Supporting Information

A Novel Alkali-Metal Hydrido-tris(pyrazolyl)borate (Tp^*) Complex. Isolation and Crystal Structure of $[(Me_2CO)_3(NaTp^*)_2]$

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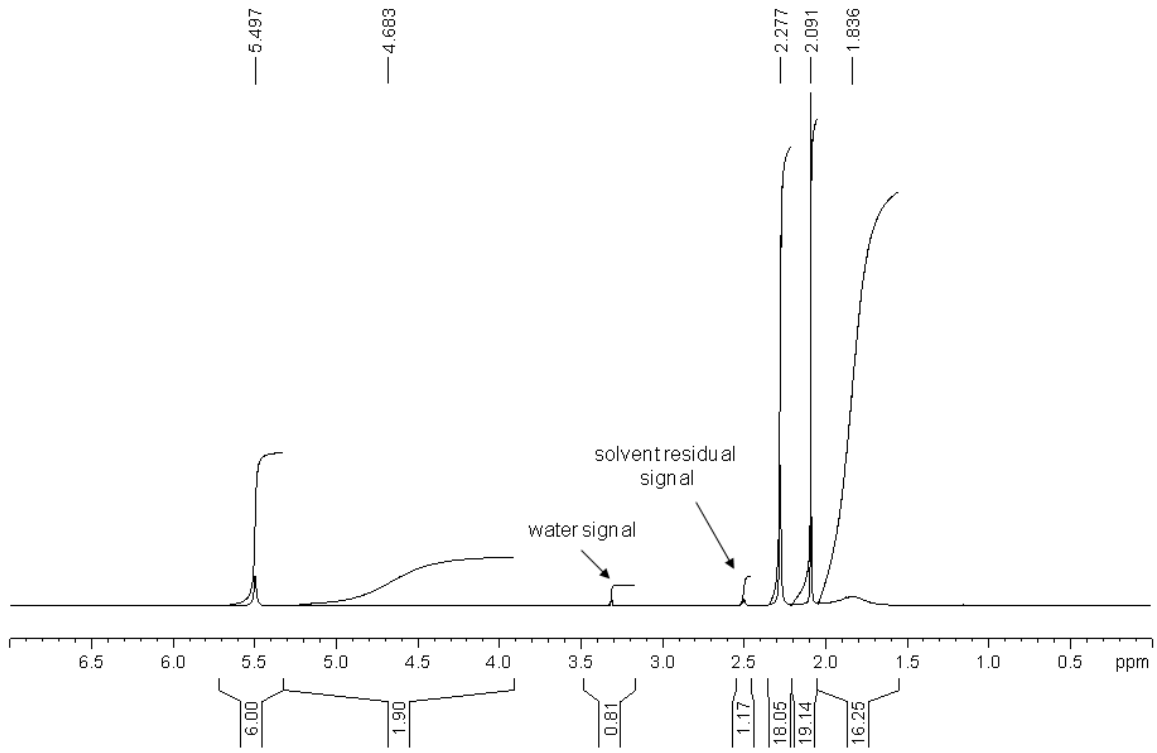

Fig. S1. ^{1}H NMR Spectrum of **2** ([D_6]DMSO, 298 K, 300.130 MHz).

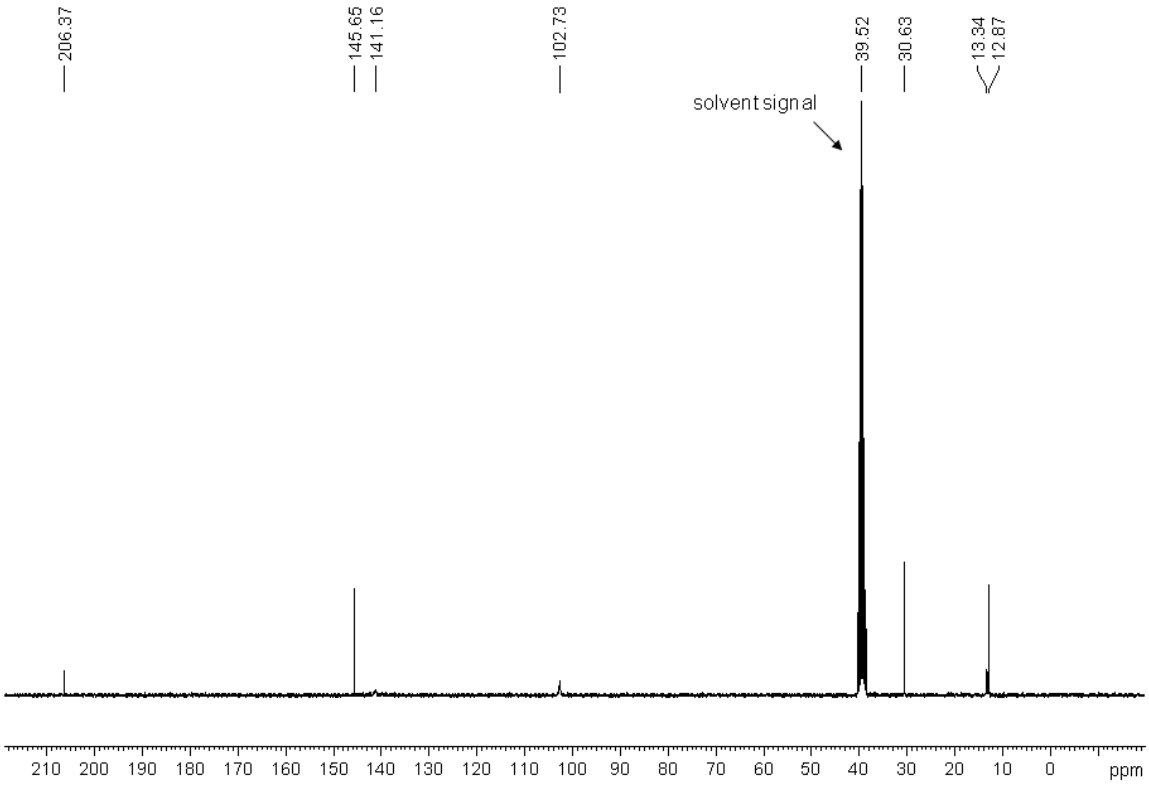

Fig. S2. $^{13}C\{^{1}H\}$ NMR Spectrum of **2** ([D_6]DMSO, 300 K, 75.467 MHz).

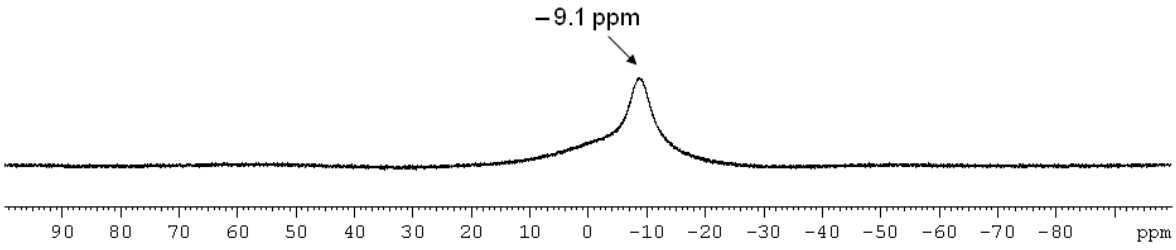

Fig. S3. ^{11}B NMR Spectrum of **2** ([D_6]DMSO, 300 K, 96.293 MHz).

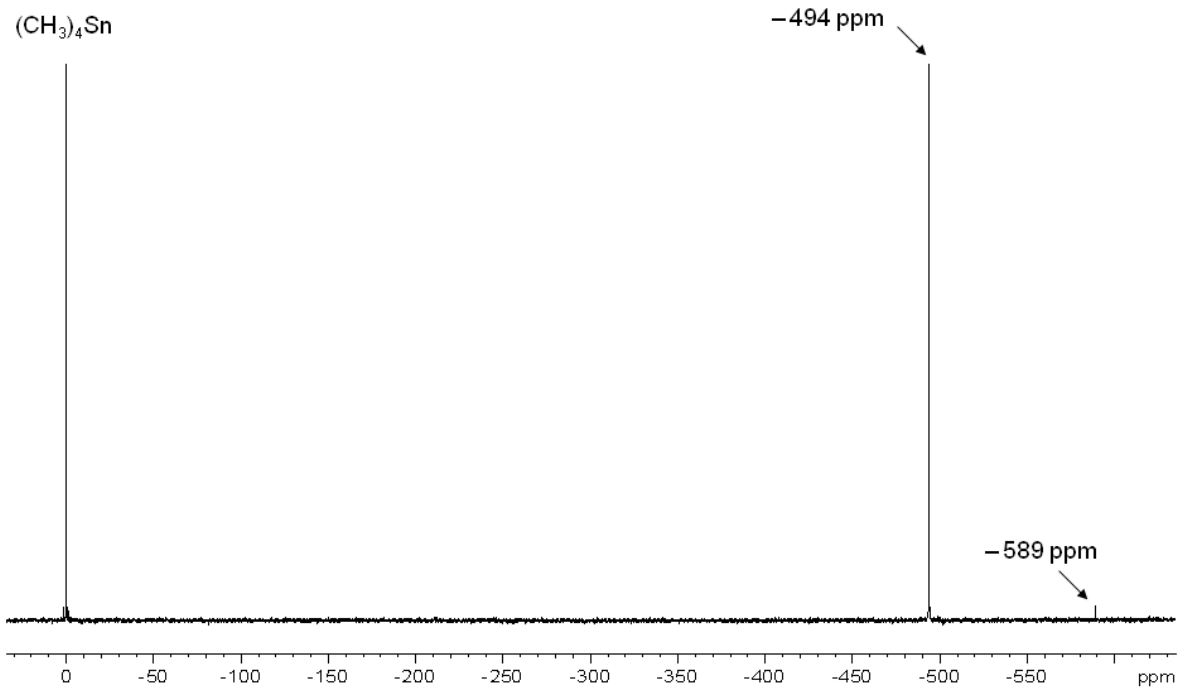

Fig. S4. $^{119}Sn\{^{1}H\}$ NMR Spectrum of tin co-products (D_2O, 300 K, 111.920 MHz).

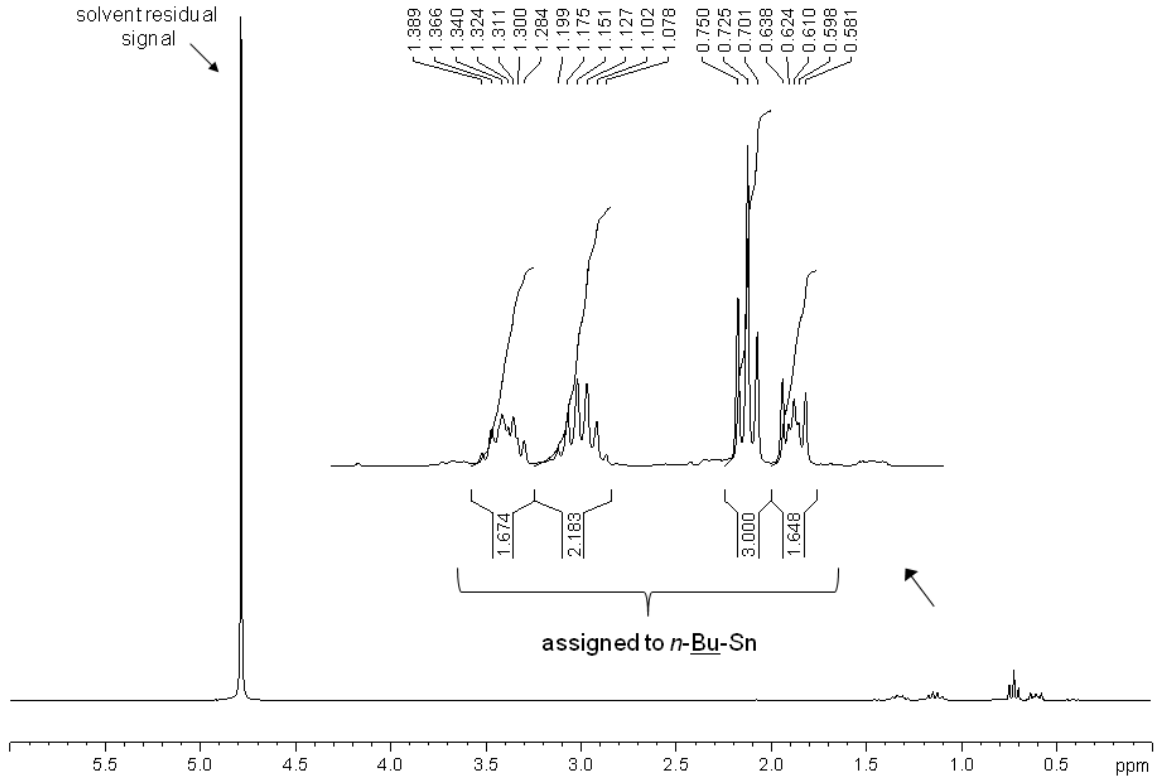

Fig. S5. ^{1}H NMR Spectrum of Spectrum of tin co-products (D_2O, 300 K, 300.130 MHz).

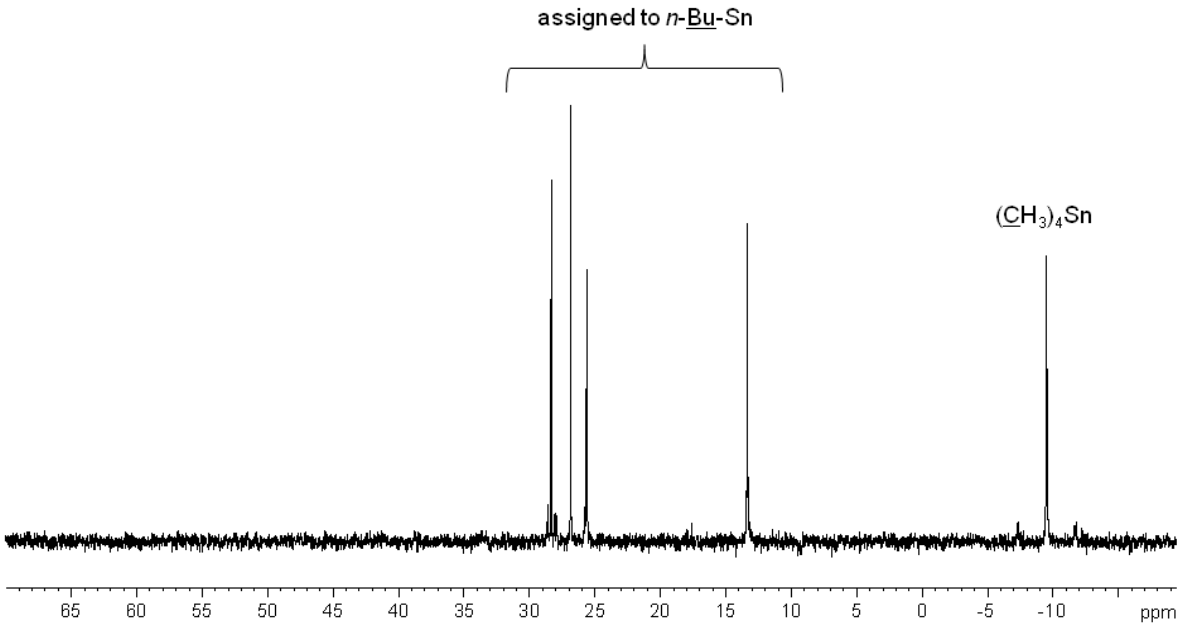

Fig. S6. $^{13}C\{^{1}H\}$ NMR Spectrum of tin coproducts (D_2O, 300 K, 75.475 MHz).

Fig. S7. X-ray structure of **2**·3$CHCl_3$ (ORTEP view with crystallographic numbering scheme).

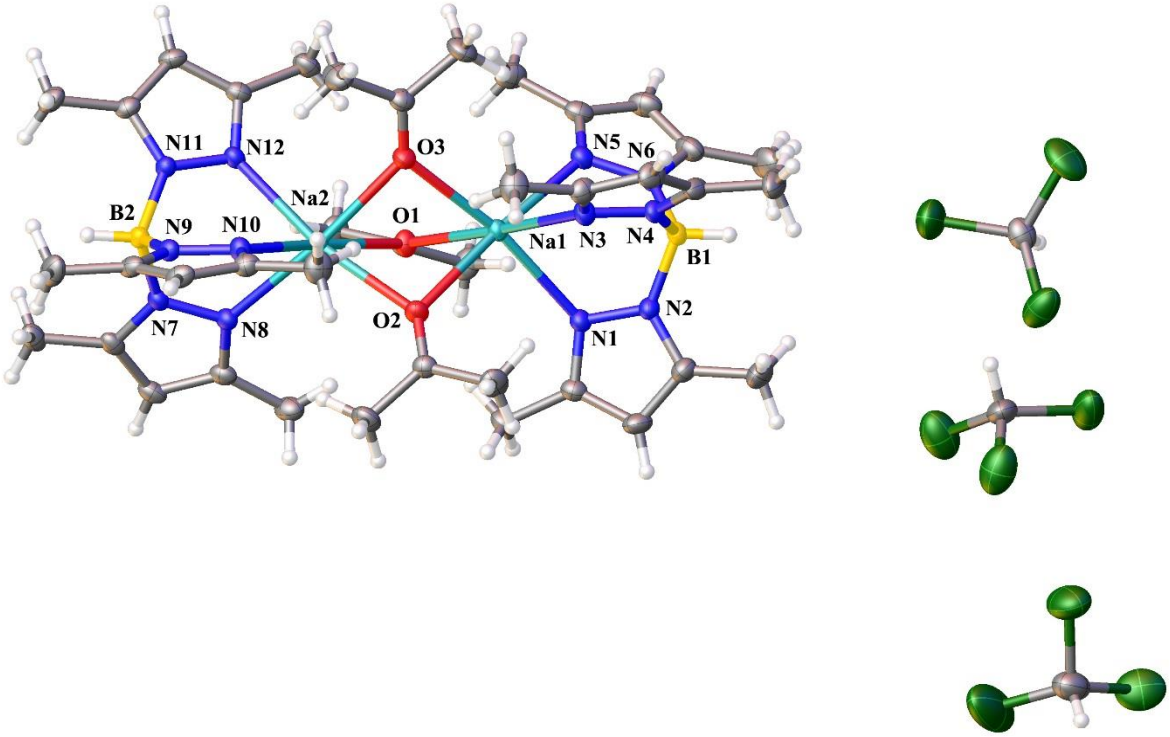

Table S8. Crystallographic data and structure refinement for **2**·3$CHCl_3$.

Empirical formula	$C_{42}H_{65}B_2Cl_9N_{12}Na_2O_3$
Formula weight	1172.71
Temperature, K	115
Crystal size, mm^3	0.37 × 0.25 × 0.25
Crystal system	triclinic
Space group	$P\bar{1}$
a, Å	13.6804(4)
b, Å	15.0269(5)
c, Å	16.3031(5)
α, deg	79.389(2)
β, deg	76.220(2)
γ, deg	67.767(2)
Volume, $Å^3$	2996.51(17)
Z	2
$\rho_{calcd.}$, mg mm^{-3}	1.300
m, mm^{-1}	0.481
F(000), e	1220.0
Radiation; wavelength, Å	MoK_α; 0.71073
2*θ* range for data collection	5.586–55.108°
Index ranges	$-17 \le h \le 17$, $-19 \le k \le 19$, $-21 \le l \le 21$
Reflections collected	56642
Independent reflections / R_{int} / R_σ	13799 / 0.0273 / 0.0235
Data / restraints / parameters	13799 / 0 / 649
Goodness-of-fit on F^2	1.037
Final indices *R*1 / *wR*2 [$I > 2\,\sigma(I)$]	0.0512 / 0.1257
Final indices *R*1 / *wR*2 [all data]	0.0636 / 0.1349
Largest diff. peak / hole, e $Å^{-3}$	0.98 / –0.80

Table S9. Fractional atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for **2**·3CHCl$_3$ (U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor).

Atom	*x*	*y*	*z*	U_{eq}
Na1	1140.1(6)	1285.2(5)	2791.6(4)	18.78(15)
Na2	2288.9(6)	–392.6(5)	1372.1(4)	18.38(15)
O1	690.5(11)	1061.8(10)	1542.4(8)	22.7(3)
O2	2842.8(10)	746(1)	1828.8(9)	23.2(3)
O3	1625.9(11)	–444.2(10)	2879.1(8)	23.4(3)
N1	928.7(13)	2999.3(11)	2514.8(10)	21.4(3)
N2	747.5(13)	3420.3(11)	3243.2(10)	21.0(3)
N3	1687.8(13)	1369.5(12)	4070.9(10)	23.2(3)
N4	1078.8(13)	2155.5(12)	4506.3(10)	21.7(3)
N5	–598.2(13)	1971.6(12)	3667.2(10)	22.5(3)
N6	–739.1(13)	2776.1(12)	4031.8(10)	22.6(3)
N7	3100.6(12)	–1274.3(11)	–466.2(10)	19.4(3)
N8	2731.8(12)	–389.0(11)	–165.4(10)	20.7(3)
N9	4166.4(12)	–2357.8(11)	650(1)	19.8(3)
N10	3976.3(13)	–1781.7(12)	1275.3(10)	22.0(3)
N11	2253.5(12)	–2290.1(11)	707.1(10)	18.6(3)
N12	1572.8(12)	–1562.2(11)	1191.3(10)	19.5(3)
C1	1432.7(15)	3477.1(14)	1902.0(12)	23.3(4)
C2	1587.5(18)	4204.1(16)	2226.5(14)	30.6(4)
C3	1145.7(17)	4144.6(15)	3079.1(13)	26.9(4)
C4	1740.7(18)	3210.1(17)	1012.7(13)	30.9(4)
C5	1076(2)	4743.3(18)	3744.2(16)	41.4(6)
C6	2331.4(17)	750.7(15)	4576.4(13)	26.1(4)
C7	2147.9(18)	1130.0(16)	5346.8(13)	29.2(4)
C8	1355.5(18)	2020.6(15)	5278.0(12)	26.2(4)
C9	3116.2(19)	–192.5(17)	4287.6(15)	35.5(5)
C10	866(2)	2762.0(17)	5896.7(14)	37.7(5)
C11	–1576.2(16)	1958.4(15)	3713.2(12)	25.7(4)
C12	–2357.6(17)	2749.6(17)	4105.7(15)	33.6(5)
C13	–1802.4(17)	3254.6(15)	4298.7(14)	30.2(4)
C14	–1716.8(19)	1157.7(17)	3382.0(15)	34.0(5)
C15	–2229(2)	4169.7(18)	4711.0(18)	44.4(6)
C16	–55.0(15)	1476.9(14)	1167.3(11)	20.4(4)
C17	–754.4(18)	2501.3(15)	1293.7(16)	32.5(5)
C18	–294.1(18)	980.3(16)	567.9(14)	29.6(4)
C19	3616.3(15)	1006.3(14)	1642.0(12)	21.9(4)
C21	3821.2(18)	1547.8(18)	2228.1(15)	33.5(5)
C22	4389.3(17)	789.9(17)	822.5(14)	31.6(5)
C23	1516.8(16)	–1068.7(14)	3444.9(12)	23.8(4)
C24	747(2)	–817.3(18)	4256.7(13)	35.4(5)

C25	2148(2)	–2111.4(16)	3348.4(16)	40.0(5)
C26	3258.6(14)	–1165.1(15)	–1329.6(12)	22.0(4)
C27	2979.0(15)	–189.6(15)	–1589.9(12)	25.1(4)
C28	2654.9(15)	265.3(14)	–843.0(12)	22.9(4)
C29	3669.0(17)	–1994.5(16)	–1855.9(13)	28.4(4)
C30	2268.1(18)	1319.6(15)	–739.8(15)	31.9(5)
C31	5199.5(15)	–2985.0(13)	551.1(13)	23.5(4)
C32	5683.2(15)	–2812.3(14)	1125.3(14)	25.6(4)
C33	4890.9(16)	–2060.4(14)	1562.4(13)	23.7(4)
C34	5660.7(17)	–3722.6(16)	–71.1(16)	34.9(5)
C35	4964.0(19)	–1593.3(17)	2269.3(15)	34.6(5)
C36	1846.0(15)	–3008.9(13)	812.8(12)	21.8(4)
C37	883.0(16)	–2738.9(14)	1374.6(13)	24.7(4)
C38	746.9(15)	–1832.5(14)	1589.5(12)	21.1(4)
C39	2402.2(17)	–3915.8(14)	389.9(15)	29.5(4)
C40	–167.4(16)	–1178.4(16)	2157.2(13)	28.2(4)
B1	218.2(18)	3035.1(16)	4114.6(13)	22.6(4)
B2	3305.5(17)	–2232.9(15)	126.8(13)	20.1(4)
Cl7	6239.3(15)	7309.0(14)	4571.7(8)	138.2(7)
Cl8	5954.7(8)	6776.4(6)	6382.1(6)	76.0(3)
Cl9	5051.1(7)	8757.0(7)	5731.8(6)	70.1(2)
C43	6116(3)	7664(2)	5554.2(18)	55.3(7)
Cl4	6771.1(7)	4325.0(6)	7507.3(7)	69.0(2)
Cl5	4577.6(7)	5445.5(7)	8095.7(6)	71.6(3)
Cl6	5165.1(7)	4410.3(8)	6619.2(6)	72.7(3)
C42	5442(2)	4413(2)	7605.8(17)	47.2(7)
Cl1	2266.2(6)	5220.0(5)	7764.7(6)	58.6(2)
Cl2	781.3(7)	4491.7(7)	8989.2(4)	67.5(2)
Cl3	1491.5(8)	3884.4(6)	7316.2(5)	65.8(2)
C41	1177.4(19)	4838.3(18)	7911.2(14)	34.9(5)

Table S10. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2**·3$CHCl_3$ (the anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Na1	19.6(3)	21.4(4)	15.9(3)	–4.5(3)	–1.9(3)	–7.5(3)
Na2	17.3(3)	19.1(3)	17.9(3)	–4.6(3)	–0.4(3)	–5.8(3)
O1	21.1(7)	25.0(7)	22.3(6)	–6.2(5)	–7.3(5)	–4.8(5)
O2	19.1(6)	27.1(7)	25.4(7)	–6.1(5)	0.0(5)	–11.0(6)
O3	28.3(7)	23.6(7)	17.9(6)	–1.8(5)	–1.4(5)	–10.4(6)
N1	24.7(8)	21.9(8)	17.5(7)	–2.9(6)	–2.3(6)	–8.7(6)
N2	25.4(8)	19.0(7)	18.7(7)	–3.0(6)	–2.6(6)	–8.3(6)
N3	25.6(8)	24.7(8)	19.6(8)	–4.9(6)	–4.6(6)	–7.7(7)
N4	28.6(8)	23.3(8)	15.4(7)	–4.1(6)	–2.5(6)	–11.4(7)
N5	23.3(8)	26.3(8)	17.8(7)	–3.1(6)	–1.5(6)	–9.6(7)
N6	22.7(8)	22.0(8)	19.2(7)	–3.7(6)	1.7(6)	–6.1(6)
N7	16.9(7)	22.4(8)	18.3(7)	–4.6(6)	0.6(6)	–7.6(6)
N8	19.5(8)	19.3(7)	20.9(8)	–3.4(6)	0.5(6)	–5.9(6)
N9	15.5(7)	17.1(7)	23.7(8)	–3.8(6)	0.0(6)	–3.6(6)
N10	18.7(8)	22.6(8)	22.8(8)	–5.8(6)	–2.4(6)	–4.4(6)
N11	17.3(7)	17.3(7)	20.7(7)	–3.5(6)	–1.5(6)	–5.9(6)
N12	17.1(7)	22.7(8)	18.1(7)	–4.6(6)	0.0(6)	–7.0(6)
C1	22.3(9)	25.0(9)	21.2(9)	1.5(7)	–3.8(7)	–8.8(8)
C2	36.6(12)	30.5(11)	29.3(11)	2.6(8)	–3.9(9)	–20.7(9)
C3	31.5(11)	23.6(9)	28.4(10)	–2.9(8)	–5.2(8)	–12.7(8)
C4	34.0(11)	36.9(11)	20.2(9)	0.4(8)	–1.5(8)	–14.2(9)
C5	58.0(16)	37.7(13)	38.9(13)	–11.1(10)	–1.7(11)	–29.6(12)
C6	28.9(10)	28.4(10)	25.4(10)	–1.8(8)	–9.8(8)	–12.4(8)
C7	40.5(12)	32.2(11)	22.4(10)	1.5(8)	–14.0(9)	–18.2(9)
C8	38.6(11)	30.4(10)	16.9(9)	–0.9(7)	–5.2(8)	–21.1(9)
C9	32.9(12)	34.2(12)	37.2(12)	–5.8(9)	–16.2(10)	–2.6(9)
C10	63.7(16)	35.6(12)	21.2(10)	–6.3(9)	–7.6(10)	–24.3(12)
C11	23.1(9)	31.9(10)	20.8(9)	3.5(8)	–3.5(7)	–11.4(8)
C12	21.5(10)	35.2(12)	37.1(12)	2.8(9)	–0.6(9)	–8.3(9)
C13	25.4(10)	28(1)	28.1(10)	–0.8(8)	3.0(8)	–5.2(8)
C14	34.0(12)	43.0(13)	32.1(11)	0.1(9)	–8.7(9)	–21.7(10)
C15	33.5(12)	32.7(12)	53.0(15)	–12.3(11)	10.0(11)	–3.3(10)
C16	18.9(9)	24.5(9)	18.2(8)	–2.3(7)	–0.9(7)	–9.4(7)
C17	26.3(10)	25.7(10)	43.7(13)	–6.1(9)	–12.3(9)	–2.6(8)
C18	30.5(11)	34.6(11)	29(1)	–5.7(8)	–13.0(8)	–11.8(9)
C19	18.2(9)	22.3(9)	23.8(9)	–0.9(7)	–4.1(7)	–6.3(7)
C21	27.5(11)	44.7(13)	36.7(12)	–10.7(10)	–4.6(9)	–19.7(10)
C22	22.3(10)	41.1(12)	29.6(11)	–6.6(9)	4.2(8)	–13.4(9)
C23	25.9(10)	27(1)	19.1(9)	0.4(7)	–4.6(7)	–10.8(8)
C24	41.2(13)	41.6(13)	20.1(10)	0.2(9)	2.8(9)	–17.6(10)

C25	47.7(14)	25.6(11)	36.4(12)	3.4(9)	–1.9(10)	–7.9(10)
C26	14.3(8)	32.5(10)	19.8(9)	–5.0(7)	–0.3(7)	–9.6(7)
C27	18.9(9)	34.4(11)	19.5(9)	1.0(8)	–2.0(7)	–9.3(8)
C28	16.0(8)	25.2(9)	24.1(9)	0.9(7)	–0.7(7)	–6.9(7)
C29	24.1(10)	41.5(12)	23.3(10)	–10.6(8)	–1.4(8)	–14.1(9)
C30	30.5(11)	25.4(10)	33.8(11)	1.6(8)	–0.6(9)	–8.6(9)
C31	17.5(9)	15.4(8)	33.1(10)	–1.1(7)	0.2(7)	–4.4(7)
C32	16.5(9)	20.0(9)	37.7(11)	1.5(8)	–5.7(8)	–5.2(7)
C33	21.3(9)	22.2(9)	27.1(10)	1.1(7)	–5.8(7)	–7.9(7)
C34	22.3(10)	26.8(10)	51.9(14)	–16.4(10)	0.8(9)	–3.3(8)
C35	31.5(11)	38.4(12)	36.6(12)	–7.5(10)	–13.6(9)	–9(1)
C36	22.1(9)	17.4(8)	25.8(9)	2.1(7)	–6.7(7)	–7.4(7)
C37	22.8(9)	22.9(9)	29(1)	3.5(8)	–4.1(8)	–11.8(8)
C38	18.2(9)	25.4(9)	19.0(9)	1.3(7)	–3.4(7)	–8.4(7)
C39	30.1(11)	17.8(9)	40.1(12)	–2.8(8)	–5.9(9)	–8.2(8)
C40	21.4(9)	36.0(11)	25.7(10)	–4.7(8)	2.6(8)	–11.8(8)
B1	27.5(11)	22(1)	17.8(10)	–5.6(8)	0.3(8)	–9.1(9)
B2	18.1(9)	19.3(9)	21.8(10)	–5.7(8)	1.2(8)	–6.4(8)
Cl7	192.2(16)	220.8(18)	63.7(6)	–61.7(9)	27.2(8)	–150.2(15)
Cl8	86.5(6)	51.6(4)	79.8(6)	4.0(4)	4.9(5)	–30.2(4)
Cl9	64.6(5)	71.7(5)	73.6(5)	18.6(4)	–36.5(4)	–21.3(4)
C43	63.5(19)	67.6(19)	43.6(15)	–4.5(14)	1.3(13)	–40.0(16)
Cl4	54.8(4)	59.6(5)	96.1(7)	–26.3(4)	–27.2(4)	–7.7(4)
Cl5	58.3(5)	71.1(5)	91.0(6)	–44.4(5)	20.1(4)	–32.9(4)
Cl6	54.3(5)	103.4(7)	64.8(5)	–30.3(5)	–10.5(4)	–23.0(5)
C42	61.0(17)	43.2(14)	44.3(14)	–10.4(11)	9.4(12)	–34.7(13)
Cl1	40.1(3)	44.7(4)	94.9(6)	–18.7(4)	–11.1(4)	–14.6(3)
Cl2	74.5(5)	85.7(6)	27.7(3)	1.8(3)	–8.6(3)	–15.9(4)
Cl3	88.8(6)	67.3(5)	55.9(4)	–28.6(4)	–0.4(4)	–41.3(5)
C41	31.8(11)	41.0(12)	29.7(11)	–6.4(9)	–8.3(9)	–7.6(10)

Table S11. Bond lengths (Å) for **2**·3$CHCl_3$.

Atom	Atom	Lengths	Atom	Atom	Lengths
Na1	Na2	3.4059(10)	C1	C2	1.400(3)
Na1	O1	2.3756(14)	C1	C4	1.495(3)
Na1	O2	2.4175(15)	C2	C3	1.379(3)
Na1	O3	2.4119(15)	C3	C5	1.496(3)
Na1	N1	2.4479(17)	C6	C7	1.404(3)
Na1	N3	2.4169(17)	C6	C9	1.496(3)
Na1	N5	2.4137(17)	C7	C8	1.372(3)
Na2	O1	2.4398(15)	C8	C10	1.495(3)
Na2	O2	2.4032(15)	C11	C12	1.399(3)
Na2	O3	2.4056(15)	C11	C14	1.497(3)
Na2	N8	2.4339(17)	C12	C13	1.375(3)
Na2	N10	2.4519(17)	C13	C15	1.493(3)
Na2	N12	2.4014(17)	C16	C17	1.495(3)
O1	C16	1.216(2)	C16	C18	1.491(3)
O2	C19	1.217(2)	C19	C21	1.497(3)
O3	C23	1.215(2)	C19	C22	1.495(3)
N1	N2	1.375(2)	C23	C24	1.491(3)
N1	C1	1.331(2)	C23	C25	1.492(3)
N2	C3	1.351(2)	C26	C27	1.378(3)
N2	B1	1.550(3)	C26	C29	1.496(3)
N3	N4	1.369(2)	C27	C28	1.402(3)
N3	C6	1.328(3)	C28	C30	1.497(3)
N4	C8	1.357(2)	C31	C32	1.377(3)
N4	B1	1.553(3)	C31	C34	1.495(3)
N5	N6	1.373(2)	C32	C33	1.400(3)
N5	C11	1.330(3)	C33	C35	1.496(3)
N6	C13	1.358(3)	C36	C37	1.377(3)
N6	B1	1.541(3)	C36	C39	1.491(3)
N7	N8	1.371(2)	C37	C38	1.402(3)
N7	C26	1.361(2)	C38	C40	1.497(3)
N7	B2	1.549(3)	Cl7	C43	1.731(3)
N8	C28	1.332(2)	Cl8	C43	1.752(3)
N9	N10	1.373(2)	Cl9	C43	1.751(4)
N9	C31	1.361(2)	Cl4	C42	1.743(3)
N9	B2	1.550(3)	Cl5	C42	1.750(3)
N10	C33	1.330(2)	Cl6	C42	1.739(3)
N11	N12	1.372(2)	Cl1	C41	1.741(3)
N11	C36	1.360(2)	Cl2	C41	1.754(2)
N11	B2	1.546(2)	Cl3	C41	1.740(2)
N12	C38	1.328(2)			

Table S12. Bond Angles (deg) for **2**·3$CHCl_3$.

Atom	Atom	Atom	Angle	Atom	Atom	Atom	Angle
O1	Na1	Na2	45.76(4)	C31	N9	B2	127.48(16)
O1	Na1	O2	75.59(5)	N9	N10	Na2	115.58(11)
O1	Na1	O3	76.72(5)	C33	N10	Na2	136.78(13)
O1	Na1	N1	100.53(6)	C33	N10	N9	106.25(15)
O1	Na1	N3	175.18(6)	N12	N11	B2	122.03(14)
O1	Na1	N5	102.69(6)	C36	N11	N12	110.12(15)
O2	Na1	Na2	44.88(4)	C36	N11	B2	127.84(16)
O2	Na1	N1	94.97(6)	N11	N12	Na2	116.35(11)
O3	Na1	Na2	44.93(3)	C38	N12	Na2	135.41(13)
O3	Na1	O2	75.13(5)	C38	N12	N11	106.28(15)
O3	Na1	N1	170.09(6)	N1	C1	C2	110.42(17)
O3	Na1	N3	98.66(6)	N1	C1	C4	120.31(18)
O3	Na1	N5	109.78(6)	C2	C1	C4	129.26(18)
N1	Na1	Na2	126.80(5)	C3	C2	C1	105.56(18)
N3	Na1	Na2	129.74(5)	N2	C3	C2	107.62(18)
N3	Na1	O2	102.05(6)	N2	C3	C5	123.06(19)
N3	Na1	N1	83.80(6)	C2	C3	C5	129.32(19)
N5	Na1	Na2	137.04(5)	N3	C6	C7	110.34(18)
N5	Na1	O2	174.44(6)	N3	C6	C9	120.34(18)
N5	Na1	N1	80.08(6)	C7	C6	C9	129.32(19)
N5	Na1	N3	80.05(6)	C8	C7	C6	105.45(18)
O1	Na2	Na1	44.23(3)	N4	C8	C7	107.78(17)
O1	Na2	N10	174.31(6)	N4	C8	C10	123.21(19)
O2	Na2	Na1	45.22(4)	C7	C8	C10	128.99(19)
O2	Na2	O1	74.67(5)	N5	C11	C12	110.51(19)
O2	Na2	O3	75.51(5)	N5	C11	C14	120.34(19)
O2	Na2	N8	111.44(6)	C12	C11	C14	129.14(19)
O2	Na2	N10	99.76(6)	C13	C12	C11	105.69(19)
O3	Na2	Na1	45.09(4)	N6	C13	C12	107.50(19)
O3	Na2	O1	75.64(5)	N6	C13	C15	123.5(2)
O3	Na2	N8	171.71(6)	C12	C13	C15	129.0(2)
O3	Na2	N10	102.02(6)	O1	C16	C17	120.76(17)
N8	Na2	Na1	136.91(5)	O1	C16	C18	120.98(18)
N8	Na2	O1	101.42(5)	C18	C16	C17	118.27(17)
N8	Na2	N10	81.60(6)	O2	C19	C21	120.88(18)
N10	Na2	Na1	130.68(5)	O2	C19	C22	120.86(18)
N12	Na2	Na1	125.75(5)	C22	C19	C21	118.26(17)
N12	Na2	O1	102.38(5)	O3	C23	C24	121.02(19)
N12	Na2	O2	169.15(6)	O3	C23	C25	121.04(19)
N12	Na2	O3	93.65(5)	C24	C23	C25	117.94(18)
N12	Na2	N8	79.31(6)	N7	C26	C27	107.53(17)
N12	Na2	N10	82.87(6)	N7	C26	C29	123.45(18)

Na1	O1	Na2	90.02(5)	C27	C26	C29	129.02(18)
C16	O1	Na1	134.82(13)	C26	C27	C28	105.58(17)
C16	O1	Na2	135.09(12)	N8	C28	C27	110.39(17)
Na2	O2	Na1	89.90(5)	N8	C28	C30	120.46(18)
C19	O2	Na1	133.20(13)	C27	C28	C30	129.15(18)
C19	O2	Na2	136.79(13)	N9	C31	C32	107.47(17)
Na2	O3	Na1	89.98(5)	N9	C31	C34	123.58(18)
C23	O3	Na1	134.59(13)	C32	C31	C34	128.94(18)
C23	O3	Na2	135.29(13)	C31	C32	C33	105.61(17)
N2	N1	Na1	112.91(11)	N10	C33	C32	110.59(18)
C1	N1	Na1	131.42(13)	N10	C33	C35	120.61(18)
C1	N1	N2	106.21(15)	C32	C33	C35	128.79(18)
N1	N2	B1	122.09(15)	N11	C36	C37	107.46(17)
C3	N2	N1	110.19(15)	N11	C36	C39	123.61(17)
C3	N2	B1	127.62(16)	C37	C36	C39	128.92(18)
N4	N3	Na1	116.64(12)	C36	C37	C38	105.52(17)
C6	N3	Na1	135.43(14)	N12	C38	C37	110.62(17)
C6	N3	N4	106.53(16)	N12	C38	C40	119.95(17)
N3	N4	B1	121.39(15)	C37	C38	C40	129.41(18)
C8	N4	N3	109.90(16)	N2	B1	N4	109.38(16)
C8	N4	B1	128.71(17)	N6	B1	N2	111.31(16)
N6	N5	Na1	115.35(11)	N6	B1	N4	111.64(16)
C11	N5	Na1	135.16(14)	N7	B2	N9	110.28(15)
C11	N5	N6	106.23(16)	N11	B2	N7	111.46(15)
N5	N6	B1	121.99(15)	N11	B2	N9	111.59(15)
C13	N6	N5	110.07(17)	Cl7	C43	Cl8	111.83(18)
C13	N6	B1	127.93(17)	Cl7	C43	Cl9	111.9(2)
N8	N7	B2	122.61(15)	Cl9	C43	Cl8	109.55(16)
C26	N7	N8	110.04(15)	Cl4	C42	Cl5	109.75(14)
C26	N7	B2	127.35(16)	Cl6	C42	Cl4	110.40(15)
N7	N8	Na2	116.05(11)	Cl6	C42	Cl5	112.06(18)
C28	N8	Na2	137.33(13)	Cl1	C41	Cl2	110.58(13)
C28	N8	N7	106.46(15)	Cl3	C41	Cl1	110.75(13)
N10	N9	B2	122.36(14)	Cl3	C41	Cl2	110.07(14)
C31	N9	N10	110.08(15)				

Table S13. Torsion angles (deg) for **2**·3$CHCl_3$.

A	B	C	D	Angle	A	B	C	D	Angle
Na1	O1	C16	C17	21.0(3)	N11	N12	C38	C40	–178.25(16)
Na1	O1	C16	C18	–159.16(14)	N11	C36	C37	C38	0.1(2)
Na1	O2	C19	C21	22.0(3)	N12	N11	C36	C37	0.1(2)
Na1	O2	C19	C22	–158.20(15)	N12	N11	C36	C39	–178.60(17)
Na1	O3	C23	C24	15.7(3)	N12	N11	B2	N7	–51.7(2)
Na1	O3	C23	C25	–164.45(16)	N12	N11	B2	N9	72.1(2)
Na1	N1	N2	C3	150.03(13)	C1	N1	N2	C3	–0.5(2)
Na1	N1	N2	B1	–26.6(2)	C1	N1	N2	B1	–177.15(17)
Na1	N1	C1	C2	–142.52(16)	C1	C2	C3	N2	–0.3(2)
Na1	N1	C1	C4	38.0(3)	C1	C2	C3	C5	–179.8(2)
Na1	N3	N4	C8	168.97(12)	C3	N2	B1	N4	–94.7(2)
Na1	N3	N4	B1	–11.0(2)	C3	N2	B1	N6	141.42(19)
Na1	N3	C6	C7	–165.45(15)	C4	C1	C2	C3	179.4(2)
Na1	N3	C6	C9	15.1(3)	C6	N3	N4	C8	0.4(2)
Na1	N5	N6	C13	162.67(13)	C6	N3	N4	B1	–179.56(17)
Na1	N5	N6	B1	–18.3(2)	C6	C7	C8	N4	0.5(2)
Na1	N5	C11	C12	–157.70(15)	C6	C7	C8	C10	–177.7(2)
Na1	N5	C11	C14	23.3(3)	C8	N4	B1	N2	125.1(2)
Na2	O1	C16	C17	–163.17(15)	C8	N4	B1	N6	–111.2(2)
Na2	O1	C16	C18	16.6(3)	C9	C6	C7	C8	179.1(2)
Na2	O2	C19	C21	–162.91(15)	C11	N5	N6	C13	–0.1(2)
Na2	O2	C19	C22	16.8(3)	C11	N5	N6	B1	178.90(16)
Na2	O3	C23	C24	–158.74(15)	C11	C12	C13	N6	–0.2(2)
Na2	O3	C23	C25	21.1(3)	C11	C12	C13	C15	179.0(2)
Na2	N8	C28	C27	–175.13(14)	C13	N6	B1	N2	–108.1(2)
Na2	N8	C28	C30	5.0(3)	C13	N6	B1	N4	129.3(2)
Na2	N10	C33	C32	–164.80(14)	C14	C11	C12	C13	179.0(2)
Na2	N10	C33	C35	16.1(3)	C26	N7	N8	Na2	176.54(11)
Na2	N12	C38	C37	–162.31(14)	C26	N7	N8	C28	0.5(2)
Na2	N12	C38	C40	19.0(3)	C26	N7	B2	N9	118.57(19)
N1	N2	C3	C2	0.5(2)	C26	N7	B2	N11	–116.90(19)
N1	N2	C3	C5	–179.9(2)	C26	C27	C28	N8	0.1(2)
N1	N2	B1	N4	81.3(2)	C26	C27	C28	C30	179.92(19)
N1	N2	B1	N6	–42.6(2)	C29	C26	C27	C28	–179.60(18)
N1	C1	C2	C3	0.0(2)	C31	N9	N10	Na2	168.44(12)
N2	N1	C1	C2	0.3(2)	C31	N9	N10	C33	–0.4(2)
N2	N1	C1	C4	–179.19(17)	C31	N9	B2	N7	–107.5(2)
N3	N4	C8	C7	–0.6(2)	C31	N9	B2	N11	128.01(18)
N3	N4	C8	C10	177.79(19)	C31	C32	C33	N10	–0.3(2)
N3	N4	B1	N2	–54.9(2)	C31	C32	C33	C35	178.7(2)
N3	N4	B1	N6	68.7(2)	C34	C31	C32	C33	–178.7(2)
N3	C6	C7	C8	–0.3(2)	C36	N11	N12	Na2	166.22(12)
N4	N3	C6	C7	–0.1(2)	C36	N11	N12	C38	–0.3(2)

N4	N3	C6	C9	–179.55(18)	C36	N11	B2	N7	126.83(19)
N5	N6	C13	C12	0.2(2)	C36	N11	B2	N9	–109.4(2)
N5	N6	C13	C15	–179.0(2)	C36	C37	C38	N12	–0.3(2)
N5	N6	B1	N2	73.1(2)	C36	C37	C38	C40	178.15(19)
N5	N6	B1	N4	–49.5(2)	C39	C36	C37	C38	178.75(19)
N5	C11	C12	C13	0.1(2)	B1	N2	C3	C2	176.90(19)
N6	N5	C11	C12	0.0(2)	B1	N2	C3	C5	–3.5(3)
N6	N5	C11	C14	–178.99(17)	B1	N4	C8	C7	179.39(18)
N7	N8	C28	C27	–0.3(2)	B1	N4	C8	C10	–2.2(3)
N7	N8	C28	C30	179.81(17)	B1	N6	C13	C12	–178.76(18)
N7	C26	C27	C28	0.2(2)	B1	N6	C13	C15	2.1(3)
N8	N7	C26	C27	–0.4(2)	B2	N7	N8	Na2	–4.2(2)
N8	N7	C26	C29	179.40(16)	B2	N7	N8	C28	179.68(16)
N8	N7	B2	N9	–60.5(2)	B2	N7	C26	C27	–179.58(17)
N8	N7	B2	N11	64.0(2)	B2	N7	C26	C29	0.2(3)
N9	N10	C33	C32	0.4(2)	B2	N9	N10	Na2	–8.7(2)
N9	N10	C33	C35	–178.66(18)	B2	N9	N10	C33	–177.47(16)
N9	C31	C32	C33	0.0(2)	B2	N9	C31	C32	177.12(17)
N10	N9	C31	C32	0.2(2)	B2	N9	C31	C34	–4.0(3)
N10	N9	C31	C34	179.07(18)	B2	N11	N12	Na2	–15.0(2)
N10	N9	B2	N7	69.0(2)	B2	N11	N12	C38	178.47(16)
N10	N9	B2	N11	–55.4(2)	B2	N11	C36	C37	–178.59(18)
N11	N12	C38	C37	0.4(2)	B2	N11	C36	C39	2.7(3)

Table S14. Hydrogen atom coordinates (Å × 10^4) and isotropic displacement parameters (Å^2 × 10^3) for **2**·3CHCl$_3$.

Atom	*x*	*y*	*z*	U_{iso}
H2	1919	4637	1929	37
H4A	2506	3021	835	46
H4B	1395	3756	642	46
H4C	1519	2682	990	46
H5A	1546	4357	4130	62
H5B	350	4971	4051	62
H5C	1286	5285	3478	62
H7	2491	839	5807	35
H9A	2970	–714	4670	53
H9B	3833	–227	4281	53
H9C	3049	–242	3726	53
H10A	103	2905	6039	57
H10B	1010	3341	5647	57
H10C	1170	2517	6402	57
H12	–3098	2902	4214	40
H14A	–1523	1214	2774	51
H14B	–2454	1199	3547	51
H14C	–1264	547	3613	51
H15A	–1960	4640	4351	67
H15B	–2002	4045	5248	67
H15C	–3000	4413	4799	67
H17A	–621	2914	788	49
H17B	–596	2692	1763	49
H17C	–1495	2555	1411	49
H18A	–970	891	795	44
H18B	264	362	493	44
H18C	–331	1368	30	44
H21A	4494	1176	2406	50
H21B	3253	1657	2717	50
H21C	3848	2157	1938	50
H22A	4329	1380	458	47
H22B	4226	361	551	47
H22C	5108	490	932	47
H24A	151	–1021	4289	53
H24B	490	–131	4277	53
H24C	1103	–1138	4727	53
H25A	2627	–2364	3747	60
H25B	2555	–2177	2781	60
H25C	1666	–2464	3454	60
H27	3001	105	–2145	30
H29A	3145	–2302	–1757	43

H29B	4327	–2453	–1703	43
H29C	3798	–1761	–2446	43
H30A	2119	1404	–148	48
H30B	1625	1650	–971	48
H30C	2812	1582	–1034	48
H32	6389	–3129	1206	31
H34A	6388	–4106	–13	52
H34B	5650	–3403	–637	52
H34C	5240	–4133	38	52
H35A	4260	–1179	2506	52
H35B	5421	–1217	2054	52
H35C	5259	–2083	2702	52
H37	420	–3085	1570	30
H39A	1937	–4286	503	44
H39B	3049	–4289	606	44
H39C	2579	–3757	–212	44
H40A	–198	–1478	2732	42
H40B	–829	–1062	1978	42
H40C	–62	–576	2126	42
H1	–52	3547	4493	27
H2A	3590	–2765	–231	24
H43	6781	7763	5564	66
H42	5344	3846	7971	57
H41	575	5379	7719	42