The digallane molecule, Ga_2H_6: experimental update giving an improved structure and estimate of the enthalpy change for the reaction $Ga_2H_6(g) \rightarrow 2GaH_3(g)$

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Supplementary Information

Table S1 Nozzle-to-film distances / mm, weighting functions / nm^{-1}, scale factors, correlation parameters and electron wavelengths / pm used in the GED study of Ga_2H_6.[a]

Nozzle-to-film distance	Δs	s_{min}	sw_1	sw_2	s_{max}	Scale factor[b]	Correlation parameter	Electron wavelength[c]
259.80	0.1	30	40	138	140	0.622(10)	0.424	5.67
201.22	0.2	120	140	155	180	0.587(32)	0.222	5.67

[a] From the $r_{a3,1}$ refinement. [b] Values in parentheses are the estimated standard deviations. [c] Determined by reference to the scattering pattern of benzene.

Table S2 Refined and calculated [MP2(full)/aug-cc-pVTZ] amplitudes of vibration (u), associated r_a distances and corresponding correction values ($r_a - r_e$) for the r_{h1} GED refinement of Ga_2H_6.[a]

	Atom pair	r_a	u_{GED}	$r_a - r_e$	$u_{calc.}$	Restraint
u_1	Ga(1)–H(4)	156.5(6)	7.8(7)	1.5	8.9	8.9(9)
u_2	Ga(1)–H(2)	174.8(7)	9.6(tied to u_1)	2.4	11.0	—
u_3	H(2)···H(3)	234.8(20)	14.4(fixed)	2.8	14.4	—
u_4	Ga(1)···Ga(6)	257.85(14)	6.2(4)	3.0	5.7	—
u_5	H(2)···H(4)	268.6(10)	16.9(fixed)	2.5	16.9	—
u_6	H(4)···H(5)	280.7(16)	14.5(fixed)	1.4	14.5	—
u_7	Ga(1)···H(7)	353.6(9)	17.9(14)	2.6	16.5	16.5(17)
u_8	H(4)···H(8)	390.5(23)	32.8(fixed)	1.4	32.8	—
u_9	H(4)···H(7)	481.3(16)	16.6(fixed)	2.3	16.6	—

[a] Distances in pm. Values in parentheses are the standard deviations on the last digits. See Figure 3 for atom numbering.

Table S3 Least-squares correlation matrix (×100) for the GED refinement of Ga_2H_6.[a]

	p_1	p_2	p_3	p_4	u_1	u_4	u_7	k_1	k_2
p_1	100								
p_2		100							
p_3			100						
p_4				100					
u_1					100				
u_4						100		62	84
u_7							100		
k_1								100	53
k_2									100

[a] Only absolute values ≥50 are shown. k_1 and k_2 are scale factors.

Table S4 GED-determined coordinates (Å) for Ga_2H_6.

	x	*y*	*z*
Ga(1)	1.2743	0.0000	0.0000
H(2)	0.0000	1.1600	0.0000
H(3)	0.0000	–1.1600	0.0000
H(4)	1.9457	0.0000	–1.3967
H(5)	1.9457	0.0000	1.3967
Ga(6)	–1.2743	0.0000	0.0000
H(7)	–1.9457	0.0000	1.3967
H(8)	–1.9457	0.0000	–1.3967

Table S5 Calculated coordinates [Å; MP2(full)/aug-cc-pVTZ] for Ga_2H_6.

	x	*y*	*z*
(1)	1.2700	0.0000	0.0000
(2)	0.0000	1.1495	0.0000
(3)	0.0000	–1.1495	0.0000
(4)	1.9247	0.0000	–1.3889
(5)	1.9247	0.0000	1.3889
(6)	–1.2700	0.0000	0.0000
(7)	–1.9247	0.0000	1.3889
(8)	–1.9247	0.0000	–1.3889

Total energy (zero-point corrected) = –3850.413904 Hartrees.

Figure S1 Molecular-scattering intensity curves from the $r_{a3,1}$ GED refinement of Ga_2H_6.