B(4)	0.87	1.5	1.103	0.516	11.42	0.08	1.618
4-*exp*	N(1) -C(1)	3.64(1)	-37.8(1)	0.717	0.431	21.62	0.00	1.149
4-*cry*	N(1) -C(1)	3.25	-27.0	0.719	0.429	24.28	0.00	1.149
4-*exp*	C(1) -C(2)	1.93(1)	-14.6(1)	0.753	0.692	12.68	0.00	1.446(1)
4-*cry*	C(1) -C(2)	1.79	-13.0	0.778	0.668	11.40	0.00	1.446
3-*exp*	N(1) -H(9)	2.66	-77.7	0.845	0.192	28.49	0.17	1.009
	N(1) -H(11)	2.67	-81.1	0.847	0.188	27.48	0.17	1.009
	N(1) -H(9)a	2.70	-79.6	0.845	0.191	28.21	0.16	1.009
	N(2) -H(10)	2.67	-78.0	0.845	0.192	28.57	0.17	1.009
	N(2) -H(12)	2.42	-68.2	0.844	0.198	29.29	0.19	1.009
	N(2) -H(10)a	2.22	-57.0	0.844	0.208	31.28	0.18	1.009
3-*cry*	N(1) -H(9)	2.35	-37.9	0.740	0.269	25.30	0.02	1.009
	N(1) -H(11)	2.39	-38.1	0.736	0.273	25.45	0.02	1.009
	N(1) -H(9)a	2.35	-37.8	0.740	0.269	25.31	0.02	1.009
	N(2) -H(10)	2.36	-36.8	0.736	0.273	25.81	0.02	1.009
	N(2) -H(12)	2.38	-37.2	0.734	0.275	25.58	0.03	1.009
	N(2) -H(10)a	2.37	-37.2	0.736	0.273	25.75	0.02	1.009
3-*gas*	N(1) -H(18)	2.32	-34.3	0.733	0.286	25.84	0.02	1.019
	N(1) -H(20)	2.31	-32.1	0.730	0.287	26.48	0.02	1.017
4-*exp*	C(2) -H(21)	1.86(1)	-19.0(1)	0.728	0.365	14.43	0.10	1.092
	C(2) -H(22)	1.78(1)	-16.7(1)	0.735	0.357	14.58	0.11	1.092
	C(2) -H(23)	2.00(1)	-24.0(1)	0.717	0.375	14.11	0.09	1.092
4-*cry*	C(2) -H(21)	1.87	-21.2	0.698	0.394	14.26	0.03	1.092
	C(2) -H(22)	1.89	-22.6	0.701	0.391	13.95	0.03	1.092
	C(2) -H(23)	1.89	-22.2	0.701	0.392	14.03	0.03	1.092

Table S10: Topological bond descriptors 7: standard modelling of **3**

bond	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	λ_3	ϵ	Rxy [Å]
B(1)-B(3)	0.81(1)	-1.6(1)	0.885	0.849	2.77	10.31	1.734
B(1)-B(5)	0.80(1)	-2.7(1)	0.963	0.935	2.48	2.19	1.899
B(1)-B(5)a	0.80(1)	-2.7(1)	0.964	0.935	2.48	2.22	1.900
B(2)-B(4)	0.82(1)	-1.6(1)	0.881	0.850	2.76	10.75	1.731
B(2)-B(6)	0.81(1)	-2.7(1)	0.961	0.938	2.47	2.28	1.899
B(3)-B(5)	0.84(1)	-2.5(1)	0.865	0.895	2.58	3.82	1.761
B(3)-B(7)	0.83(1)	-2.6(1)	0.894	0.871	2.61	2.16	1.764
B(2)-B(6)a	0.81(1)	-2.7(1)	0.962	0.938	2.47	2.31	1.900
B(3)-B(5)a	0.84(1)	-2.5(1)	0.866	0.895	2.58	3.83	1.761
B(3)-B(7)a	0.83(1)	-2.6(1)	0.894	0.871	2.61	2.16	1.764
B(4)-B(6)	0.84(1)	-2.5(1)	0.862	0.893	2.57	3.71	1.754
B(4)-B(7)	0.83(1)	-2.5(1)	0.897	0.873	2.63	2.22	1.771
B(4)-B(6)a	0.84(1)	-2.5(1)	0.862	0.893	2.56	3.72	1.754
B(4)-B(7)a	0.83(1)	-2.5(1)	0.897	0.873	2.63	2.22	1.771
B(5)-B(7)	0.82(1)	-2.2(1)	0.885	0.901	2.80	2.03	1.786
B(6)-B(7)	0.83(1)	-2.2(1)	0.887	0.898	2.81	2.02	1.785
B(7)-B(7)a	0.74(1)	-1.4(1)	0.913	0.913	2.74	3.66	1.827
B(5)a-B(7)a	0.82(1)	-2.2(1)	0.885	0.901	2.80	2.03	1.786
B(6)a-B(7)a	0.83(1)	-2.2(1)	0.887	0.898	2.81	2.02	1.785
B(1)-H(1)	1.26(1)	-10.7(1)	0.523	0.667	6.80	0.20	1.190
B(2)-H(2)	1.24(1)	-11.6(1)	0.532	0.659	5.47	0.20	1.190
B(3)-H(3)	1.24(1)	-14.6(1)	0.604	0.587	1.55	0.01	1.190
B(4)-H(4)	1.26(1)	-15.2(1)	0.610	0.581	1.31	0.00	1.190
B(5)-H(5)	1.23(1)	-14.0(1)	0.596	0.595	1.84	0.13	1.190
B(5)-H(8)	0.91(1)	-6.5(1)	0.623	0.715	1.28	0.93	1.339
B(6)-H(6)	1.27(1)	-13.9(1)	0.561	0.630	2.59	0.14	1.190
B(6)-H(8)	0.92(1)	-6.7(1)	0.624	0.714	1.25	0.86	1.338
B(7)-H(7)	1.23(1)	-13.4(1)	0.639	0.551	2.48	0.00	1.190
B(5)a-H(5)a	1.23(1)	-14.0(1)	0.596	0.595	1.84	0.13	1.190
B(5)a-H(8)a	0.91(1)	-6.5(1)	0.623	0.715	1.28	0.93	1.339
B(6)a-H(6)a	1.27(1)	-13.9(1)	0.561	0.630	2.59	0.14	1.190
B(6)a-H(8)a	0.92(1)	-6.7(1)	0.624	0.714	1.25	0.86	1.338
B(7)a-H(7)a	1.23(1)	-13.4(1)	0.639	0.551	2.48	0.00	1.190
N(1)-B(1)	0.97(1)	6.3(1)	1.101	0.490	18.99	0.17	1.591
N(2)-B(2)	0.96(1)	5.8(1)	1.106	0.492	18.30	0.18	1.598
N(1)-H(9)	2.79(1)	-71.0(7)	0.799	0.230	25.22	0.14	1.029
N(1)-H(11)	2.92(1)	-77.4(5)	0.794	0.233	24.27	0.14	1.027
N(1)-H(9)a	2.82(1)	-72.6(2)	0.799	0.229	24.99	0.14	1.028
N(2)-H(10)	2.92(1)	-70.2(7)	0.786	0.245	25.08	0.15	1.031
N(2)-H(12)	2.85(1)	-62.0(5)	0.773	0.264	26.99	0.17	1.037
N(2)-H(10)a	2.57(1)	-54.9(2)	0.784	0.257	27.79	0.14	1.041

Table S11: Topological descriptors of ring and cage critical points 1: **1** and **2**

model	atoms	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	d_3 [Å]	λ_1 [eÅ^{-5}]	λ_2 [eÅ^{-5}]	λ_3 [eÅ^{-5}]
1-*exp*	B(1) B(4) B(5)	0.73	-0.3	1.030	1.036	1.025	-3.31	1.45	1.55
	B(1) B(4) B(6)	0.73	-0.3	1.029	1.037	1.028	-3.31	1.45	1.57
	B(2) B(3) B(4)	0.73	-0.2	1.031	1.035	1.025	-3.32	1.50	1.58
	B(2) B(4) B(6)	0.73	-0.3	1.032	1.043	1.024	-3.33	1.42	1.57
	B(3) B(4) B(5)	0.73	-0.4	1.033	1.046	1.017	-3.33	1.38	1.60
	B(1)a B(2) B(3)	0.73	-0.3	1.021	1.037	1.036	-3.35	1.47	1.56
	B(1) B(2)a B(5)	0.73	-0.3	1.031	1.029	1.032	-3.34	1.44	1.58
	B(1) B(3)a B(6)	0.73	-0.3	1.028	1.030	1.036	-3.34	1.43	1.60
	B(2) B(5)a B(6)	0.73	-0.3	1.034	1.027	1.035	-3.34	1.44	1.60
	B(3) B(5) B(6)a	0.73	-0.3	1.033	1.029	1.032	-3.34	1.41	1.62
1-*cry*	B(1) B(4) B(5)	0.74	-0.5	1.031	1.035	1.025	-3.25	1.34	1.45
	B(1) B(4) B(6)	0.74	-0.4	1.032	1.039	1.025	-3.24	1.32	1.47
	B(2) B(3) B(4)	0.74	-0.5	1.025	1.029	1.037	-3.27	1.34	1.42
	B(2) B(4) B(6)	0.73	-0.4	1.031	1.037	1.030	-3.22	1.35	1.45
	B(3) B(4) B(5)	0.74	-0.5	1.029	1.038	1.027	-3.24	1.32	1.47
	B(1)a B(2) B(3)	0.74	-0.5	1.033	1.031	1.029	-3.24	1.36	1.40
	B(1) B(2)a B(5)	0.74	-0.5	1.028	1.036	1.030	-3.24	1.37	1.39
	B(1) B(3)a B(6)	0.74	-0.5	1.027	1.039	1.030	-3.23	1.35	1.41
	B(2) B(5)a B(6)	0.74	-0.5	1.027	1.042	1.028	-3.24	1.35	1.42
	B(3) B(5) B(6)a	0.74	-0.5	1.026	1.029	1.041	-3.24	1.33	1.43
1-*gas*	B B B	0.72	0.1	1.030	1.030	1.030	-3.13	1.59	1.61
2-*exp*	B(1) B(4) B(6)	0.69	-0.1	1.008	1.010	1.132	-2.95	1.06	1.84
	B(6) B(7) B(4)	0.68	0.0	1.014	1.009	1.146	-2.89	1.03	1.89
	B(4) B(3) B(7)	0.68	0.0	1.010	1.009	1.152	-2.88	1.01	1.90
	B(7) B(8) B(3)	0.68	0.0	1.015	1.005	1.141	-2.89	1.02	1.87
	B(3) B(2) B(8)	0.67	0.0	1.007	1.015	1.149	-2.86	1.00	1.88
	B(8) B(5) B(2)	0.68	0.0	1.009	1.011	1.145	-2.90	1.03	1.87
	B(2) B(1) B(5)	0.68	0.0	1.013	1.013	1.142	-2.89	1.04	1.87
	B(5) B(6) B(1)	0.68	0.0	1.010	1.013	1.147	-2.89	1.03	1.88
2-*cry*	B(1) B(4) B(6)	0.66	0.1	1.014	1.021	1.117	-2.98	1.25	1.78
	B(6) B(7) B(4)	0.65	0.1	1.025	1.017	1.127	-2.92	1.23	1.83
	B(4) B(3) B(7)	0.65	0.1	1.018	1.023	1.129	-2.91	1.21	1.84
	B(7) B(8) B(3)	0.65	0.1	1.019	1.017	1.126	-2.95	1.22	1.82
	B(3) B(2) B(8)	0.65	0.1	1.020	1.020	1.130	-2.92	1.21	1.84
	B(8) B(5) B(2)	0.65	0.1	1.018	1.019	1.127	-2.93	1.23	1.81
	B(2) B(1) B(5)	0.65	0.1	1.021	1.020	1.129	-2.91	1.23	1.81
	B(5) B(6) B(1)	0.65	0.1	1.021	1.022	1.127	-2.91	1.22	1.82
2-*gas*	$B_{cenA}B_{cenA}B_{cenB}$	0.65	0.5	1.020	1.020	1.129	-2.71	1.28	1.96
1-*exp*	cage	0.08	2.0	3.398	1.699	1.699	0.66	0.67	0.68
1-*cry*	cage	0.07	2.2	3.398	1.699	1.699	0.71	0.72	0.73
1-*gas*	cage	0.11	1.9	3.391	1.696	1.696	0.64	0.64	0.64
2-*exp*	cage	0.18	3.0	3.717	1.861	1.856	0.45	1.29	1.31
2-*cry*	cage	0.14	3.1	3.717	1.859	1.858	0.62	1.21	1.22
2-*gas*	cage	0.19	2.9	3.711	1.855	1.855	0.52	1.21	1.21

Table S12: Topological descriptors of ring and cage critical points 2: **3** and **4**

model	atoms	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	d_3 [Å]	λ_1 [eÅ^{-5}]	λ_2 [eÅ^{-5}]	λ_3 [eÅ^{-5}]
3-*exp*	B(1) B(3) B(5)	0.79	-1.2	1.026	1.024	1.046	-3.85	0.98	1.68
	B(1) B(3) B(5)a	0.79	-1.2	1.028	1.026	1.043	-3.82	0.98	1.66
	B(2) B(4) B(6)	0.80	-1.2	1.021	1.025	1.044	-3.88	0.95	1.69
	B(2) B(4) B(6)a	0.80	-1.2	1.023	1.026	1.041	-3.85	0.95	1.67
4-*exp*	B(1) B(2) B(3)	0.77	-0.5	1.067	1.010	1.028	-3.60	1.21	1.92
	B(1) B(2) B(4)	0.76	-0.4	1.070	1.017	1.023	-3.56	1.16	1.95
3-*cry*	B(1) B(3) B(5)	0.77	-1.0	1.066	0.977	1.049	-3.58	1.03	1.53
	B(1) B(3) B(5)a	0.77	-1.0	1.066	0.977	1.049	-3.58	1.03	1.53
	B(2) B(4) B(6)	0.78	-1.1	1.058	0.980	1.047	-3.61	1.05	1.51
	B(2) B(4) B(6)a	0.78	-1.1	1.058	0.980	1.047	-3.62	1.05	1.51
4-*cry*	B(1) B(2) B(3)	0.77	-0.9	1.095	0.960	1.048	-3.54	1.08	1.53
	B(1) B(2) B(4)	0.74	-0.9	1.037	1.023	1.050	-3.41	1.07	1.47
3-*gas*	B0-B2-B1	0.75	-0.4	1.054	1.006	1.024	-3.40	1.35	1.63
3-*exp*	B(3) B(5) B(7)	0.78	-0.2	0.999	1.027	1.032	-3.57	1.65	1.71
	B(4) B(6) B(7)	0.78	-0.2	0.997	1.029	1.029	-3.58	1.66	1.69
4-*exp*	B(2) B(3) B(5)a	0.79	-0.3	1.011	1.059	0.997	-3.44	1.31	1.86
	B(2) B(4) B(5)	0.78	-0.3	1.014	1.055	1.001	-3.43	1.28	1.88
3-*cry*	B(3) B(5) B(7)	0.77	-0.7	0.980	1.008	1.074	-3.49	0.96	1.83
	B(4) B(6) B(7)	0.77	-0.7	0.981	1.011	1.065	-3.50	1.00	1.77
4-*cry*	B(2) B(3) B(5)a	0.77	-0.7	0.998	1.017	1.052	-3.47	1.03	1.71
	B(2) B(4) B(5)	0.77	-0.7	1.000	1.011	1.059	-3.45	0.98	1.74
3-*gas*	B2-B1-B3	0.75	-0.1	1.017	0.995	1.039	-3.27	1.29	1.92
3-*exp*	B(3) B(7) B(7)a	0.72	-0.2	1.186	0.968	0.968	-3.33	0.57	2.60
	B(4) B(7) B(7)a	0.72	-0.2	1.185	0.971	0.971	-3.34	0.57	2.59
4-*exp*	B(2) B(5) B(5)a	0.75	-0.2	1.084	1.006	1.008	-3.42	1.37	1.88
3-*cry*	B(3) B(7) B(7)a	0.72	-0.3	1.096	1.001	1.001	-3.23	1.13	1.81
	B(4) B(7) B(7)a	0.72	-0.3	1.096	1.004	1.004	-3.21	1.16	1.80
4-*cry*	B(2) B(5) B(5)a	0.73	-0.4	1.107	0.998	0.999	-3.23	1.00	1.80
3-*gas*	B2-B3-B3	0.71	0.1	1.118	0.989	0.989	-3.08	1.09	2.07
3-*exp*	B(5) B(6) B(7)	0.67	0.7	0.995	0.996	1.167	-2.98	1.24	2.44
4-*exp*	B(4) B(3)a B(5)	0.69	0.8	0.981	0.984	1.222	-3.13	0.92	3.06
3-*cry*	B(5) B(6) B(7)	0.68	0.1	0.988	0.987	1.193	-3.03	0.68	2.44
4-*cry*	B(4) B(3)a B(5)	0.67	0.1	0.976	0.982	1.232	-3.02	0.65	2.45
3-*gas*	B1-B1-B3	0.65	0.7	0.991	0.991	1.189	-2.76	0.88	2.57
3-*exp*	cage	0.04	1.0	3.492	1.748	1.744	0.07	0.44	0.49
4-*exp*	cage	0.03	1.0	3.335	1.668	1.668	0.11	0.28	0.56
3-*cry*	cage	0.04	0.8	3.408	1.701	1.707	0.06	0.32	0.46
4-*cry*	cage	0.04	0.9	3.328	1.664	1.664	0.08	0.23	0.62
3-*gas*	cage	0.05	0.8	3.310	1.655	1.655	0.08	0.16	0.58

Table S13: Source Function contributions in free $B_{12}H_{12}^{2-}$, model **1**-*gas*

atom	B(1)-B(2) [eÅ^{-3}] (%)	B(1)-H(13) [eÅ^{-3}] (%)	B(1)-B(2)-B(3) [eÅ^{-3}] (%)
B(1)	0.186(23.9)	0.373(32.2)	0.124(17.2)
B(2)	0.184(23.6)	0.012	0.121(16.8)
B(3)	0.034(5.1)	0.012	0.121(16.8)
B(4)	0.016(2.0)	0.007	0.021(2.9)
B(5)	0.017(2.2)	0.015(1.3)	0.022(3.1)
B(6)	0.017(2.2)	0.016(1.4)	0.014(2.0)
B(7)	0.042(5.4)	0.015(1.3)	0.022 3.1)
B(8)	0.011	0.008	0.014(1.9)
B(9)	0.007	0.007	0.008
B(10)	0.009	0.007	0.008
B(11)	0.017(2.2)	0.008	0.014(1.9)
B(12)	0.010	0.007	0.010
H(13)	0.052(6.7)	0.545(47.0)	0.044(6.1)
H(14)	0.052(6.7)	0.014	0.043(6.0)
H(15)	0.025(3.2)	0.014	0.043(6.0)
H(16)	0.014(1.9)	0.007	0.017(2.4)
H(17)	0.014(1.9)	0.014	0.017(2.4)
H(18)	0.014(1.9)	0.014	0.013(1.8)
H(19)	0.025(3.2)	0.014	0.017(2.4)
H(20)	0.011	0.007	0.013(1.8)
H(21)	0.009	0.007	0.010
H(22)	0.011	0.007	0.010
H(23)	0.014(1.9)	0.007	0.013(1.8)
H(24)	0.009	0.006	0.010
sum	0.808208(103.6)	1.147262(98.9)	0.748184(103.9)

Table S14: Source Function contributions in free $B_{10}H_{10}^{2-}$, model **2**-*gas*

atom	B(1)-B(10) [eÅ^{-3}] (%)	B(1)-B(5) [eÅ^{-3}] (%)	B(1)-H(11) [eÅ^{-3}] (%)	B(10)-H(20) [eÅ^{-3}] (%)	B(1)-B(2)-B(5) [eÅ^{-3}] (%)	B(1)-B(2)† [eÅ^{-3}] (%)
B(1)	0.240(26.9)	0.167(22.5)	0.381(33.4)	0.018(1.5)	0.099(15.2)	0.140(19.7)
B(2)	0.044(4.9)	0.028(3.8)	0.011	0.018	0.099(15.2)	0.140(19.7)
B(3)	0.022(2.5)	0.007	0.007	0.018	0.011	0.016
B(4)	0.044(4.9)	0.011	0.011	0.018	0.011	0.016
B(5)	0.015	0.176(23.8)	0.012	0.007	0.094(14.5)	0.038(5.3)
B(6)	0.011	0.016	0.008	0.007	0.019(2.9)	0.016
B(7)	0.011	0.012	0.008	0.007	0.011	0.010
B(8)	0.015	0.035(4.7)	0.012	0.007	0.019(2.9)	0.016
B(9)	0.005	0.010	0.005	0.005	0.005	-0.014
B(10)	0.249(28.0)	0.032(4.3)	0.026(2.3)	0.368(32.3)	0.041(6.4)	0.064(9.0)
H(11)	0.054(6.1)	0.051(6.9)	0.582(51.0)	0.014(1.3)	0.043(6.6)	0.048(6.7)
H(12)	0.025(2.8)	0.024(3.2)	0.013	0.014	0.043(6.6)	0.048(6.7)
H(13)	0.017	0.012	0.008	0.014	0.015	0.016
H(14)	0.025(2.8)	0.015	0.013	0.014	0.015	0.016
H(15)	0.014	0.051(6.9)	0.014	0.007	0.040(6.1)	0.025(3.5)
H(16)	0.011	0.015	0.008	0.007	0.017(2.6)	0.015
H(17)	0.015	0.012	0.008	0.007	0.012	0.011
H(18)	0.014	0.024(3.2)	0.014	0.007	0.017(2.6)	0.015
H(19)	0.008	0.015	0.008	0.005	0.013	0.010
H(20)	0.052(5.9)	0.015	0.016	0.522(45.8)	0.019(2.9)	0.027(3.8)
sum	0.888(99.8)	0.728(98.4)	1.165(102.2)	1.131(99.2)	0.639(98.3)	0.671(94.4)

† For B(1)-B(2) no bcp is found, therefore the midpoint between B(1) and B(2) was chosen as reference point in the calculation of the Source Function.

Table S15: Source Function contributions in free bis-amino-*arachno*-borane 1, model *gas*: B-B

atom	B(3)-B(7) [eÅ^{-3}] (%)	B(3)-B(5) [eÅ^{-3}] (%)	B(5)-B(7) [eÅ^{-3}] (%)	B(7)-B(9) [eÅ^{-3}] (%)	B(5)-B(9) [eÅ^{-3}] (%)	B(9)-B(24) [eÅ^{-3}] (%)	B(7)-B(8)† [eÅ^{-3}] (%)
B(3)	0.194(25.2)	0.215(26.2)	0.048(6.0)	0.015	0.017	0.009	0.007
B(4)	0.002	0.002	0.003	0.006	0.006	0.009	0.007
B(5)	0.060(7.7)	0.192(23.4)	0.186(23.2)	0.054(6.7)	0.205(25.0)	0.053(7.2)	0.018(2.6)
B(6)	0.008	0.009	0.011	0.018	0.020	0.053(7.2)	0.018(2.6)
B(7)	0.181(23.5)	0.034(4.1)	0.190(23.7)	0.183(22.9)	0.040(4.9)	0.010	0.087(12.5)
B(8)	0.001	-0.000	0.004	0.020	0.009	0.010	0.087(12.5)
B(9)	0.019	0.017	0.044(5.5)	0.196(24.5)	0.204(24.9)	0.151(20.7)	0.046(6.2)
B(22)	0.007	0.034	0.009	0.003	0.010	0.010	-0.000
B(23)	-0.002	-0.000	-0.000	0.001	0.003	0.010	-0.000
B(24)	0.011	0.017	0.016	0.016	0.035(4.3)	0.151(20.7)	0.010
H(10)	0.050(6.5)	0.047(5.7)	0.025(3.1)	0.013	0.013	0.009	0.009
H(11)	0.001	0.002	0.004	0.006	0.006	0.009	0.009
H(12)	0.033(4.2)	0.060(7.3)	0.054(6.8)	0.027(3.4)	0.050(6.1)	0.026(3.5)	0.015(2.1)
H(13)	0.009	0.009	0.011	0.014	0.015	0.026(3.5)	0.015(2.1)
H(14)	0.051(6.6)	0.025(3.0)	0.053(6.6)	0.053(6.6)	0.026(3.2)	0.015	0.051(7.4)
H(15)	0.013	0.010	0.014	0.023	0.015	0.015	0.051(7.4)
H(16)	0.015	0.015	0.026(3.2)	0.054(6.8)	0.057(6.9)	0.053(7.2)	0.026(3.8)
H(17)	0.024(3.1)	0.010(1.2)	0.025(3.1)	0.037(4.6)	0.017(2.1)	0.011(1.5)	0.184(26.7)
H(25)	0.015	0.025	0.015	0.011	0.014	0.015	0.009
H(26)	0.009	0.010	0.009	0.009	0.011	0.015	0.009
H(27)	0.011	0.015	0.015	0.015	0.025	0.053(7.2)	0.011(1.5)
H(28)	0.004	0.010	0.006	0.005	0.008	0.011	0.002
N(1)	0.016	0.020	0.006	0.003	0.003	0.002	0.003
N(2)	0.002	0.002	0.002	0.002	0.002	0.002	0.003
H(18)	0.010	0.010	0.004	0.002	0.001	0.001	0.003
H(19)	0.002	0.002	0.002	0.002	0.001	0.001	0.003
H(20)	0.011	0.013	0.007	0.004	0.005	0.004	0.003
H(21)	0.002	0.002	0.002	0.003	0.003	0.004	0.003
H(29)	0.012	0.013	0.009	0.006	0.006	0.004	0.005
H(30)	0.003	0.002	0.003	0.004	0.003	0.004	0.005
sum	0.772(100.3)	0.819(99.9)	0.802(100.2)	0.804(100.5)	0.830(101.3)	0.740(101.4)	0.691(100.1)

† For B(7)-B(8) no bcp is found, therefore the midpoint between B(7) and B(8) was chosen as reference point in the calculation of the Source Function.

Table S16: Source Function contributions in free bis-amino-*arachno*-borane 2, model *gas*: B-N and B-H

atom	B(3)-N(1) [eÅ^{-3}] (%)	B(3)-H(10) [eÅ^{-3}] (%)	B(7)-H(14) [eÅ^{-3}] (%)	B(5)-H(12) [eÅ^{-3}] (%)	B(9)-H(16) [eÅ^{-3}] (%)	B(7)-H(17) [eÅ^{-3}] (%)
B(3)	0.229(26.4)	0.415(34.0)	0.011	0.021(1.7)	0.006	0.012
B(4)	0.001	0.001	0.003	0.002	0.006	0.003
B(5)	0.020	0.019	0.018	0.391(32.9)	0.020	0.020(2.3)
B(6)	0.007	0.007	0.009	0.010	0.020(1.6)	0.012
B(7)	0.006	0.003	0.410(33.9)	0.011	0.008(1.6)	0.227(26.7)
B(8)	-0.001	-0.002	0.003	0.001	0.008	0.021(2.4)
B(9)	0.008	0.008	0.015	0.016	0.423(34.4)	0.026(3.0)
B(22)	0.006	0.003	0.001	0.011	0.003	0.000
B(23)	-0.001	-0.002	-0.000	0.001	0.003	-0.001
B(24)	0.008	0.008	0.007	0.016	0.012	0.009
H(10)	0.094(10.8)	0.584(47.9)	0.013	0.017	0.006	0.013
H(11)	-0.002	-0.004	0.002	0.003	0.006	0.004
H(12)	0.016	0.014	0.013	0.604(50.7)	0.013	0.015
H(13)	0.006	0.007	0.007	0.008	0.013	0.011
H(14)	0.014	0.016	0.601(49.6)	0.015	0.014	0.08710.2)
H(15)	0.007	0.009	0.013	0.008	0.014	0.028(3.3)
H(16)	0.008	0.008	0.014	0.015	0.621(50.5)	0.019
H(17)	0.003	-0.001	0.037(3.1)	0.008	0.013	0.279(32.8)
H(25)	0.014	0.016	0.007	0.015	0.007	0.009
H(26)	0.007	0.009	0.006	0.008	0.007	0.008
H(27)	0.008	0.008	0.007	0.015	0.013	0.009
H(28)	0.003	-0.001	0.002	0.008	0.005	0.001
N(1)	0.310(35.7)	0.039(3.2)	-0.000	0.003	0.001	0.003
N(2)	0.001	0.002	0.001	0.001	0.001	0.002
H(18)	0.033(3.8)	0.015	0.004	-0.001	0.000	0.004
H(19)	0.002	0.003	0.002	0.001	0.000	0.003
H(20)	0.034(3.9)	0.015	0.003	0.009	0.003	0.003
H(21)	0.002	0.002	0.001	0.002	0.003	0.002
H(29)	0.034(3.9)	0.015	0.007	0.009	0.004	0.006
H(30)	0.002	0.002	0.003	0.002	0.004	0.004
sum	0.879(101.2)	1.218(99.8)	1.222(101.0)	1.229(103.3)	1.258(102.3)	0.841(98.9)

Table S17: Source Function contributions in free bis-amino-*arachno*-borane 3, model *gas*: rcp and ccp

atom	B(3)-B(5)-B(7) [eÅ^{-3}] (%)	B(7)-B(8)-B(9) [eÅ^{-3}] (%)	B(5)-B(7)-B(9) [eÅ^{-3}] (%)	B(5)-B(9)-B(24) [eÅ^{-3}] (%)	ccp [eÅ^{-3}] (%)
B(3)	0.144(19.2)	0.008	0.023	0.013	-0.017
B(4)	0.002	0.008	0.005	0.007	-0.017
B(5)	0.126(16.8)	0.022	0.135(18.0)	0.111(15.7)	0.005
B(6)	0.009	0.022	0.016	0.031	0.005
B(7)	0.134(17.8)	0.081(12.4)	0.134(17.9)	0.014	-0.017
B(8)	0.001	0.081(12.4)	0.010	0.007	-0.017
B(9)	0.023	0.079(12.1)	0.124(16.6)	0.123(17.3)	0.009
B(22)	0.012	0.001	0.007	0.014	-0.017
B(23)	-0.001	0.001	0.001	0.007	-0.017
B(24)	0.014	0.012	0.019	0.123(17.3)	0.009
H(10)	0.041(5.5)	0.009	0.016	0.011	-0.006
H(11)	0.002	0.009	0.005	0.007	-0.006
H(12)	0.048(6.3)	0.016	0.044(5.9)	0.038(5.3)	0.015
H(13)	0.010	0.016	0.013	0.019	0.015
H(14)	0.044(5.9)	0.047(7.2)	0.046(6.1)	0.017	0.018
H(15)	0.012	0.047(7.2)	0.017	0.013	0.018
H(16)	0.018	0.037(5.7)	0.044(5.9)	0.048(6.7)	0.013
H(17)	0.020(2.7)	0.087(13.3)	0.026(3.5)	0.011	-0.008
H(25)	0.017	0.009	0.013	0.017	0.018
H(26)	0.009	0.009	0.010	0.013	0.018
H(27)	0.013	0.012	0.017	0.048(6.7)	0.013
H(28)	0.005	0.003	0.006	0.011	-0.008
N(1)	0.013	0.002	0.004	0.003	0.006
N(2)	0.002	0.002	0.002	0.002	0.006
H(18)	0.008	0.003	0.002	0.001	0.005
H(19)	0.002	0.003	0.002	0.001	0.005
H(20)	0.010	0.003	0.005	0.005	0.005
H(21)	0.002	0.003	0.003	0.003	0.005
H(29)	0.011	0.005	0.007	0.005	0.005
H(30)	0.003	0.005	0.003	0.003	0.005
sum	0.753(100.5)	0.641(98.6)	0.757(101.0)	0.727(102.4)	0.066(132.6)

Table S18: ELI of free $B_{12}H_{12}^{2-}$, model **1**-*gas*

no.	V_{001} [Å^3]	ELI-D$_{pop}$ [e]	max	basin	Δ_{ELI-D} [Å]
1	0.24	2.07	13.46	C(B12)	-
2	0.24	2.07	13.46	C(B1)	-
3	0.25	2.08	14.76	C(B7)	-
4	0.25	2.08	13.23	C(B11)	-
5	0.25	2.08	15.01	C(B10)	-
6	0.25	2.08	14.77	C(B4)	-
7	0.25	2.08	13.25	C(B6)	-
8	0.25	2.08	14.17	C(B3)	-
9	0.25	2.08	13.93	C(B8)	-
10	0.25	2.08	16.48	C(B5)	-
11	0.25	2.08	13.92	C(B2)	-
12	0.25	2.08	15.30	C(B9)	-
13	1.91	0.80	1.52	V_2(B12,B10)	0.097
14	1.91	0.80	1.51	V_2(B6,B10)	0.085
15	1.92	0.80	1.51	V_2(B2,B1)	0.106
16	1.92	0.81	1.52	V_2(B6,B1)	0.104
17	1.92	0.81	1.51	V_2(B9,B8)	0.129
18	1.92	0.81	1.51	V_2(B7,B6)	0.116
19	1.92	0.81	1.52	V_2(B4,B2)	0.111
20	1.92	0.81	1.52	V_2(B3,B5)	0.112
21	1.92	0.81	1.52	V_2(B2,B11)	0.119
22	1.92	0.81	1.51	V_2(B10,B11)	0.105
23	1.92	0.81	1.51	V_2(B11,B7)	0.093
24	1.92	0.81	1.51	V_2(B8,B4)	0.103
25	1.92	0.81	1.52	V_2(B2,B7)	0.102
26	1.92	0.81	1.51	V_2(B3,B2)	0.102
27	1.92	0.81	1.51	V_2(B8,B5)	0.119
28	1.92	0.81	1.51	V_2(B9,B10)	0.115
29	1.92	0.81	1.51	V_2(B4,B11)	0.115
30	1.92	0.81	1.52	V_2(B11,B12)	0.103
31	1.92	0.81	1.52	V_2(B6,B5)	0.110
32	1.92	0.81	1.52	V_2(B5,B9)	0.093
33	1.93	0.81	1.52	V_2(B5,B1)	0.099
34	1.93	0.81	1.52	V_2(B7,B10)	0.104
35	1.93	0.81	1.52	V_2(B12,B8)	0.096
36	1.93	0.81	1.52	V_2(B7,B1)	0.102
37	1.93	0.81	1.52	V_2(B3,B8)	0.109
38	1.93	0.81	1.52	V_2(B12,B4)	0.097
39	1.93	0.81	1.52	V_2(B3,B1)	0.100
40	1.94	0.81	1.51	V_2(B9,B6)	0.094
41	1.94	0.81	1.52	V_2(B3,B4)	0.118
42	1.94	0.81	1.52	V_2(B9,B12)	0.105
43	15.46	2.02	8.31	V_1(B2,H14)	-
44	15.47	2.02	8.16	V_1(B12,H24)	-
45	15.47	2.02	8.16	V_1(B1,H13)	-
46	15.47	2.02	8.19	V_1(B4,H16)	-
47	15.47	2.02	8.24	V_1(B10,H22)	-
48	15.47	2.02	8.31	V_1(B11,H23)	-
49	15.47	2.02	8.26	V_1(B7,H19)	-
50	15.47	2.02	8.23	V_1(B6,H18)	-
51	15.47	2.02	8.19	V_1(B9,H21)	-
52	15.47	2.02	8.29	V_1(B8,H20)	-
53	15.48	2.02	8.26	V_1(B3,H15)	-
54	15.48	2.02	8.24	V_1(B5,H17)	-
sum	246.31	73.4610			

Table S19: ELI of free $B_{10}H_{10}^{2-}$, model **2**-*gas*

no.	V_{001} [Å^3]	ELI-D$_{pop}$† [e]	max	basin	Δ_{ELI-D} [Å]
1	0.24	2.08(2.08)	13.37	C(B9)	-
2	0.24	2.08(2.08)	13.37	C(B10)	-
3	0.25	2.08(2.08)	15.24	C(B4)	-
4	0.25	2.07(2.08)	13.46	C(B7)	-
5	0.25	2.07(2.08)	13.46	C(B8)	-
6	0.25	2.08(2.08)	13.59	C(B1)	-
7	0.25	2.08(2.08)	13.59	C(B3)	-
8	0.25	2.08(2.08)	14.78	C(B6)	-
9	0.25	2.08(2.08)	14.78	C(B5)	-
10	0.25	2.08(2.08)	12.37	C(B2)	-
11	1.23	0.46(0.47)	1.47	V_2(B5,B8)	0.327
12	1.25	0.47(0.47)	1.47	V_2(B4,B1)	0.323
13	1.25	0.47(0.47)	1.47	V_2(B4,B3)	0.323
14	1.25	0.47(0.47)	1.47	V_2(B3,B2)	0.327
15	1.25	0.47(0.47)	1.47	V_2(B1,B2)	0.327
16	1.25	0.47(0.47)	1.47	V_2(B5,B6)	0.358
17	1.26	0.48(0.48)	1.47	V_2(B7,B8)	0.293
18	1.26	0.48(0.48)	1.47	V_2(B6,B7)	0.356
19	2.28	0.90(0.92)	1.52	V_2(B2,B5)	0.080
20	2.30	0.91(0.92)	1.52	V_2(B1,B8)	0.104
21	2.30	0.91(0.92)	1.52	V_2(B3,B7)	0.104
22	2.32	0.92(0.92)	1.52	V_2(B7,B4)	0.099
23	2.35	0.93(0.92)	1.52	V_2(B2,B6)	0.080
24	2.36	0.93(0.92)	1.52	V_2(B3,B6)	0.075
25	2.36	0.93(0.92)	1.52	V_2(B1,B5)	0.075
26	2.37	0.94(0.92)	1.52	V_2(B8,B4)	0.099
27	3.32	1.14(1.17)	1.55	V_2(B2,B10)	0.168
28	3.34	1.15(1.17)	1.55	V_2(B7,B9)	0.169
29	3.38	1.16(1.17)	1.55	V_2(B5,B9)	0.177
30	3.40	1.17(1.17)	1.55	V_2(B3,B10)	0.162
31	3.40	1.17(1.17)	1.55	V_2(B1,B10)	0.162
32	3.43	1.18(1.17)	1.55	V_2(B8,B9)	0.169
33	3.45	1.18(1.17)	1.55	V_2(B6,B9)	0.177
34	3.49	1.19(1.17)	1.55	V_2(B4,B10)	0.176
35	15.77	2.01(2.02)	7.96	V_1(B2,H12)	-
36	15.78	2.02(2.02)	7.90	V_1(B3,H13)	-
37	15.78	2.02(2.02)	7.91	V_1(B1,H11)	-
38	15.78	2.02(2.02)	7.86	V_1(B4,H14)	-
39	15.79	2.02(2.02)	7.92	V_1(B6,H16)	-
40	15.79	2.02(2.02)	7.91	V_1(B5,H15)	-
41	15.79	2.02(2.02)	7.87	V_1(B7,H17)	-
42	15.79	2.02(2.02)	7.86	V_1(B8,H18)	-
43	16.76	2.04(2.04)	7.88	V_1(B9,H19)	-
44	16.76	2.04(2.04)	7.88	V_1(B10,H20)	-
sum	218.12	61.48(61.49)			

† values in brackets belong to calculations with a grid size of 0.05 a.u. (DGRID-4.5).

Table S20: ELI of free bis-amino-arachno-borane, model **3**-*gas*

no.	V_{001} [Å^3]	ELI-D$_{pop}$† [e]	max	basin	Δ_{ELI-D} [Å]
1	0.07	2.11(2.11)	9.38	C(N1)	-
2	0.07	2.11(2.11)	8.93	C(N2)	-
3	0.24	2.07(2.08)	13.32	C(B5)	-
4	0.24	2.07(2.08)	13.95	C(B6)	-
5	0.24	2.08(2.08)	15.91	C(B9)	-
6	0.24	2.08(2.08)	15.91	C(B24)	-
7	0.25	2.08(2.08)	14.72	C(B22)	-
8	0.25	2.08(2.08)	14.72	C(B7)	-
9	0.25	2.08(2.08)	14.33	C(B23)	-
10	0.25	2.08(2.08)	14.33	C(B8)	-
11	0.25	2.08(2.08)	14.16	C(B3)	-
12	0.25	2.08(2.08)	14.54	C(B4)	-
13	1.12	0.53(0.53)	1.47	V_2(B9,B24)	0.166
14	1.87	0.84(0.85)	1.53	V_2(B5,B24)	0.188
15	1.89	0.84(0.85)	1.53	V_2(B6,B24)	0.188
16	1.95	0.87(0.87)	1.53	V_2(B6,B9)	0.188
17	1.96	0.87(0.87)	1.53	V_2(B5,B9)	0.188
18	2.79	1.96(1.96)	1.89	V_2(N1,B3)	0.009
19	2.79	1.96(1.96)	1.89	V_2(N2,B4)	0.009
20	3.21	1.37(1.38)	1.56	V_2(B8,B9)	0.239
21	3.21	1.38(1.38)	1.56	V_2(B23,B24)	0.239
22	3.29	1.41(1.40)	1.56	V_2(B22,B24)	0.239
23	3.29	1.41(1.40)	1.56	V_2(B7,B9)	0.239
24	4.94	1.83(1.84)	1.78	V_2(B3,B22)	0.249
25	4.94	1.83(1.84)	1.78	V_2(B4,B23)	0.249
26	5.03	1.88(1.87)	1.78	V_2(B3,B7)	0.249
27	5.03	1.88(1.87)	1.78	V_2(B4,B8)	0.249
28	7.49	1.95(1.95)	4.54	V_1(N2,H19)	-
29	7.50	1.95(1.95)	4.58	V_1(N1,H18)	-
30	7.59	1.96(1.96)	4.84	V_2(H28)	-
31	7.59	1.96(1.96)	4.84	V_2(H17)	-
32	8.09	1.93(1.94)	4.68	V_1(N2,H21)	-
33	8.11	1.94(1.94)	4.64	V_1(N1,H29)	-
34	8.11	1.94(1.94)	4.64	V_1(N1,H20)	-
35	8.13	1.95(1.95)	4.68	V_1(N2,H30)	-
36	12.20	1.99(1.99)	7.39	V_1(B4,H11)	-
37	12.27	1.99(1.99)	7.42	V_1(B3,H10)	-
38	13.26	1.99(1.99)	8.32	V_1(B5,H12)	-
39	13.26	1.99(1.99)	8.26	V_1(B6,H13)	-
40	14.50	2.02(2.02)	8.44	V_1(B9,H16)	-
41	14.55	2.02(2.02)	8.44	V_1(B24,H27)	-
42	14.75	2.02(2.02)	8.27	V_1(B8,H15)	-
43	14.76	2.02(2.02)	8.27	V_1(B23,H26)	-
44	14.77	2.02(2.02)	8.21	V_1(B7,H14)	-
45	14.77	2.02(2.02)	8.21	V_1(B22,H25)	-
sum	251.58	81.53(81.54)			

† values in brackets belong to calculations with a grid size of 0.05 a.u. (DGRID-4.5).

Table S21: ELI of free bis-acetonitrile-arachno-borane, model **4**-*gas*

no.	V_{001} [Å^3]	ELI-D$_{pop}$ [e]	max	basin	Δ_{ELI-D} [Å]
1	0.06	2.11	10.16	C(N2)	-
2	0.06	2.11	10.16	C(N1)	-
3	0.12	2.09	12.59	C(C25)	-
4	0.12	2.09	12.59	C(C26)	-
5	0.12	2.10	11.39	C(C31)	-
6	0.12	2.10	11.39	C(C27)	-
7	0.24	2.08	14.42	C(B5)	-
8	0.24	2.08	14.42	C(B6)	-
9	0.24	2.08	15.68	C(B9)	-
10	0.24	2.08	15.68	C(B20)	-
11	0.25	2.08	15.88	C(B19)	-
12	0.25	2.08	15.88	C(B18)	-
13	0.25	2.08	15.90	C(B8)	-
14	0.25	2.08	15.90	C(B7)	-
15	0.25	2.08	15.29	C(B4)	-
16	0.25	2.08	15.29	C(B3)	-
17	1.29	0.61	1.49	V_2(B9,B20)	0.161
18	1.74	0.79	1.53	V_2(B6,B20)	0.176
19	1.74	0.79	1.53	V_2(B5,B20)	0.176
20	1.79	0.81	1.53	V_2(B6,B9)	0.176
21	1.79	0.81	1.53	V_2(B5,B9)	0.176
22	3.37	1.45	1.57	V_2(B8,B9)	0.243
23	3.37	1.45	1.57	V_2(B18,B20)	0.243
24	3.45	1.48	1.57	V_2(B19,B20)	0.243
25	3.45	1.48	1.57	V_2(B7,B9)	0.243
26	4.32	2.25	1.95	V_2(C25,C27)	0.008
27	4.32	2.25	1.95	V_2(C26,C31)	0.008
28	4.66	1.71	1.75	V_2(B3,B18)	0.237
29	4.66	1.71	1.75	V_2(B4,B19)	0.237
30	4.73	1.74	1.75	V_2(B4,B8)	0.237
31	4.73	1.74	1.75	V_2(B3,B7)	0.237
32	5.44	2.82	1.87	V_2(N1,B3)	0.017
33	5.44	2.82	1.87	V_2(N2,B4)	0.017
34	7.60	1.97	4.95	V_2(H24)	-
35	7.60	1.97	4.95	V_2(H17)	-
36	8.37	2.08	1.56	V_2(N1,C26)	0.658
37	8.37	2.08	1.56	V_2(N2,C25)	0.658
38	9.86	1.93	6.18	V_1(C31,H33)	-
39	9.86	1.93	6.18	V_1(C27,H28)	-
40	9.91	1.93	6.17	V_2(N2,C25)	-
41	9.91	1.93	6.17	V_2(N1,C26)	-
42	9.91	1.93	6.17	V_1(C31,H32)	-
43	9.91	1.93	6.17	V_1(C27,H29)	-
44	10.78	2.80	1.56	V_1(C27,H30)	0.656
45	10.78	2.80	1.56	V_1(C31,H34)	0.656
46	11.82	1.96	7.46	V_1(B3,H10)	-
47	11.83	1.96	7.46	V_1(B4,H11)	-
48	13.47	2.00	8.62	V_1(B5,H12)	-
49	13.47	2.00	8.62	V_1(B6,H13)	-
50	14.44	2.02	8.56	V_1(B20,H23)	-
51	14.47	2.02	8.56	V_1(B9,H16)	-
52	14.51	2.02	8.53	V_1(B7,H14)	-
53	14.51	2.02	8.53	V_1(B19,H22)	-
54	14.52	2.02	8.53	V_1(B8,H15)	-
55	14.52	2.02	8.53	V_1(B18,H21)	-
sum	313.77	105.40			

Table S22: Hirshfeld rigid-bond test for **1**

ATOM	ATOM	DMSDA	ATOM	DMSDA	ATOM	DMSDA∗
N(1)	C(2)	2	C(3)	1	H(1)	61
C(2)	C(5)	-1	C(7)	7		
C(3)	C(4)	0	C(8)	13		
C(4)	C(6)	1	H(4)	52		
C(5)	C(6)	3	H(5)	56		
C(6)	H(6)	50				
C(7)	H(71)	60	H(72)	57	H(73)	58
C(8)	H(81)	56	H(82)	60	H(83)	52
B(1)	B(4)	0	B(5)	1	B(6)	-2
	H(91)	50				
B(2)	B(3)	-1	B(4)	0	B(6)	-1
	H(92)	49				
B(3)	B(4)	0	B(5)	4	H(93)	52
B(4)	B(5)	2	B(6)	2	H(94)	51
B(5)	H(95)	49				
B(6)	H(96)	50				

∗ DMSDA = difference mean square dispalcement amplitude

Table S23: Hirshfeld rigid-bond test for **2**

ATOM	ATOM	DMSDA	ATOM	DMSDA	ATOM	DMSDA∗
N(100)	C(101)	12	C(105)	2	H(100)	54
N(111)	C(106)	-4	C(110)	8		
N(200)	C(201)	5	C(205)	1	H(200)	56
N(211)	C(206)	1	C(210)	1		
C(101)	C(102)	1	H(101)	48		
C(102)	C(103)	-2	H(102)	48		
C(103)	C(104)	7	H(103)	44		
C(104)	C(105)	-8	H(104)	47		
C(105)	C(106)	1				
C(106)	C(107)	0				
C(107)	C(108)	4	H(107)	53		
C(108)	C(109)	2	H(108)	54		
C(109)	C(110)	-10	H(109)	52		
C(110)	H(110)	47				
C(201)	C(202)	3	H(201)	51		
C(202)	C(203)	1	H(202)	45		
C(203)	C(204)	-3	H(203)	50		
C(204)	C(205)	-4	H(204)	50		
C(205)	C(206)	1				
C(206)	C(207)	2				
C(207)	C(208)	-2	H(207)	51		
C(208)	C(209)	-3	H(208)	53		
C(209)	C(210)	2	H(209)	48		
C(210)	H(210)	51				
B(1)	B(2)	-3	B(4)	-1	B(5)	-1
	B(6)	2	B(9)	2	H(1)	52
B(2)	B(3)	-1	B(5)	2	B(8)	1
	B(9)	-1	H(2)	51		
B(3)	B(4)	2	B(7)	-1	B(8)	1
	B(9)	-2	H(3)	53		
B(4)	B(6)	0	B(7)	1	B(9)	0
	H(4)	52				
B(5)	B(6)	2	B(8)	1	B(10)	2
	H(5)	52				
B(6)	B(7)	-2	B(10)	0	H(6)	52
B(7)	B(8)	0	B(10)	-2	H(7)	51
B(8)	B(10)	3	H(8)	54		
B(9)	H(9)	53				
B(10)	H(10)	53				

∗ DMSDA = difference mean square dispalcement amplitude

Table S24: Hirshfeld rigid-bond test for **3**

ATOM	ATOM	DMSDA	ATOM	DMSDA	ATOM	DMSDA∗
N(1)	B(1)	3				
N(2)	B(2)	0				
B(1)	B(3)	2	H(1)	85		
B(2)	B(4)	5	H(2)	188		
B(3)	B(5)	-5	B(7)	3	H(3)	61
B(4)	B(6)	-3	B(7)	0	H(4)	203
B(5)	B(7)	-4	H(5)	216		
B(6)	B(7)	0	H(6)	235		
B(7)	H(7)	199				

∗ DMSDA = difference mean square dispalcement amplitude

Table S25: Hirshfeld rigid-bond test for **4**

ATOM	ATOM	DMSDA	ATOM	DMSDA	ATOM	DMSDA∗
N(1)	C(1)	0	B(1)	6		
C(1)	C(2)	8				
C(2)	H(21)	155	H(22)	82	H(23)	258
B(1)	B(2)	1	B(3)	0	B(4)	4
	H(1)	204				
B(2)	B(3)	0	B(4)	-2	B(5)	1
	H(2)	197				
B(3)	H(3)	208	H(6)	31		
B(4)	B(5)	-1	H(4)	60		
B(5)	H(5)	251				

∗ DMSDA = difference mean square dispalcement amplitude

Table S26: Topological bond descriptors for new data reduction: B-B and B-H bonds of **1**

bond	$\rho(\mathbf{r}_{bcp})$ [eÅ^{-3}]	$\nabla^2\rho(\mathbf{r}_{bcp})$ [eÅ^{-5}]	d_1 [Å]	d_2 [Å]	λ_3	ϵ	Rxy [Å]	Rbp [Å]	Δ_{bcp} [Å]
B(1)-B(4)	0.79(1)	-1.9(1)	0.890	0.893	2.76	2.46	1.782(7)	1.784	0.019
B(1)-B(5)	0.78(1)	-1.7(1)	0.894	0.890	2.77	2.70	1.783(6)	1.786	0.019
B(1)-B(6)	0.77(1)	-1.7(1)	0.896	0.891	2.77	2.72	1.786(6)	1.787	0.020
B(1)-B(2)a	0.77(1)	-1.7(1)	0.892	0.892	2.83	2.58	1.784(6)	1.786	0.021
B(1)-B(3)a	0.77(1)	-1.6(1)	0.900	0.888	2.78	2.67	1.786(7)	1.790	0.019
B(2)-B(3)	0.77(1)	-1.7(1)	0.899	0.885	2.72	2.72	1.783(6)	1.786	0.020
B(2)-B(4)	0.78(1)	-1.8(1)	0.893	0.894	2.80	2.57	1.787(6)	1.790	0.025
B(2)-B(6)	0.77(1)	-1.7(1)	0.897	0.892	2.79	2.72	1.789(6)	1.791	0.017
B(2)-B(5)a	0.77(1)	-1.7(1)	0.894	0.892	2.82	2.59	1.785(7)	1.788	0.020
B(3)-B(4)	0.78(1)	-1.8(1)	0.883	0.899	2.72	2.58	1.781(7)	1.784	0.024
B(3)-B(5)	0.76(1)	-1.6(1)	0.890	0.901	2.74	2.81	1.791(6)	1.794	0.016
B(3)-B(6)a	0.77(1)	-1.7(1)	0.886	0.896	2.75	2.62	1.781(6)	1.784	0.019
B(4)-B(5)	0.78(1)	-1.8(1)	0.894	0.891	2.77	2.60	1.785(6)	1.787	0.019
B(4)-B(6)	0.78(1)	-1.8(1)	0.895	0.891	2.77	2.60	1.786(7)	1.788	0.018
B(5)-B(6)a	0.77(1)	-1.7(1)	0.893	0.891	2.80	2.55	1.783(6)	1.786	0.019
B(1)-H(91)	1.23(1)	-10.5(1)	0.527	0.664	6.79	0.00	1.190	1.190	0.007
B(2)-H(92)	1.22(1)	-10.7(1)	0.529	0.661	6.45	0.00	1.190	1.190	0.001
B(3)-H(93)	1.17(1)	-9.7(1)	0.532	0.659	6.07	0.01	1.190	1.191	0.020
B(4)-H(94)	1.27(1)	-8.2(1)	0.511	0.679	10.20	0.00	1.190	1.190	0.008
B(5)-H(95)	1.21(1)	-10.8(1)	0.531	0.660	6.09	0.00	1.190	1.191	0.024
B(6)-H(96)	1.21(1)	-9.5(1)	0.524	0.666	7.43	0.00	1.190	1.190	0.005

The results refer to Figure S9, right side. They are virtually identical to the results which were used in this work, see Tables S4 and S7.

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