Supplementary Material (ESI) for Dalton Transactions

Synthetic and Structural Studies on C-Ethynyl- and C-Bromo-Carboranes. Gas Phase Electron Diffraction Studies of C-Ethynyl- and C-Trimethylsilylethynyl-*para*-carbaboranes.

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Data for Electronic Supplementary Information

Table S1 Least-squares correlation matrix (x100) for GED structure refinement of 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$.[a]

Table S2 Least-squares correlation matrix (x100) for GED structure refinement of 1-HCC-1,12-$C_2B_{10}H_{11}$.[a]

Table S3 Distances, amplitudes of vibration, r_{h1} corrections and original amplitudes of vibration from the GED structure refinement of 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$. All distances are in pm.

Table S4 Distances, amplitudes of vibration, r_{h1} corrections and original amplitudes of vibration from the GED structure refinement of 1-HCC-1,12-$C_2B_{10}H_{11}$. All distances are in pm.

Table S5 Cartesian coordinates for the GED structure of 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$.

Table S6 Cartesian coordinates for the GED structure of 1-HCC-1,12-$C_2B_{10}H_{11}$.

Table S7 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$.

Table S8 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-HCC-1,12-$C_2B_{10}H_{11}$.

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Table S10 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1,12-$(HCC)_2$-1,12-$C_2B_{10}H_{10}$.

Table S11 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-F-1,12-$C_2B_{10}H_{11}$.

Table S12 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-Cl-1,12- $C_2B_{10}H_{11}$.

Table S13 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-HO_2C-1,12- $C_2B_{10}H_{11}$.

Table S14 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-H_3C-1,12- $C_2B_{10}H_{11}$.

Table S15 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-NC-1,12- $C_2B_{10}H_{11}$.

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Table S17 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1,12-Ph_2-1,12- $C_2B_{10}H_{10}$.

Table S18 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-(1'-1',12'- $C_2B_{10}H_{11}$)-1,12- $C_2B_{10}H_{11}$ – C,C'-bis(para-carborane).

Table S19 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-HCC-1,2-$C_2B_{10}H_{11}$.

Table S20 Non-bond distances (r_a/Å) and amplitudes of vibration (u/Å) obtained in the GED refinement of **5**.

Table S21 Non-bond distances (r_a/Å) and amplitudes of vibration (u/Å) obtained in the GED refinement of **6**.

Table S22 Calculated (r_e) and experimental (r_{h1}) structure of 1,12-$C_2B_{10}H_{11}$-C≡CH. All bond lengths in pm and all angles in °.

Figure S1 Experimental and final weighted difference (experimental-theoretical) molecular scattering intensities for 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$.

Figure S2 Experimental and final weighted difference (experimental-theoretical) molecular scattering intensities for 1-HCC-1,12-$C_2B_{10}H_{11}$.

Table S1 Least-squares correlation matrix (x100) for GED structure refinement of 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$.[a]

	p_4	p_8	p_{10}	u_5	u_9	u_{12}	u_{18}	u_{26}	u_{32}	u_{49}	u_{84}	k_2
p_1	79	-68	89	60	56							
p_4		-64	95	79						54		
p_8			-62	-53	-71							
p_9						-52						
p_{10}				79						51		
p_{15}							63					
u_5										56		
u_9						67		58	65			
u_{23}								81	61			
u_{26}									82			
u_{76}											59	

[a] Only elements with the absolute values > 50% are shown; k_2 is a scale factor

Table S2 Least-squares correlation matrix (x100) for GED structure refinement of 1-HCC-1,12-$C_2B_{10}H_{11}$.[a]

	p_4	p_8	p_{11}	u_3	u_9	u_{12}	u_{20}	u_{37}	u_{40}	k_2
p_1	69	88			52					
p_2			-62							
p_3				-50					52	
p_4		93			65					
p_8					64					
p_9								51		
p_{11}						-57				
u_9										51
u_{12}							69			

[a] Only elements with the absolute values > 50% are shown k_2 is a scale factor

Table S3 Distances, amplitudes of vibration, r_{h1} corrections and original amplitudes of vibration from the GED structure refinement of 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$. All distances are in pm.

	Atom pair	Distance	Amplitude	r_{h1} correction	Original amplitude
u_1	C(1)-H(29)	108.6(4)	8.2(4)	0.4	7.5
u_2	B(2)-H(19)	119.9(6)	9.0(Tied to u_1)	0.4	8.2
u_3	C(13)-C(14)	122.6(5)	3.9(Tied to u_1)	0.1	3.6
u_4	C(12)-C(13)	144.2(5)	4.1(4)	0.2	4.7
u_5	C(1)-B(2)	170.9(7)	8.2(5)	0.3	6.9
u_6	B(7)-C(12)	171.9(6)	8.6(Tied to u_5)	-0.2	7.1
u_7	B(2)-B(7)	176.4(8)	7.2(Tied to u_9)	0.2	6.7
u_{12}	H(30)...H(31)	177.6(13)	12.7(fixed)	-0.2	12.7
u_9	B(7)-B(8)	179.3(6)	7.4(3)	0.7	6.9
u_8	B(2)-B(3)	179.3(7)	7.2(Tied to u_9)	0.4	6.8
u_{10}	C(14)-Si(15)	184.0(5)	5.4(5)	0.2	5.3
u_{11}	Si(15)-C(16)	187.4(5)	6.6(4)	0.2	5.5
u_{13}	B(2)...H(29)	240.0(9)	11.7(fixed)	-0.3	11.7
u_{14}	Si(15)...H(30)	244.5(12)	10.0(7)	0.0	12.8
u_{16}	C(12)...H(24)	251.5(12)	11.4(Tied to u_{17})	-0.8	12.2
u_{15}	C(1)...H(19)	252.1(12)	11.2(Tied to u_{17})	-0.4	12.1
u_{18}	B(7)...H(25)	259.3(7)	11.8()	0.1	12.7
u_{17}	B(2)...H(20)	259.3(8)	11.8(9)	-0.3	12.7
u_{20}	C(12)...C(14)	265.6(6)	4.8(Tied to u_{17})	-1.1	5.2
u_{21}	B(2)...H(24)	266.0(14)	11.3(Tied to u_{17})	-0.3	12.2
u_{19}	B(7)...H(19)	266.1(12)	11.2(Tied to u_{17})	-0.4	12.1
u_{22}	B(7)...C(13)	271.5(9)	10.4(Tied to u_{23})	-0.1	9.0
u_{23}	C(1)...B(7)	273.2(7)	7.9(4)	0.1	6.8
u_{24}	B(2)...C(12)	275.9(6)	8.0(Tied to u_{23})	-0.3	6.9
u_{25}	H(19)...H(29)	278.2(17)	18.8(fixed)	-0.4	18.8
u_{26}	B(2)...B(8)	288.3(3)	7.9(4)	0.4	7.1
u_{28}	B(7)...B(9)	289.6(9)	8.5(Tied to u_{26})	0.4	7.7
u_{27}	B(2)...B(4)	290.0(11)	8.2(Tied to u_{26})	0.3	7.5

u_{29}	H(24)...H(25)	295.3(13)	20.2(fixed)	0.0	20.2
u_{30}	H(19)...H(20)	295.4(14)	20.2(fixed)	-0.4	20.2
u_{31}	C(13)...H(24)	297.2(18)	18.3(Tied to u_{32})	0.0	17.3
u_{32}	C(14)...C(16)	302.3(9)	12.5(8)	-0.8	11.9
u_{33}	C(13)...Si(15)	304.3(6)	6.4(Tied to u_{32})	-2.2	6.1
u_{36}	H(31)...H(35)	305.1(31)	39.7(fixed)	7.3	39.7
u_{35}	C(16)...C(17)	305.6(12)	13.0(Tied to u_{32})	0.5	12.3
u_{38}	H(30)...H(33)	305.9(37)	40.0(fixed)	9.0	40.0
u_{34}	C(1)...C(12)	307.6(9)	7.0(Tied to u_{32})	-0.5	6.6
u_{39}	C(14)...H(31)	319.6(17)	27.8(fixed)	0.4	27.8
u_{37}	H(19)...H(24)	320.6(27)	19.2(fixed)	-0.5	19.2
u_{40}	C(16)...H(35)	322.2(16)	27.8(fixed)	1.3	27.8
u_{41}	C(16)...H(33)	322.4(21)	27.6(fixed)	1.9	27.6
u_{42}	B(2)...B(9)	339.2(3)	8.2(4)	0.2	7.3
u_{43}	H(30)...H(35)	346.2(24)	44.0(fixed)	0.4	44.0
u_{44}	B(7)...H(29)	367.7(9)	10.6(fixed)	-0.7	10.6
u_{46}	C(14)...H(24)	371.9(21)	23.2(fixed)	-4.8	23.2
u_{45}	B(7)...C(14)	375.3(10)	15.9(15)	-4.0	12.4
u_{47}	C(1)...H(24)	385.8(11)	11.9(Tied to u_{50})	-0.8	10.8
u_{48}	C(12)...H(19)	388.3(10)	12.0(Tied to u_{50})	-1.2	10.9
u_{50}	B(7)...H(26)	390.5(11)	13.1(4)	-0.6	12.0
u_{49}	B(2)...H(21)	391.0(13)	13.0(Tied to u_{50})	-0.7	11.9
u_{53}	C(14)...H(30)	391.4(11)	14.3(Tied to u_{50})	-4.5	13.1
u_{56}	C(16)...H(34)	394.8(13)	14.5(Tied to u_{50})	-3.5	13.2
u_{52}	B(2)...H(25)	395.5(7)	12.6(Tied to u_{50})	-0.6	11.5
u_{51}	B(7)...H(21)	395.6(6)	12.6(Tied to u_{50})	-0.6	11.5
u_{55}	B(2)...C(13)	403.7(6)	9.9(6)	-0.7	8.3
u_{54}	C(13)...C(16)	407.1(11)	18.6(23)	-1.7	18.2
u_{57}	C(13)...H(31)	409.5(19)	37.2(Tied to u_{54})	0.5	36.4
u_{58}	C(12)...H(29)	415.5(10)	9.7(fixed)	-1.5	9.7
u_{59}	H(31)...H(34)	416.1(21)	26.4(fixed)	-4.0	26.4
u_{60}	H(30)...H(34)	417.0(25)	25.9(fixed)	-2.7	25.9

u_{61}	C(12)...Si(15)	446.4(7)	9.1(5)	-4.2	7.1
u_{62}	C(1)...C(13)	451.2(9)	9.0(Tied to u_{61})	-1.0	7.1
u_{63}	B(2)...H(26)	457.2(6)	13.5(Tied to u_{61})	-1.0	10.6
u_{64}	B(7)...H(22)	457.3(6)	13.5(Tied to u_{61})	-1.0	10.6
u_{65}	H(24)...H(29)	472.7(13)	14.5(fixed)	-1.7	14.5
u_{68}	H(31)...H(38)	473.6(21)	15.9(fixed)	-7.6	15.9
u_{66}	H(24)...H(26)	477.8(21)	16.4(fixed)	-1.6	16.4
u_{67}	H(19)...H(21)	478.5(22)	16.3(fixed)	-1.7	16.3
u_{69}	H(25)...H(35)	483.6(23)	75.1(fixed)	1.4	75.1
u_{74}	H(25)...H(34)	491.0(22)	81.4(fixed)	-8.4	81.4
u_{71}	H(24)...H(31)	492.7(23)	68.4(fixed)	6.3	68.4
u_{70}	H(19)...H(25)	494.4(11)	15.6(fixed)	-1.5	15.6
u_{73}	C(13)...H(30)	501.6(12)	17.7(fixed)	-7.2	17.7
u_{72}	C(13)...H(19)	506.3(12)	14.4(Tied to u_{76})	-1.5	13.1
u_{75}	H(26)...H(34)	515.2(23)	76.2(fixed)	8.0	76.2
u_{76}	B(2)...C(14)	516.5(5)	12.5(6)	-3.4	11.3
u_{77}	Si(15)...H(24)	519.1(20)	33.6(Tied to u_{76})	-8.4	30.4
u_{78}	C(17)...H(25)	520.9(21)	59.8(fixed)	-8.4	59.8
u_{79}	C(12)...H(31)	528.0(20)	43.1(fixed)	-4.1	43.1
u_{80}	C(12)...C(16)	536.8(12)	26.0(Tied to u_{83})	-5.3	23.7
u_{84}	H(24)...H(35)	536.8(23)	70.0(fixed)	-9.5	70.0
u_{81}	H(24)...H(32)	540.4(21)	73.1(fixed)	3.4	73.1
u_{82}	C(16)...H(24)	543.9(21)	51.0(fixed)	-1.3	51.0
u_{83}	B(7)...Si(15)	544.8(8)	18.8(6)	-7.9	17.1
u_{85}	B(8)...H(35)	554.0(17)	63.1(fixed)	-5.6	63.1
u_{87}	C(13)...H(29)	559.0(9)	10.0(fixed)	-2.1	10.0
u_{88}	B(8)...H(34)	559.7(17)	65.2(fixed)	-9.5	65.2
u_{86}	B(7)...H(31)	560.9(18)	58.2(fixed)	-0.9	58.2
u_{89}	C(17)...H(26)	565.1(20)	60.6(fixed)	-2.9	60.6
u_{92}	B(9)...H(34)	571.5(18)	63.9(fixed)	-1.2	63.9
u_{90}	C(1)...C(14)	571.9(9)	7.5(fixed)	-3.1	7.5
u_{93}	H(26)...H(35)	572.8(21)	81.5(fixed)	-4.8	81.5

u_{91}	H(19)...H(26)	575.8(12)	13.1(fixed)	-2.3	13.1
u_{95}	B(8)...C(17)	582.7(12)	44.6(fixed)	-10.7	44.6
u_{96}	B(7)...H(35)	584.2(19)	55.9(fixed)	-10.5	55.9
u_{99}	C(17)...H(24)	585.5(20)	47.0(fixed)	-15.1	47.0
u_{97}	H(25)...H(31)	585.8(23)	68.2(fixed)	-4.2	68.2
u_{94}	B(7)...H(32)	588.3(16)	61.4(fixed)	-0.7	61.4
u_{98}	B(7)...C(16)	596.5(11)	39.2(fixed)	-5.2	39.2
u_{102}	B(9)...H(35)	604.2(16)	64.5(fixed)	-8.2	64.5
u_{104}	H(24)...H(34)	605.3(20)	56.9(fixed)	-20.3	56.9
u_{101}	B(9)...C(17)	607.0(11)	44.9(fixed)	-7.5	44.9
u_{100}	C(14)...H(19)	612.6(12)	17.3(fixed)	-4.6	17.3
u_{103}	B(8)...H(31)	614.0(19)	53.3(fixed)	-5.6	53.3
u_{106}	C(16)...H(25)	617.4(20)	50.4(fixed)	-12.6	50.4
u_{105}	B(7)...C(17)	618.9(10)	33.4(fixed)	-14.2	33.4
u_{107}	H(25)...H(38)	621.2(23)	48.7(fixed)	-13.7	48.7
u_{108}	B(7)...H(34)	623.2(16)	49.5(fixed)	-16.4	49.5
u_{109}	C(12)...H(30)	634.0(13)	22.9(fixed)	-11.8	22.9
u_{110}	B(8)...H(38)	636.5(19)	42.1(fixed)	-8.9	42.1
u_{111}	B(8)...C(16)	639.3(10)	33.8(fixed)	-10.9	33.8
u_{112}	H(24)...H(30)	640.4(21)	54.3(fixed)	-10.4	54.3
u_{116}	H(25)...H(32)	643.4(21)	64.1(fixed)	-16.1	64.1
u_{113}	C(17)...H(27)	648.1(20)	46.6(fixed)	-7.4	46.6
u_{114}	B(8)...H(32)	649.0(16)	52.3(fixed)	-11.2	52.3
u_{115}	B(8)...C(18)	654.2(9)	21.3(fixed)	-11.9	21.3
u_{119}	H(24)...H(37)	656.3(23)	62.2(fixed)	-9.5	62.2
u_{117}	B(7)...H(37)	658.0(19)	52.6(fixed)	-5.8	52.6
u_{120}	H(26)...H(33)	658.7(20)	63.0(fixed)	-11.1	63.0
u_{121}	C(17)...H(28)	660.0(20)	29.3(fixed)	-13.9	29.3
u_{118}	B(7)...C(18)	664.8(9)	29.2(fixed)	-10.4	29.2
u_{123}	B(8)...H(37)	665.1(17)	39.5(fixed)	-11.2	39.5
u_{125}	C(16)...H(26)	666.1(20)	31.3(fixed)	-13.2	31.3
u_{124}	B(9)...H(31)	667.5(18)	41.9(fixed)	-10.4	41.9

u_{122}	B(9)...C(16)	667.9(9)	21.1(fixed)	-11.3	21.1
u_{128}	H(25)...H(37)	668.9(21)	39.1(fixed)	-18.0	39.1
u_{127}	B(7)...H(38)	670.3(17)	42.7(fixed)	-11.3	42.7
u_{129}	H(26)...H(31)	676.3(22)	48.5(fixed)	-12.6	48.5
u_{133}	H(24)...H(33)	677.2(20)	49.0(fixed)	-20.4	49.0
u_{131}	H(24)...H(38)	678.1(22)	45.9(fixed)	-17.3	45.9
u_{126}	C(14)...H(29)	679.5(10)	10.4(fixed)	-4.3	10.4
u_{132}	B(8)...H(33)	683.7(12)	45.2(fixed)	-18.6	45.2
u_{130}	B(2)...Si(15)	690.3(6)	20.4(7)	-7.3	16.8
u_{134}	B(7)...H(30)	695.6(12)	40.7(fixed)	-13.6	40.7
u_{135}	B(4)...H(34)	699.8(19)	67.4(fixed)	-7.3	67.4
u_{137}	B(3)...H(35)	702.5(20)	62.2(fixed)	-11.0	62.2
u_{140}	H(25)...H(30)	703.3(19)	52.8(fixed)	-19.4	52.8
u_{138}	B(9)...H(33)	704.9(11)	45.4(fixed)	-15.2	45.4
u_{136}	B(2)...H(31)	706.4(19)	62.9(fixed)	-5.2	62.9
u_{139}	B(4)...H(35)	713.1(18)	66.8(fixed)	-9.6	66.8
u_{142}	B(7)...H(33)	715.6(11)	33.3(fixed)	-20.3	33.3
u_{141}	B(3)...H(31)	722.0(20)	56.8(fixed)	-5.7	56.8
u_{148}	H(25)...H(36)	724.3(19)	35.8(fixed)	-22.0	35.8
u_{144}	B(3)...H(34)	726.3(18)	60.9(fixed)	-15.2	60.9
u_{147}	B(8)...H(30)	732.3(10)	34.6(fixed)	-18.2	34.6
u_{145}	B(4)...C(17)	733.5(13)	46.5(fixed)	-11.6	46.5
u_{143}	B(2)...C(16)	736.2(13)	43.4(fixed)	-6.1	43.4
u_{149}	B(3)...C(17)	739.5(13)	40.7(fixed)	-15.1	40.7
u_{155}	H(24)...H(36)	740.5(20)	41.7(fixed)	-19.5	41.7
u_{146}	B(4)...H(38)	743.7(20)	50.1(fixed)	-3.5	50.1
u_{152}	B(8)...H(36)	745.6(11)	22.4(fixed)	-18.5	22.4
u_{158}	H(26)...H(30)	747.7(20)	35.1(fixed)	-18.0	35.1
u_{150}	C(1)...Si(15)	751.0(6)	9.2(fixed)	-8.0	9.2
u_{156}	B(2)...H(35)	752.1(20)	50.3(fixed)	-15.5	50.3
u_{151}	B(3)...H(32)	754.3(18)	60.2(fixed)	-7.7	60.2
u_{159}	B(7)...H(36)	755.0(11)	29.2(fixed)	-17.0	29.2

u_{153}	B(3)...C(16)	757.3(12)	37.1(fixed)	-10.3	37.1
u_{161}	B(9)...H(30)	758.2(11)	21.8(fixed)	-17.3	21.8
u_{154}	H(21)...H(34)	760.4(26)	77.2(fixed)	-5.8	77.2
u_{160}	H(20)...H(35)	764.7(26)	70.9(fixed)	-11.0	70.9
u_{157}	H(19)...H(31)	768.0(25)	73.0(fixed)	-4.6	73.0
u_{162}	B(4)...C(18)	773.9(12)	27.8(fixed)	-8.9	27.8
u_{163}	B(4)...H(37)	775.1(17)	47.7(fixed)	-7.9	47.7
u_{165}	B(4)...H(31)	775.6(20)	50.2(fixed)	-10.6	50.2
u_{164}	Si(15)...H(19)	779.8(14)	25.0(fixed)	-8.5	25.0
u_{167}	B(2)...C(17)	780.1(11)	26.0(fixed)	-16.3	26.0
u_{169}	B(2)...H(34)	780.9(18)	45.4(fixed)	-17.4	45.4
u_{166}	H(21)...H(35)	781.2(24)	77.0(fixed)	-8.6	77.0
u_{170}	B(3)...H(38)	790.6(19)	42.0(fixed)	-10.4	42.0
u_{168}	H(20)...H(31)	792.1(26)	63.8(fixed)	-5.1	63.8
u_{171}	B(4)...C(16)	793.2(11)	28.0(fixed)	-13.4	28.0
u_{173}	B(4)...H(32)	793.9(18)	47.9(fixed)	-12.6	47.9
u_{174}	B(3)...H(37)	798.7(19)	47.7(fixed)	-8.7	47.7
u_{177}	H(20)...H(34)	799.7(22)	69.2(fixed)	-18.4	69.2
u_{175}	B(3)...C(18)	800.5(11)	23.0(fixed)	-12.0	23.0
u_{176}	C(17)...H(21)	803.4(20)	57.0(fixed)	-11.6	57.0
u_{172}	C(16)...H(19)	805.3(20)	53.5(fixed)	-5.4	53.5
u_{178}	C(1)...H(31)	809.2(18)	51.8(fixed)	-9.8	51.8
u_{179}	C(17)...H(20)	812.1(19)	49.7(fixed)	-17.1	49.7
u_{180}	H(21)...H(38)	821.0(25)	56.5(fixed)	-5.2	56.5
u_{181}	C(1)...C(16)	829.1(12)	31.3(fixed)	-10.6	31.3
u_{185}	B(4)...H(33)	833.3(14)	47.6(fixed)	-20.3	47.6
u_{184}	B(2)...H(30)	836.2(14)	45.4(fixed)	-15.0	45.4
u_{182}	C(16)...H(20)	837.0(18)	45.6(fixed)	-11.9	45.6
u_{186}	H(19)...H(35)	838.5(24)	54.4(fixed)	-18.4	54.4
u_{183}	H(20)...H(32)	838.7(21)	68.5(fixed)	-9.9	68.5
u_{187}	B(3)...H(33)	838.9(13)	40.9(fixed)	-23.0	40.9
u_{190}	B(3)...H(30)	854.2(13)	38.3(fixed)	-19.0	38.3

u_{189}	Si(15)...H(29)	858.2(8)	11.7(fixed)	-9.6	11.7
u_{188}	C(17)...H(22)	858.5(17)	50.6(fixed)	-11.2	50.6
u_{191}	H(21)...H(37)	867.5(21)	49.3(fixed)	-12.2	49.3
u_{193}	B(4)...H(36)	869.6(12)	28.5(fixed)	-16.8	28.5
u_{192}	H(21)...H(31)	870.8(24)	57.0(fixed)	-13.2	57.0
u_{194}	C(17)...H(19)	872.4(16)	29.3(fixed)	-19.3	29.3
u_{195}	B(2)...H(33)	875.7(12)	25.2(fixed)	-22.7	25.2
u_{196}	H(19)...H(34)	880.5(21)	44.6(fixed)	-21.9	44.6
u_{199}	B(4)...H(30)	886.4(11)	28.3(fixed)	-20.9	28.3
u_{197}	C(16)...H(21)	889.9(15)	34.5(fixed)	-16.8	34.5
u_{198}	H(20)...H(38)	890.8(23)	41.3(fixed)	-15.3	41.3
u_{202}	B(3)...H(36)	892.9(11)	22.4(fixed)	-19.7	22.4
u_{201}	H(21)...H(32)	896.8(21)	49.6(fixed)	-17.6	49.6
u_{200}	C(17)...H(23)	899.4(15)	29.2(fixed)	-15.9	29.2
u_{203}	H(19)...H(30)	904.3(21)	57.5(fixed)	-15.0	57.5

Table S4 Distances, amplitudes of vibration, r_{h1} corrections and original amplitudes of vibration from the GED structure refinement of 1-HCC-1,12-$C_2B_{10}H_{11}$. All distances are in pm.

	Atom pair	Distance	Amplitude	r_{h1} correction	Original amplitude
u_1	C(25)-H(26)	109.9(12)	7.3(fixed)	0.22	7.3
u_2	C(1)-H(13)	110.0(12)	7.5(fixed)	0.33	7.5
u_3	C(24)-C(25)	123.3(5)	3.7(3)	0.05	3.5
u_4	C(4)-C(24)	143.0(5)	4.0(5)	0.03	4.6
u_5	C(1)-B(2)	170.4(5)	7.1(Tied to u_9)	0.35	6.7
u_6	B(2)-B(11)	178.9(6)	7.0(Tied to u_9)	0.12	6.6
u_7	B(3)-C(4)	173.0(5)	7.3(Tied to u_9)	0.36	6.9
u_8	B(3)-B(5)	179.8(6)	7.1(Tied to u_9)	0.19	6.7
u_9	B(3)-B(2)	177.4(4)	7.0(1)	-0.14	6.6
u_{10}	B(3)-H(23)	118.1(3)	8.7(Tied to u_3)	0.39	8.2
u_{11}	B(2)-H(18)	118.2(3)	8.7(Tied to u_3)	0.4	8.2
u_{12}	C(1)...B(3)	273.9(6)	7.2(3)	0.16	6.6
u_{13}	C(1)...C(4)	308.3(5)	6.5(8)	0.57	6.4
u_{14}	C(1)...H(14)	250.3(9)	11.4(Tied to u_{37})	-0.56	11.9
u_{15}	C(1)...H(19)	384.8(10)	12.7(Tied to u_{40})	-0.73	10.7
u_{16}	C(1)...C(24)	450.9(5)	6.8(fixed)	-0.04	6.8
u_{17}	C(1)...C(25)	572.4(6)	7.1(fixed)	-1.82	7.1
u_{18}	C(1)...H(26)	679.7(12)	10.1(fixed)	-4.6	10.1
u_{19}	B(2)...C(4)	276.9(6)	7.3(Tied to u_{12})	0.03	6.7
u_{20}	B(2)...B(6)	288.9(1)	7.5(2)	-0.23	7.0
u_{21}	B(2)...B(7)	340.0(1)	7.8(3)	-0.29	7.1
u_{22}	B(2)...B(9)	289.3(10)	7.9(Tied to u_{20})	-0.13	7.3
u_{23}	B(2)...H(13)	240.4(10)	11.0(Tied to u_{37})	0.11	11.5
u_{24}	B(2)...H(14)	257.6(6)	11.8(Tied to u_{37})	-0.5	12.3
u_{25}	B(2)...H(15)	388.8(10)	13.7(Tied to u_{40})	-1.11	11.6
u_{26}	B(2)...H(19)	394.6(4)	13.3(Tied to u_{40})	-1.16	11.3
u_{27}	B(2)...H(20)	456.5(3)	10.5(fixed)	-1.41	10.5
u_{28}	B(2)...H(22)	265.8(10)	11.5(Tied to u_{37})	-0.65	12.0

u_{29}	B(2)...C(24)	403.6(4)	9.1(Tied to u_{40})	-0.5	7.7
u_{30}	B(2)...C(25)	518.3(4)	10.9(4)	-2.13	10.0
u_{31}	B(2)...H(26)	621.8(12)	13.9(fixed)	-4.74	13.9
u_{32}	B(3)...B(6)	290.8(9)	8.1(Tied to u_{20})	-0.01	7.5
u_{33}	B(3)...H(13)	369.3(12)	14.0(Tied to u_{40})	-0.62	10.5
u_{34}	B(3)...H(14)	265.1(9)	11.5(Tied to u_{37})	-0.67	12.0
u_{35}	B(3)...H(15)	394.4(4)	13.3(Tied to u_{40})	-1.18	11.3
u_{36}	B(3)...H(16)	456.5(3)	10.5(fixed)	-1.41	10.5
u_{37}	B(3)...H(19)	258.3(5)	11.8(6)	-0.46	12.4
u_{38}	B(3)...H(20)	390.1(9)	13.9(Tied to u_{40})	-1.02	11.7
u_{39}	B(3)...C(24)	270.9(6)	9.4(Tied to u_{12})	0.1	8.7
u_{40}	B(3)...C(25)	377.6(6)	13.9(4)	-1.2	11.8
u_{41}	B(3)...H(26)	478.2(11)	15.9(fixed)	-3.44	15.9
u_{42}	C(4)...H(13)	417.4(11)	9.5(fixed)	-0.37	9.5
u_{43}	C(4)...H(14)	387.3(9)	12.8(Tied to u_{40})	-0.86	10.8
u_{44}	C(4)...H(19)	251.1(8)	11.5(Tied to u_{37})	-0.54	12.1
u_{45}	C(4)...C(25)	265.3(6)	5.4(6)	-1.08	5.1
u_{46}	C(4)...H(26)	373.2(13)	10.2(Tied to u_{40})	-3.1	8.7
u_{47}	H(13)...H(14)	277.4(14)	18.5(fixed)	-0.33	18.5
u_{48}	H(13)...H(19)	473.0(15)	14.3(fixed)	-1.52	14.3
u_{49}	H(13)...C(24)	559.9(12)	9.8(fixed)	-1.08	9.8
u_{50}	H(13)...C(25)	681.3(12)	10.0(fixed)	-3.01	10.0
u_{51}	H(13)...H(26)	788.5(23)	12.4(fixed)	-5.97	12.4
u_{52}	H(14)...H(15)	293.3(10)	19.8(fixed)	-0.63	19.8
u_{53}	H(14)...H(16)	475.1(16)	16.1(fixed)	-2.06	16.1
u_{54}	H(14)...H(19)	319.5(21)	18.9(fixed)	-0.7	18.9
u_{55}	H(14)...H(20)	492.0(8)	15.4(fixed)	-2.06	15.4
u_{56}	H(14)...H(21)	573.2(6)	13.0(fixed)	-2.62	13.0
u_{57}	H(14)...C(24)	504.7(10)	12.6(fixed)	-1.37	12.6
u_{58}	H(14)...C(25)	613.0(10)	15.7(fixed)	-3.04	15.7
u_{59}	H(14)...H(26)	712.2(15)	20.1(fixed)	-5.7	20.1
u_{60}	H(19)...H(20)	293.9(9)	19.8(fixed)	-0.61	19.8

u_{61}	H(19)...H(21)	476.1(14)	16.2(fixed)	-2.02	16.2
u_{62}	H(19)...C(24)	296.0(14)	16.9(fixed)	-0.38	16.9
u_{63}	H(19)...C(25)	374.7(16)	26.4(Tied to u_{40})	-1.19	22.3
u_{64}	H(19)...H(26)	461.1(18)	27.5(fixed)	-3.03	27.5
u_{65}	C(24)...H(26)	231.6(12)	7.8(fixed)	-1.58	7.8

Table S5 Cartesian coordinates for the GED structure of 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C(1)	-7.5909	0.0000	0.0000	H(20)	-7.4756	0.7810	2.4037
B(2)	-6.8139	1.5242	0.0000	H(21)	-7.4756	-2.0447	1.4856
B(3)	-6.8139	0.4710	1.4496	H(22)	-7.4756	-2.0447	-1.4856
B(4)	-6.8139	-1.2331	0.8959	H(23)	-7.4756	0.7810	-2.4037
B(5)	-6.8139	-1.2331	-0.8959	H(24)	-4.6566	2.0412	1.4830
B(6)	-6.8139	0.4710	-1.4496	H(25)	-4.6566	-0.7797	2.3996
B(7)	-5.3208	1.2309	0.8943	H(26)	-4.6566	-2.5231	0.0000
B(8)	-5.3208	-0.4702	1.4470	H(27)	-4.6566	-0.7797	-2.3996
B(9)	-5.3208	-1.5215	0.0000	H(28)	-4.6566	2.0412	-1.4830
B(10)	-5.3208	-0.4702	-1.4470	H(29)	-8.6793	0.0000	0.0000
B(11)	-5.3208	1.2309	-0.8943	H(30)	1.7193	1.7444	0.0000
C(12)	-4.5079	0.0000	0.0000	H(31)	0.2621	2.2654	0.8935
C(13)	-3.0664	0.0000	0.0000	H(32)	0.2621	2.2654	-0.8935
C(14)	-1.8398	0.0000	0.0000	H(33)	1.7193	-0.8722	1.5107
Si(15)	0.0000	0.0000	0.0000	H(34)	0.2621	-1.9065	1.5152
C(16)	0.6310	1.7650	0.0000	H(35)	0.2621	-0.3589	2.4086
C(17)	0.6310	-0.8825	1.5285	H(36)	1.7193	-0.8722	-1.5107
C(18)	0.6310	-0.8825	-1.5285	H(37)	0.2621	-0.3589	-2.4086
H(19)	-7.4756	2.5274	0.0000	H(38)	0.2621	-1.9065	-1.5152

Table S6 Cartesian coordinates for the GED structure of 1-HCC-1,12-$C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*
C(1)	-5.7433	0.0000	0.0000
B(2)	-4.9789	1.5227	0.0000
B(3)	-3.4713	1.2377	0.8992
C(4)	-2.6647	0.0000	0.0000
B(5)	-3.4713	1.2377	-0.8992
B(6)	-3.4713	-0.4728	-1.4550
B(7)	-3.4713	-1.5299	0.0000
B(8)	-3.4713	-0.4728	1.4550
B(9)	-4.9789	-1.2319	0.8950
B(10)	-4.9789	-1.2319	-0.8950
B(11)	-4.9789	0.4706	-1.4482
B(12)	-4.9789	0.4706	1.4482
H(13)	-6.8448	0.0000	0.0000
H(14)	-5.6299	0.7761	2.3887
H(15)	-5.6299	-2.0320	1.4763
H(16)	-5.6299	-2.0320	-1.4763
H(17)	-5.6299	0.7761	-2.3887
H(18)	-5.6299	2.5117	0.0000
H(19)	-2.8172	-0.7777	2.3935
H(20)	-2.8172	-2.5167	0.0000
H(21)	-2.8172	-0.7777	-2.3935
H(22)	-2.8172	2.0361	-1.4793
H(23)	-2.8172	2.0361	1.4793
C(24)	-1.2333	0.0000	0.0000
C(25)	0.0000	0.0000	0.0000
H(26)	1.1015	0.0000	0.0000

Table S7 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C(1)	-3.9577	-0.0032	0.0003	H(20)	-3.8081	1.1662	2.2333
B(2)	-3.1793	1.4897	-0.2533	H(21)	-3.8069	-1.7656	1.8024
B(3)	-3.1787	0.6994	1.3414	H(22)	-3.8070	-2.2617	-1.1190
B(4)	-3.1780	-1.0614	1.0825	H(23)	-3.8084	0.3635	-2.4936
B(5)	-3.1781	-1.3593	-0.6721	H(24)	-1.0504	2.2546	1.1182
B(6)	-3.1789	0.2173	-1.4976	H(25)	-1.0491	-0.3682	2.4916
B(7)	-1.6882	1.3581	0.6741	H(26)	-1.0485	-2.4848	0.4216
B(8)	-1.6874	-0.2230	1.5020	H(27)	-1.0494	-1.1702	-2.2312
B(9)	-1.6871	-1.4990	0.2542	H(28)	-1.0506	1.7590	-1.8006
B(10)	-1.6876	-0.7065	-1.3450	H(29)	-5.0453	-0.0037	0.0004
B(11)	-1.6883	1.0593	-1.0854	H(30)	5.3140	1.7802	0.4616
C(12)	-0.8819	-0.0019	-0.0001	H(31)	3.8592	2.0252	1.4385
C(13)	0.5555	-0.0013	-0.0003	H(32)	3.8592	2.4692	-0.2729
C(14)	1.7899	-0.0009	-0.0003	H(33)	5.3151	-1.2892	1.3103
Si(15)	3.6370	-0.0001	-0.0002	H(34)	3.8609	-2.2586	1.0344
C(16)	4.2202	1.7308	0.4489	H(35)	3.8603	-0.9985	2.2746
C(17)	4.2212	-1.2541	1.2742	H(36)	5.3151	-0.4894	-1.7721
C(18)	4.2212	-0.4764	-1.7235	H(37)	3.8603	0.2333	-2.4735
H(19)	-3.8090	2.4820	-0.4217	H(38)	3.8609	-1.4708	-2.0023
Energy	-814.4935						

Table S8 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-HCC-1,12-$C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*
C(1)	0.0000	0.0000	-2.0592
B(2)	0.8897	1.2246	-1.2807
B(3)	0.0000	1.5180	0.2099
C(4)	0.0000	0.0000	1.0135
B(5)	1.4437	0.4691	0.2099
B(6)	0.8922	-1.2281	0.2099
B(7)	-0.8922	-1.2281	0.2099
B(8)	-1.4437	0.4691	0.2099
B(9)	-1.4396	-0.4678	-1.2807
B(10)	0.0000	-1.5137	-1.2807
B(11)	1.4396	-0.4678	-1.2807
B(12)	-0.8897	1.2246	-1.2807
H(13)	0.0000	0.0000	-3.1468
H(14)	-1.4815	2.0390	-1.9098
H(15)	-2.3970	-0.7788	-1.9098
H(16)	0.0000	-2.5204	-1.9098
H(17)	2.3970	-0.7788	-1.9098
H(18)	1.4815	2.0390	-1.9098
H(19)	-2.3943	0.7779	0.8490
H(20)	-1.4797	-2.0367	0.8490
H(21)	1.4797	-2.0367	0.8490
H(22)	2.3943	0.7779	0.8490
H(23)	0.0000	2.5175	0.8490
C(24)	0.0000	0.0000	2.4523
C(25)	0.0000	0.0000	3.6731
H(26)	0.0000	0.0000	4.7406
Energy	-406.7747		

Table S9 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1,12-$(Me_3SiCC)_2$-1,12-$C_2B_{10}H_{10}$.

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C(1)	0.0002	-1.5526	0.0000	H(27)	0.7787	1.3799	-2.3959
B(2)	-1.5168	-0.7443	0.0000	H(28)	-2.0384	1.3794	-1.4806
B(3)	-0.4687	-0.7443	1.4430	H(29)	-1.8372	7.7494	0.0000
B(4)	1.2274	-0.7441	0.8917	H(30)	-2.3217	6.2953	0.8840
B(5)	1.2274	-0.7441	-0.8917	H(31)	-2.3217	6.2953	-0.8840
B(6)	-0.4687	-0.7443	-1.4430	H(32)	0.9198	7.7487	1.5913
B(7)	-1.2273	0.7440	0.8917	H(33)	1.9263	6.2935	1.5692
B(8)	0.4688	0.7442	1.4430	H(34)	0.3947	6.2950	2.4527
B(9)	1.5169	0.7443	0.0000	H(35)	0.9198	7.7487	-1.5913
B(10)	0.4688	0.7442	-1.4430	H(36)	0.3947	6.2950	-2.4527
B(11)	-1.2273	0.7440	-0.8917	H(37)	1.9263	6.2935	-1.5692
C(12)	-0.0001	1.5526	0.0000	C(38)	0.0004	-2.9891	0.0000
C(13)	-0.0003	2.9891	0.0000	C(39)	0.0004	-4.2237	0.0000
C(14)	-0.0004	4.2237	0.0000	Si(40)	-0.0001	-6.0707	0.0000
Si(15)	0.0000	6.0707	0.0000	C(41)	1.7876	-6.6556	0.0000
C(16)	-1.7877	6.6555	0.0000	C(42)	-0.8941	-6.6546	-1.5485
C(17)	0.8940	6.6548	1.5484	C(43)	-0.8941	-6.6546	1.5485
C(18)	0.8940	6.6548	-1.5484	H(44)	1.8371	-7.7495	0.0000
H(19)	-2.5189	-1.3798	0.0000	H(45)	2.3216	-6.2954	-0.8841
H(20)	-0.7785	-1.3799	2.3959	H(46)	2.3216	-6.2954	0.8841
H(21)	2.0384	-1.3794	1.4807	H(47)	-0.9199	-7.7485	-1.5915
H(22)	2.0384	-1.3794	-1.4807	H(48)	-1.9263	-6.2934	-1.5692
H(23)	-0.7785	-1.3799	-2.3959	H(49)	-0.3948	-6.2948	-2.4527
H(24)	-2.0384	1.3794	1.4806	H(50)	-0.9199	-7.7485	1.5915
H(25)	0.7787	1.3799	2.3959	H(51)	-0.3948	-6.2948	2.4527
H(26)	2.5190	1.3799	0.0000	H(52)	-1.9263	-6.2934	1.5692
Energy	-1298.1249						

Table S10 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1,12-$(HCC)_2$-1,12-$C_2B_{10}H_{10}$.

Atom	*x*	*y*	*z*
C(1)	0.0000	0.0000	1.5497
B(2)	0.0000	1.5174	0.7440
B(3)	0.8919	1.2276	-0.7440
C(4)	0.0000	0.0000	-1.5497
B(5)	-0.8919	1.2276	-0.7440
B(6)	-1.4432	-0.4689	-0.7440
B(7)	0.0000	-1.5174	-0.7440
B(8)	1.4432	-0.4689	-0.7440
B(9)	0.8919	-1.2276	0.7440
B(10)	-0.8919	-1.2276	0.7440
B(11)	-1.4432	0.4689	0.7440
B(12)	1.4432	0.4689	0.7440
H(13)	2.3959	0.7785	1.3797
H(14)	1.4807	-2.0380	1.3797
H(15)	-1.4807	-2.0380	1.3797
H(16)	-2.3959	0.7785	1.3797
H(17)	0.0000	2.5192	1.3797
H(18)	2.3959	-0.7785	-1.3797
H(19)	0.0000	-2.5192	-1.3797
H(20)	-2.3959	-0.7785	-1.3797
H(21)	-1.4807	2.0380	-1.3797
H(22)	1.4807	2.0380	-1.3797
C(23)	0.0000	0.0000	2.9880
C(24)	0.0000	0.0000	4.2088
H(25)	0.0000	0.0000	5.2764
C(26)	0.0000	0.0000	-2.9880
C(27)	0.0000	0.0000	-4.2088
H(28)	0.0000	0.0000	-5.2764
Energy	-482.6872		

Table S11 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-F-1,12-$C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*
C(1)	0.0000	0.0000	-1.8087
B(2)	0.8903	1.2254	-1.0308
B(3)	0.0000	1.5174	0.4599
C(4)	0.0000	0.0000	1.2314
B(5)	1.4431	0.4689	0.4599
B(6)	0.8919	-1.2276	0.4599
B(7)	-0.8919	-1.2276	0.4599
B(8)	-1.4431	0.4689	0.4599
B(9)	-1.4405	-0.4680	-1.0308
B(10)	0.0000	-1.5146	-1.0308
B(11)	1.4405	-0.4680	-1.0308
B(12)	-0.8903	1.2254	-1.0308
H(13)	0.0000	0.0000	-2.8959
H(14)	-1.4818	2.0396	-1.6595
H(15)	-2.3976	-0.7790	-1.6595
H(16)	0.0000	-2.5210	-1.6595
H(17)	2.3976	-0.7790	-1.6595
H(18)	1.4818	2.0396	-1.6595
H(19)	-2.3832	0.7743	1.1151
H(20)	-1.4729	-2.0273	1.1151
H(21)	1.4729	-2.0273	1.1151
H(22)	2.3832	0.7743	1.1151
H(23)	0.0000	2.5058	1.1151
F(24)	0.0000	0.0000	2.5947
Energy	-429.8637		

Table S12 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-Cl-1,12-$C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*
C(1)	0.0000	0.0000	-2.1161
B(2)	0.8899	1.2248	-1.3378
B(3)	0.0000	1.5176	0.1537
C(4)	0.0000	0.0000	0.9374
B(5)	1.4434	0.4690	0.1537
B(6)	0.8921	-1.2278	0.1537
B(7)	-0.8921	-1.2278	0.1537
B(8)	-1.4434	0.4690	0.1537
B(9)	-1.4398	-0.4678	-1.3378
B(10)	0.0000	-1.5139	-1.3378
B(11)	1.4398	-0.4678	-1.3378
B(12)	-0.8899	1.2248	-1.3378
H(13)	0.0000	0.0000	-3.2035
H(14)	-1.4820	2.0397	-1.9654
H(15)	-2.3978	-0.7791	-1.9654
H(16)	0.0000	-2.5212	-1.9654
H(17)	2.3978	-0.7791	-1.9654
H(18)	1.4820	2.0397	-1.9654
H(19)	-2.3893	0.7763	0.7990
H(20)	-1.4766	-2.0324	0.7990
H(21)	1.4766	-2.0324	0.7990
H(22)	2.3893	0.7763	0.7990
H(23)	0.0000	2.5122	0.7990
Cl(24)	0.0000	0.0000	2.6889
Energy	-789.8829		

Table S13 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-HO_2C-1,12- $C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*
C(1)	-0.0266	-2.3409	0.0000
B(2)	0.4538	-1.5684	1.4401
B(3)	1.2386	-0.0931	0.8896
C(4)	0.0210	0.7161	0.0000
C(5)	0.1186	2.2248	0.0000
B(6)	1.4996	-1.5895	0.0000
B(7)	1.2386	-0.0931	-0.8896
B(8)	-0.4633	-0.0623	-1.4412
B(9)	-1.5134	-0.0536	0.0000
B(10)	-0.4633	-0.0623	1.4412
B(11)	-1.2396	-1.5457	0.8896
B(12)	-1.2396	-1.5457	-0.8896
B(13)	0.4538	-1.5684	-1.4401
H(14)	2.4942	-2.2370	0.0000
H(15)	0.7543	-2.2015	-2.3981
H(16)	-2.0628	-2.1631	-1.4812
H(17)	-2.0628	-2.1631	1.4812
H(18)	0.7543	-2.2015	2.3981
H(19)	2.0546	0.5328	-1.4783
H(20)	-0.7608	0.5806	-2.3936
H(21)	-2.5126	0.5812	0.0000
H(22)	-0.7608	0.5806	2.3936
H(23)	2.0546	0.5328	1.4783
H(24)	-0.0438	-3.4283	0.0000
O(25)	1.1681	2.8381	0.0000
O(26)	-1.1025	2.8027	0.0000
H(27)	-0.9370	3.7703	0.0000
Energy	-518.9470		

Table S14 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-H_3C-1,12- $C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*
C(1)	1.2314	0.0000	-0.0002
B(2)	0.4222	-1.4361	-0.4666
B(3)	-1.0684	-0.8891	-1.2249
B(4)	-1.0684	0.8901	-1.2242
C(5)	-1.8469	0.0000	0.0002
B(6)	-1.0691	-1.4397	0.4673
B(7)	0.4254	-0.8883	1.2195
B(8)	-1.0676	-0.0007	1.5137
B(9)	-1.0691	1.4393	0.4685
B(10)	0.4254	0.8872	1.2202
B(11)	0.4222	1.4365	-0.4654
B(12)	0.4269	0.0007	-1.5081
H(13)	1.0620	0.0011	-2.5124
H(14)	1.0576	-2.3901	-0.7783
H(15)	-1.6995	-1.4785	-2.0399
H(16)	-1.6995	1.4802	-2.0386
H(17)	1.0576	2.3908	-0.7763
H(18)	1.0607	-1.4771	2.0326
H(19)	-1.7005	-2.3958	0.7787
H(20)	-2.9343	0.0000	0.0003
H(21)	-1.7005	2.3951	0.7807
H(22)	1.0607	1.4753	2.0339
H(23)	-1.6982	-0.0011	2.5198
C(24)	2.7556	0.0000	0.0000
H(25)	3.1317	-0.0004	1.0255
H(26)	3.1322	-0.8879	-0.5131
H(27)	3.1322	0.8883	-0.5124
Energy	-370.0333		

Table S15 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-NC-1,12- $C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*
C(1)	0.5498	-0.2204	0.8262
B(2)	-1.1228	-0.6004	0.8650
B(3)	-1.5096	-0.9775	-0.8103
B(4)	-0.0156	-0.8630	-1.7737
C(5)	-1.1030	0.4424	-1.6579
B(6)	-1.8611	0.6373	-0.1456
B(7)	-0.5482	1.0933	0.9346
B(8)	-0.5844	1.7499	-0.6982
B(9)	0.5562	0.8227	-1.7044
B(10)	0.9530	1.2084	-0.0334
B(11)	1.3062	-0.4142	-0.7013
B(12)	0.0233	-1.5322	-0.1461
H(13)	0.3082	-2.6408	0.1639
H(14)	-1.5863	-1.1007	1.8352
H(15)	-2.3984	-1.6727	-1.1772
H(16)	0.0880	-1.4820	-2.7806
H(17)	2.4288	-0.7929	-0.7540
H(18)	-0.6365	1.6991	1.9503
H(19)	-2.9834	1.0150	-0.0709
H(20)	-1.6912	0.6782	-2.5420
H(21)	1.0397	1.3234	-2.6653
H(22)	1.8449	1.8894	0.3501
H(23)	-0.8586	2.8667	-0.9906
C(24)	1.3308	-0.5338	2.0004
N(25)	1.9707	-0.7905	2.9623
Energy	-422.8615		

Table S16 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-Ph-1,12-$C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C(1)	2.1801	1.2131	-0.0103	C(18)	-3.1397	-0.0110	0.0438
C(2)	1.4624	0.0083	-0.0341	H(19)	-4.2268	-0.0184	0.0726
C(3)	2.1674	-1.2044	-0.0094	H(20)	-2.9176	-0.1766	2.5542
C(4)	3.5624	-1.2087	0.0028	H(21)	-2.9505	-2.4535	0.6564
C(5)	4.2727	-0.0072	0.0098	H(22)	-3.0330	-1.3558	-2.0918
C(6)	3.5752	1.2016	0.0042	H(23)	-3.0484	1.6048	-1.8954
C(7)	-0.0443	0.0105	-0.0374	H(24)	-2.9759	2.3315	0.9725
B(8)	-0.8753	-1.3949	-0.5808	H(25)	1.6308	-2.1476	-0.0011
B(9)	-0.8277	-0.9619	1.1429	H(26)	4.0933	-2.1575	0.0171
B(10)	-0.8357	0.8125	1.2606	H(27)	5.3598	-0.0130	0.0213
B(11)	-0.8911	1.4673	-0.3908	H(28)	4.1164	2.1446	0.0188
B(12)	-0.9031	0.1054	-1.5289	H(29)	1.6549	2.1622	-0.0030
B(13)	-2.3977	0.9600	-1.1399	H(30)	-0.3018	0.1760	-2.5503
B(14)	-2.3537	1.3978	0.5842	H(31)	-0.3232	2.4687	-0.6731
B(15)	-2.3180	-0.1048	1.5318	H(32)	-0.1865	1.3515	2.0960
B(16)	-2.3384	-1.4704	0.3940	H(33)	-0.1755	-1.5988	1.9034
B(17)	-2.3885	-0.8098	-1.2572	H(34)	-0.2875	-2.3385	-0.9931
Energy	-561.1689						

Table S17 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1,12-Ph_2-1,12- $C_2B_{10}H_{10}$.

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C(1)	3.7693	-1.1956	-0.0005	C(23)	-5.1636	1.2159	-0.0006
C(2)	3.0766	0.0249	0.0001	C(24)	-3.7689	1.1955	-0.0007
C(3)	3.8076	1.2217	0.0007	H(25)	-3.2940	-2.1769	0.0011
C(4)	5.2027	1.1945	0.0006	H(26)	-5.7552	-2.1310	0.0012
C(5)	5.8872	-0.0218	-0.0001	H(27)	-6.9742	0.0400	0.0001
C(6)	5.1641	-1.2156	-0.0006	H(28)	-5.6840	2.1706	-0.0011
C(7)	1.5708	0.0327	0.0002	H(29)	-3.2205	2.1324	-0.0012
B(8)	0.7083	1.5214	0.0002	H(30)	-1.3605	-0.8107	-2.3970
B(9)	0.7409	0.4832	-1.4380	H(31)	-1.3957	2.0071	-1.4936
B(10)	0.7707	-1.1999	-0.8887	H(32)	-1.3961	2.0071	1.4935
B(11)	0.7703	-1.2000	0.8887	H(33)	-1.3611	-0.8108	2.3966
B(12)	0.7406	0.4831	1.4382	H(34)	-1.2566	-2.5730	-0.0004
B(13)	-0.7407	-0.4835	1.4381	H(35)	3.2934	2.1765	0.0013
B(14)	-0.7086	-1.5216	-0.0001	H(36)	5.7544	2.1315	0.0010
B(15)	-0.7404	-0.4834	-1.4383	H(37)	6.9742	-0.0391	-0.0002
B(16)	-0.7704	1.1999	-0.8887	H(38)	5.6846	-2.1702	-0.0012
B(17)	-0.7706	1.1999	0.8887	H(39)	3.2213	-2.1327	-0.0009
C(18)	-1.5709	-0.0326	-0.0002	H(40)	1.3610	0.8110	2.3966
C(19)	-3.0768	-0.0254	-0.0002	H(41)	1.3963	-2.0070	1.4933
C(20)	-3.8080	-1.2219	0.0006	H(42)	1.3967	-2.0069	-1.4933
C(21)	-5.2031	-1.1942	0.0007	H(43)	1.3614	0.8112	-2.3962
C(22)	-5.8872	0.0223	0.0000	H(44)	1.2559	2.5730	0.0002
Energy	-791.4757						

Table S18 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-(1'-1',12'- $C_2B_{10}H_{11}$)-1,12- $C_2B_{10}H_{11}$ – C,C'-bis(para-carborane).

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C(1)	-0.7678	-0.0064	-0.0418	B(24)	1.6060	0.1020	1.5212
B(2)	-1.6053	0.1625	-1.5150	H(25)	-1.0202	0.2642	-2.5398
B(3)	-1.6038	-1.3874	-0.6265	H(26)	0.9989	2.4561	0.6252
B(4)	-1.5926	-1.0118	1.1126	H(27)	-1.0098	-2.3268	-1.0353
B(5)	-1.5916	0.7512	1.3056	H(28)	-0.9810	-1.6845	1.8716
B(6)	-3.0816	-0.1609	1.5070	H(29)	-0.9741	1.2613	2.1780
B(7)	-3.0896	-1.4772	0.3171	H(30)	-0.9987	2.4794	-0.5263
B(8)	-3.0979	-0.7514	-1.3056	H(31)	-3.7288	-1.2500	-2.1787
C(9)	-3.8715	0.0014	0.0081	H(32)	-3.7113	-2.4665	0.5265
B(10)	-3.0879	1.3782	0.6266	H(33)	-3.6944	-0.2723	2.5175
B(11)	-3.0922	1.0170	-1.1126	H(34)	-3.7050	2.3035	1.0414
B(12)	-1.5986	1.4849	-0.2950	H(35)	-3.7189	1.6944	-1.8593
C(13)	0.7675	-0.0079	0.0433	H(36)	-4.9591	0.0025	0.0120
B(14)	1.5986	1.4717	0.3534	H(37)	0.9724	1.3460	-2.1257
B(15)	1.5904	0.8018	-1.2746	H(38)	0.9802	-1.6101	-1.9351
B(16)	1.5919	-0.9672	-1.1509	H(39)	1.0114	-2.3658	0.9441
B(17)	1.6050	-1.4110	0.5718	H(40)	1.0217	0.1634	2.5496
B(18)	3.0898	-1.4632	-0.3755	H(41)	3.7036	2.3431	-0.9509
B(19)	3.0804	-0.1015	-1.5128	H(42)	3.6925	-0.1726	-2.5275
B(20)	3.0871	1.4019	-0.5726	H(43)	3.7114	-2.4434	-0.6245
C(21)	3.8715	0.0022	-0.0091	H(44)	3.7311	-1.3344	2.1266
B(22)	3.0992	-0.8018	1.2745	H(45)	3.7197	1.6203	1.9234
B(23)	3.0926	0.9728	1.1510	H(46)	4.9592	0.0036	-0.0140
Energy	-660.5611						

Table S19 Cartesian coordinates for the MP2(fc)/6-31G* optimised structure of 1-HCC-1,2-$C_2B_{10}H_{11}$.

Atom	*x*	*y*	*z*
B(1)	-2.2408	0.0001	-0.0655
H(2)	-3.4280	0.0001	-0.1443
B(3)	-1.3260	-1.4478	0.4411
H(4)	-1.8386	-2.4823	0.7272
B(5)	-1.3711	-0.0026	1.4878
H(6)	-1.9240	-0.0047	2.5416
B(7)	-1.3256	1.4462	0.4458
H(8)	-1.8388	2.4792	0.7362
B(9)	-1.2533	0.8920	-1.2399
H(10)	-1.5961	1.4864	-2.2096
B(11)	-1.2530	-0.8877	-1.2430
H(12)	-1.5950	-1.4797	-2.2144
B(13)	0.2096	-1.4513	-0.4180
H(14)	0.9080	-2.3269	-0.8061
B(15)	0.1451	-0.8949	1.2677
H(16)	0.7930	-1.4849	2.0686
B(17)	0.1452	0.8909	1.2707
H(18)	0.7920	1.4779	2.0746
B(19)	0.2097	1.4531	-0.4135
H(20)	0.9085	2.3300	-0.7980
C(21)	0.1808	0.0023	-1.3300
H(22)	0.8077	0.0037	-2.2185
C(23)	0.9994	-0.0003	0.0937
C(24)	2.4327	-0.0005	0.0311
C(25)	3.6524	0.0005	-0.0230
H(26)	4.7201	-0.0014	-0.0546
Energy	-406.7443		

Table S20 Non-bond distances (r_a/Å) and amplitudes of vibration (u/Å) obtained in the GED refinement of **5**.

Number	Atom pair	r_a	Amplitude	Restraint
u_{14}	Si(15)...H(30)	2.445(12)	0.100(7)	
u_{15}	C(12)...H(7)	2.521(12)	0.112	Tied to u_{17}
u_{16}	C(1)...H(2)	2.515(12)	0.114	Tied to u_{17}
u_{17}	B(7)...H(8)	2.593(8)	0.118(9)	
u_{18}	B(2)...H(3)	2.593(7)	0.118	Tied to u_{17}
u_{19}	B(2)...H(7)	2.661(12)	0.112	Tied to u_{17}
u_{20}	C(1)...C(14)	2.656(6)	0.048	Tied to u_{17}
u_{21}	B(7)...H(2)	2.660(14)	0.113	Tied to u_{17}
u_{22}	B(2)...C(13)	2.715(9)	0.104	Tied to u_{23}
u_{23}	C(12)...B(2)	2.732(7)	0.079(4)	
u_{26}	B(2)...B(8)	2.883(3)	0.079(4)	
u_{27}	B(7)...B(9)	2.900(11)	0.082	Tied to u_{26}
u_{28}	B(2)...B(4)	2.896(9)	0.085	Tied to u_{26}
u_{31}	C(13)...H(2)	2.972(18)	0.183	Tied to u_{32}
u_{32}	C(14)...C(16)	3.023(9)	0.125(8)	
u_{33}	C(13)...Si(15)	3.043(6)	0.064	Tied to u_{32}
u_{34}	C(1)...C(12)	3.076(9)	0.070	Tied to u_{32}
u_{35}	C(16)...C(17)	3.056(11)	0.130	Tied to u_{32}
u_{42}	B(2)...B(9)	3.392(3)	0.082(4)	
u_{45}	B(2)...C(14)	3.753(9)	0.159(15)	
u_{47}	C(12)...H(2)	3.858(11)	0.119	Tied to u_{50}
u_{48}	C(1)...H(7)	3.883(10)	0.120	Tied to u_{50}
u_{49}	B(7)...H(9)	3.910(13)	0.130	Tied to u_{50}
u_{50}	B(2)...H(4)	3.905(11)	0.131(4)	
u_{51}	B(2)...H(8)	3.956(6)	0.126	Tied to u_{50}
u_{52}	B(7)...H(4)	3.955(7)	0.126	Tied to u_{50}
u_{53}	C(14)...H(30)	3.914(11)	0.143	Tied to u_{50}
u_{54}	C(13)...C(16)	4.071(11)	0.186(23)	
u_{55}	B(7)...C(13)	4.037(6)	0.099(6)	
u_{56}	C(16)...H(34)	3.948(13)	0.145	Tied to u_{50}
u_{57}	C(13)...H(31)	4.095(19)	0.372	Tied to u_{54}
u_{61}	C(1)...Si(15)	4.464(7)	0.091(5)	

u_{62}	C(12)...C(13)	4.512(9)	0.090	Tied to u_{61}
u_{63}	B(7)...H(5)	4.572(6)	0.135	Tied to u_{61}
u_{64}	B(2)...H(9)	4.573(6)	0.135	Tied to u_{61}
u_{72}	C(13)...H(7)	5.063(12)	0.144	Tied to u_{76}
u_{76}	B(7)...C(14)	5.165(5)	0.125(6)	
u_{77}	Si(15)...H(2)	5.191(20)	0.336	Tied to u_{76}
u_{80}	C(1)...C(16)	5.368(12)	0.260	Tied to u_{83}
u_{83}	B(2)...Si(15)	5.448(8)	0.188(6)	
u_{130}	B(7)...Si(15)	6.903(6)	0.204(7)	

Table S21 Non-bond distances (r_a/Å) and amplitudes of vibration (u/Å) obtained in the GED refinement of **6**.

Number	Atom pair	r_a	Amplitude	Restraint
u_{12}	C(12)...B(2)	2.739(6)	0.072(3)	
u_{13}	C(1)...C(12)	3.083(5)	0.065(6)	
u_{14}	C(12)...H(7)	2.503(9)	0.114	Tied to u_{37}
u_{15}	C(12)...H(2)	3.848(10)	0.127	Tied to u_{40}
u_{19}	B(7)...C(1)	2.769(6)	0.073	Tied to u_{12}
u_{20}	B(2)...B(8)	2.889(1)	0.075(2)	
u_{21}	B(2)...B(9)	3.400(1)	0.078(3)	
u_{22}	B(2)...B(5)	2.893(10)	0.079	Tied to u_{20}
u_{23}	B(7)...H(12)	2.404(10)	0.110	Tied to u_{37}
u_{24}	B(7)...H(8)	2.576(6)	0.118	Tied to u_{37}
u_{25}	B(7)...H(9)	3.888(10)	0.137	Tied to u_{40}
u_{26}	B(7)...H(4)	3.946(4)	0.133	Tied to u_{40}
u_{28}	B(7)...H(2)	2.658(10)	0.115	Tied to u_{37}
u_{29}	B(7)...C(13)	4.036(4)	0.091	Tied to u_{40}
u_{30}	B(7)...C(14)	5.183(4)	0.109(4)	
u_{32}	B(2)...B(4)	2.908(9)	0.08076	Tied to u_{20}
u_{33}	B(2)...H(12)	3.693(12)	0.140	Tied to u_{40}
u_{34}	B(2)...H(8)	2.651(9)	0.115	Tied to u_{37}
u_{35}	B(2)...H(9)	3.944(4)	0.133	Tied to u_{40}
u_{37}	B(2)...H(4)	2.583(5)	0.118(6)	
u_{38}	B(2)...H(5)	3.901(9)	0.139	Tied to u_{40}
u_{39}	B(2)...C(13)	2.709(6)	0.094	Tied to u_{12}
u_{40}	B(2)...C(14)	3.776(6)	0.139(4)	
u_{43}	C(1)...H(12)	3.873(9)	0.128	Tied to u_{40}
u_{44}	C(1)...H(2)	2.511(8)	0.115	Tied to u_{37}
u_{45}	C(1)...C(14)	2.653(6)	0.054(6)	
u_{46}	C(1)...H(14)	3.732(13)	0.102	Tied to u_{40}
u_{63}	H(2)...C(14)	3.747(15)	0.264	Tied to u_{40}

Table S22 Calculated (r_e) and experimental (r_{h1}) structure of 1,12-$C_2B_{10}H_{11}$-C≡CH. All bond lengths in pm and all angles in °.

Parameter	HF/6-31G*	HF/6-31+G*	HF/6-311G*	HF/6-311+G*	GED
C(12)-B(7)	170.8	170.7	171.0	171.0	170.4(5)
C(12)-H(12)	107.3	107.3	107.2	107.2	110.2(12)
B(2)-B(7)	177.1	177.1	177.3	177.2	177.8(4)
B(7)-H(7)	117.9	117.9	117.9	117.9	118.4(3)
B(2)-C(1)	172.4	172.4	172.6	172.6	173.0(5)
B(2)-H(2)	117.7	117.7	117.7	117.7	118.4(3)
C(1)-C(13)	145.0	145.0	144.8	144.8	143.1(5)
C(13)-C(14)	**118.5**	**118.7**	**118.2**	**118.3**	**123.3(5)**
C(14)-H(14)	105.7	105.8	105.6	105.6	110.2(12)
C(1)...C(12)	306.6	306.5	306.7	306.8	307.9(5)
B(7)-C(12)-H(12)	116.9	116.8	116.8	116.8	116.7(2)
C(12)-B(7)-H(7)	120.6	120.6	120.5	120.6	120.0(7)
C(1)-B(2)-H(2)	119.7	119.6	119.5	119.6	118.7(7)
C(13)-C(1)-B(2)	117.5	117.5	117.4	117.5	117.8(3)
	MP2/6-31G*	MP2/6-31+G*	MP2/6-311G*	MP2/cc-pVDZ	GED
C(12)-B(7)	170.2	170.4	171.0	171.9	170.4(5)
C(12)-H(12)	108.8	108.9	108.6	109.4	110.2(12)
B(2)-B(7)	176.1	176.2	176.8	178.2	177.8(4)
B(7)-H(7)	118.7	118.8	118.6	119.5	118.4(3)
B(2)-C(1)	171.8	172.0	172.4	173.3	173.0(5)
B(2)-H(2)	118.6	118.7	118.6	119.4	118.4(3)
C(1)-C(13)	143.9	144.0	143.8	144.6	143.1(5)

C(13)-C(14)	**122.1**	**122.3**	**122.0**	**123.3**	**123.3(5)**			
C(14)-H(14)	106.8	106.9	106.6	107.6	110.2(12)			
C(1)...C(12)	307.3	307.5	307.9	309.3	307.9(5)			
B(7)-C(12)-H(12)	117.2	117.2	117.1	117.0	116.7(2)			
C(12)-B(7)-H(7)	120.8	120.8	120.6	120.7	120.0(7)			
C(1)-B(2)-H(2)	119.5	119.5	119.2	119.3	118.7(7)			
C(13)-C(1)-B(2)	117.9	117.9	117.8	117.6	117.8(3)			
	B3LYP/ 6-31G*	B3LYP/ 6-31+G*	B3LYP/ 6-311G*	B3LYP/ 6-311+G*	B3LYP/ 6-311+G**	B3LYP/ cc-pVDZ	B3LYP/ Aug-cc-pVDZ	GED
C(12)-B(7)	170.8	170.8	170.7	170.7	170.7	171.0	171.0	170.4(5)
C(12)-H(12)	108.4	108.5	108.1	108.1	108.1	108.8	108.7	110.2(12)
B(2)-B(7)	176.4	176.5	176.4	176.4	176.4	177.1	176.9	177.8(4)
B(7)-H(7)	118.4	118.4	118.1	118.1	117.9	119.1	118.6	118.4(3)
B(2)-C(1)	172.7	172.8	172.7	172.7	172.7	172.9	172.8	173.0(5)
B(2)-H(2)	118.3	118.3	118.0	118.0	117.7	118.9	118.5	118.4(3)
C(1)-C(13)	144.0	144.2	143.7	143.8	143.8	144.3	144.2	143.1(5)
C(13)-C(14)	**120.6**	**120.7**	**120.0**	**120.1**	**120.1**	**121.1**	**121.0**	**123.3(5)**
C(14)-H(14)	106.7	106.8	106.4	106.4	106.3	107.3	106.9	110.2(12)
C(1)...C(12)	308.7	308.9	308.7	308.7	308.6	308.7	308.5	307.9(5)
B(7)-C(12)-H(12)	117.3	117.3	117.3	117.3	117.2	117.1	117.1	116.7(2)
C(12)-B(7)-H(7)	120.7	120.7	120.7	120.7	120.9	120.9	120.9	120.0(7)
C(1)-B(2)-H(2)	119.6	119.6	119.5	119.6	119.7	119.7	119.6	118.7(7)
C(13)-C(1)-B(2)	118.0	118.1	118.0	118.0	118.0	117.9	117.9	117.8(3)

Figure S1 Experimental and final weighted difference (experimental-theoretical) molecular scattering intensities for 1-Me_3SiCC-1,12-$C_2B_{10}H_{11}$.

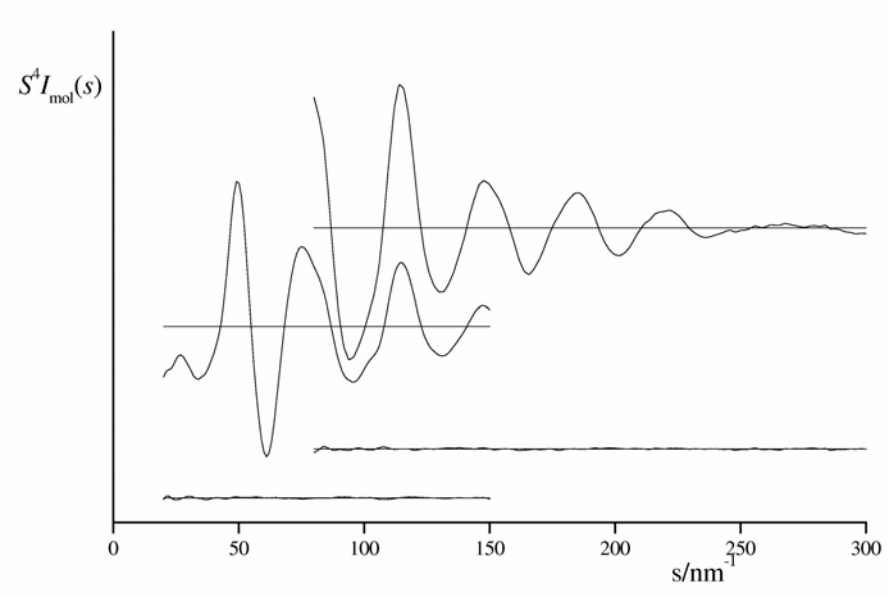

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Figure S2 Experimental and final weighted difference (experimental-theoretical) molecular scattering intensities for 1-HCC-1,12-$C_2B_{10}H_{11}$.