Supplementary data for *Dalton Transactions*

The gas-phase structure of 1-selena-*closo*-dodecaborane(11), 1-$SeB_{11}H_{11}$, determined by the concerted use of electron diffraction and computational methods

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Electronic Supplementary Information

Table S1 Nozzle-to-film distances / mm, weighting functions / nm^{-1}, scale factors, correlation parameters and electron wavelengths / pm used in the electron diffraction study of $SeB_{11}H_{11}$.

Nozzle-to-film distance[a]	Δs	s_{min}	sw_1	sw_2	s_{max}	Scale factor[b]	Correlation parameter	Electron wavelength
249.9	1	20	40	129	150	0.805(7)	0.493	6.18
87.8	2	100	120	300	350	2.040(50)	0.309	6.18

[a] Determined by reference to the scattering pattern of benzene. [b] Values in parentheses are the estimated standard deviations.

Table S2 Interatomic distances (r_a / pm), refined and calculated amplitudes of vibration (u / pm) and perpendicular corrections (k / pm) for the SARACEN-restrained GED structure of $SeB_{11}H_{11}$.[a]

	Atom pair	r_a	u(exp.)[b]	k	u(calc.)
u_1	B(2)–H(2)	119.2(2)	5.7(2)	1.2	8.0
u_2	B(12)–H(12)	119.2(2)	5.7(tied to u_1)	1.3	8.1
u_3	B(7)–H(7)	119.2(2)	5.7(tied to u_1)	1.3	8.1
u_4	B(2)–B(7)	176.0(2)	6.5(1)	0.1	6.7
u_5	B(7)–B(12)	178.0(2)	6.5(tied to u_4)	0.0	6.8
u_6	B(7)–B(8)	179.1(3)	6.5(tied to u_4)	0.1	6.8
u_7	B(2)–B(3)	192.1(2)	7.6(4)	–0.1	8.4
u_8	Se(1)–B(2)	213.3(2)	7.9(2)	0.4	7.4
u_9	B(2)...H(7)	253.6(9)	12.1(tied to u_{15})	0.4	12.4
u_{10}	B(7)...H(12)	259.9(4)	11.9(tied to u_{15})	0.4	12.1
u_{11}	B(7)...H(8)	261.5(4)	11.9(tied to u_{15})	0.2	12.1
u_{12}	B(12)...H(7)	261.7(10)	11.8(tied to u_{15})	0.2	12.1
u_{13}	B(7)...H(2)	266.1(8)	11.5(tied to u_{15})	0.5	11.8
u_{14}	B(2)...H(3)	271.7(5)	12.8(tied to u_{15})	0.1	13.0
u_{15}	Se(1)...H(2)	276.0(14)	12.5(5)	0.2	12.7
u_{16}	B(2)...B(12)	288.8(6)	7.7(tied to u_{18})	–0.1	7.1
u_{17}	B(7)...B(9)	289.7(4)	7.8(tied to u_{18})	0.1	7.2
u_{18}	B(2)...B(9)	294.1(2)	8.2(1)	–0.2	7.5
u_{19}	H(7)...H(12)	303.0(16)	19.1(fixed)	–0.1	19.1
u_{20}	H(2)...H(7)	304.5(18)	19.0(fixed)	0.3	19.0
u_{21}	H(7)...H(8)	303.2(9)	19.3(fixed)	–0.5	19.3
u_{22}	H(2)...H(3)	310.8(11)	19.8(fixed)	–0.7	19.8
u_{23}	B(2)...B(4)	310.9(4)	10.8(tied to u_{24})	–0.2	8.8
u_{24}	Se(1)...B(7)	321.1(2)	8.6(1)	0.4	7.0
u_{25}	B(2)...B(10)	347.6(2)	9.4(tied to u_{24})	–0.3	7.7
u_{26}	Se(1)...B(12)	374.6(6)	8.2(8)	0.2	6.8
u_{27}	B(2)...H(12)	392.1(6)	12.9(tied to u_{33})	0.3	11.3
u_{28}	B(7)...H(9)	395.6(6)	12.8(tied to u_{33})	0.3	11.3
u_{29}	B(12)...H(2)	399.1(9)	12.5(tied to u_{33})	0.2	11.0
u_{30}	B(2)...H(9)	398.3(3)	13.2(tied to u_{33})	0.1	11.6
u_{31}	B(7)...H(3)	401.2(3)	12.9(tied to u_{33})	0.2	11.3
u_{32}	B(2)...H(4)	413.6(8)	13.9(tied to u_{33})	0.4	12.2
u_{33}	Se(1)...H(7)	422.9(9)	12.8(7)	0.8	11.3
u_{34}	B(7)...H(4)	465.8(3)	12.2(tied to u_{33})	0.4	10.7
u_{35}	B(2)...H(10)	465.7(3)	12.2(tied to u_{33})	–0.1	10.8
u_{36}	Se(1)...H(12)	492.9(6)	11.5(tied to u_{33})	0.5	10.1
u_{37}	H(7)...H(9)	491.7(15)	15.3(fixed)	0.3	15.3
u_{38}	H(2)...H(12)	493.9(11)	15.1(fixed)	0.5	15.1
u_{39}	H(2)...H(9)	495.6(5)	15.4(fixed)	–0.1	15.4
u_{40}	H(2)...H(4)	504.3(18)	15.9(fixed)	0.2	15.9
u_{41}	H(2)...H(10)	583.3(4)	13.1(fixed)	0.0	13.1

[a] Estimated standard deviations, as obtained in the least squares refinement, are given in parentheses. [b] Amplitudes not refined were fixed at the values obtained using the force field calculated at the RHF/AE1 level (see main text for basis set definition).

Table S3 Least-squares correlation matrix (×100) for $SeB_{11}H_{11}$.[a]

	p_3	p_4	p_5	u_4	u_8	u_{18}	u_{33}	k_2
p_1	51							–56
p_2	85	–81	–82	50				
p_3	100	–70	–73			–58		
p_4		100	84					
u_4				100	67			83
u_8					100			68
u_{26}							52	

[a] Only elements with absolute values ≥ 50% are shown.

Table S4 GED Cartesian coordinates (in Å) for $SeB_{11}H_{11}$.

Atom	*x*	*y*	*z*
S(1)	0.0000	0.0000	1.3633
B(2)	–0.9612	–1.3229	0.0000
B(3)	0.9612	–1.3229	0.0000
B(4)	1.5552	0.5053	0.0000
B(5)	0.0000	1.6352	0.0000
B(6)	–1.5552	0.5053	0.0000
B(7)	–1.4482	–0.4706	–1.4589
B(8)	0.0000	–1.5228	–1.4589
B(9)	1.4482	–0.4706	–1.4589
B(10)	0.8951	1.2319	–1.4589
B(11)	–0.8951	1.2319	–1.4589
B(12)	0.0000	0.0000	–2.3810
H(2)	–1.5577	–2.1440	0.6009
H(3)	1.5577	–2.1440	0.6009
H(4)	2.5204	0.8189	0.6009
H(5)	0.0000	2.6501	0.6009
H(6)	–2.5204	0.8189	0.6009
H(7)	–2.4571	–0.7983	–1.9747
H(8)	0.0000	–2.5835	–1.9747
H(9)	2.4571	–0.7983	–1.9747
H(10)	1.5185	2.0901	–1.9747
H(11)	–1.5185	2.0901	–1.9747
H(12)	0.0000	0.0000	–3.5605

Table S5 Calculated Cartesian coordinates [MP2/962(d)] (in Å) for $SeB_{11}H_{11}$.

Atom	*x*	*y*	*z*
S(1)	0.0000	0.0000	1.4992
B(2)	0.0000	1.6242	0.1193
B(3)	–1.5447	0.5019	0.1193
B(4)	–0.9547	–1.3140	0.1193
B(5)	0.9547	–1.3140	0.1193
B(6)	1.5447	0.5019	0.1193
B(7)	0.8939	1.2304	–1.3414
B(8)	–0.8939	1.2304	–1.3414
B(9)	–1.4464	–0.4700	–1.3414
B(10)	0.0000	–1.5209	–1.3414
B(11)	1.4464	–0.4700	–1.3414
B(12)	0.0000	0.0000	–2.2664
H(2)	0.0000	2.6501	0.7195
H(3)	–2.5204	0.8189	0.7195
H(4)	–1.5577	–2.1439	0.7195
H(5)	1.5577	–2.1439	0.7195
H(6)	2.5204	0.8189	0.7195
H(7)	1.5281	2.1033	–1.8458
H(8)	–1.5281	2.1033	–1.8458
H(9)	–2.4726	–0.8034	–1.8458
H(10)	0.0000	–2.5998	–1.8458
H(11)	2.4726	–0.8034	–1.8458
H(12)	0.0000	0.0000	–3.4574

Energy = –2678.8879 Hartrees (not corrected for ZPE).

Figure S1 Experimental and difference (experimental minus theoretical) molecular-scattering intensities for $SeB_{11}H_{11}$.