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The molecular structure of [Sn($P_2C_2Bu^t_2$)] using gas-phase electron diffraction and DFT calculations

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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 [Sn($P_2C_2Bu^t_2$)], **2b**.

Nozzle-to-film distance[a]	Δs	s_{min}	sw_1	sw_2	s_{max}	Scale factor[b]	Correlation parameter	Electron wavelength
86.06	4	80	120	230	250	0.801(42)	0.393	6.020
255.26	2	20	40	102	110	0.857(14)	0.119	6.020

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

Table S2 Selected interatomic distances (r_a/pm) and amplitudes of vibration (u_{h1}/pm) for the restrained GED structure of [Sn($P_2C_2Bu^t_2$)], **2b**.[a]

	Atom pair	r_a/pm	u_{h1}/pm[b]	Restraint
$u_{1–9}$	C–H	110.2(3)	7.1(3)	7.7(8)
u_{10}	C(3)–C(6)	152.1(4)	4.0(6)	—
$u_{11–12}$	C(6)–C(8/9)	154.8(2)	4.1(tied to u_{10})	—
u_{13}	C(6)–C(7)	155.6(2)	4.1(tied to u_{10})	—
$u_{14–15}$	P(2)–C(3/5)	180.2(3)	5.2(4)	—
u_{16}	Sn(1)–C(3)	240.7(11)	10.5(11)	10.1(10)
u_{17}	C(3)…C(7)	249.1(10)	7.1(8)	8.0(8)
$u_{18–19}$	C(7)…C(8)	250.6(23)	7.1(tied to u_{17})	—
$u_{20–21}$	C(3)…C(9)	252.6(8)	6.8(tied to u_{17})	—
u_{22}	Sn(1)–P(2)	261.4(7)	7.5(8)	7.7(8)
u_{23}	P(2)…P(4)	269.8(17)	5.1(6)	5.6(6)
u_{24}	P(2)…C(6)	300.0(14)	9.0(7)	8.2(8)
u_{25}	P(2)…C(19)	304.7(16)	9.0(tied to u_{24})	—
u_{26}	P(2)…C(8)	336.7(38)	18.7(18)	19.1(19)
u_{27}	P(2)…C(22)	341.8(39)	18.7(tied to u_{26})	—
u_{28}	Sn(1)…C(6)	352.7(11)	12.1(12)	12.4(12)
u_{29}	P(2)…C(7)	362.0(28)	18.0(25)	—
u_{30}	P(2)…C(20)	369.3(40)	18.0(tied to u_{29})	—
$u_{31–32}$	Sn(1)…C(8/9)	393.5(32)	22.7(17)	—
u_{33}	P(2)…C(9)	424.1(12)	9.8(9)	—
u_{34}	P(2)…C(21)	426.6(14)	9.9(tied to u_{33})	—
u_{35}	Sn(1)…C(7)	480.7(11)	13.8(12)	12.0(12)

[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 B3PW91/LanL2DZ on Sn and 6-31G* on P, C, and H. Other amplitudes were also included and fixed at this level but are not shown here.

Table S3 Least-squares correlation matrix (×100) for [Sn($P_2C_2Bu^t_2$)], **2b**.[a]

	p_2	p_{10}	p_{21}	u_6	k_1	k_2
p_1	–50				–58	
p_5		–52				
p_{12}				–75		
p_{18}			81			
u_1						62

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

Table S4 GED coordinates for [Sn($P_2C_2Bu^t_2$)], **2b**.[a]

Atom	*x*	*y*	*z*
Sn(1)	0.0000	2.2002	0.0000
P(2)	0.0000	0.0000	1.3626
C(3)	1.1809	0.0986	0.0000
P(4)	0.0000	0.0000	–1.3626
C(5)	–1.1809	0.0986	0.0000
C(6)	2.7139	–0.1401	0.0000
C(7)	2.9627	–1.6776	0.0009
C(8)	3.3627	0.4916	–1.2673
C(9)	3.3649	0.4990	1.2625
H(10)	4.0667	–1.9066	0.0111
H(11)	2.5158	–2.1588	–0.9161
H(12)	2.4985	–2.1599	0.9082
H(13)	4.4785	0.3295	–1.2714
H(14)	3.1718	1.6022	–1.3060
H(15)	2.9405	0.0327	–2.2067
H(16)	4.4815	0.3422	1.2625
H(17)	2.9488	0.0412	2.2052
H(18)	3.1689	1.6088	1.2982
C(19)	–2.7139	–0.1401	0.0000
C(20)	–2.9627	–1.6776	–0.0009
C(21)	–3.3627	0.4916	1.2671
C(22)	–3.3649	0.4990	–1.2625
H(23)	–4.0667	–1.9066	–0.0111
H(24)	–2.5158	–2.1581	0.9161
H(25)	–2.4985	–2.1599	–0.9082
H(26)	–4.4785	0.3295	1.2714
H(27)	–3.1718	1.6022	1.3060
H(28)	–2.9405	0.0327	2.2067
H(29)	–4.4815	0.3422	–1.2625
H(30)	–2.9488	0.0412	–2.2052
H(31)	–3.1689	1.6088	–1.2982

[a] All coordinates are r_a in Å.

Table S5 Calculated coordinates (B3PW91/6-31G*/LanL2DZ) for [Sn($P_2C_2Bu^t_2$)], **2b**.

Atom	*x*	*y*	*z*
Sn(1)	0.0000	0.0000	1.5772
P(2)	1.3678	0.0000	–0.6732
C(3)	0.0000	–1.1813	–0.5416
P(4)	–1.3678	–0.0000	–0.6732
C(5)	–0.0000	1.1813	–0.5416
C(6)	0.0000	–2.6845	–0.7173
C(7)	0.0000	–2.9910	–2.2308
C(8)	1.2554	–3.3041	–0.0845
C(9)	–1.2553	–3.3043	–0.0845
H(10)	0.8868	–2.5675	–2.7158
H(11)	0.0001	–4.0747	–2.4041
H(12)	–0.8867	–2.5675	–2.7158
H(13)	1.2710	–3.1461	1.0005
H(14)	1.2852	–4.3848	–0.2700
H(15)	2.1710	–2.8689	–0.5029
H(16)	–2.1709	–2.8689	–0.5028
H(17)	–1.2850	–4.3849	–0.2699
H(18)	–1.2709	–3.1461	1.0005
C(19)	–0.0000	2.6845	–0.7173
C(20)	–0.0000	2.9910	–2.2308
C(21)	–1.2554	3.3041	–0.0845
C(22)	1.2553	3.3043	–0.0845
H(23)	–0.8868	2.5675	–2.7158
H(24)	–0.0001	4.0747	–2.4041
H(25)	0.8867	2.5675	–2.7158
H(26)	–1.2710	3.1461	1.0005
H(27)	–1.2852	4.3848	–0.2700
H(28)	–2.1710	2.8689	–0.5029
H(29)	2.1709	2.8689	–0.5028
H(30)	1.2850	4.3849	–0.2699
H(31)	1.2709	3.1461	1.0005

Energy = –1077.502038 Hartrees (corrected for ZPE).
All coordinates are in Å.

Table S6 Calculated coordinates (B3PW91/6-31G*/LanL2DZ) for [Sn($P_2C_2H_2$)], **3**.

Atom	*x*	*y*	*z*
Sn(1)	0.0000	0.0000	1.0351
P(2)	0.0000	1.3710	–1.2177
C(3)	1.1613	0.0000	–1.0797
P(4)	0.0000	–1.3710	–1.2177
C(5)	–1.1613	0.0000	–1.0797
H(6)	2.2453	0.0000	–1.1341
H(7)	–2.2453	0.0000	–1.1341

Energy = –763.324630 Hartrees (corrected for ZPE).
All coordinates are in Å.

Table S7 Calculated coordinates (B3PW91/6-31G*) for [$P_2C_2Bu^t_2$], **4**.

Atom	*x*	*y*	*z*
P(1)	1.3795	–0.0122	0.0000
C(2)	–0.1428	1.1642	0.0000
P(3)	–1.3797	0.0122	0.0000
C(4)	0.1428	–1.1642	0.0000
C(5)	–0.1458	2.6577	0.0000
C(6)	–1.5778	3.2086	0.0000
C(7)	0.6035	3.1488	1.2573
C(8)	0.6035	3.1488	–1.2573
H(9)	–2.1292	2.8754	0.8870
H(10)	–1.5679	4.3049	0.0000
H(11)	–2.1292	2.8754	–0.8869
H(12)	1.6307	2.7673	1.2871
H(13)	0.6508	4.2447	1.2601
H(14)	0.0925	2.8242	2.1701
H(15)	0.0925	2.8242	–2.1701
H(16)	0.6508	4.2447	–1.2601
H(17)	1.6307	2.7673	–1.2871
C(18)	0.1458	–2.6577	0.0000
C(19)	1.5778	–3.2086	0.0000
C(20)	–0.6035	–3.1488	1.2573
C(21)	–0.6035	–3.1488	–1.2573
H(22)	2.1292	–2.8754	0.8870
H(23)	1.5679	–4.3049	0.0000
H(24)	2.1292	–2.8754	–0.8869
H(25)	–1.6307	–2.7673	1.2871
H(26)	–0.6508	–4.2447	1.2601
H(27)	–0.0925	–2.8242	2.1701
H(28)	–0.0925	–2.8242	–2.1701
H(29)	–0.6508	–4.2447	–1.2601
H(30)	–1.6307	–2.7673	–1.2871

Energy = –1074.038806 Hartrees (corrected for ZPE).
All coordinates are in Å.

Table S8 Calculated coordinates (B3PW91/6-31G*/LanL2DZ) for [Sn($C_4Bu^t_2H_2$)], **5**.

Atom	*x*	*y*	*z*
Sn(1)	–1.5890	–0.0002	0.0057
C(2)	0.5256	–1.0284	–0.0020
C(3)	0.5163	0.0000	–1.0447
C(4)	0.5253	1.0285	–0.0020
C(5)	0.5231	0.0000	1.0410
C(6)	0.8581	0.0002	–2.5111
C(7)	2.3981	0.0004	–2.6389
C(8)	0.3008	–1.2557	–3.1956
C(9)	0.3005	1.2560	–3.1955
H(10)	2.8300	–0.8858	–2.1604
H(11)	2.6990	0.0005	–3.6945
H(12)	2.8298	0.8866	–2.1603
H(13)	–0.7948	–1.2682	–3.1648
H(14)	0.6139	–1.2909	–4.2464
H(15)	0.6640	–2.1687	–2.7091
H(16)	0.6634	2.1691	–2.7089
H(17)	0.6136	1.2914	–4.2462
H(18)	–0.7951	1.2683	–3.1647
C(19)	0.8750	0.0000	2.5050
C(20)	2.4158	0.0002	2.6223
C(21)	0.3221	1.2557	3.1933
C(22)	0.3224	–1.2560	3.1931
H(23)	2.8443	0.8865	2.1408
H(24)	2.7240	0.0002	3.6758
H(25)	2.8445	–0.8859	2.1407
H(26)	–0.7737	1.2680	3.1699
H(27)	0.6423	1.2910	4.2418
H(28)	0.6817	2.1688	2.7042
H(29)	0.6823	–2.1689	2.7040
H(30)	0.6427	–1.2913	4.2417
H(31)	–0.7734	–1.2686	3.1698
H(32)	0.6564	–2.1033	–0.0026
H(33)	0.6559	2.1034	–0.0024

Energy = –472.194130 Hartrees (corrected for ZPE).
All coordinates are in Å.

Table S9 Calculated coordinates (B3PW91/6-31G*) for $[Li_2(P_2C_2Bu^t_2)]$, **6**.

Atom	*x*	*y*	*z*
Li(1)	0.0000	0.0000	–1.9281
P(2)	0.0000	–1.3843	–0.0649
C(3)	1.1816	0.0000	–0.0807
P(4)	0.0000	1.3843	–0.0648
C(5)	–1.1816	0.0000	–0.0807
C(6)	2.6982	0.0000	0.0140
C(7)	3.1455	0.0000	1.4933
C(8)	3.2746	–1.2534	–0.6636
C(9)	3.2746	1.2535	–0.6635
H(10)	2.7667	–0.8930	2.0093
H(11)	4.2399	–0.0000	1.5919
H(12)	2.7667	0.8928	2.0093
H(13)	3.0331	–1.2653	–1.7339
H(14)	4.3670	–1.2903	–0.5611
H(15)	2.8640	–2.1688	–0.2205
H(16)	2.8640	2.1688	–0.2204
H(17)	4.3670	1.2903	–0.5611
H(18)	3.0331	1.2654	–1.7338
C(19)	–2.6982	0.0000	0.0140
C(20)	–3.1455	0.0000	1.4933
C(21)	–3.2746	1.2535	–0.6635
C(22)	–3.2746	–1.2534	–0.6636
H(23)	–2.7667	0.8929	2.0093
H(24)	–4.2399	0.0000	1.5919
H(25)	–2.7667	–0.8930	2.0093
H(26)	–3.0331	1.2654	–1.7338
H(27)	–4.3670	1.2903	–0.5610
H(28)	–2.8640	2.1688	–0.2204
H(29)	–2.8640	–2.1688	–0.2205
H(30)	–4.3670	–1.2903	–0.5611
H(31)	–3.0331	–1.2653	–1.7339
Li(32)	0.0000	–0.0000	1.7920

Energy = –1089.185305 Hartrees (corrected for ZPE).
All coordinates are in Å.

Figure S1 Molecular-scattering intensity and final weighted difference curves for [Sn($P_2C_2Bu^t_2$)], **2b**, at nozzle-to-film distances of (*a*) 255 mm and (*b*) 86 mm.