Silicion(II) Cation $Cp^*Si:^+ X^-$: A New Efficient Catalyst in Organosilicon Chemistry

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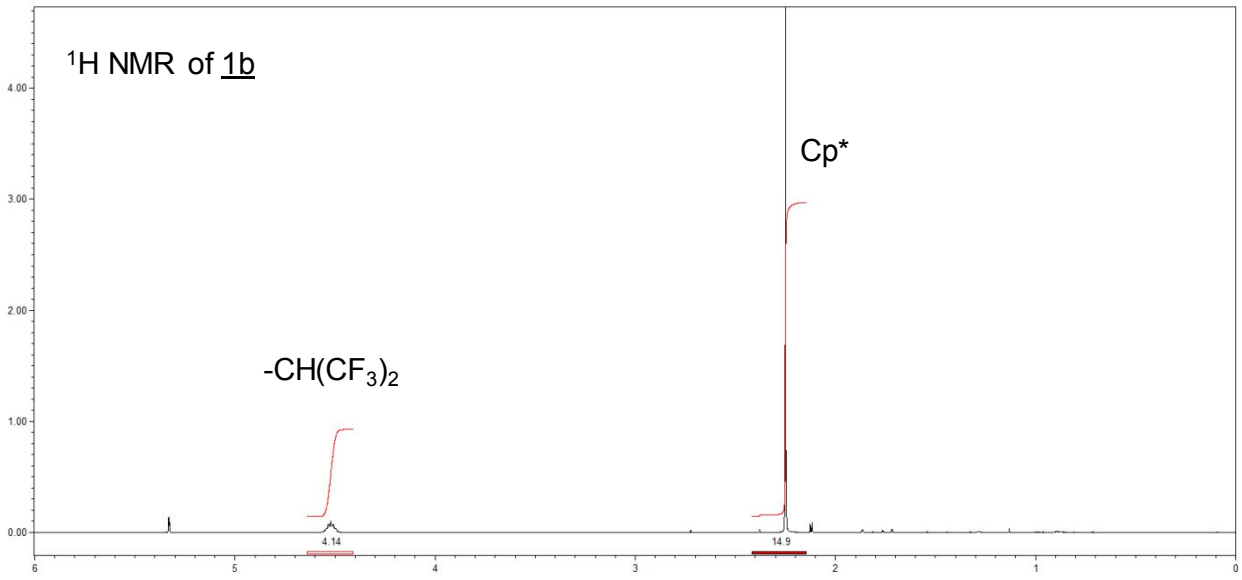
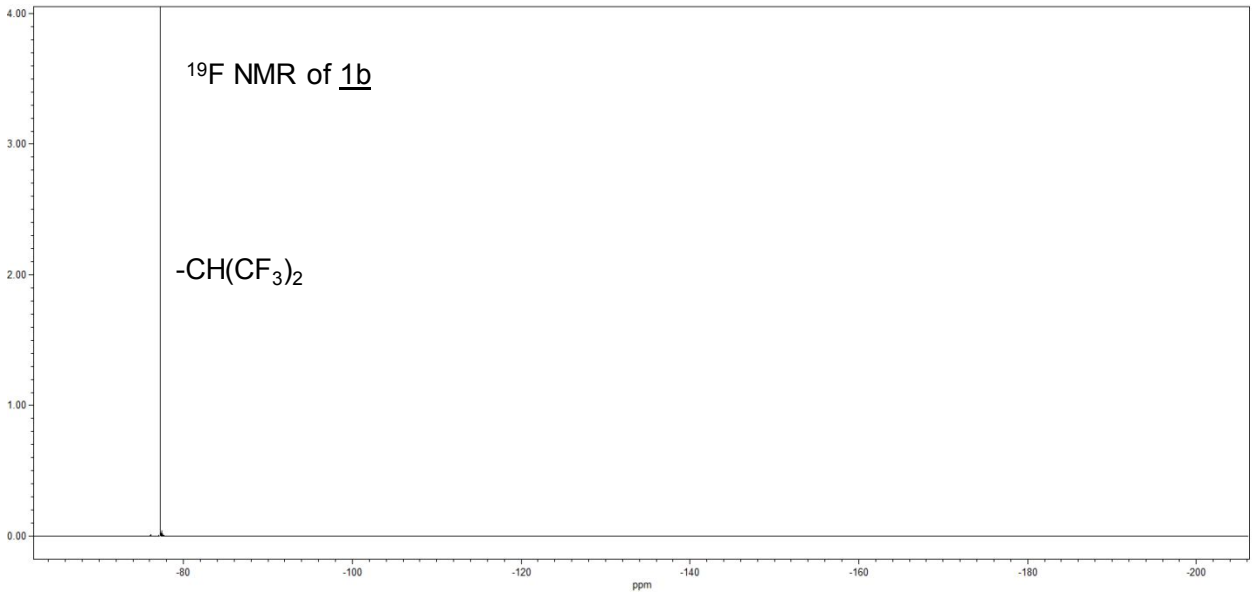
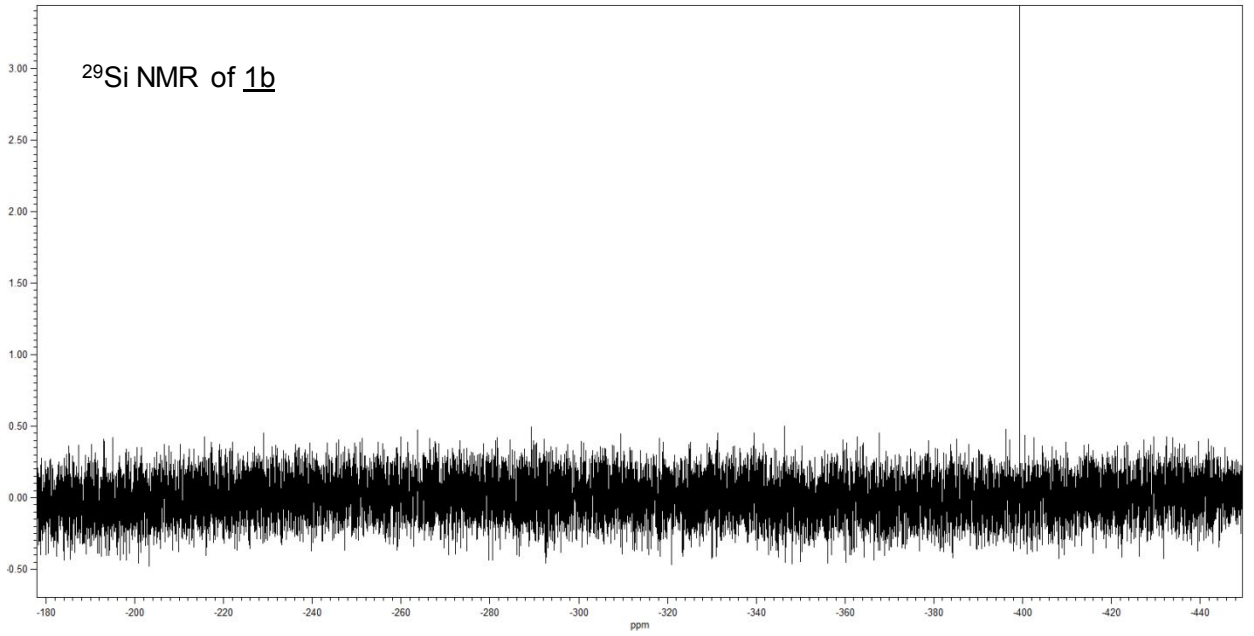
Supporting Information

NMR spectra of the new compounds 1b, 1c, 1d and 1e (in CD_2Cl_2)

1) NMR spectra of 1b

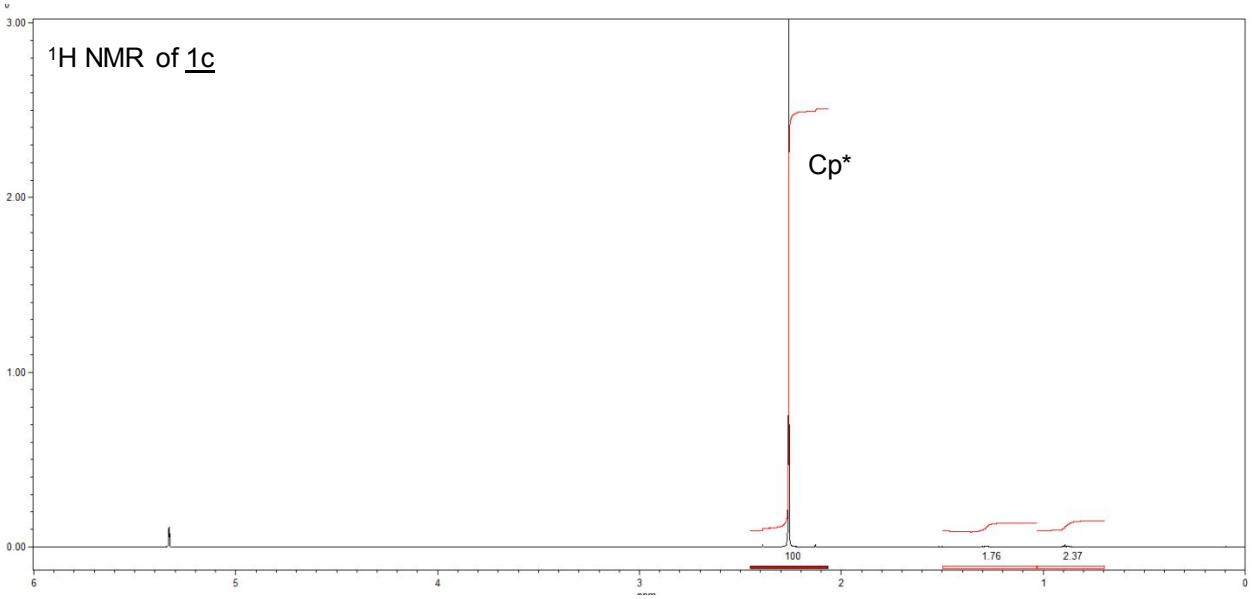




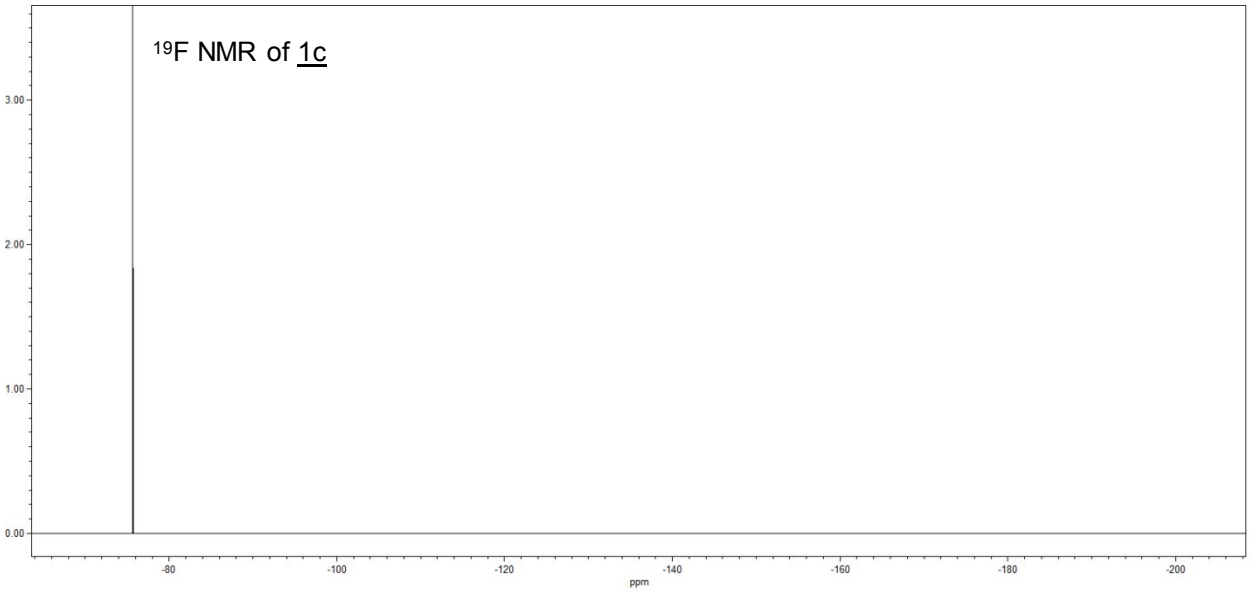


2) NMR spectra of 1c

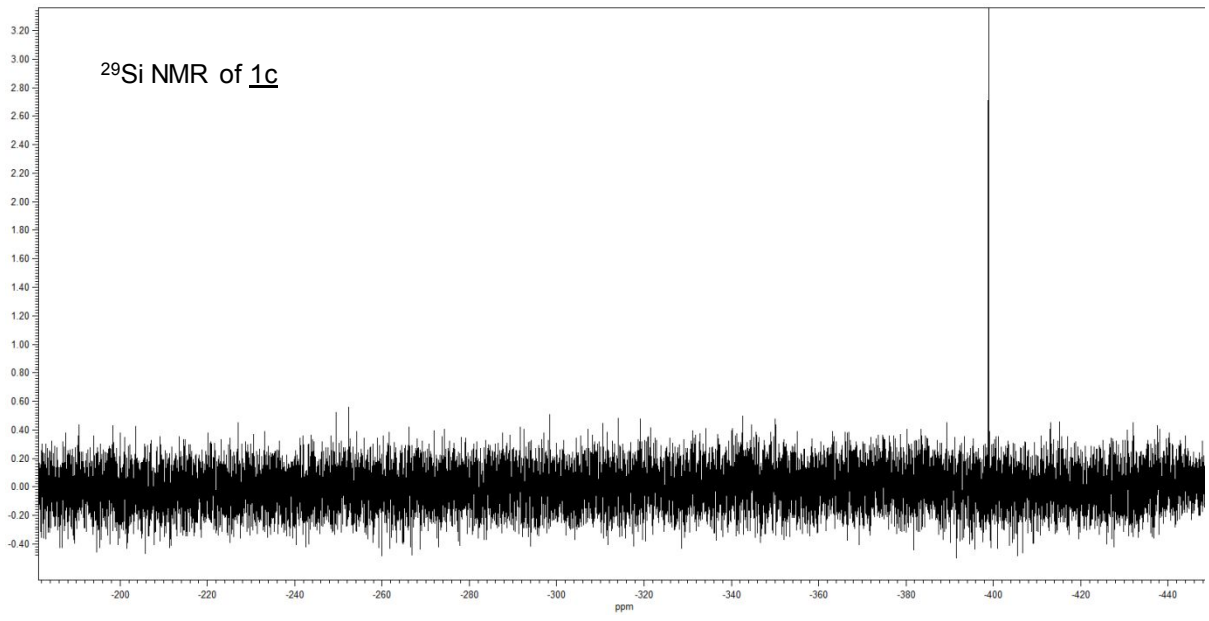
^{1}H NMR of 1c



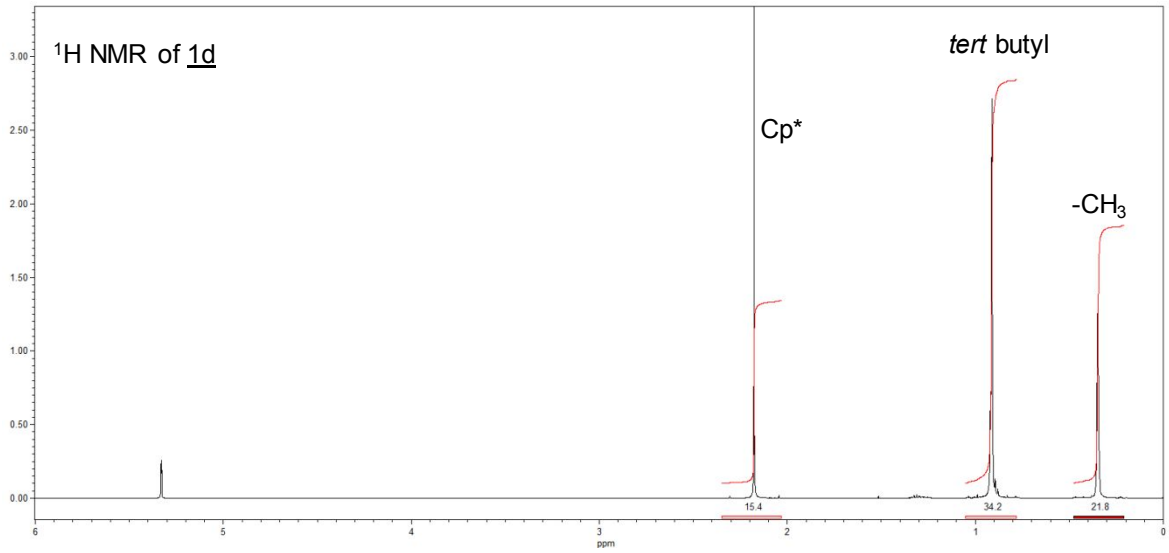
^{19}F NMR of 1c

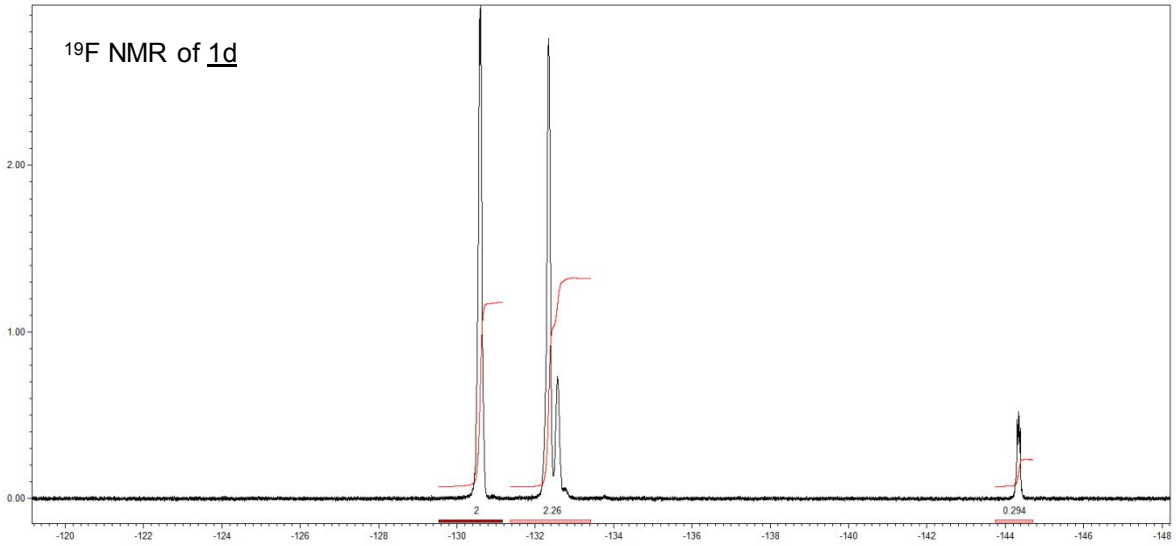


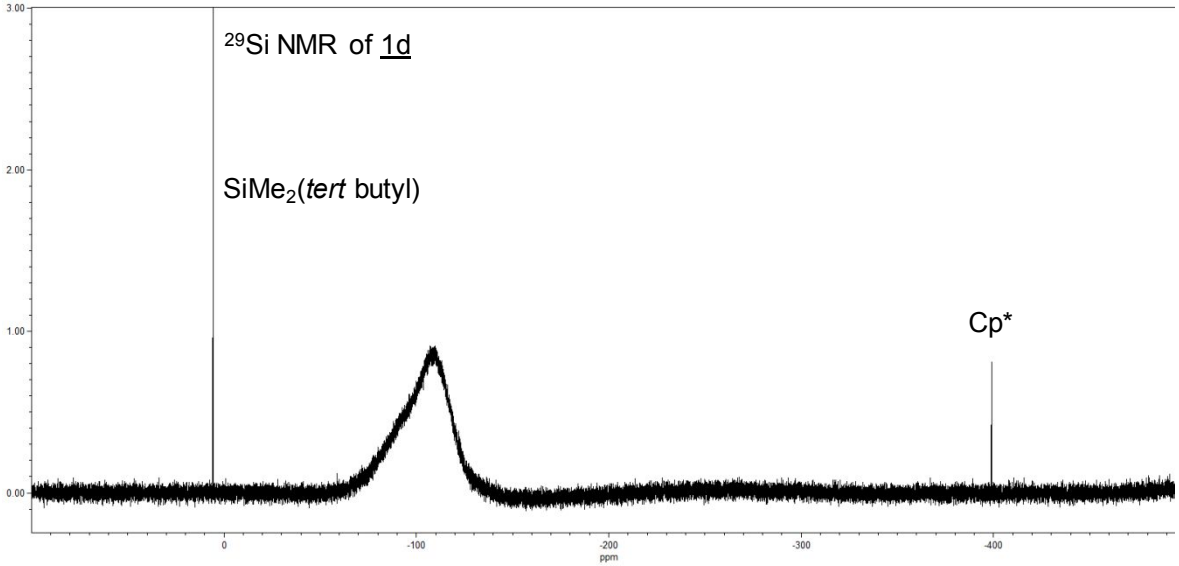
^{29}Si NMR of 1c



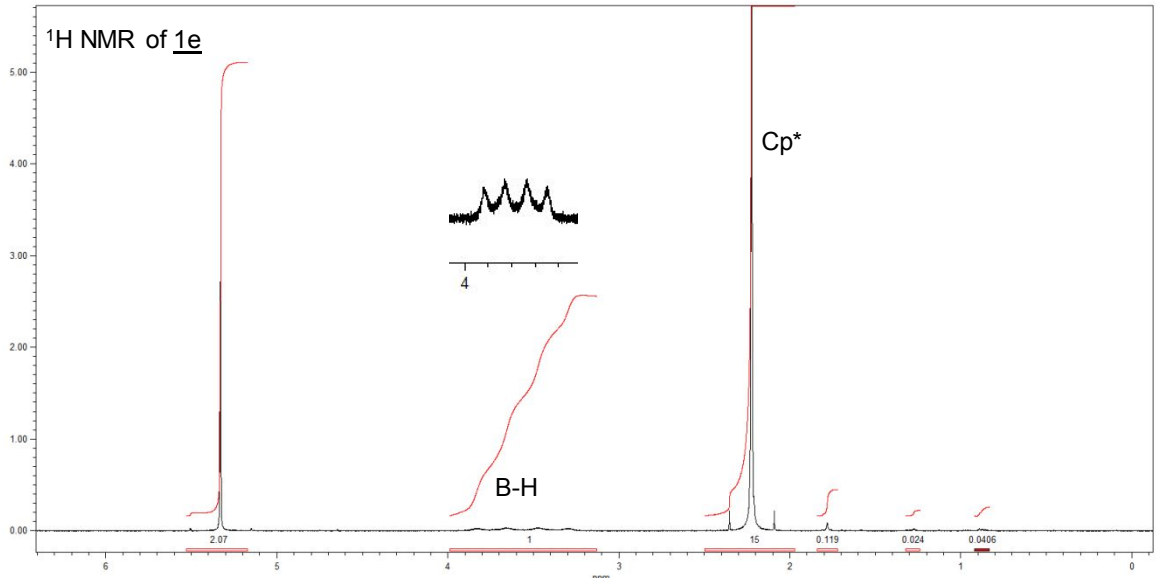
3) NMR spectra of 1d

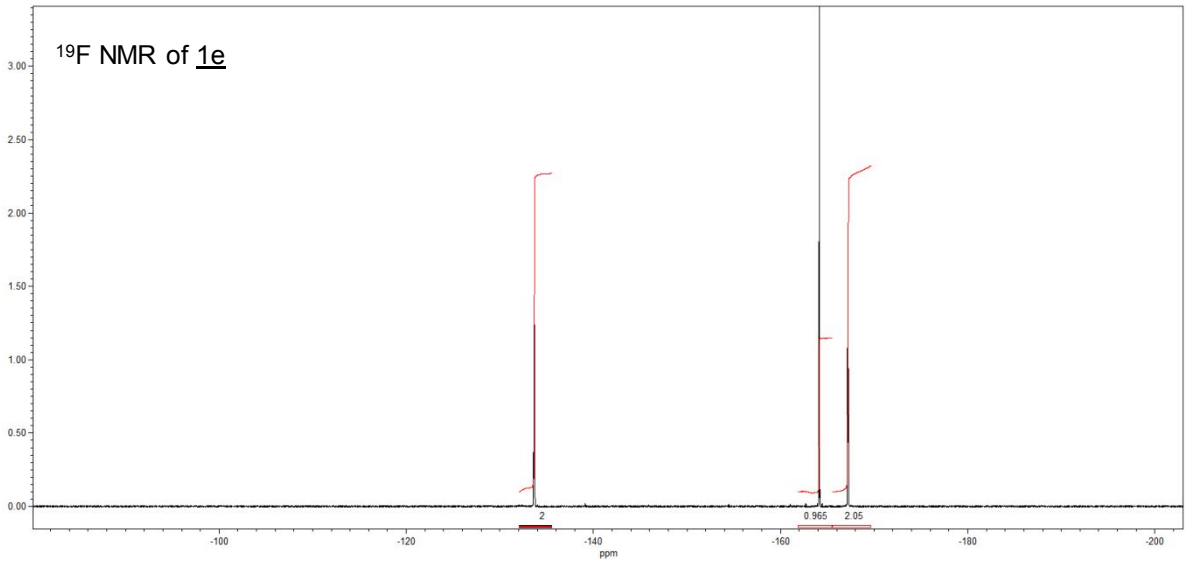


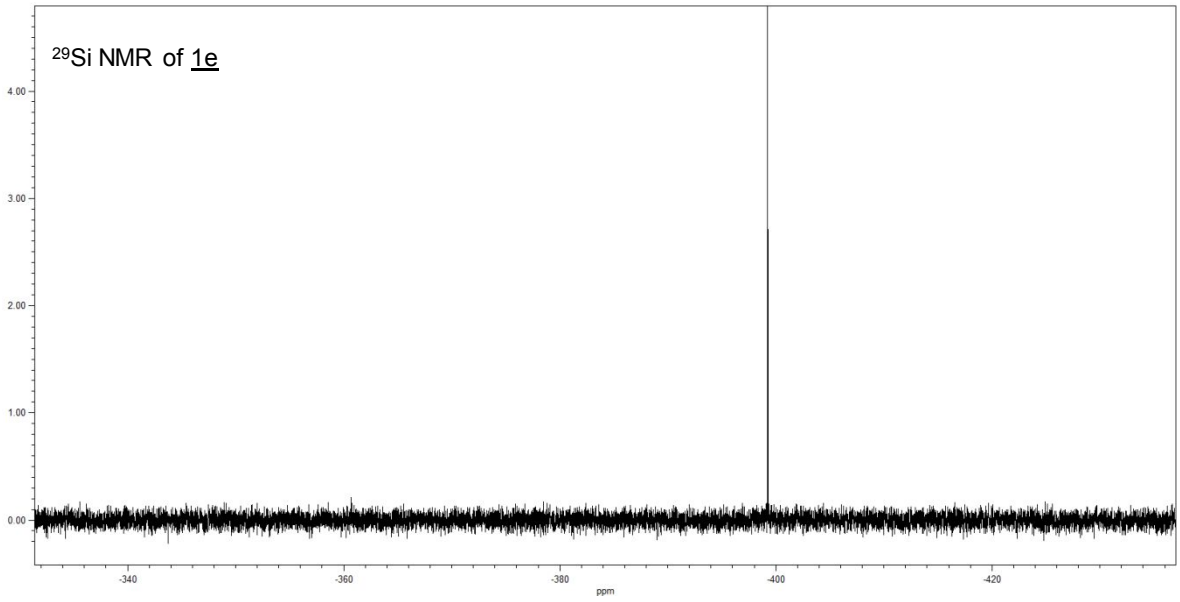


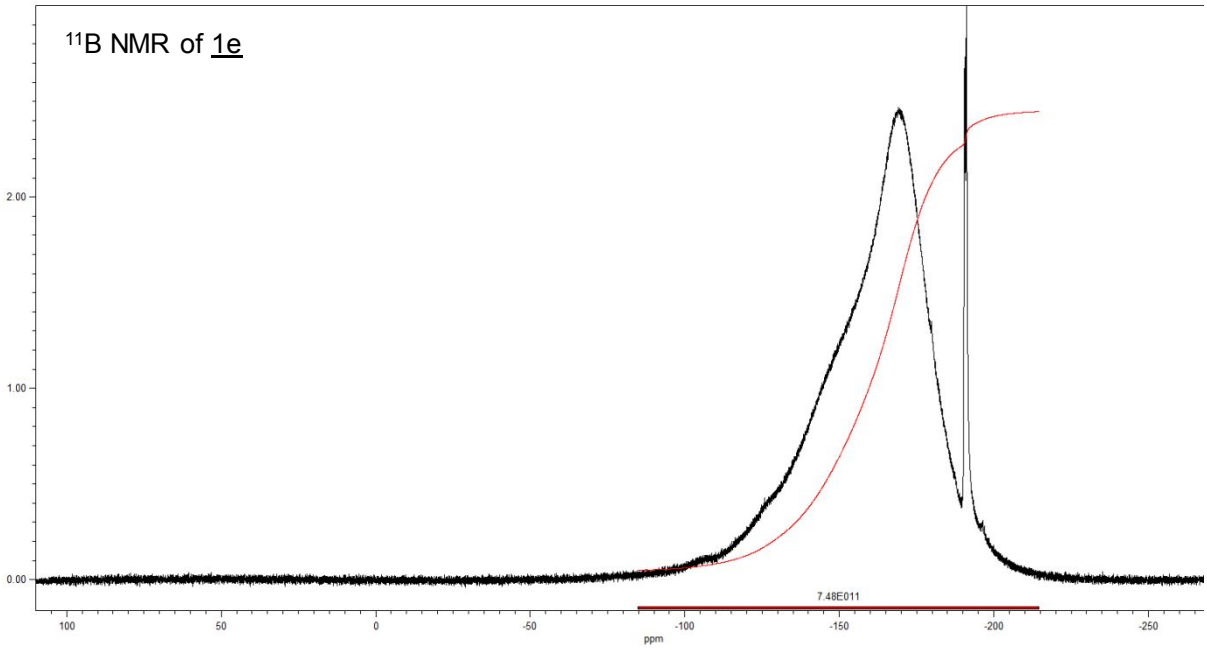


4) NMR spectra of 1e

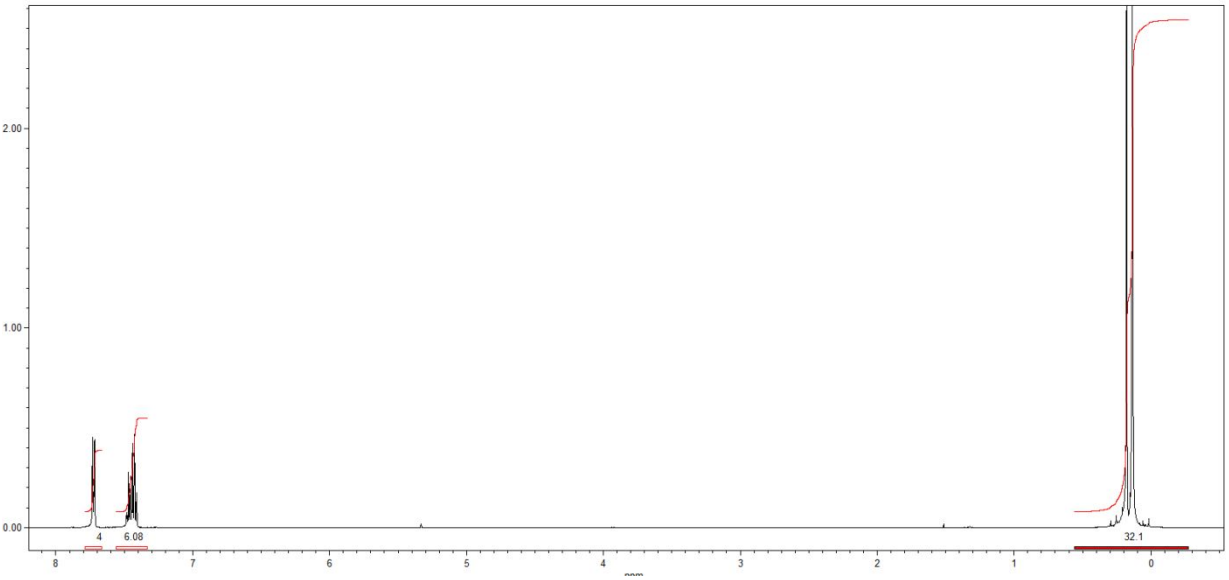


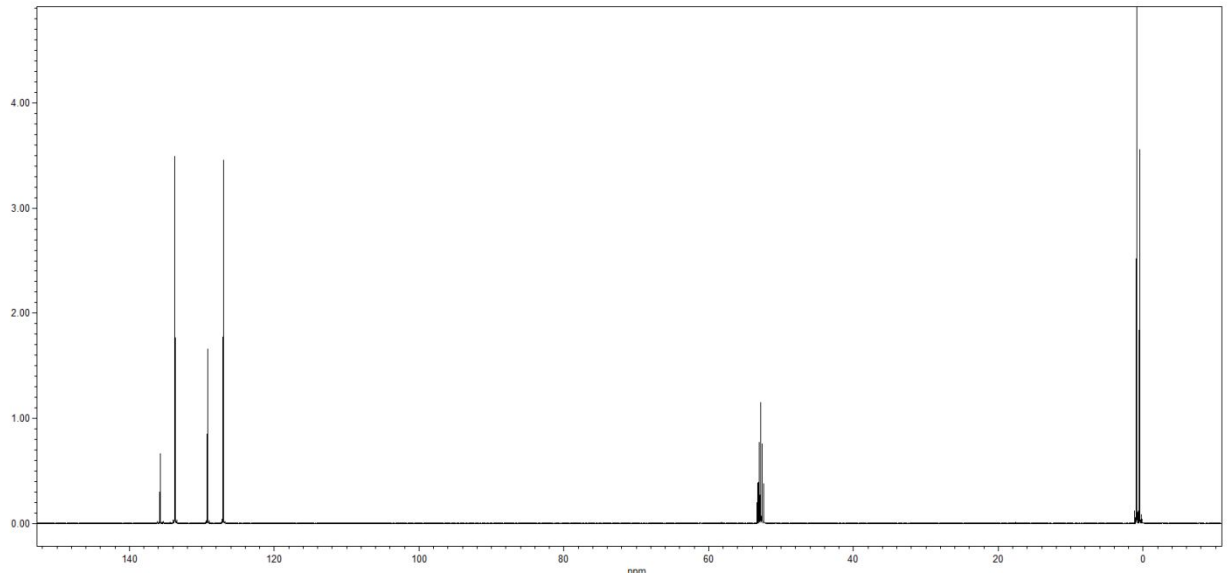


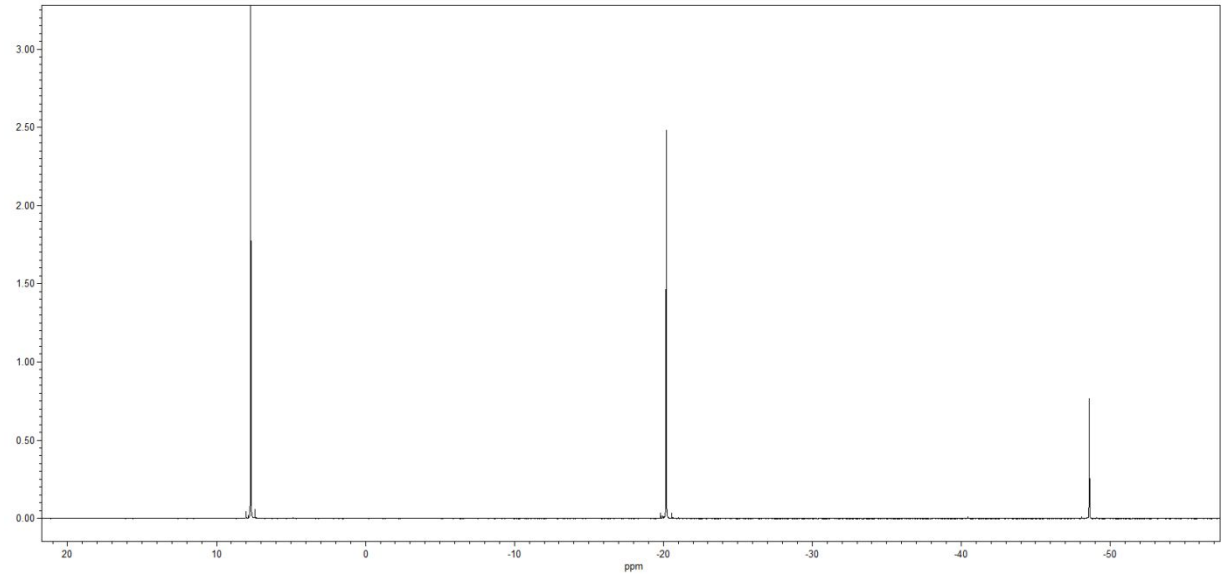




^{1}H, ^{13}C and ^{29}Si NMR spectra of 4 (in CD_2Cl_2)







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Crystal Data of 1e (internal name wes-si16-b).

Compound	**wes-si16-b**	**Compound**	**wes-si16-b**
Formula	$C_{28}H_{16}BF_{15}Si$	V/Å^3	1351.59(7)
$D_{calc.}$/ g cm^{-3}	1.662	Z	2
μ/mm^{-1}	1.925	Z'	1
Formula Weight	676.31	Θ_{min}/°	4.642
Colour	colourless	Θ_{max}/°	76.573
Shape	block	Measured Refl.	43502
Max Size/mm	0.12	Independent Refl.	5645
Mid Size/mm	0.12	Reflections Used	4999
Min Size/mm	0.08	R_{int}	0.0384
T/K	123.00(10)	Parameters	470
Crystal System	triclinic	Restraints	0
Space Group	P-1	Largest Peak	0.294
a/Å	9.4778(3)	Deepest Hole	-0.232
b/Å	10.3906(3)	GooF	1.018
c/Å	14.9750(4)	wR_2 (all data)	0.1018
α/°	99.913(2)	wR_2	0.0972
β/°	91.410(2)	R_1 (all data)	0.0408
γ/°	110.858(3)	R_1	0.0358

Experimental. Single colourless block-shaped crystals of (**wes-si16-b**) were obtained by recrystallisation from dichloromethane. A suitable crystal (0.12×0.12×0.08) was selected and mounted on a MITIGEN holder with inert oil on a SuperNova, Single source at offset, Atlas diffractometer. The crystal was kept at T = 123.00(10) K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program, using the Unknown solution method. The model was refined with version 2014/7 of **ShelXL** (Sheldrick, 2015) using Least Squares minimisation.

Crystal Data. $C_{28}H_{16}BF_{15}Si$, M_r = 676.31, triclinic, P-1 (No. 2), a = 9.4778(3) Å, b = 10.3906(3) Å, c = 14.9750(4) Å, α =9 9.913(2)°, β = 91.410(2)°, γ = 110.858(3)°, V = 1351.59(7) Å^3, T = 123.00(10) K, Z = 2, Z' = 1, μ(CuK$_\alpha$) = 1.925, 43502 reflections measured, 5645 unique (R_{int} = 0.0384) which were used in all calculations. The final wR_2 was 0.1018 (all data) and R_1 was 0.0358 (I > 2(I)).

Structure Quality Indicators

Reflections:	d min (Cu) 0.79	I/σ 26.4	Rint 3.84%	complete 100%
Refinement:	Shift 0.001	Max Peak 0.3	Min Peak -0.2	GooF 1.018

Data were measured using scans scans of 1.0° per frame for 1.5 s using CuK$_\alpha$ radiation (50 kV, 0.8 mA). The total number of runs and images was based on the strategy calculation from the program CrysAlisPro (Rigaku Oxford Diffraction). The actually achieved resolution was Θ =

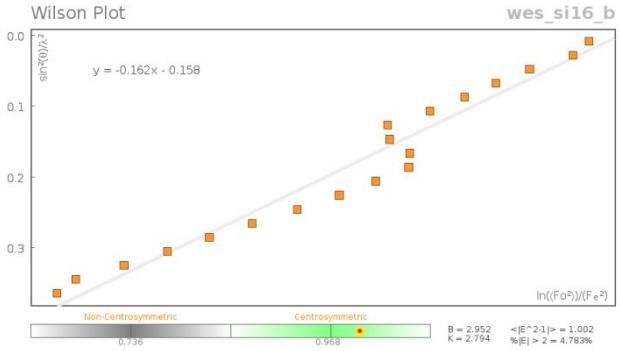
76.573.

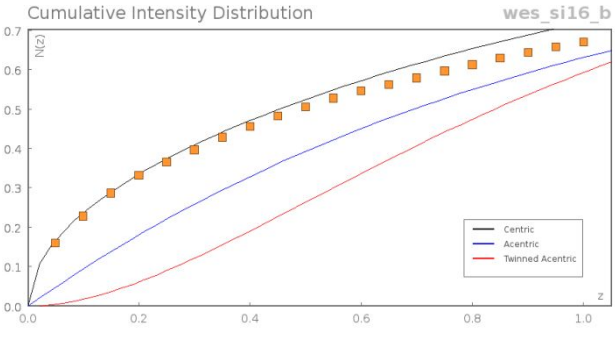
Cell parameters were retrieved using the CrysAlisPro (Rigaku Oxford Diffraction) software and refined using CrysAlisPro (Rigaku Oxford Diffraction) on 19471 reflections, 45 of the observed reflections. Data reduction was performed using the CrysAlisPro (Rigaku Oxford Diffraction) software which corrects for Lorentz polarisation. The final completeness is 100.00 out to 76.573 in Θ. The absorption coefficient (μ) of this material is 1.925 and the minimum and maximum transmissions are 0.960 and 0.977.

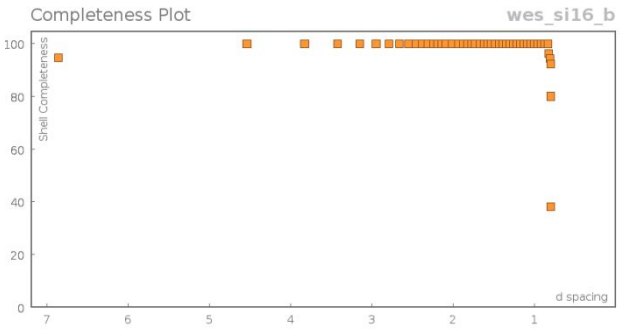
The structure was solved in the space group P-1 (# 2) by intrinsic phasing using the **ShelXT** (Sheldrick, 2015) structure solution program and refined by Least Squares using version 2014/7 of **ShelXL** (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 2 and Z' is 1.

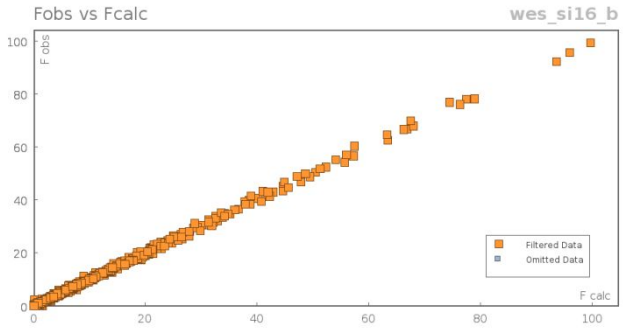
Data Plots: Diffraction Data







Data Plots: Refinement and Data



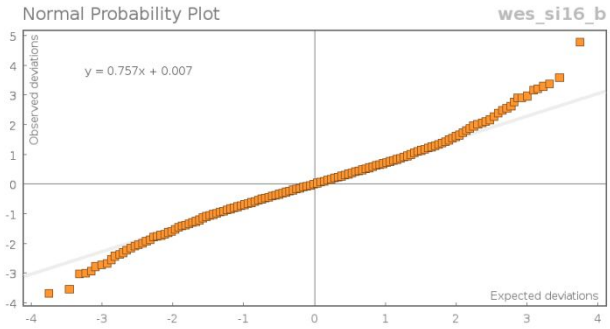


Table S1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **wes_si16_b**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Si1	5360.9(5)	-1041.0(4)	7323.1(3)	34.86(11)
F6	5521.5(11)	1715(1)	8868.4(6)	38.2(2)
F1	790.6(11)	28.2(9)	8087.6(7)	40.9(2)
F5	4615.8(11)	4536.1(9)	8358.2(7)	42.6(2)
F7	8493.7(12)	3107.5(12)	9199.7(7)	46.0(2)
F3	985.3(12)	3693.1(12)	10454.8(7)	44.2(2)
F10	5675.8(11)	3112.3(12)	6012.1(7)	46.1(2)
F4	3465.9(12)	5452.7(10)	9819.4(8)	47.6(3)
F15	2050.3(14)	3378.1(12)	6713.8(7)	50.8(3)
F2	-359.4(11)	989.9(11)	9547.8(8)	46.1(2)
F11	3509.3(15)	-505.8(11)	5722.7(7)	52.0(3)
F8	10117.9(12)	4474.8(14)	7942.5(8)	54.3(3)
F9	8629.4(12)	4408.4(14)	6332.0(8)	56.2(3)
F13	828.1(15)	938.0(15)	3696.6(8)	67.7(4)
F12	2187.2(17)	-839.8(13)	4064.9(7)	64.6(4)
F14	782.3(16)	3047.5(16)	5041.2(9)	66.8(4)
C11	2804.2(16)	2210.3(15)	8159(1)	28.6(3)
C12	1512.3(16)	1386.6(15)	8498.7(10)	30.6(3)
C3	5254.8(18)	-2202.2(15)	8387.1(10)	31.7(3)
C17	2791.5(17)	1420.9(16)	6316.5(10)	33.1(3)
C16	3395.7(17)	3591.5(15)	8631.7(10)	31.3(3)
C13	885.2(16)	1852.2(17)	9253.7(11)	33.2(3)
C23	5419.4(17)	2358.7(15)	7433.7(10)	29.6(3)
C4	5847.2(19)	-2804.0(15)	7631.4(11)	33.7(3)
C24	6306.1(18)	3058.5(16)	6817.4(10)	33.5(3)
C2	3766.4(18)	-2302.9(15)	8104.8(11)	33.6(3)
C15	2815.2(17)	4104.9(16)	9392.1(11)	34.0(3)
C28	6250.8(18)	2393.9(15)	8218.5(10)	31.3(3)
C27	7790.8(18)	3084.6(17)	8406.8(10)	34.9(3)
C14	1552.6(17)	3223.7(17)	9710.9(10)	33.3(3)
C5	4744(2)	-3258.8(15)	6878.9(11)	37.9(3)
C26	8616.7(18)	3776.5(18)	7771.1(12)	38.9(3)
C18	2091.3(19)	2292.9(18)	6084.3(11)	38.4(3)
C22	2806(2)	387.2(17)	5597.5(11)	38.5(3)
C7	3458.6(19)	-2947.8(17)	7159.1(11)	38.8(4)
C19	1439(2)	2156(2)	5219.0(13)	46.2(4)
C20	1469(2)	1097(2)	4538.2(12)	48.4(5)
C25	7863.8(19)	3744.9(18)	6965.9(11)	38.3(3)
C21	2162(2)	203.5(19)	4726.8(11)	45.2(4)
C1	2716(3)	-1855(2)	8701.7(16)	51.3(5)
C10	6065(2)	-1578(2)	9320.6(12)	47.7(4)
C6	4900(3)	-3967(2)	5943.6(13)	58.2(6)
C9	7368(2)	-2939(2)	7660.1(16)	50.4(5)
B1	3575.2(19)	1536.6(17)	7325.9(11)	30.3(3)

Atom	x	y	z	U_{eq}
C8	2034(3)	-3270(3)	6570.0(18)	61.6(6)

Table S2: Anisotropic Displacement Parameters (×10⁴) **wes_si16_b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	42.2(2)	25.72(19)	36.2(2)	10.92(16)	7.71(17)	9.26(16)
F6	45.0(5)	45.1(5)	27.7(4)	13.5(4)	6.1(4)	17.1(4)
F1	35.6(5)	28.1(4)	50.5(6)	5.8(4)	-0.6(4)	2.6(4)
F5	39.5(5)	26.8(4)	57.2(6)	7.5(4)	18.6(4)	6.4(4)
F7	42.7(5)	67.0(7)	35.1(5)	10.4(5)	-1.8(4)	28.1(5)
F3	43.2(5)	60.9(6)	33.2(5)	6.3(4)	8.8(4)	25.7(5)
F10	40.9(5)	59.7(6)	35.3(5)	24.7(5)	1.8(4)	8.5(4)
F4	41.1(5)	36.2(5)	54.8(6)	-10.7(4)	5.5(4)	10.1(4)
F15	71.7(7)	49.5(6)	41.8(5)	11.5(5)	1.7(5)	33.7(5)
F2	35.2(5)	47.8(6)	60.4(6)	27.3(5)	17.7(4)	12.7(4)
F11	80.2(8)	43.0(5)	36.9(5)	5.3(4)	10.9(5)	28.1(5)
F8	31.2(5)	75.2(8)	52.5(6)	13.5(6)	3.4(4)	14.1(5)
F9	39.9(5)	74.8(8)	48.3(6)	28.6(6)	11.5(5)	6.2(5)
F13	60.0(7)	83.8(9)	34.0(6)	22.4(6)	-13.1(5)	-8.0(6)
F12	90.0(9)	51.7(6)	29.9(5)	-2.8(5)	9.0(5)	4.0(6)
F14	68.5(8)	83.7(9)	59.5(7)	33.0(7)	-6.5(6)	33.2(7)
C11	30.9(7)	29.1(7)	25.6(6)	6.8(5)	1.2(5)	10.1(5)
C12	29.6(7)	26.6(7)	33.1(7)	8.1(5)	-3.0(6)	6.7(5)
C3	39.0(8)	27.6(7)	28.1(7)	8.6(5)	7.4(6)	10.0(6)
C17	33.5(7)	31.1(7)	28.5(7)	7.8(6)	2.6(6)	3.3(6)
C16	28.5(7)	28.4(7)	35.5(7)	8.3(6)	4.5(6)	7.5(5)
C13	25.7(7)	39.8(8)	37.7(8)	18.6(6)	5.2(6)	11.2(6)
C23	35.4(7)	26.9(6)	28.0(7)	4.8(5)	5.0(6)	13.2(6)
C4	43.0(8)	25.1(6)	35.2(8)	11.5(6)	12.5(6)	11.9(6)
C24	38.3(8)	35.7(7)	28.0(7)	8.4(6)	2.5(6)	14.5(6)
C2	37.7(8)	28.4(7)	35.2(8)	11.6(6)	9.3(6)	9.8(6)
C15	31.4(7)	31.9(7)	35.4(8)	0.1(6)	-1.0(6)	11.1(6)
C28	39.5(8)	31.0(7)	27.3(7)	6.3(5)	7.2(6)	17.0(6)
C27	39.3(8)	42.7(8)	29.3(7)	5.4(6)	1.9(6)	23.6(7)
C14	32.0(7)	44.7(8)	27.3(7)	6.9(6)	2.6(6)	19.1(6)
C5	53.8(9)	24.4(7)	29.4(7)	7.0(6)	9.4(7)	5.9(6)
C26	30.4(7)	46.2(9)	40.6(9)	5.5(7)	4.2(6)	16.1(7)
C18	39.0(8)	38.0(8)	34.2(8)	10.2(6)	3.2(6)	7.8(6)
C22	44.2(9)	34.2(8)	30.8(8)	9.1(6)	6.3(6)	5.3(6)
C7	41.0(8)	32.0(7)	36.4(8)	14.6(6)	-0.8(6)	1.5(6)
C19	37.6(8)	52.6(10)	46.2(10)	24.5(8)	-0.3(7)	7.5(7)
C20	39.6(9)	56.7(10)	29.3(8)	16.9(7)	-5.3(6)	-9.2(8)
C25	38.0(8)	41.8(8)	36.3(8)	12.7(7)	10.8(6)	13.2(7)
C21	50.1(10)	40.1(9)	27.1(8)	4.5(6)	5.3(7)	-4.6(7)
C1	51.3(11)	51.0(11)	61.9(12)	20.1(10)	26.2(10)	25.7(9)
C10	53.8(11)	49.4(10)	31.2(8)	7.5(7)	-1.1(7)	9.0(8)
C6	89.5(17)	41.7(10)	31.1(9)	1.6(8)	16.1(10)	11(1)
C9	48.5(10)	47.3(10)	66.9(13)	24.6(9)	22.4(9)	23.9(8)
B1	36.4(8)	26.6(7)	26.6(7)	6.4(6)	4.4(6)	9.3(6)
C8	48.5(11)	60.8(13)	63.2(14)	28.9(11)	-13.3(10)	-1.2(10)

Table S3: Bond Lengths in Å for **wes_si16_b**.

Atom	Atom	Length/Å
Si1	C3	2.1420(15)
Si1	C4	2.1595(15)
Si1	C2	2.1395(15)
Si1	C5	2.1421(16)
Si1	C7	2.1221(16)
F6	C28	1.3582(17)

Atom	Atom	Length/Å
F1	C12	1.3534(17)
F5	C16	1.3497(17)
F7	C27	1.3395(18)
F3	C14	1.3406(17)
F10	C24	1.3512(18)
F4	C15	1.3446(18)

Atom	Atom	Length/Å
F15	C18	1.352(2)
F2	C13	1.3405(17)
F11	C22	1.355(2)
F8	C26	1.341(2)
F9	C25	1.3439(19)
F13	C20	1.343(2)
F12	C21	1.344(2)
F14	C19	1.343(2)
C11	C12	1.387(2)
C11	C16	1.390(2)
C11	B1	1.640(2)
C12	C13	1.384(2)
C3	C4	1.423(2)
C3	C2	1.425(2)
C3	C10	1.498(2)
C17	C18	1.381(2)
C17	C22	1.388(2)
C17	B1	1.634(2)
C16	C15	1.384(2)
C13	C14	1.379(2)
C23	C24	1.386(2)
C23	C28	1.387(2)
C23	B1	1.639(2)
C4	C5	1.412(2)
C4	C9	1.497(2)
C24	C25	1.385(2)
C2	C7	1.433(2)
C2	C1	1.496(2)
C15	C14	1.377(2)
C28	C27	1.374(2)
C27	C26	1.381(2)
C5	C7	1.423(3)
C5	C6	1.503(2)
C26	C25	1.375(2)
C18	C19	1.384(2)
C22	C21	1.379(2)
C7	C8	1.494(3)
C19	C20	1.374(3)
C20	C21	1.374(3)

Table S4: Bond Angles in ° for **wes_si16_b**.

Atom	Atom	Atom	Angle/°
C3	Si1	C4	38.63(6)
C3	Si1	C5	64.70(6)
C2	Si1	C3	38.87(6)
C2	Si1	C4	65.00(6)
C2	Si1	C5	65.24(6)
C5	Si1	C4	38.31(7)
C7	Si1	C3	65.33(6)
C7	Si1	C4	64.99(7)
C7	Si1	C2	39.29(6)
C7	Si1	C5	38.98(7)
C12	C11	C16	113.38(13)
C12	C11	B1	121.30(13)
C16	C11	B1	125.19(13)
F1	C12	C11	119.74(14)
F1	C12	C13	115.87(13)
C13	C12	C11	124.39(14)
C4	C3	Si1	71.35(8)
C4	C3	C2	108.42(14)
C4	C3	C10	125.46(16)
C2	C3	Si1	70.47(8)
C2	C3	C10	126.12(15)
C10	C3	Si1	124.26(12)
C18	C17	C22	114.00(15)
C18	C17	B1	125.74(14)
C22	C17	B1	120.25(14)
F5	C16	C11	120.32(13)
F5	C16	C15	115.33(13)
C15	C16	C11	124.35(14)
F2	C13	C12	121.03(14)
F2	C13	C14	119.52(14)
C14	C13	C12	119.45(14)
C24	C23	C28	113.25(14)
C24	C23	B1	127.56(14)
C28	C23	B1	119.19(13)
C3	C4	Si1	70.02(8)
C3	C4	C9	124.74(16)
C5	C4	Si1	70.17(9)
C5	C4	C3	107.94(14)
C5	C4	C9	127.31(16)
C9	C4	Si1	126.24(11)
F10	C24	C23	120.86(14)
F10	C24	C25	115.15(14)
C25	C24	C23	123.99(15)
C3	C2	Si1	70.66(8)
C3	C2	C7	107.28(14)
C3	C2	C1	125.74(16)
C7	C2	Si1	69.70(9)
C7	C2	C1	126.95(17)
C1	C2	Si1	126.33(12)
F4	C15	C16	120.77(14)
F4	C15	C14	119.77(14)
C14	C15	C16	119.46(14)
F6	C28	C23	119.17(14)
F6	C28	C27	115.84(13)
C27	C28	C23	124.99(14)
F7	C27	C28	120.94(14)
F7	C27	C26	119.79(15)
C28	C27	C26	119.26(15)
F3	C14	C13	120.62(14)
F3	C14	C15	120.46(14)
C15	C14	C13	118.92(14)
C4	C5	Si1	71.51(9)
C4	C5	C7	108.50(14)
C4	C5	C6	125.56(19)
C7	C5	Si1	69.75(9)
C7	C5	C6	125.93(19)
C6	C5	Si1	125.12(12)
F8	C26	C27	120.50(15)
F8	C26	C25	120.94(15)
C25	C26	C27	118.55(15)
F15	C18	C17	120.02(15)
F15	C18	C19	116.12(16)
C17	C18	C19	123.84(17)
F11	C22	C17	120.12(15)

Atom	Atom	Atom	Angle/°
F11	C22	C21	115.64(16)
C21	C22	C17	124.23(17)
C2	C7	Si1	71.01(9)
C2	C7	C8	126.52(19)
C5	C7	Si1	71.27(9)
C5	C7	C2	107.84(15)
C5	C7	C8	125.62(19)
C8	C7	Si1	124.26(13)
F14	C19	C18	120.60(19)
F14	C19	C20	119.97(17)
C20	C19	C18	119.43(18)
F13	C20	C19	120.3(2)
F13	C20	C21	120.37(19)
C21	C20	C19	119.35(16)
F9	C25	C24	119.84(15)
F9	C25	C26	120.23(15)
C26	C25	C24	119.91(15)
F12	C21	C22	121.23(19)
F12	C21	C20	119.63(16)
C20	C21	C22	119.14(17)
C17	B1	C11	113.53(13)
C17	B1	C23	113.10(12)
C23	B1	C11	110.59(12)

Table S5: Torsion Angles in ° for **wes_si16_b**.

Atom	Atom	Atom	Atom	Angle/°
Si1	C3	C4	C5	-60.20(10)
Si1	C3	C4	C9	120.89(15)
Si1	C3	C2	C7	60.37(10)
Si1	C3	C2	C1	-121.39(16)
Si1	C4	C5	C7	-60.22(11)
Si1	C4	C5	C6	120.44(16)
Si1	C2	C7	C5	62.13(10)
Si1	C2	C7	C8	-119.07(18)
Si1	C5	C7	C2	-61.96(10)
Si1	C5	C7	C8	119.22(17)
F6	C28	C27	F7	-2.0(2)
F6	C28	C27	C26	178.73(13)
F1	C12	C13	F2	0.1(2)
F1	C12	C13	C14	-179.95(13)
F5	C16	C15	F4	-1.0(2)
F5	C16	C15	C14	178.77(14)
F7	C27	C26	F8	-0.2(2)
F7	C27	C26	C25	-179.48(15)
F10	C24	C25	F9	0.5(2)
F10	C24	C25	C26	178.84(15)
F4	C15	C14	F3	-1.3(2)
F4	C15	C14	C13	178.83(14)
F15	C18	C19	F14	-1.4(2)
F15	C18	C19	C20	178.54(15)
F2	C13	C14	F3	1.3(2)
F2	C13	C14	C15	-178.88(14)
F11	C22	C21	F12	2.8(2)
F11	C22	C21	C20	-177.97(15)
F8	C26	C25	F9	0.6(3)
F8	C26	C25	C24	-177.75(15)
F13	C20	C21	F12	-0.5(2)
F13	C20	C21	C22	-179.75(15)
F14	C19	C20	F13	-0.7(3)
F14	C19	C20	C21	179.16(16)
C11	C12	C13	F2	-179.34(13)
C11	C12	C13	C14	0.6(2)
C11	C16	C15	F4	179.08(14)
C11	C16	C15	C14	-1.2(2)
C12	C11	C16	F5	-

Atom	Atom	Atom	Atom	Angle/°
				177.22(13)
C12	C11	C16	C15	2.7(2)
C12	C11	B1	C17	83.97(16)
C12	C11	B1	C23	-147.66(13)
C12	C13	C14	F3	-178.66(13)
C12	C13	C14	C15	1.2(2)
C3	C4	C5	Si1	60.10(10)
C3	C4	C5	C7	-0.12(17)
C3	C4	C5	C6	-179.46(15)
C3	C2	C7	Si1	-60.99(10)
C3	C2	C7	C5	1.14(17)
C3	C2	C7	C8	179.94(16)
C17	C18	C19	F14	-179.73(16)
C17	C18	C19	C20	0.3(3)
C17	C22	C21	F12	-178.54(15)
C17	C22	C21	C20	0.7(3)
C16	C11	C12	F1	178.13(13)
C16	C11	C12	C13	-2.4(2)
C16	C11	B1	C17	-100.53(17)
C16	C11	B1	C23	27.84(19)
C16	C15	C14	F3	178.94(14)
C16	C15	C14	C13	-0.9(2)
C23	C24	C25	F9	-179.34(15)
C23	C24	C25	C26	-1.0(3)
C23	C28	C27	F7	177.40(14)
C23	C28	C27	C26	-1.8(2)
C4	C3	C2	Si1	-61.59(10)
C4	C3	C2	C7	-1.22(16)
C4	C3	C2	C1	177.02(15)
C4	C5	C7	Si1	61.33(10)
C4	C5	C7	C2	-0.64(17)
C4	C5	C7	C8	-179.45(16)
C24	C23	C28	F6	-178.30(12)
C24	C23	C28	C27	2.3(2)
C24	C23	B1	C11	-121.34(16)
C24	C23	B1	C17	7.3(2)
C2	C3	C4	Si1	61.03(10)
C2	C3	C4	C5	0.84(16)
C2	C3	C4	C9	-178.08(14)
C28	C23	C24	F10	179.30(13)
C28	C23	C24	C25	-0.8(2)
C28	C23	B1	C11	58.66(17)

Atom	Atom	Atom	Atom	Angle/°
C28	C23	B1	C17	-172.74(13)
C28	C27	C26	F8	179.10(14)
C28	C27	C26	C25	-0.2(2)
C27	C26	C25	F9	179.87(15)
C27	C26	C25	C24	1.6(2)
C18	C17	C22	F11	177.41(14)
C18	C17	C22	C21	-1.2(2)
C18	C17	B1	C11	28.8(2)
C18	C17	B1	C23	-98.22(18)
C18	C19	C20	F13	179.29(15)
C18	C19	C20	C21	-0.8(3)
C22	C17	C18	F15	-177.49(14)
C22	C17	C18	C19	0.7(2)
C22	C17	B1	C11	-151.86(14)
C22	C17	B1	C23	81.07(17)
C19	C20	C21	F12	179.63(15)
C19	C20	C21	C22	0.4(3)
C1	C2	C7	Si1	120.80(17)
C1	C2	C7	C5	-177.07(15)
C1	C2	C7	C8	1.7(3)
C10	C3	C4	Si1	-119.28(16)
C10	C3	C4	C5	-179.47(15)
C10	C3	C4	C9	1.6(2)
C10	C3	C2	Si1	118.72(16)
C10	C3	C2	C7	179.09(15)
C10	C3	C2	C1	-2.7(3)
C6	C5	C7	Si1	-119.33(17)
C6	C5	C7	C2	178.70(15)
C6	C5	C7	C8	-0.1(3)
C9	C4	C5	Si1	-121.02(16)
C9	C4	C5	C7	178.76(15)
C9	C4	C5	C6	-0.6(3)
B1	C11	C12	F1	-5.9(2)
B1	C11	C12	C13	173.58(14)
B1	C11	C16	F5	7.0(2)
B1	C11	C16	C15	-173.09(14)
B1	C17	C18	F15	1.8(2)
B1	C17	C18	C19	-179.94(15)
B1	C17	C22	F11	-2.0(2)
B1	C17	C22	C21	179.41(14)
B1	C23	C24	F10	-0.7(2)
B1	C23	C24	C25	179.16(15)
B1	C23	C28	F6	1.7(2)

Atom	Atom	Atom	Atom	Angle/°
B1	C23	C28	C27	-177.70(14)

Table S6: Hydrogen Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **wes_si16_b**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H1	3410(20)	440(20)	7436(13)	35(5)
H8A	1500(20)	-2700(20)	6861(14)	38(5)
H10A	5830(30)	-2310(30)	9670(17)	56(6)
H9A	7330(30)	-3780(30)	7928(18)	64(7)
H10B	7180(30)	-1070(30)	9280(20)	77(8)
H6A	4470(30)	-4950(30)	5891(17)	59(7)
H9B	7560(30)	-3180(30)	7025(19)	68(7)
H6B	4090(30)	-3840(30)	5570(20)	80(9)
H8B	2210(40)	-3210(30)	5930(20)	83(9)
H8C	1340(40)	-4240(30)	6530(20)	81(9)
H10C	5690(30)	-840(30)	9640(20)	81(9)
H1A	2270(40)	-2490(40)	9050(20)	102(11)
H9C	8200(40)	-2020(30)	8000(20)	83(9)
H1B	1880(40)	-1750(40)	8350(20)	99(11)
H6C	5880(40)	-3530(40)	5720(20)	97(10)
H1C	3240(40)	-1100(40)	9160(30)	106(12)

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