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Gas-phase electron diffraction studies of the icosahedral carbaboranes, *ortho-*, *meta-* and *para*-$C_2B_{10}H_{12}$

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Parameters used to define gas-phase structures

Closo-1,2-$C_2B_{10}H_{12}$ (*ortho*-carbaborane)

The model for *ortho*-carbaborane was constructed in C_{2v} symmetry, reflecting the structure found in the theoretical calculations. Twenty-two geometrical parameters described the structure. The C(1)–C(2) bond length is p_1 (*r*CC). The distance from the midpoint of the C–C bond (corresponding to the *x* axis) to the projection of the B(3) position onto the *y* axis (point a) is p_2, and p_3 is the distance from a to B(3) along the *z* axis. Parameter p_4 is the distance from a to the projection of the B(4) position onto the *y* axis (point b), p_5 is the distance from b to B(4) along the *x* axis, and p_6 is the distance from b to B(4) along the *z* axis. The distance from b to the projection of the B(8) position onto the *y* axis (point c) is p_7 and p_8 is the distance from c to B(8) along the *z* axis, while p_9 is the distance from c to the midpoint of the B(9)–B(12) bond and p_{10} is the B(9)–B(12) bond distance. The C–H bond distance is p_{11}, while p_{12}–p_{16} define the four distinct B–H distances: p_{12} is the average B–H distance and p_{13}–p_{16} are the differences from this average distance. Strictly speaking, one of these five parameters used to define four distinct distances is redundant, but in practice the differences were all held fixed at the *ab initio* values throughout the refinement, while the average distance was allowed to refine. The positions of the hydrogen atoms were defined by projecting straight lines from the centre of mass (c.o.m.) of the C_2B_{10} core through the corresponding heavy atoms and out the appropriate distance. Parameters p_{17}–p_{22} define the angle of deviations from straight lines drawn from the c.o.m. through the heavy atoms, for the C–H and four distinct B–H bonds. All of the hydrogens except H(16) and its symmetry equivalents lie on a mirror plane [H(13) and H(21) on the *xy* plane, H(15) and H(20) on the *yz* plane], and so they require just one angle to describe their position. Each angle is defined in terms of displacement away from a mirror plane on which it does not lie, a positive angle indicating movement away from that plane. The refined parameter values are listed in Table 2.

Closo-1,7-$C_2B_{10}H_{12}$ (*meta*-carbaborane)

The model for the *meta* carbaborane was constructed in C_{2v} symmetry, reflecting the structure found in the theoretical calculations. Twenty-two geometrical parameters described the structure. The B(2)–B(3) bond length is p_1 (*r*B2B3), the distance from

the midpoint of the B(2)–B(3) bond (corresponding to the *x* axis) to the projection of the C(1) position onto the *y* axis (point a) is p_2 (*r*BBa) and p_3 (*r*aC1) is the distance from a to C(1) along the *z* axis. The distance from a to the projection of the B(4) position onto the *y* axis (point b) is p_4 (*r*ab), p_5 (*r*bB4x) is the distance from b to B(4) along the *x* axis, and p_6 (*r*bB4z) is the distance from b to B(4) along the *z* axis. The distance from b to the projection of the B(5) position onto the *y* axis (point c) is p_7 (*r*bc) and p_8 (*r*cB5) is the distance from c to B(5) along the *z* axis. The distance from c to the midpoint of the B(9)–B(10) bond is p_9 (*r*cBB) and p_{10} (*r*B9B10) is the B(9)–B(10) bond distance. The C–H bond distance is p_{11}, while p_{12}–p_{16} define the four distinct B–H distances: p_{12} is the average B–H distance and p_{13}–p_{16} are the differences from this average distance, which were fixed at the *ab initio* values throughout the refinement while the average distance was allowed to refine. The position of each of the hydrogen atoms was defined by projecting a straight line from the c.o.m. of the C_2B_{10} core through the corresponding heavy atom and out the appropriate distance. Parameters p_{17}–p_{22} define the angles of deviation from straight lines, from the c.o.m. through the heavy atoms, for the C–H and four B–H bonds. All of the hydrogens except H(16) and its symmetry equivalents lie on a mirror plane [H(14) and H(21) on the *xy* plane, H(13) and H(17) on the *yz* plane], and so they require just one angle to describe their position. Each angle is defined in terms of displacement away from a mirror plane on which it does not lie, a positive angle indicating movement away from that plane. The refined parameter values are listed in **Error! Reference source not found.**3.

***Closo*-1,12-$C_2B_{10}H_{12}$ (*para*-carbaborane)**

The molecular model was constructed in D_{5d} symmetry, reflecting the structure of the molecule found in the theoretical calculations. The positions of all the atoms were defined with reference to the centre of mass (c.o.m.) of the molecule. Six geometrical parameters were required to describe the structure. First, p_1 (*r*AC) was defined to be the distance from the point A (the position of the boron atoms projected onto the C_5 axis) to the carbon atoms, p_2 (*r*CH) the C–H bond length, p_3 (*r*OA) the distance from the c.o.m. (O) to A, p_4 (*r*AB) the distance from A to the boron atoms in a line perpendicular to the C_5 axis, and p_5 (*r*BH) to be the B–H bond length. The position of each hydrogen atom was defined by projecting a straight line from the c.o.m. through

the corresponding heavy atom and out by the appropriate distance defined by p_2 or p_5. The parameter p_6 (ψ) gives the deviation from a straight line (at the corresponding boron atom) for the hydrogens bonded to the boron atoms. A positive angle indicates that the hydrogen is moved further away from the C_5 axis. The parameters and their refined values are listed in **Error! Reference source not found.**4.

Table S1. Reported[Error! Bookmark not defined.] GED data for *ortho*-carbaborane.

		Models		
Bond	**3-parameter**	**4-parameter**	**5-parameter**	**Overall**
C(1)–C(2)	1.635(14)	1.651(16)	1.620(17)	1.653(49)
C(1)–B(3)/B(6), C(2)–B(3)/B(6)	1.707(4)	1.707(5)	1.710(4)	1.711(14)
C(1)–B(4)/B(5), C(2)–B(7)/B(11)	1.707(4)	1.707(5)	1.710(4)	1.711(14)
B(3)–B(4)/B(7), B(6)–B(5)/B(11)	1.791(1)	1.800(4)	1.800(5)	1.802(13)
B(4)–B(5), B(7)–B(11)	1.791(1)	1.800(4)	1.800(5)	1.802(13)
B(3)–B(8), B(6)–B(10)	1.791(1)	1.787(3)	1.810(8)	1.789(9)
B(4)/B(5)–B(9), B(7)/B(11)–B(12)	1.791(1)	1.787(3)	1.810(8)	1.789(9)
B(4)/B(7)–B(8), B(5)/B(11)–B(10)	1.791(1)	1.787(3)	1.810(8)	1.789(9)
B(8)–B(9)/B(12), B(10)–B(9)/B(12)	1.791(1)	1.787(3)	1.745(11)	1.789(9)
B(9)–B(12)	1.791(1)	1.787(3)	1.745(11)	1.789(9)

Table S2. Reported[Error! Bookmark not defined.] GED data for *meta*-carbaborane.

			Models			
Bond	**2-parameter**	**3-parameter**	**4-parameter**	**5-parameter**	**6-parameter**	**Overall**
C(1)–B(2)/B(3), C(7)–B(2)/B(3)	1.724(2)	1.720(3)	1.719(2)	1.720(2)	1.719(5)	1.720(9)
C(1)–B(4)/B(6), C(7)–B(8)/B(11)	1.724(2)	1.720(3)	1.719(2)	1.720(2)	1.719(5)	1.720(9)
C(1)–B(5), C(7)–B(12)	1.724(2)	1.720(3)	1.719(2)	1.720(2)	1.719(5)	1.720(9)
B(2)–B(3)	1.803(1)	1.798(3)	1.830(17)	1.835(16)	1.834(17)	1.831(52)
B(2)–B(6)/B(11), B(3)–B(4)/B(8)	1.803(1)	1.798(3)	1.790(4)	1.771(8)	1.777(13)	1.791(15)
B(5)–B(4)/B(6), B(12)–B(8)/B(11)	1.803(1)	1.798(3)	1.790(4)	1.803(8)	1.798(10)	1.791(15)
B(9)–B(4)/B(8), B(10)–B(6)/B(11)	1.803(1)	1.812(4)	1.816(4)	1.818(3)	*1.812(14)*	1.817(13)
B(5)–B(9)/B(10), B(12)–B(9)/B(10)	1.803(1)	1.812(4)	1.816(4)	1.818(3)	*1.812(14)*	1.817(13)
B(4)–B(8), B(6)–B(11)	1.803(1)	1.812(4)	1.816(4)	1.818(3)	*1.826(12)*	1.817(13)
B(9)–B(10)	1.803(1)	1.812(4)	1.816(4)	1.818(3)	*1.826(12)*	1.817(13)

Table S3. Distances (r_a), r.m.s. amplitudes of vibration (u_{h1}), and distance corrections (k_{h1}) for *closo*-1,2-dicarborane (*ortho*-carbaborane). Numbers in parentheses indicate the estimated standard deviation (e.s.d.) in the last digits.

	Atom Pair	r_a / Å	u_{h1} / Å	Constraint/Restraint		k_{h1} / Å	Area / %
u_1	C(2)-B(7)	1.700(6)	0.069(2)		0.070(7)	0.002	100.0
u_2	C(1)-B(3)	1.734(7)	0.070	Tied to u_1		0.003	98.0
u_3	B(3)-B(8)	1.773(9)	0.068	Tied to u_1		0.002	79.9
u_4	B(4)-B(9)	1.787(6)	0.069	Tied to u_1		0.002	79.3
u_5	B(3)-B(4)	1.788(6)	0.068	Tied to u_1		0.003	79.2
u_6	B(4)-B(8)	1.796(6)	0.069	Tied to u_1		0.002	78.9
u_7	B(8)-B(9)	1.807(8)	0.069	Tied to u_1		0.002	78.4
u_8	C(1)-C(2)	1.622(8)	0.068	Tied to u_1		0.001	62.9
u_9	C(2)...B(4)	2.752(6)	0.082(2)		0.074(7)	0.000	61.8
u_{10}	C(1)...B(8)	2.762(7)	0.078	Tied to u_9		0.000	61.5
u_{11}	B(4)...B(12)	2.890(6)	0.082	Tied to u_9		0.001	49.0
u_{12}	B(3)...B(9)	2.890(9)	0.082	Tied to u_9		0.001	49.0
u_{13}	B(4)...B(7)	2.891(12)	0.082	Tied to u_9		0.001	49.0
u_{14}	B(3)...B(5)	2.912(5)	0.086	Tied to u_9		0.001	48.6
u_{15}	B(4)...B(10)	2.916(7)	0.082	Tied to u_9		0.001	48.6
u_{16}	B(4)...B(11)	3.402(10)	0.080(5)		0.075(7)	0.000	41.6
u_{17}	B(3)...B(10)	3.438(10)	0.080	Tied to u_{16}		0.000	41.2
u_{18}	B(9)-B(12)	1.787(9)	0.069	Tied to u_1		0.002	39.6
u_{19}	B(4)-B(5)	1.794(8)	0.068	Tied to u_1		0.003	39.5
u_{20}	C(1)...B(9)	2.741(7)	0.078	Tied to u_9		0.000	31.0
u_{21}	C(1)...B(12)	3.226(6)	0.077	Tied to u_{16}		-0.001	26.3
u_{22}	B(8)...B(10)	2.944(19)	0.083	Tied to u_9		0.001	24.1
u_{23}	B(3)...B(6)	2.948(15)	0.093	Tied to u_9		0.002	24.0
u_{24}	B(3)-H(15)	1.190(3)	0.088	Tied to u_{26}		0.004	23.8
u_{25}	B(4)-H(16)	1.192(3)	0.088	Tied to u_{26}		0.004	23.8
u_{26}	B(8)-H(20)	1.193(3)	0.088(5)		0.083(8)	0.004	23.7
u_{27}	C(1)-H(13)	1.091(8)	0.081(7)		0.075(8)	0.004	15.6
u_{28}	C(1)...H(16)	2.483(12)	0.137	Tied to u_9		-0.005	13.7
u_{29}	C(1)...H(15)	2.511(13)	0.138	Tied to u_9		-0.004	13.5
u_{30}	B(9)-H(21)	1.194(3)	0.088	Tied to u_{26}		0.004	11.9
u_{31}	B(3)...H(13)	2.401(10)	0.134	Tied to u_9		-0.003	11.8
u_{32}	B(4)...H(13)	2.442(13)	0.131	Tied to u_9		-0.003	11.6
u_{33}	B(3)...H(16)	2.557(14)	0.143	Tied to u_9		-0.004	11.1
u_{34}	B(3)...H(20)	2.571(14)	0.142	Tied to u_9		-0.004	11.0
u_{35}	B(4)...H(17)	2.588(18)	0.141	Tied to u_9		-0.004	10.9
u_{36}	B(4)...H(21)	2.597(13)	0.142	Tied to u_9		-0.004	10.9
u_{37}	B(4)...H(20)	2.617(8)	0.141	Tied to u_9		-0.004	10.8
u_{38}	B(8)...H(21)	2.626(9)	0.141	Tied to u_9		-0.004	10.8
u_{39}	B(7)...H(15)	2.639(9)	0.123	Tied to u32		-0.009	10.7
u_{40}	B(4)...H(15)	2.643(9)	0.138	Tied to u_9		-0.004	10.7
u_{41}	B(9)...H(20)	2.654(16)	0.141	Tied to u_9		-0.004	10.7
u_{42}	B(8)...H(16)	2.680(15)	0.137	Tied to u_9		-0.004	10.6
u_{43}	B(9)...H(16)	2.692(12)	0.136	Tied to u_9		-0.004	10.5

u_{44}	B(8)...H(15)	2.711(16)	0.134	Tied to u_9		-0.004	10.4
u_{45}	C(1)...H(15)	3.761(10)	0.120(5)		0.117(12)	-0.010	9.0
u_{46}	C(1)...H(20)	3.824(9)	0.116	Tied to u_{45}		-0.010	8.9
u_{47}	B(4)...H(14)	3.665(12)	0.114	Tied to u_{45}		-0.008	7.7
u_{48}	B(8)...H(13)	3.719(10)	0.110	Tied to u_{45}		-0.009	7.6
u_{49}	C(1)...H(14)	2.315(17)	0.127	Tied to u_9		-0.004	7.3
u_{50}	B(3)...H(18)	3.902(18)	0.128	Tied to u_{45}		-0.009	7.3
u_{51}	B(3)...H(17)	3.907(11)	0.124	Tied to u_{45}		-0.009	7.3
u_{52}	B(4)...H(18)	3.925(8)	0.122	Tied to u_{45}		-0.009	7.2
u_{53}	B(3)...H(21)	3.939(10)	0.119	Tied to u_{45}		-0.009	7.2
u_{54}	B(4)...H(19)	3.951(15)	0.119	Tied to u_{45}		-0.009	7.2
u_{55}	B(4)...H(24)	3.954(10)	0.119	Tied to u_{45}		-0.009	7.2
u_{56}	B(4)...H(22)	3.977(10)	0.119	Tied to u_{45}		-0.009	7.1
u_{57}	B(8)...H(17)	3.987(12)	0.118	Tied to u_{45}		-0.009	7.1
u_{58}	B(9)...H(15)	4.001(11)	0.115	Tied to u_{45}		-0.009	7.1
u_{59}	B(9)...H(19)	4.004(10)	0.115	Tied to u_{45}		-0.010	7.1
u_{60}	B(8)...H(22)	4.015(23)	0.119	Tied to u_{45}		-0.009	7.1
u_{61}	B(9)...H(24)	2.624(17)	0.140	Tied to u_9		-0.004	5.4
u_{62}	C(1)...H(21)	3.803(11)	0.116	Tied to u_{45}		-0.010	4.5
u_{63}	B(9)...H(13)	3.731(13)	0.108	Tied to u_{45}		-0.009	3.8
u_{64}	H(13)...H(15)	2.737(19)	0.215	Tied to u_9		-0.004	2.1
u_{65}	H(13)...H(16)	2.811(23)	0.212	Tied to u_9		-0.005	2.0
u_{66}	H(15)...H(16)	3.000(21)	0.225	Tied to u_9		-0.005	1.9
u_{67}	H(20)...H(21)	3.078(20)	0.226	Tied to u_9		-0.006	1.8
u_{68}	H(16)...H(20)	3.125(23)	0.222	Tied to u_9		-0.006	1.8
u_{69}	H(16)...H(21)	3.130(24)	0.221	Tied to u_9		-0.006	1.8
u_{70}	H(15)...H(20)	3.148(28)	0.218	Tied to u_9		-0.006	1.8
u_{71}	H(13)...H(14)	2.578(41)	0.199	Tied to u_9		-0.004	1.1
u_{72}	H(16)...H(17)	2.951(45)	0.228	Tied to u_9		-0.005	1.0
u_{73}	H(21)...H(24)	3.066(42)	0.224	Tied to u_9		-0.006	0.9

Table S4. Molecular scattering intensities for *closo*-1,2-$C_2B_{10}H_{12}$ (*ortho*-carbaborane) at the short camera distance.

s / nm^{-1}	Experimental	Theoretical	Difference
80.00	138.28147	138.87326	-0.29590
84.00	67.30301	65.85699	0.72301
88.00	-5.96275	-9.56189	1.79957
92.00	-66.10872	-63.08278	-1.51297
96.00	-101.95907	-95.21527	-3.37190
100.00	-121.85433	-118.71973	-1.56730
104.00	-101.27670	-107.44871	3.08600
108.00	-13.56403	-19.38812	2.91204
112.00	110.87464	106.73194	2.07135
116.00	158.14567	162.12209	-1.98821
120.00	100.82738	101.80546	-0.48904
124.00	-6.88581	-5.53818	-0.67382
128.00	-76.37663	-72.85127	-1.76268
132.00	-82.82793	-79.14704	-1.84045
136.00	-55.25433	-53.15565	-1.04934
140.00	-18.95212	-22.19802	1.62295
144.00	6.12051	6.47558	-0.17753
148.00	37.91573	33.98532	1.96520
152.00	56.33914	52.80464	1.76725
156.00	50.89924	47.43045	1.73440
160.00	15.95374	13.39577	1.27899
164.00	-33.67642	-31.58410	-1.04616
168.00	-60.38752	-57.98857	-1.19947
172.00	-48.32979	-47.58874	-0.37053
176.00	-10.54758	-9.99866	-0.27446
180.00	25.86158	26.96760	-0.55301
184.00	40.26033	43.06615	-1.40291
188.00	31.66787	36.64610	-2.48911
192.00	13.10348	16.59663	-1.74658
196.00	-8.99040	-6.53954	-1.22543
200.00	-21.39836	-23.89312	1.24738
204.00	-26.68208	-30.48360	1.90076
208.00	-19.74957	-25.33051	2.79047
212.00	-6.49060	-9.44664	1.47802
216.00	11.74865	11.91666	-0.08401
220.00	26.67219	26.70299	-0.01540
224.00	26.26147	24.58124	0.84011
228.00	9.22092	8.75271	0.23411
232.00	-6.56350	-7.24241	0.33946
236.00	-13.20700	-14.07315	0.43307
240.00	-14.43032	-13.00858	-0.71087
244.00	-11.23116	-9.01262	-1.10927
248.00	-4.65253	-3.37073	-0.64090
252.00	2.63046	4.59193	-0.98073

256.00	9.94146	12.00862	-1.03358
260.00	10.81692	12.99867	-1.09087
264.00	3.64224	5.39456	-0.87616
268.00	-4.04567	-5.44465	0.69949
272.00	-8.14872	-11.39270	1.62199
276.00	-7.70083	-9.27261	0.78589
280.00	0.14170	-2.61480	1.37825
284.00	3.18217	3.17304	0.00456
288.00	5.42184	5.57234	-0.07525
292.00	4.27085	5.25062	-0.48988
296.00	1.96697	3.56796	-0.80049
300.00	0.70473	1.08023	-0.18775
304.00	-2.01627	-1.85029	-0.08299
308.00	-3.30172	-4.17256	0.43542

Table S5. Molecular scattering intensities for *closo*-1,2-$C_2B_{10}H_{12}$ (*ortho*-carbaborane) at the long camera distance.

s / nm^{-1}	Experimental	Theoretical	Difference
20.00	-58.38028	-57.32746	-0.52641
22.00	-52.28136	-55.24945	1.48405
24.00	-48.58452	-47.43269	-0.57592
26.00	-41.17524	-39.11301	-1.03111
28.00	-34.03234	-34.15040	0.05903
30.00	-32.99885	-34.29998	0.65056
32.00	-37.45142	-39.01049	0.77953
34.00	-45.68610	-45.28386	-0.20112
36.00	-48.57431	-47.92088	-0.32672
38.00	-42.22473	-40.75365	-0.73554
40.00	-18.88906	-19.12090	0.11592
42.00	17.50542	17.24540	0.13001
44.00	60.70525	62.51381	-0.90428
46.00	104.02811	105.45324	-0.71257
48.00	133.38949	132.67508	0.35721
50.00	136.29960	133.22570	1.53695
52.00	104.85555	102.82086	1.01734
54.00	47.38508	46.12474	0.63017
56.00	-24.12719	-23.82737	-0.14991
58.00	-89.45376	-89.18315	-0.13530
60.00	-132.52932	-132.92497	0.19782
62.00	-143.70040	-144.61391	0.45676
64.00	-123.12249	-123.81246	0.34498
66.00	-79.92927	-79.57534	-0.17697
68.00	-28.09707	-26.20049	-0.94829
70.00	19.73886	22.50032	-1.38073
72.00	54.82005	57.62690	-1.40342
74.00	74.29797	76.52560	-1.11381
76.00	79.52999	81.25140	-0.86071
78.00	75.49183	75.78365	-0.14591
80.00	64.85623	63.82593	0.51515
82.00	49.00031	48.02705	0.48663
84.00	31.39508	30.26777	0.56366
86.00	12.74665	12.23581	0.25542
88.00	-3.81421	-4.39463	0.29021
90.00	-16.91280	-18.29435	0.69077
92.00	-27.10899	-28.99275	0.94188
94.00	-35.28929	-37.08098	0.89585
96.00	-41.12356	-43.76079	1.31861
98.00	-47.89330	-49.81676	0.96173
100.00	-53.56584	-54.56340	0.49878
102.00	-55.53885	-55.54066	0.00091
104.00	-50.80893	-49.38326	-0.71283
106.00	-36.04358	-33.69191	-1.17584
108.00	-11.88405	-8.91075	-1.48665
110.00	18.57166	20.90470	-1.16652

112.00	48.30133	49.05383	-0.37625
114.00	68.34040	68.50933	-0.08447
116.00	75.16193	74.51105	0.32544
118.00	67.06180	66.22848	0.41666
120.00	46.74815	46.78963	-0.02074
122.00	21.17897	21.84051	-0.33077
124.00	-3.54593	-2.54534	-0.50030
126.00	-22.11314	-21.73657	-0.18828
128.00	-33.17757	-33.48233	0.15238
130.00	-37.15437	-37.83204	0.33884
132.00	-35.16612	-36.37586	0.60487
134.00	-29.32457	-31.26243	0.96893
136.00	-22.86399	-24.43025	0.78313
138.00	-17.05673	-17.19973	0.07150
140.00	-12.87864	-10.20217	-1.33823

Table S6. Refined molecular co-ordinates for *closo*-1,2-$C_2B_{10}H_{12}$ (*ortho*-carbaborane). All values are in Å.

Atom	x	y	z
C	-0.81195	-1.30101	0.00000
C	0.81195	-1.30101	0.00000
B	0.00000	-0.88130	1.47433
B	-1.44622	-0.00314	0.89698
B	-1.44622	-0.00314	-0.89698
B	0.00000	-0.88130	-1.47433
B	1.44622	-0.00314	0.89698
B	0.00000	0.89245	1.47267
B	-0.89357	1.44056	0.00000
B	0.00000	0.89245	-1.47267
B	1.44622	-0.00314	-0.89698
B	0.89357	1.44056	0.00000
H	-1.29824	-2.28028	0.00000
H	1.29824	-2.28028	0.00000
H	0.00000	-1.68165	2.35777
H	-2.46972	-0.17501	1.48688
H	-2.46972	-0.17501	-1.48688
H	0.00000	-1.68165	-2.35777
H	2.46972	-0.17501	1.48688
H	0.00000	1.48388	2.51136
H	-1.54367	2.44429	0.00000
H	0.00000	1.48388	-2.51136
H	2.46972	-0.17501	-1.48688
H	1.54367	2.44429	0.00000

Table S7. List of distances (r_a), RMS amplitudes of vibration (u_{h1}), and distance corrections (k_{h1}) for *closo*-1,7-$C_2B_{10}H_{12}$ (*meta*-carbaborane). Numbers in parentheses indicate the estimated standard deviation (e.s.d.) in the last digits.

	Atom Pair	r_a / Å	u_{h1} / Å	Constraint/Restraint		k_{h1} / Å	Area / %
u_1	C(1)–B(3)	1.678(5)	0.064(1)		0.068(7)	0.002	100.0
u_2	C(1)–B(4)	1.730(5)	0.066	Tied to u_1		0.002	97.0
u_3	B(3)–B(8)	1.771(6)	0.065	Tied to u_1		0.003	78.9
u_4	B(4)–B(8)	1.778(9)	0.065	Tied to u_1		0.002	78.6
u_5	B(4)–B(9)	1.780(6)	0.066	Tied to u_1		0.002	78.5
u_6	B(5)–B(9)	1.783(6)	0.066	Tied to u_1		0.002	78.4
u_7	B(5)–B(4)	1.802(5)	0.065	Tied to u_1		0.003	77.6
u_8	C(1)...B(9)	2.739(5)	0.069	Tied to u_9		0.000	61.2
u_9	C(1)...B(8)	2.750(5)	0.069(2)		0.070(7)	0.000	61.0
u_{10}	C(1)–B(5)	1.703(8)	0.066	Tied to u_1		0.002	49.3
u_{11}	B(3)...B(9)	2.847(8)	0.071	Tied to u_9		0.001	49.1
u_{12}	B(5)...B(3)	2.853(5)	0.073	Tied to u_9		0.001	49.0
u_{13}	B(4)...B(12)	2.891(5)	0.071	Tied to u_9		0.001	48.4
u_{14}	B(4)...B(2)	2.897(5)	0.074	Tied to u_9		0.001	48.3
u_{15}	B(4)...B(10)	2.906(6)	0.072	Tied to u_9		0.001	48.1
u_{16}	B(3)...B(10)	3.362(7)	0.078	Tied to u_{18}		0.000	41.6
u_{17}	B(4)...B(11)	3.438(7)	0.078(6)		0.074(7)	0.000	40.7
u_{18}	C(1)...C(7)	2.573(9)	0.065	Tied to u_9		-0.001	39.1
u_{19}	B(3)–B(2)	1.787(9)	0.065	Tied to u_1		0.003	39.1
u_{20}	B(9)–B(10)	1.794(9)	0.067	Tied to u_1		0.002	39.0
u_{21}	C(1)...B(12)	3.209(6)	0.076	Tied to u_{18}		-0.001	26.1
u_{22}	B(5)...B(12)	2.877(13)	0.071	Tied to u_9		0.001	24.3
u_{23}	B(4)...B(6)	2.944(7)	0.074	Tied to u_9		0.001	23.7
u_{24}	B(3)–H(15)	1.191(3)	0.093	Tied to u_{26}		0.004	23.5
u_{25}	B(4)–H(16)	1.193(3)	0.093	Tied to u_{26}		0.004	23.4
u_{26}	B(9)–H(21)	1.195(3)	0.094(5)		0.083(8)	0.004	23.4
u_{27}	C(1)–H(13)	1.083(5)	0.079(7)		0.075(8)	0.004	15.5
u_{28}	C(1)...H(15)	2.535(7)	0.125	Tied to u_9		-0.005	13.2
u_{29}	C(1)...H(16)	2.536(12)	0.127	Tied to u_9		-0.004	13.2
u_{30}	H(13)...B(3)	2.364(12)	0.122	Tied to u_9		-0.003	11.8
u_{31}	B(5)–H(17)	1.193(3)	0.093	Tied to u_{26}		0.004	11.7
u_{32}	H(13)...B(4)	2.411(7)	0.123	Tied to u_9		-0.003	11.6
u_{33}	H(16)...B(3)	2.546(13)	0.131	Tied to u_9		-0.004	11.0
u_{34}	B(3)...H(14)	2.546(14)	0.132	Tied to u_9		-0.004	11.0
u_{35}	H(17)...B(4)	2.584(7)	0.130	Tied to u_9		-0.004	10.8
u_{36}	B(4)...H(21)	2.592(13)	0.130	Tied to u_9		-0.004	10.8
u_{37}	B(5)...H(21)	2.611(8)	0.130	Tied to u_9		-0.004	10.7
u_{38}	B(9)...H(22)	2.623(17)	0.130	Tied to u_9		-0.004	10.7
u_{39}	B(4)...H(15)	2.628(12)	0.127	Tied to u_9		-0.004	10.6
u_{40}	B(5)...H(16)	2.633(15)	0.130	Tied to u_9		-0.004	10.6
u_{41}	B(4)...H(20)	2.648(17)	0.127	Tied to u_9		-0.004	10.6
u_{42}	H(17)...B(9)	2.679(11)	0.127	Tied to u_9		-0.004	10.4
u_{43}	H(16)...B(9)	2.698(11)	0.127	Tied to u_9		-0.004	10.4

Table S8. Molecular scattering intensities for *closo*-1,7-$C_2B_{10}H_{12}$ (*meta*-carbaborane) at the short camera distance.

s / nm^{-1}	Experimental	Theoretical	Difference
80.00	146.02756	145.34507	0.34124
84.00	78.61909	80.84234	-1.11163
88.00	5.35927	0.14016	2.60955
92.00	-62.53081	-61.78073	-0.37504
96.00	-100.12310	-93.75281	-3.18514
100.00	-117.86460	-116.07598	-0.89431
104.00	-110.88107	-112.50364	0.81129
108.00	-26.68429	-33.14759	3.23165
112.00	98.31130	95.76849	1.27141
116.00	162.13540	163.05011	-0.45735
120.00	109.62845	111.49627	-0.93391
124.00	0.97808	4.70479	-1.86335
128.00	-69.23580	-65.78079	-1.72751
132.00	-79.07562	-76.27049	-1.40257
136.00	-56.95370	-57.05732	0.05181
140.00	-27.15296	-33.18586	3.01645
144.00	-2.63535	-5.94976	1.65720
148.00	30.63372	27.72680	1.45346
152.00	58.37806	56.90286	0.73760
156.00	60.93203	60.80746	0.06228
160.00	27.57726	29.36733	-0.89504
164.00	-25.12794	-23.39811	-0.86492
168.00	-65.15387	-63.88831	-0.63278
172.00	-62.10615	-62.06590	-0.02013
176.00	-21.32239	-21.00289	-0.15975
180.00	21.14207	24.20557	-1.53175
184.00	41.85750	43.79473	-0.96861
188.00	35.46140	37.49280	-1.01570
192.00	19.43419	20.45898	-0.51239
196.00	0.54436	2.41306	-0.93435
200.00	-11.84593	-14.08549	1.11978
204.00	-24.51784	-26.65309	1.06762
208.00	-29.44042	-30.70956	0.63457
212.00	-19.72293	-21.20571	0.74139
216.00	0.98670	1.22929	-0.12130
220.00	26.23399	24.15961	1.03719
224.00	33.49928	30.96925	1.26501
228.00	21.05022	18.04732	1.50145
232.00	0.95431	-1.75565	1.35498
236.00	-14.32906	-14.02047	-0.15430
240.00	-17.64366	-15.50796	-1.06785
244.00	-14.00850	-11.46223	-1.27313
248.00	-5.92868	-5.96795	0.01963
252.00	1.07194	1.07288	-0.00047

256.00	6.11258	9.12639	-1.50691
260.00	7.05119	13.64321	-3.29601
264.00	8.41978	10.09075	-0.83548
268.00	1.08692	0.14995	0.46849
272.00	-5.96253	-8.81723	1.42735
276.00	-7.22760	-10.79766	1.78503
280.00	-6.21798	-6.15273	-0.03262
284.00	-0.44078	0.21211	-0.32644
288.00	4.00353	4.04848	-0.02248
292.00	7.02039	4.68727	1.16656
296.00	3.97331	3.80931	0.08200
300.00	2.34739	2.58757	-0.12009
304.00	0.10410	0.72481	-0.31036
308.00	-2.71470	-2.01886	-0.34792

Table S9. Molecular scattering intensities for *closo*-1,7-$C_2B_{10}H_{12}$ (*meta*-carbaborane) at the long camera distance.

s / nm^{-1}	Experimental	Theoretical	Difference
20.00	-56.04765	-55.18716	-0.43025
22.00	-52.24844	-54.64185	1.19671
24.00	-49.77199	-48.59923	-0.58638
26.00	-42.99872	-41.34622	-0.82625
28.00	-36.00306	-36.23002	0.11348
30.00	-33.89444	-35.26374	0.68465
32.00	-37.71796	-38.69419	0.48811
34.00	-45.19209	-44.30070	-0.44570
36.00	-47.79052	-47.21785	-0.28633
38.00	-42.09733	-41.14029	-0.47852
40.00	-20.41819	-21.02333	0.30257
42.00	14.01535	13.85476	0.08030
44.00	56.74094	58.17871	-0.71888
46.00	99.79211	101.29707	-0.75248
48.00	131.31926	130.26695	0.52615
50.00	136.77880	134.08103	1.34889
52.00	109.66521	107.65771	1.00375
54.00	54.49765	54.28983	0.10391
56.00	-15.14134	-14.34136	-0.39999
58.00	-81.45387	-81.03793	-0.20797
60.00	-127.50644	-128.39460	0.44408
62.00	-143.22120	-144.75712	0.76796
64.00	-127.31123	-128.26189	0.47533
66.00	-87.82012	-86.95492	-0.43260
68.00	-37.86855	-34.82390	-1.52232
70.00	10.34703	14.08455	-1.86876
72.00	47.71319	50.47582	-1.38132
74.00	70.80373	71.44185	-0.31906
76.00	79.79566	78.92898	0.43334
78.00	78.37813	76.72213	0.82800
80.00	70.16499	68.01854	1.07323
82.00	55.70383	54.67638	0.51372
84.00	37.65364	37.83257	-0.08946
86.00	17.89004	18.91705	-0.51351
88.00	-0.33369	0.06559	-0.19964
90.00	-15.74003	-16.38272	0.32135
92.00	-27.50017	-28.91212	0.70598
94.00	-36.37110	-37.59026	0.60958
96.00	-42.64295	-43.87441	0.61573
98.00	-48.62946	-49.38394	0.37724
100.00	-54.17380	-54.32120	0.07370
102.00	-56.42007	-56.63417	0.10705
104.00	-52.84645	-52.64942	-0.09852
106.00	-39.65321	-39.11358	-0.26982

108.00	-16.80471	-15.51240	-0.64615
110.00	13.70779	14.70148	-0.49685
112.00	44.10704	44.81770	-0.35533
114.00	66.38898	67.23066	-0.42084
116.00	76.03314	76.30414	-0.13550
118.00	70.60016	70.39583	0.10216
120.00	52.21176	52.17799	0.01689
122.00	26.90036	27.30107	-0.20036
124.00	1.73157	2.20174	-0.23509
126.00	-18.05154	-18.01813	-0.01671
128.00	-30.62775	-30.78407	0.07816
130.00	-35.75155	-36.09302	0.17073
132.00	-34.85676	-35.69304	0.41814
134.00	-30.62726	-31.91222	0.64248
136.00	-25.42936	-26.70167	0.63615
138.00	-20.71319	-21.15790	0.22235
140.00	-17.80645	-15.53031	-1.13807

Table S10. Refined molecular co-ordinates for *closo*-1,7-$C_2B_{10}H_{12}$ (*meta*-carbaborane). All values are in Å.

Atom	x	y	z
C(1)	0.00000	-0.81447	1.28745
B(2)	-0.89295	-1.41511	0.00000
B(3)	0.89295	-1.41511	0.00000
B(4)	1.47239	0.00228	0.88896
B(5)	0.00000	0.88251	1.43890
B(6)	-1.47239	0.00228	0.88896
C(7)	0.00000	-0.81447	-1.28745
B(8)	1.47239	0.00228	-0.88896
B(9)	0.89725	1.43292	0.00000
B(10)	-0.89725	1.43292	0.00000
B(11)	-1.47239	0.00228	-0.88896
B(12)	0.00000	0.88251	-1.43890
H(13)	0.00000	-1.40267	2.19942
H(14)	-1.43103	-2.48068	0.00000
H(15)	1.43103	-2.48068	0.00000
H(16)	2.43548	-0.13331	1.58470
H(17)	0.00000	1.36410	2.53422
H(18)	-2.43548	-0.13331	1.58470
H(19)	0.00000	-1.40267	-2.19942
H(20)	2.43548	-0.13331	-1.58470
H(21)	1.53358	2.44750	0.00000
H(22)	-1.53358	2.44750	0.00000
H(23)	-2.43548	-0.13331	-1.58470
H(24)	0.00000	1.36410	-2.53422

Table S11. List of distances (r_a), RMS amplitudes of vibration (u_h1), and distance corrections (k_h1) for *closo*-1,12-$C_2B_{10}H_{12}$ (*para*-carbaborane). Numbers in parentheses indicate the estimated standard deviation (e.s.d.) in the last digits.

	Atom Pair	r_a / Å	u_{h1} / Å	Constraint/Restraint	k_{h1} / Å	Area / %
u_1	C(1)-B(2)	1.697(3)	0.068(2)		0.002	100.0
u_2	B(2)-B(7)	1.773(4)	0.067	Tied to u_1	0.002	79.7
u_3	B(2)-B(3)	1.783(1)	0.067	Tied to u_1	0.002	79.3
u_4	C(1)...B(7)	2.726(2)	0.073(2)		0.000	62.2
u_5	B(2)...B(8)	2.879(1)	0.077	Tied to u_4	0.001	49.1
u_6	B(2)...B(4)	2.885(2)	0.081	Tied to u_4	0.001	49.0
u_7	B(2)-H(14)	1.187(3)	0.096(6)		0.004	23.8
u_8	B(2)...H(19)	2.598(26)	0.134	Tied to u_4	-0.004	21.8
u_9	B(2)...H(15)	2.602(9)	0.138	Tied to u_4	-0.004	21.7
u_{10}	B(2)...B(9)	3.386(1)	0.077(3)		0.000	20.9
u_{11}	B(2)...H(20)	3.932(7)	0.120(6)		-0.008	14.4
u_{12}	B(2)...H(16)	3.934(16)	0.125	Tied to u_{11}	-0.008	14.4
u_{13}	C(1)...H(14)	2.577(28)	0.134	Tied to u_4	-0.004	13.2
u_{14}	B(2)...H(13)	2.387(7)	0.130	Tied to u_4	-0.003	11.8
u_{15}	C(1)...H(19)	3.800(19)	0.115	Tied to u_{11}	-0.009	8.9
u_{16}	B(2)...H(24)	3.677(7)	0.113	Tied to u_{11}	-0.008	7.7
u_{17}	C(1)...C(12)	3.026(5)	0.071	Tied to u_4	-0.002	6.7
u_{18}	C(1)-H(13)	1.091(8)	0.087	Tied to u_7	0.004	6.2
u_{19}	B(2)...H(21)	4.565(3)	0.117(8)		-0.010	6.2
u_{20}	H(13)...H(14)	2.876(44)	0.207	Tied to u_4	-0.004	2.0
u_{21}	H(14)...H(15)	3.009(28)	0.232	Tied to u_4	-0.005	1.9
u_{22}	H(14)...H(19)	3.016(75)	0.221	Tied to u_4	-0.006	1.9
u_{23}	C(1)...H(24)	4.110(9)	0.099	Tied to u_{11}	-0.010	1.7
u_{24}	H(13)...H(19)	4.655(27)	0.160	Tied to u_{19}	-0.017	1.2
u_{25}	H(14)...H(16)	4.879(45)	0.188	Tied to u_{19}	-0.019	1.2
u_{26}	H(14)...H(20)	4.883(19)	0.179	Tied to u_{19}	-0.019	1.2
u_{27}	H(14)...H(21)	5.741(6)	0.150	Tied to u_{19}	-0.024	0.5
u_{28}	H(13)...H(24)	5.194(16)	0.133	Tied to u_{19}	-0.021	0.1

Table S12. Molecular scattering intensities for *closo*-1,12-$C_2B_{10}H_{12}$ (*para*-carbaborane) at the short camera distance.

s / nm^{-1}	Experimental	Theoretical	Difference
100.00	-99.53073	-107.21247	3.84087
102.00	-122.64739	-118.45550	-2.09594
104.00	-123.24769	-116.39261	-3.42754
106.00	-95.23672	-92.63366	-1.30153
108.00	-44.47453	-45.38827	0.45687
110.00	22.34503	17.93369	2.20567
112.00	87.58288	82.66864	2.45712
114.00	136.92415	132.38593	2.26911
116.00	156.75231	155.08405	0.83413
118.00	146.94433	147.19933	-0.12750
120.00	109.15933	113.90184	-2.37126
122.00	61.54683	66.14821	-2.30069
124.00	12.55626	16.34973	-1.89674
126.00	-28.19273	-25.57006	-1.31133
128.00	-55.71144	-54.28093	-0.71525
130.00	-68.82158	-69.10838	0.14340
132.00	-71.78360	-72.64276	0.42958
134.00	-66.97817	-68.74096	0.88139
136.00	-59.53216	-60.82634	0.64709
138.00	-50.39266	-50.93243	0.26989
140.00	-38.51338	-39.58053	0.53357
142.00	-23.91020	-26.29393	1.19187
144.00	-6.66032	-10.45651	1.89810
146.00	11.32172	7.82975	1.74599
148.00	30.58818	27.17427	1.70696
150.00	45.51672	44.89882	0.30895
152.00	54.94715	57.67264	-1.36275
154.00	59.86562	62.57331	-1.35385
156.00	54.19433	58.13000	-1.96784
158.00	41.18874	44.86512	-1.83819
160.00	21.56020	25.13596	-1.78788
162.00	-0.87335	2.41848	-1.64591
164.00	-21.61385	-19.59085	-1.01150
166.00	-40.21573	-37.69440	-1.26066
168.00	-50.28393	-49.60707	-0.33843
170.00	-54.53584	-54.11843	-0.20871
172.00	-50.99918	-51.12380	0.06231
174.00	-40.42121	-41.56728	0.57303
176.00	-23.84926	-27.25814	1.70444
178.00	-6.39967	-10.52597	2.06315
180.00	11.76921	6.22932	2.76995
182.00	26.48166	20.95084	2.76541
184.00	36.21031	32.15825	2.02603
186.00	41.80103	38.98332	1.40886

188.00	41.22655	41.06500	0.08077
190.00	36.47387	38.44769	-0.98691
192.00	28.56763	31.57032	-1.50135
194.00	18.49943	21.31863	-1.40960
196.00	4.80492	9.03560	-2.11534
198.00	-5.77409	-3.61903	-1.07753
200.00	-17.20047	-14.97181	-1.11433
202.00	-25.48152	-23.69068	-0.89542
204.00	-30.29419	-29.03482	-0.62969
206.00	-30.96806	-30.86904	-0.04951
208.00	-28.67801	-29.47384	0.39792
210.00	-23.66417	-25.28579	0.81081
212.00	-16.39981	-18.73922	1.16971
214.00	-7.62667	-10.30836	1.34085
216.00	2.12366	-0.67852	1.40109
218.00	10.82073	9.10780	0.85646
220.00	19.30283	17.68570	0.80857
222.00	24.60156	23.63572	0.48292
224.00	26.30286	25.89612	0.20337
226.00	23.33242	24.12590	-0.39674
228.00	17.58508	18.86250	-0.63871
230.00	10.44894	11.38361	-0.46733
232.00	1.87082	3.32454	-0.72686
234.00	-6.20693	-3.79222	-1.20735
236.00	-11.09988	-8.95323	-1.07332
238.00	-14.01365	-11.83523	-1.08921
240.00	-13.95037	-12.73646	-0.60696
242.00	-13.59713	-12.31183	-0.64265
244.00	-12.20289	-11.22723	-0.48783
246.00	-9.95051	-9.88202	-0.03425
248.00	-8.64156	-8.29613	-0.17272
250.00	-6.97180	-6.19777	-0.38702
252.00	-3.53247	-3.26204	-0.13521
254.00	1.11549	0.61075	0.25237
256.00	7.04624	5.10309	0.97158
258.00	10.76921	9.47115	0.64903
260.00	12.36413	12.73243	-0.18415
262.00	13.06397	13.98526	-0.46065
264.00	11.25557	12.73956	-0.74199
266.00	8.97989	9.12018	-0.07015
268.00	4.32255	3.87199	0.22528
270.00	-0.01711	-1.84365	0.91327
272.00	-4.67381	-6.78339	1.05479
274.00	-7.15330	-9.96674	1.40672
276.00	-8.25620	-10.92258	1.33319
278.00	-7.64920	-9.76218	1.05649
280.00	-5.04945	-7.07704	1.01380
282.00	-2.83334	-3.71479	0.44073
284.00	-1.02694	-0.51420	-0.25637
286.00	0.17676	1.91575	-0.86950

288.00	1.69566	3.31111	-0.80773
290.00	1.37866	3.74778	-1.18456
292.00	3.23620	3.53381	-0.14880
294.00	2.17517	3.05248	-0.43866
296.00	2.66285	2.61373	0.02456
298.00	2.02239	2.35943	-0.16852
300.00	2.11912	2.24886	-0.06487
302.00	2.04877	2.11451	-0.03287
304.00	0.58630	1.75751	-0.58560
306.00	0.27655	1.04519	-0.38432
308.00	-0.32711	-0.02632	-0.15039
310.00	-1.86781	-1.31979	-0.27401
312.00	-2.80192	-2.59340	-0.10426
314.00	-3.30374	-3.56991	0.13308
316.00	-3.41676	-4.01339	0.29832
318.00	-2.32763	-3.79077	0.73157

Table S13. Molecular scattering intensities for *closo*-1,12-$C_2B_{10}H_{12}$ (*para*-carbaborane) at the long camera distance.

s / nm^{-1}	Experimental	Theoretical	Difference
20.00	-50.47723	-52.60294	1.06285
21.00	-52.97327	-53.72950	0.37811
22.00	-54.59419	-52.45043	-1.07188
23.00	-53.80903	-50.44357	-1.68273
24.00	-50.00090	-47.04671	-1.47709
25.00	-44.36653	-43.87137	-0.24758
26.00	-38.50727	-40.26445	0.87859
27.00	-34.17286	-37.55575	1.69144
28.00	-31.54284	-35.13578	1.79647
29.00	-30.64401	-34.03525	1.69562
30.00	-30.83895	-33.63870	1.39987
31.00	-32.97490	-34.66989	0.84749
32.00	-37.13313	-36.34291	-0.39511
33.00	-40.50621	-39.02766	-0.73928
34.00	-44.30337	-41.61517	-1.34410
35.00	-46.24387	-44.12602	-1.05893
36.00	-48.66647	-45.18576	-1.74035
37.00	-47.92054	-44.59660	-1.66197
38.00	-43.69957	-41.03704	-1.33126
39.00	-36.16653	-34.39009	-0.88822
40.00	-25.37407	-23.86071	-0.75668
41.00	-10.44486	-9.71161	-0.36662
42.00	7.01470	7.92313	-0.45421
43.00	27.23485	28.28613	-0.52564
44.00	49.24752	50.21777	-0.48512
45.00	73.10926	72.57696	0.26615
46.00	95.10960	93.45486	0.82737
47.00	114.62808	111.65186	1.48811
48.00	129.55843	125.06479	2.24682
49.00	137.18651	132.85045	2.16803
50.00	137.25851	133.36653	1.94599
51.00	129.66246	126.52946	1.56650
52.00	113.75189	111.73164	1.01013
53.00	91.59650	89.88900	0.85375
54.00	62.98863	61.71918	0.63473
55.00	30.20544	29.10294	0.55125
56.00	-5.31475	-6.07251	0.37888
57.00	-39.80764	-41.37924	0.78580
58.00	-72.40011	-74.38576	0.99282
59.00	-100.58575	-102.86702	1.14063
60.00	-122.43687	-124.76372	1.16342
61.00	-136.78141	-138.82726	1.02292
62.00	-142.74149	-144.16852	0.71351
63.00	-140.78336	-140.95292	0.08478

64.00	-131.26874	-129.73871	-0.76502
65.00	-115.01101	-111.96225	-1.52438
66.00	-93.78711	-89.26031	-2.26340
67.00	-69.05873	-63.65980	-2.69946
68.00	-43.36939	-37.07842	-3.14548
69.00	-17.91082	-11.32204	-3.29439
70.00	5.62903	12.17859	-3.27478
71.00	26.45795	32.40158	-2.97182
72.00	43.38885	48.76704	-2.68909
73.00	55.94193	61.12101	-2.58954
74.00	65.45699	69.61251	-2.07776
75.00	71.86176	74.65155	-1.39489
76.00	75.24901	76.73190	-0.74144
77.00	76.34700	76.39039	-0.02169
78.00	75.37358	74.09557	0.63900
79.00	72.26739	70.23858	1.01440
80.00	67.73059	65.09883	1.31588
81.00	61.85520	58.89115	1.48203
82.00	55.15945	51.76777	1.69584
83.00	47.51094	43.87489	1.81802
84.00	39.20668	35.37805	1.91431
85.00	30.41360	26.49014	1.96173
86.00	21.15985	17.46922	1.84532
87.00	11.82740	8.61172	1.60784
88.00	3.31070	0.22084	1.54493
89.00	-4.54890	-7.43091	1.44101
90.00	-11.85047	-14.13609	1.14281
91.00	-18.04313	-19.79740	0.87714
92.00	-23.02506	-24.43040	0.70267
93.00	-27.66508	-28.18370	0.25931
94.00	-30.85357	-31.29784	0.22213
95.00	-33.90870	-34.07621	0.08375
96.00	-36.89621	-36.81874	-0.03874
97.00	-39.87126	-39.76220	-0.05453
98.00	-42.77699	-43.01247	0.11774
99.00	-45.88698	-46.52002	0.31652
100.00	-48.87546	-50.02466	0.57460
101.00	-51.69423	-53.12840	0.71709
102.00	-53.40727	-55.27058	0.93166
103.00	-53.86580	-55.85799	0.99610
104.00	-52.76257	-54.30805	0.77274
105.00	-49.38637	-50.17933	0.39648
106.00	-43.30285	-43.22227	-0.04029
107.00	-34.59322	-33.45383	-0.56969
108.00	-23.43890	-21.17788	-1.13051
109.00	-10.36146	-6.96855	-1.69645
110.00	4.21412	8.36775	-2.07681
111.00	19.07036	23.88225	-2.40595
112.00	33.86937	38.57266	-2.35164
113.00	47.25089	51.47228	-2.11069

114.00	58.25356	61.77043	-1.75844
115.00	66.22589	68.84710	-1.31060
116.00	71.02573	72.36123	-0.66775
117.00	71.74448	72.23945	-0.24748
118.00	68.98842	68.68227	0.15308
119.00	62.99318	62.11648	0.43835
120.00	54.48172	53.14587	0.66792
121.00	44.05364	42.48006	0.78679
122.00	32.38555	30.86433	0.76061
123.00	20.61211	19.03367	0.78922
124.00	8.84212	7.62868	0.60672
125.00	-1.72016	-2.82112	0.55048
126.00	-11.30064	-11.93083	0.31510
127.00	-19.02140	-19.46571	0.22216
128.00	-25.12664	-25.32714	0.10025
129.00	-29.33768	-29.54842	0.10537
130.00	-31.70785	-32.24553	0.26884
131.00	-32.90546	-33.62116	0.35785
132.00	-32.96828	-33.89465	0.46319
133.00	-32.34289	-33.30822	0.48267
134.00	-31.29436	-32.07410	0.38987
135.00	-29.73903	-30.38625	0.32361
136.00	-28.01992	-28.38118	0.18063
137.00	-26.16606	-26.15938	-0.00334
138.00	-24.32934	-23.76475	-0.28230
139.00	-22.34146	-21.20925	-0.56610
140.00	-20.23131	-18.46802	-0.88164

Table S14. Refined molecular co-ordinates for *closo*-1,12-$C_2B_{10}H_{12}$ (*para*-carbaborane). All values are in Å.

Atom	x	y	z
C(1)	0.00000	0.00000	1.51434
B(2)	1.51716	0.00000	0.75283
B(3)	0.46883	-1.44291	0.75283
B(4)	-1.22741	-0.89177	0.75283
B(5)	-1.22741	0.89177	0.75283
B(6)	0.46883	1.44291	0.75283
B(7)	1.22741	-0.89177	-0.75283
B(8)	-0.46883	-1.44291	-0.75283
B(9)	-1.51716	0.00000	-0.75283
B(10)	-0.46883	1.44291	-0.75283
B(11)	1.22741	0.89177	-0.75283
C(12)	0.00000	0.00000	-1.51434
H(13)	0.00000	0.00000	2.60878
H(14)	2.57845	0.00000	1.29331
H(15)	0.79678	-2.45225	1.29331
H(16)	-2.08601	-1.51557	1.29331
H(17)	-2.08601	1.51557	1.29331
H(18)	0.79678	2.45225	1.29331
H(20)	2.08601	-1.51557	-1.29331
H(21)	-0.79678	-2.45225	-1.29331
H(22)	-2.57845	0.00000	-1.29331
H(23)	-0.79678	2.45225	-1.29331
H(24)	2.08601	1.51557	-1.29331
H(25)	0.00000	0.00000	-2.60878

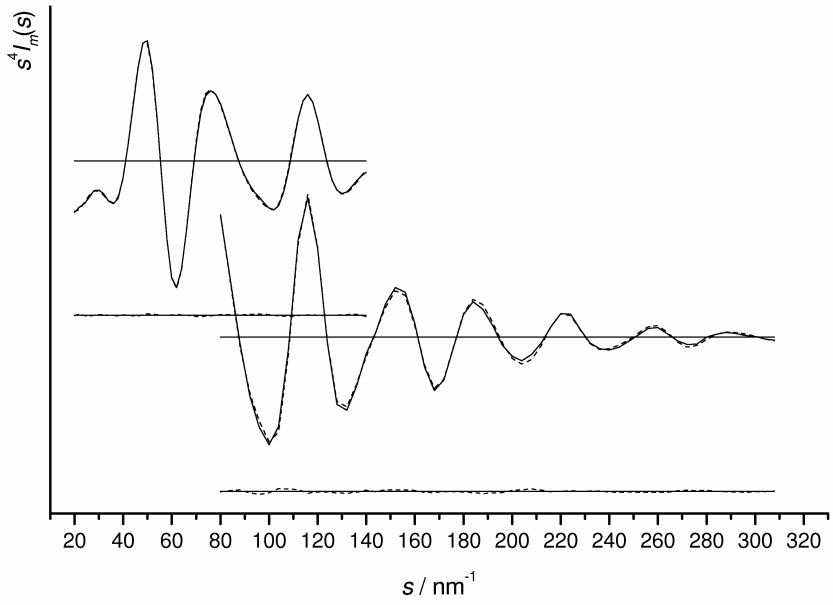

Figure S1. Molecular scattering intensities and difference curves for *closo*-1,2-$C_2B_{10}H_{12}$ (*ortho*-carbaborane) at the short and long camera distances. Solid curves: observed molecular scattering intensity; dashed curves: calculated molecular scattering intensity at refined geometry; lower dashed curves: difference between the observed and calculated molecular scattering intensities.

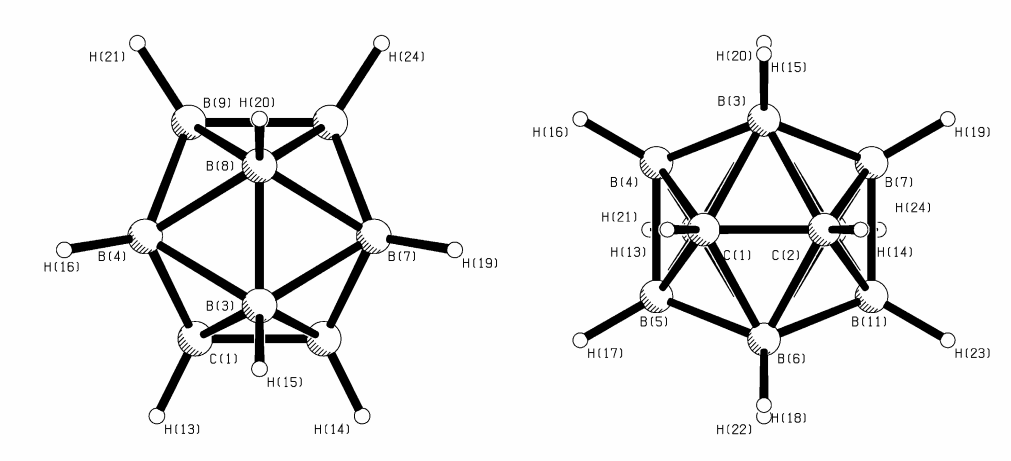

Figure S2. Refined structure of *closo*-1,2-$C_2B_{10}H_{12}$ (*ortho*-carbaborane).

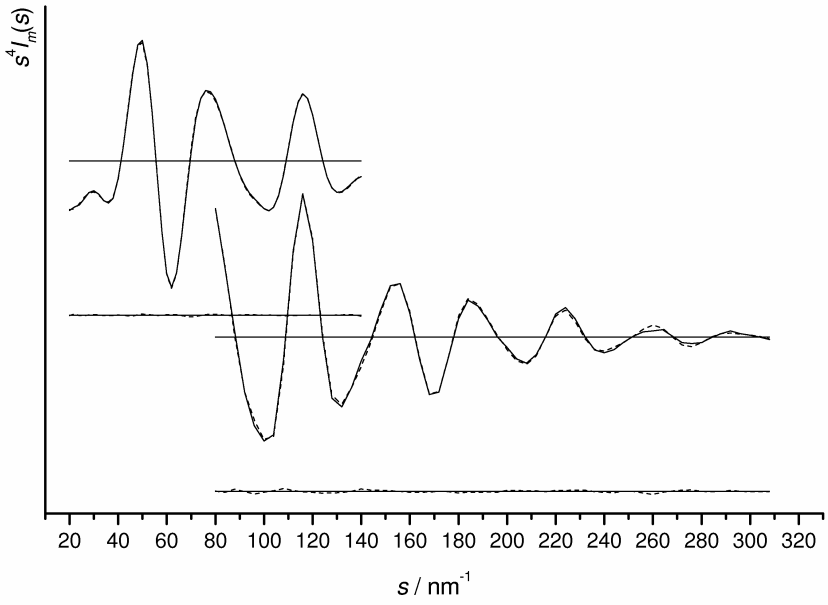

Figure S3. Molecular scattering intensities and difference curves for *closo*-1,7-$C_2B_{10}H_{12}$ (*meta*-carbaborane) at the short and the long camera distances. Solid curves: observed molecular scattering intensity; dashed curves: calculated molecular scattering intensity at refined geometry; lower dashed curves: difference between the observed and calculated molecular scattering intensities.

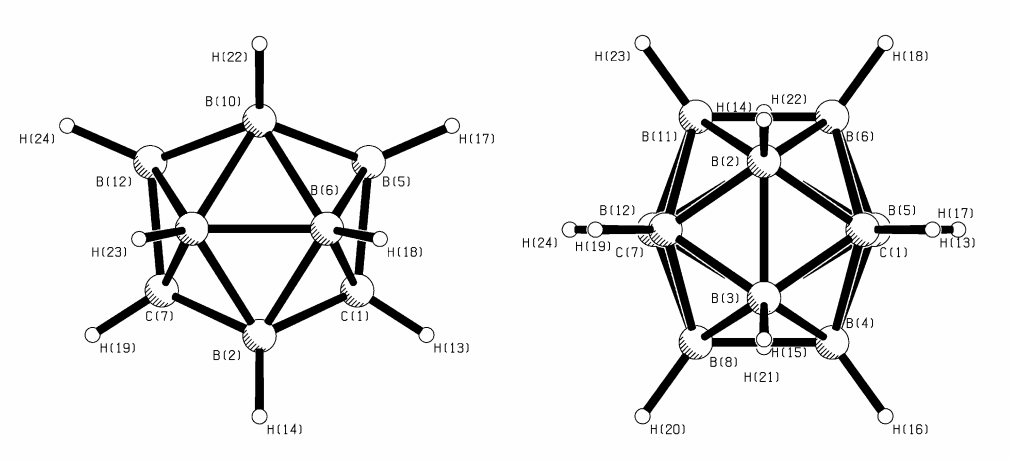

Figure S4. Refined structure of *closo*-1,7-$C_2B_{10}H_{12}$ (*meta*-carbaborane).

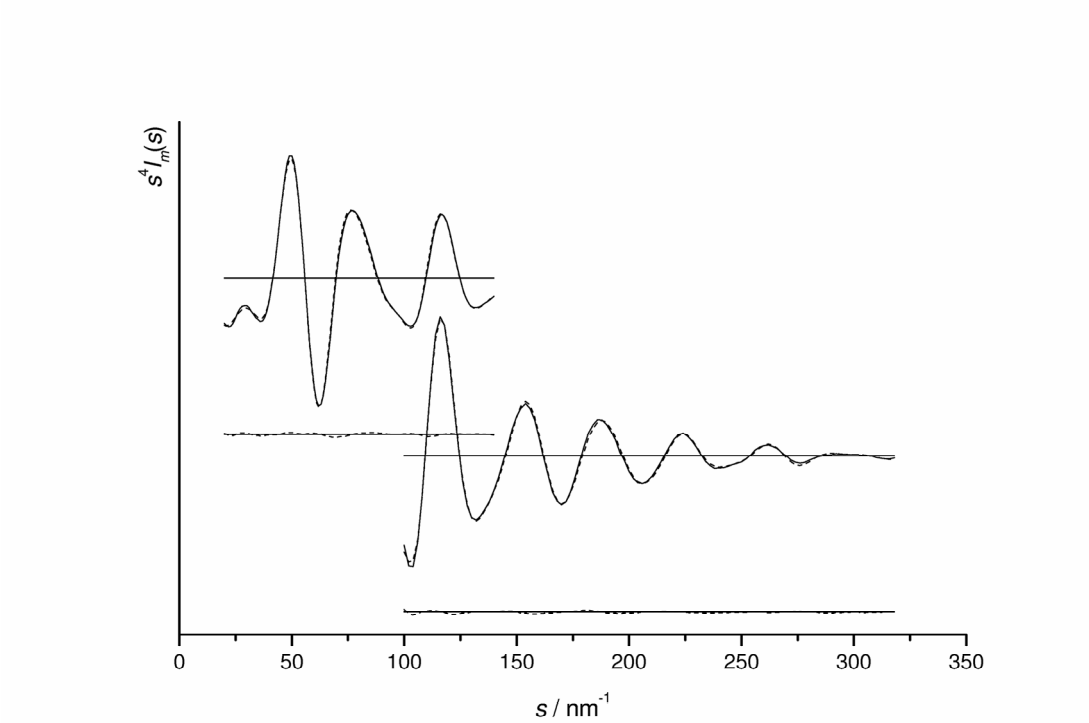

Figure S5. Molecular scattering intensities and difference curves for *closo*-1,12-$C_2B_{10}H_{12}$ (*para*-carbaborane) at the short and the long camera distances. Solid curves: observed molecular scattering intensity; dashed curves: calculated molecular scattering intensity at refined geometry; lower dashed curves: difference between the observed and calculated molecular scattering intensities.

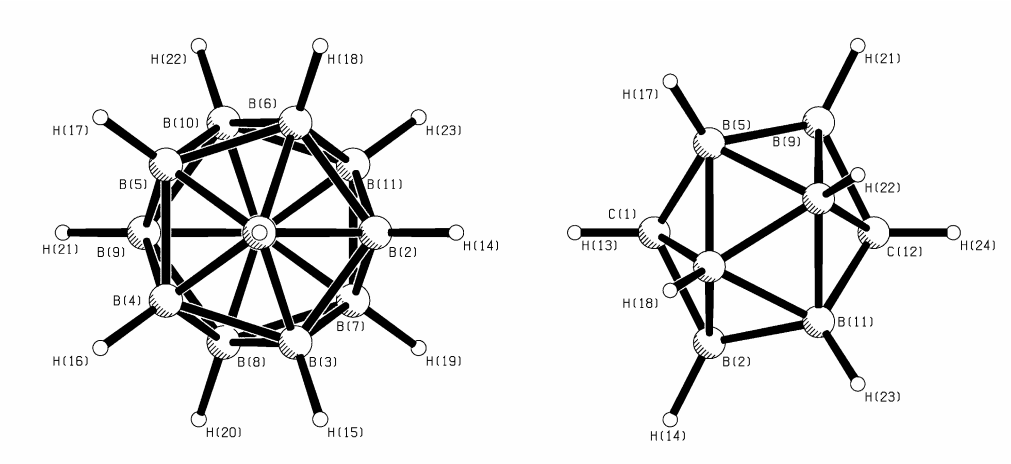

Figure S6. Refined structure of *closo*-1,12-$C_2B_{10}H_{12}$ (*para*-carbaborane).