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Supplementary Data

Manuscript name: Reactions of Tungsten Alkylidynes with Thionyl Chloride

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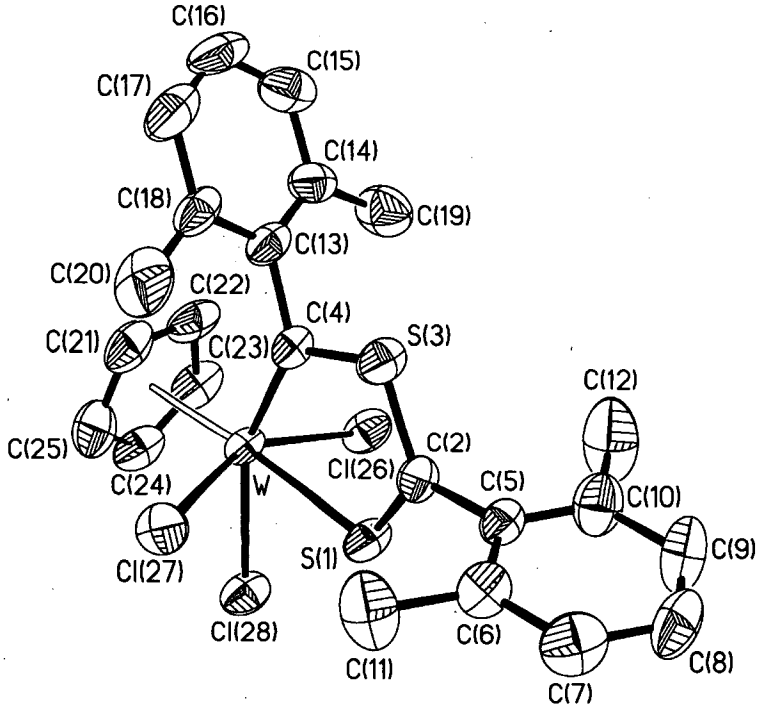
C(16)
C(15)
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S(3)
C(12)
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C(2)
Cl(26)
C(24)
W
C(5)
C(10)
Cl(27)
S(1)
C(9)
Cl(28)
C(6)
C(11)
C(8)
C(7)

Fig. S1

Table 1. Crystal data and structure refinement for **2**

Identification code	Compound **2**
Empirical formula	$C_{23}H_{23}S_2Cl_3W$
Formula weight	653.73
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 18.858(6) Å α = 90 deg. b = 8.336(2) Å β = 92.30(3) deg. c = 30.285(6) Å γ = 90 deg.
Volume	4757.2(20) $Å^3$
Z, Calculated density	8, 1.826 Mg/m^3
Absorption coefficient	5.377 mm^{-1}
F(000)	2544
Crystal size	0.47 x 0.47 x 0.22 mm
Theta range for data collection	2.16 to 25.00 deg.
Limiting indices	0<=h<=22, 0<=k<=9, -35<=l<=35
Reflections collected / unique	4318 / 4186 [R(int) = 0.0334]
Absorption correction	Face-indexed numerical
Max. and min. transmission	0.3750 and 0.1322
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4175 / 0 / 254
Goodness-of-fit on F^2	1.050
Final R indices [I>2σ(I)]	R1 = 0.0323, wR2 = 0.0745
R indices (all data)	R1 = 0.0472, wR2 = 0.0854
Extinction coefficient	0.00009(2)
Largest diff. peak and hole	0.698 and -0.570 $e.A^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
W	3687(1)	3381(1)	805(1)	35(1)
S(1)	3167(1)	2146(2)	1479(1)	44(1)
C(2)	3810(3)	1886(7)	1846(2)	37(1)
S(3)	4661(1)	2313(2)	1719(1)	46(1)
C(4)	4599(3)	3009(7)	1178(2)	37(1)
C(5)	3674(3)	1268(7)	2296(2)	38(1)
C(6)	3456(3)	2329(8)	2616(2)	44(2)
C(7)	3288(4)	1714(9)	3022(2)	59(2)
C(8)	3343(4)	101(10)	3109(2)	60(2)
C(9)	3563(5)	-917(9)	2794(3)	68(2)
C(10)	3740(4)	-359(8)	2383(2)	57(2)
C(11)	3408(5)	4121(9)	2534(2)	70(2)
C(12)	3993(7)	-1514(10)	2038(3)	101(4)
C(13)	5379(3)	3292(8)	1093(2)	42(2)
C(14)	5779(3)	2100(9)	903(2)	48(2)
C(15)	6486(4)	2417(11)	818(2)	64(2)
C(16)	6781(4)	3888(12)	928(3)	71(3)
C(17)	6395(4)	5024(11)	1129(3)	70(2)
C(18)	5696(3)	4765(9)	1222(2)	51(2)
C(19)	5484(4)	454(9)	801(3)	75(2)
C(20)	5293(4)	6041(9)	1463(3)	73(2)
C(21)	4443(2)	5091(6)	460(1)	54(2)
C(22)	4517(2)	3551(6)	267(2)	58(2)
C(23)	3873(3)	3180(5)	29(1)	56(2)
C(24)	3401(2)	4491(7)	75(2)	58(2)
C(25)	3753(3)	5672(5)	341(2)	65(2)
Cl(26)	3569(1)	522(2)	626(1)	57(1)
Cl(27)	3387(1)	5636(2)	1270(1)	53(1)
Cl(28)	2376(1)	3291(2)	706(1)	52(1)

Table 3. Bond lengths [Å] and angles [deg] for **2**.

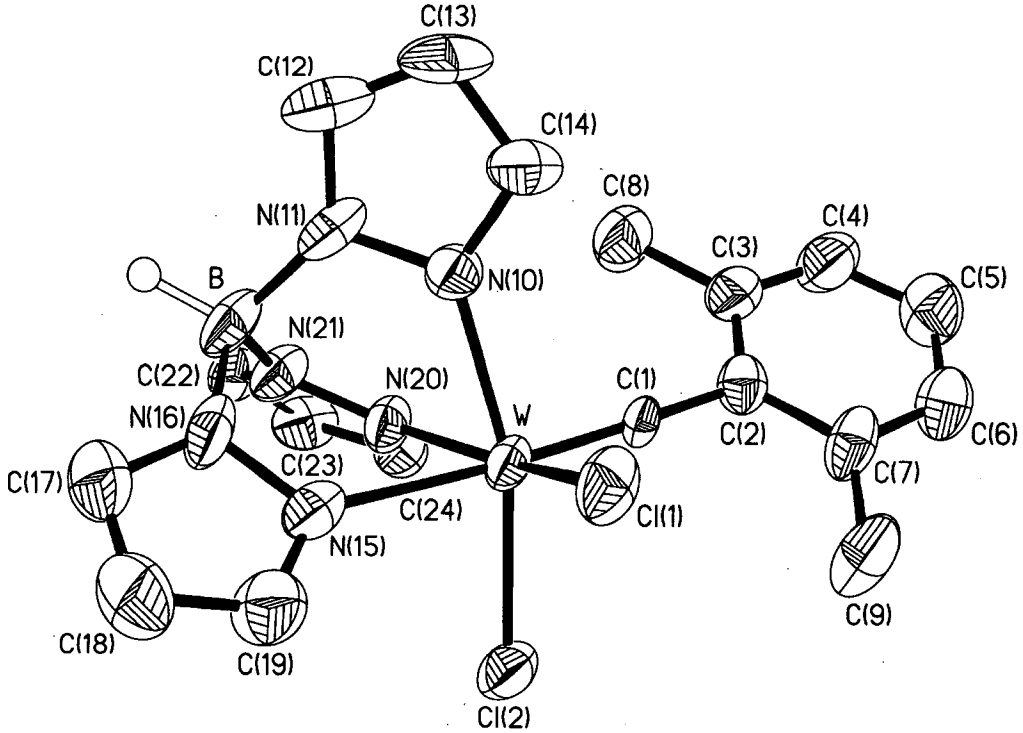
W-C(4)	2.043(6)
W-C(21)	2.297(4)
W-C(22)	2.310(4)
W-C(25)	2.377(5)
W-C(23)	2.396(4)
W-Cl(27)	2.429(2)
W-C(24)	2.436(4)
W-Cl(26)	2.453(2)
W-Cl(28)	2.479(2)
W-S(1)	2.520(2)
S(1)-C(2)	1.626(6)
C(2)-C(5)	1.488(8)
C(2)-S(3)	1.701(6)
S(3)-C(4)	1.740(6)
C(4)-C(13)	1.520(8)
C(5)-C(10)	1.387(9)
C(5)-C(6)	1.388(9)
C(6)-C(7)	1.380(9)
C(6)-C(11)	1.517(10)
C(7)-C(8)	1.373(10)
C(8)-C(9)	1.353(11)
C(9)-C(10)	1.383(10)
C(10)-C(12)	1.511(10)
C(13)-C(14)	1.388(9)
C(13)-C(18)	1.414(9)
C(14)-C(15)	1.393(9)
C(14)-C(19)	1.508(10)
C(15)-C(16)	1.382(12)
C(16)-C(17)	1.354(12)
C(17)-C(18)	1.376(10)
C(18)-C(20)	1.511(11)
C(21)-C(25)	1.42
C(21)-C(22)	1.42
C(22)-C(23)	1.42
C(23)-C(24)	1.42
C(24)-C(25)	1.42
C(4)-W-C(21)	79.7(2)
C(4)-W-C(22)	79.6(2)
C(21)-W-C(22)	35.90(6)
C(4)-W-C(25)	112.6(2)
C(21)-W-C(25)	35.32(6)
C(22)-W-C(25)	58.69(7)
C(4)-W-C(23)	112.2(2)
C(21)-W-C(23)	58.57(7)
C(22)-W-C(23)	35.06(6)
C(25)-W-C(23)	57.55(7)
C(4)-W-Cl(27)	90.4(2)
C(21)-W-Cl(27)	86.98(14)
C(22)-W-Cl(27)	122.85(14)
C(25)-W-Cl(27)	74.93(12)
C(23)-W-Cl(27)	132.05(13)
C(4)-W-C(24)	135.2(2)
C(21)-W-C(24)	57.99(8)
C(22)-W-C(24)	57.83(7)
C(25)-W-C(24)	34.29(6)
C(23)-W-C(24)	34.16(6)

Cl(27)-W-C(24)	100.61(14)
C(4)-W-Cl(26)	92.4(2)
C(21)-W-Cl(26)	123.66(14)
C(22)-W-Cl(26)	87.75(13)
C(25)-W-Cl(26)	131.01(12)
C(23)-W-Cl(26)	74.34(11)
Cl(27)-W-Cl(26)	149.23(6)
C(24)-W-Cl(26)	98.81(14)
C(4)-W-Cl(28)	151.2(2)
C(21)-W-Cl(28)	126.68(13)
C(22)-W-Cl(28)	128.08(12)
C(25)-W-Cl(28)	91.64(13)
C(23)-W-Cl(28)	93.64(13)
Cl(27)-W-Cl(28)	80.77(6)
C(24)-W-Cl(28)	73.64(11)
Cl(26)-W-Cl(28)	82.10(6)
C(4)-W-S(1)	80.6(2)
C(21)-W-S(1)	153.05(10)
C(22)-W-S(1)	153.36(11)
C(25)-W-S(1)	146.98(12)
C(23)-W-S(1)	147.46(11)
Cl(27)-W-S(1)	74.89(6)
C(24)-W-S(1)	144.18(10)
Cl(26)-W-S(1)	75.38(6)
Cl(28)-W-S(1)	70.56(6)
C(2)-S(1)-W	107.7(2)
C(5)-C(2)-S(1)	121.3(5)
C(5)-C(2)-S(3)	118.5(4)
S(1)-C(2)-S(3)	120.2(4)
C(2)-S(3)-C(4)	104.8(3)
C(13)-C(4)-S(3)	100.5(4)
C(13)-C(4)-W	133.1(4)
S(3)-C(4)-W	126.4(3)
C(10)-C(5)-C(6)	121.1(6)
C(10)-C(5)-C(2)	119.7(6)
C(6)-C(5)-C(2)	119.1(5)
C(7)-C(6)-C(5)	118.1(6)
C(7)-C(6)-C(11)	119.9(6)
C(5)-C(6)-C(11)	122.0(6)
C(8)-C(7)-C(6)	121.1(7)
C(9)-C(8)-C(7)	120.1(7)
C(8)-C(9)-C(10)	121.0(7)
C(9)-C(10)-C(5)	118.5(7)
C(9)-C(10)-C(12)	120.2(7)
C(5)-C(10)-C(12)	121.3(7)
C(14)-C(13)-C(18)	120.4(6)
C(14)-C(13)-C(4)	120.3(6)
C(18)-C(13)-C(4)	119.3(6)
C(13)-C(14)-C(15)	118.8(7)
C(13)-C(14)-C(19)	122.3(6)
C(15)-C(14)-C(19)	118.9(7)
C(16)-C(15)-C(14)	120.1(8)
C(17)-C(16)-C(15)	120.8(7)
C(16)-C(17)-C(18)	121.3(8)
C(17)-C(18)-C(13)	118.6(8)
C(17)-C(18)-C(20)	119.5(7)
C(13)-C(18)-C(20)	122.0(6)
C(25)-C(21)-C(22)	108.0
C(25)-C(21)-W	75.4(2)
C(22)-C(21)-W	72.5(2)
C(23)-C(22)-C(21)	108.0

C(23)-C(22)-W	75.8(2)
C(21)-C(22)-W	71.6(2)
C(22)-C(23)-C(24)	108.0
C(22)-C(23)-W	69.1(2)
C(24)-C(23)-W	74.5(2)
C(23)-C(24)-C(25)	108.0
C(23)-C(24)-W	71.4(2)
C(25)-C(24)-W	70.6(2)
C(21)-C(25)-C(24)	108.0
C(21)-C(25)-W	69.3(2)
C(24)-C(25)-W	75.2(2)

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2**.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[\ h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12}\ ]$

	U11	U22	U33	U23	U13	U12
W	33(1)	45(1)	26(1)	2(1)	-1(1)	-11(1)
S(1)	35(1)	63(1)	33(1)	7(1)	-1(1)	-13(1)
C(2)	43(3)	38(3)	30(3)	1(3)	0(3)	-4(3)
S(3)	38(1)	63(1)	37(1)	9(1)	-2(1)	-8(1)
C(4)	36(3)	40(3)	34(3)	1(3)	3(3)	-9(3)
C(5)	36(3)	43(3)	34(3)	3(3)	0(3)	-7(3)
C(6)	50(4)	49(4)	33(3)	-7(3)	0(3)	-6(3)
C(7)	67(5)	72(5)	37(4)	-11(4)	3(3)	-2(4)
C(8)	74(5)	73(5)	34(4)	16(4)	2(4)	-16(4)
C(9)	99(6)	51(4)	53(5)	15(4)	3(4)	-14(4)
C(10)	76(5)	53(4)	42(4)	1(3)	3(4)	-4(4)
C(11)	114(7)	52(4)	43(4)	-6(4)	1(4)	13(5)
C(12)	190(12)	57(5)	59(6)	-7(4)	31(7)	23(6)
C(13)	37(3)	55(4)	35(3)	10(3)	1(3)	-12(3)
C(14)	37(3)	66(4)	41(4)	8(3)	3(3)	3(3)
C(15)	46(4)	107(7)	41(4)	22(4)	12(3)	14(4)
C(16)	37(4)	118(7)	57(5)	38(5)	0(4)	-21(5)
C(17)	54(5)	89(6)	67(5)	37(5)	-17(4)	-33(5)
C(18)	42(4)	65(4)	46(4)	23(4)	-15(3)	-23(3)
C(19)	70(5)	65(5)	89(6)	-15(5)	8(5)	10(4)
C(20)	76(6)	52(4)	88(6)	-12(4)	-21(5)	-26(4)
C(21)	59(4)	72(5)	33(3)	13(4)	1(3)	-21(4)
C(22)	47(4)	97(6)	33(4)	17(4)	11(3)	-13(4)
C(23)	61(4)	85(5)	21(3)	-3(3)	-2(3)	-24(4)
C(24)	54(4)	92(6)	27(3)	17(4)	-4(3)	-16(4)
C(25)	84(6)	64(5)	47(4)	23(4)	2(4)	-3(4)
Cl(26)	58(1)	54(1)	60(1)	-14(1)	8(1)	-19(1)
Cl(27)	55(1)	52(1)	53(1)	-8(1)	2(1)	-4(1)
Cl(28)	38(1)	75(1)	44(1)	5(1)	-7(1)	-13(1)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C(12)
C(14)
C(8)
N(11)
C(4)
C(3)
B
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N(21)
C(22)
N(20)
C(1)
N(16)
W
C(2)
C(6)
C(23)
C(17)
C(7)
C(24)
Cl(1)
N(15)
C(9)
C(18)
C(19)
Cl(2)

Fig. S2

Table 5. Crystal data and structure refinement for **3a**

Identification code	Compound **3a**
Empirical formula	$C_{18.50}H_{20}BCl_3N_6W$
Formula weight	627.42
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.704(4) Å α = 90 deg. b = 13.587(4) Å β = 98.00(3) deg. c = 20.393(7) Å γ = 90 deg.
Volume	2388.4(16) $Å^3$
Z, Calculated density	4, 1.745 Mg/m^3
Absorption coefficient	5.189 mm^{-1}
F(000)	1212
Crystal size	0.23 x 0.17 x 0.03 mm
Theta range for data collection	1.81 to 25.00 deg.
Limiting indices	0<=h<=10, 0<=k<=16, -24<=l<=24
Reflections collected / unique	4492 / 4197 [R(int) = 0.0792]
Absorption correction	Semi-empirical
Max. and min. transmission	0.8326 and 0.5570
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4171 / 6 / 289
Goodness-of-fit on F^2	1.020
Final R indices [I>2σ(I)]	R1 = 0.0532, wR2 = 0.1044
R indices (all data)	R1 = 0.1011, wR2 = 0.3649
Largest diff. peak and hole	0.723 and -0.753 $e.Å^{-3}$

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
W	2614(1)	1373(1)	7932(1)	34(1)
Cl(1)	4113(4)	2671(2)	7595(2)	51(1)
Cl(2)	3989(4)	70(2)	7544(2)	51(1)
C(1)	3509(11)	1324(9)	8781(6)	34(2)
C(2)	4205(13)	1344(10)	9463(6)	41(3)
C(3)	3277(15)	1331(12)	9971(7)	51(3)
C(4)	3990(16)	1403(14)	10622(8)	64(4)
C(5)	5570(20)	1563(13)	10762(8)	68(5)
C(6)	6484(17)	1545(11)	10257(8)	58(4)
C(7)	5832(14)	1465(11)	9601(8)	51(3)
C(8)	1535(16)	1164(13)	9825(8)	68(5)
C(9)	6837(16)	1423(16)	9075(8)	73(5)
N(10)	840(13)	2393(7)	8100(6)	42(3)
N(11)	-662(12)	2351(8)	7789(7)	48(3)
C(12)	-1435(19)	3116(11)	7978(10)	62(5)
C(13)	-504(19)	3692(12)	8399(9)	66(4)
C(14)	914(17)	3208(10)	8490(9)	52(4)
N(15)	1310(11)	1458(8)	6839(6)	43(2)
N(16)	-267(11)	1506(9)	6724(6)	51(3)
C(17)	-723(19)	1533(13)	6065(8)	65(4)
C(18)	572(20)	1496(14)	5769(7)	71(4)
C(19)	1769(18)	1461(13)	6250(8)	63(4)
N(20)	707(12)	392(7)	8044(6)	39(3)
N(21)	-766(12)	529(8)	7722(6)	45(3)
C(22)	-1605(14)	-228(9)	7846(7)	42(3)
C(23)	-746(15)	-875(9)	8234(8)	48(3)
C(24)	716(16)	-447(9)	8368(7)	44(3)
B	-1151(14)	1481(12)	7315(9)	52(4)
C(30)	6399(59)	-328(35)	5210(29)	130(24)
Cl(31)	6967(28)	784(16)	4567(11)	191(9)
Cl(32)	5697(25)	-35(16)	6018(14)	135(8)
Cl(33)	4936(69)	-981(46)	5676(32)	149(19)

Table 7. Bond lengths [Å] and angles [deg] for **3a**

W-C(1)	1.800(11)
W-N(10)	2.138(10)
W-N(20)	2.166(10)
W-Cl(2)	2.336(3)
W-Cl(1)	2.352(3)
W-N(15)	2.359(11)
C(1)-C(2)	1.44(2)
C(2)-C(3)	1.40(2)
C(2)-C(7)	1.41(2)
C(3)-C(4)	1.39(2)
C(3)-C(8)	1.52(2)
C(4)-C(5)	1.38(2)
C(5)-C(6)	1.39(2)
C(6)-C(7)	1.38(2)
C(7)-C(9)	1.48(2)
N(10)-C(14)	1.36(2)
N(10)-N(11)	1.373(15)
N(11)-C(12)	1.33(2)
N(11)-B	1.55(2)
C(12)-C(13)	1.35(2)
C(13)-C(14)	1.39(2)
N(15)-C(19)	1.32(2)
N(15)-N(16)	1.361(13)
N(16)-C(17)	1.35(2)
N(16)-B	1.52(2)
C(17)-C(18)	1.35(2)
C(18)-C(19)	1.33(2)
N(20)-C(24)	1.32(2)
N(20)-N(21)	1.369(14)
N(21)-C(22)	1.31(2)
N(21)-B	1.55(2)
C(22)-C(23)	1.34(2)
C(23)-C(24)	1.39(2)
C(30)-Cl(32)	1.88(7)
C(30)-Cl(33)	1.91(8)
C(30)-Cl(31)	2.10(5)
Cl(31)-Cl(33)#1	1.68(6)
Cl(33)-Cl(31)#1	1.68(6)
C(1)-W-N(10)	95.5(5)
C(1)-W-N(20)	96.3(5)
N(10)-W-N(20)	78.5(3)
C(1)-W-Cl(2)	97.1(4)
N(10)-W-Cl(2)	164.0(3)
N(20)-W-Cl(2)	90.3(3)
C(1)-W-Cl(1)	97.2(4)
N(10)-W-Cl(1)	90.2(3)
N(20)-W-Cl(1)	163.1(3)
Cl(2)-W-Cl(1)	97.97(12)
C(1)-W-N(15)	176.8(4)
N(10)-W-N(15)	81.8(4)
N(20)-W-N(15)	81.7(4)
Cl(2)-W-N(15)	85.4(3)
Cl(1)-W-N(15)	84.3(3)
C(2)-C(1)-W	176.7(11)
C(3)-C(2)-C(7)	121.3(12)
C(3)-C(2)-C(1)	120.5(10)

C(7)-C(2)-C(1)	118.0(12)
C(4)-C(3)-C(2)	118.7(12)
C(4)-C(3)-C(8)	119.8(13)
C(2)-C(3)-C(8)	121.3(12)
C(5)-C(4)-C(3)	120.5(15)
C(4)-C(5)-C(6)	120.1(15)
C(7)-C(6)-C(5)	121.3(14)
C(6)-C(7)-C(2)	117.8(14)
C(6)-C(7)-C(9)	120.0(12)
C(2)-C(7)-C(9)	122.0(13)
C(14)-N(10)-N(11)	105.6(11)
C(14)-N(10)-W	130.2(10)
N(11)-N(10)-W	124.1(8)
C(12)-N(11)-N(10)	108.8(13)
C(12)-N(11)-B	132.4(13)
N(10)-N(11)-B	118.8(10)
N(11)-C(12)-C(13)	110.9(15)
C(12)-C(13)-C(14)	104.8(14)
N(10)-C(14)-C(13)	109.8(15)
C(19)-N(15)-N(16)	105.7(12)
C(19)-N(15)-W	134.0(9)
N(16)-N(15)-W	120.4(9)
C(17)-N(16)-N(15)	108.8(13)
C(17)-N(16)-B	132.9(12)
N(15)-N(16)-B	118.3(11)
N(16)-C(17)-C(18)	107.3(14)
C(19)-C(18)-C(17)	106.7(14)
N(15)-C(19)-C(18)	111.5(14)
C(24)-N(20)-N(21)	107.4(10)
C(24)-N(20)-W	129.4(9)
N(21)-N(20)-W	123.1(8)
C(22)-N(21)-N(20)	108.1(11)
C(22)-N(21)-B	132.6(11)
N(20)-N(21)-B	119.3(10)
N(21)-C(22)-C(23)	110.4(12)
C(22)-C(23)-C(24)	105.2(12)
N(20)-C(24)-C(23)	108.7(12)
N(16)-B-N(11)	110.7(11)
N(16)-B-N(21)	110.4(12)
N(11)-B-N(21)	106.5(12)
Cl(32)-C(30)-Cl(31)	121.9(30)
Cl(33)-C(30)-Cl(31)	151.0(34)
Cl(33)#1-Cl(31)-C(30)	89.5(28)
Cl(31)#1-Cl(33)-C(30)	118.5(37)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1

Table 8. Anisotropic displacement parameters ($A^2 \times 10^3$) for **3a**
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
W	22(1)	33(1)	45(1)	0(1)	0(1)	-1(1)
Cl(1)	37(2)	42(2)	72(3)	4(2)	2(2)	-11(1)
Cl(2)	33(2)	45(2)	76(3)	-10(2)	5(2)	6(1)
C(1)	18(4)	37(5)	45(7)	-9(6)	-3(4)	-2(5)
C(2)	40(6)	41(6)	40(7)	5(7)	-3(5)	-1(6)
C(3)	44(6)	54(7)	53(8)	-1(8)	3(6)	10(7)
C(4)	46(7)	83(10)	63(10)	-1(11)	6(7)	15(9)
C(5)	68(10)	89(13)	44(9)	8(9)	-7(8)	4(9)
C(6)	50(7)	67(10)	51(9)	12(8)	-11(7)	4(7)
C(7)	34(6)	46(7)	67(9)	17(8)	-10(6)	3(6)
C(8)	44(7)	98(14)	65(10)	-10(9)	12(7)	-4(8)
C(9)	38(7)	115(13)	67(10)	22(12)	5(7)	4(10)
N(10)	37(6)	30(5)	58(8)	-8(5)	3(5)	1(4)
N(11)	27(5)	44(6)	74(9)	16(6)	10(6)	10(4)
C(12)	59(9)	44(8)	91(13)	9(8)	38(9)	18(7)
C(13)	75(10)	32(7)	97(13)	-6(9)	36(9)	15(8)
C(14)	48(8)	37(6)	76(11)	-9(7)	27(8)	-6(6)
N(15)	32(5)	41(5)	57(7)	2(6)	7(5)	5(5)
N(16)	31(5)	54(7)	62(7)	5(6)	-15(5)	6(5)
C(17)	63(9)	86(12)	43(8)	1(9)	-5(7)	8(9)
C(18)	81(10)	96(13)	35(8)	8(9)	9(7)	2(11)
C(19)	62(9)	78(10)	48(9)	13(10)	3(7)	23(9)
N(20)	28(5)	33(5)	52(7)	-1(5)	-3(5)	-2(4)
N(21)	27(5)	46(6)	63(8)	3(6)	9(5)	2(4)
C(22)	27(6)	43(7)	59(9)	-8(6)	11(6)	-11(5)
C(23)	50(7)	21(5)	79(11)	-3(7)	23(7)	-9(6)
C(24)	47(7)	41(7)	43(8)	1(6)	3(6)	6(6)
B	21(5)	50(8)	83(12)	9(9)	2(6)	-1(6)
C(30)	99(34)	109(34)	160(53)	71(36)	-58(36)	-41(28)
Cl(31)	207(21)	173(16)	182(19)	-12(15)	-11(17)	49(16)
Cl(32)	105(14)	134(17)	173(23)	20(16)	52(15)	4(12)
Cl(33)	130(24)	151(25)	159(25)	11(18)	-4(18)	-3(18)

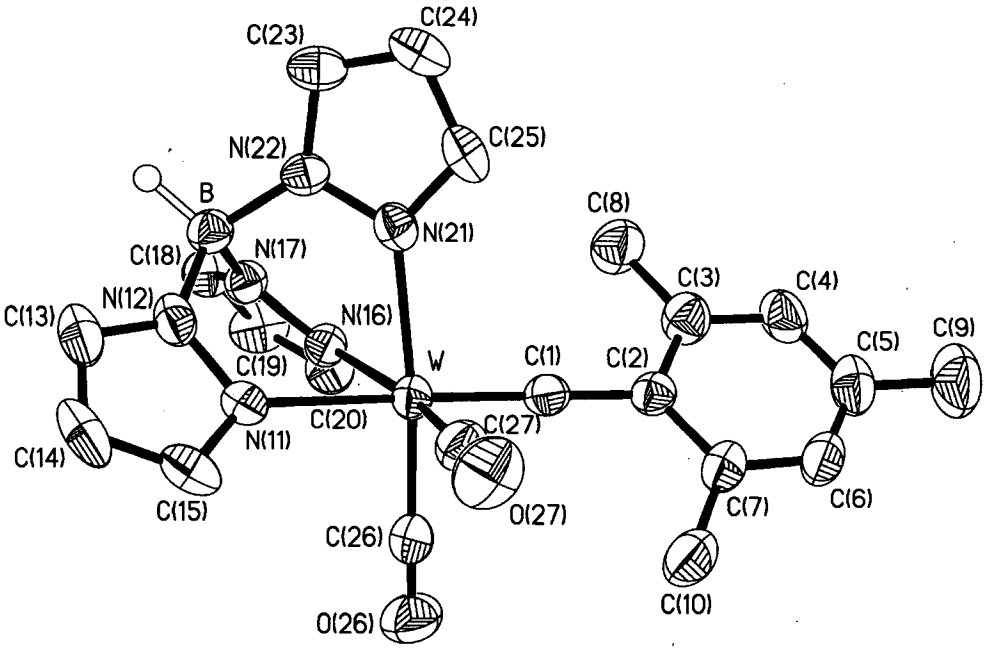
C(23)
C(24)
C(25)
N(22)
B
N(21)
C(8)
C(18)
N(17)
C(3)
C(4)
N(12)
C(13)
N(16)
C(5)
C(9)
C(19)
W
C(1)
C(2)
C(20)
C(27)
N(11)
C(14)
C(15)
O(27)
C(7)
C(6)
C(26)
C(10)
O(26)

Fig. S3

Table 9. Crystal data and structure refinement for **1e**

Identification code	Compound **1e**
Empirical formula	$C_{21}H_{21}N_6O_2BW$
Formula weight	584.10
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, $P\bar{1}$
Unit cell dimensions	a = 8.543(2) Å α = 76.26(2) deg. b = 11.608(3) Å β = 83.80(2) deg. c = 11.779(2) Å γ = 83.001(15) deg.
Volume	1122.5(4) $Å^3$
Z, Calculated density	2, 1.728 Mg/m^3
Absorption coefficient	5.175 mm^{-1}
F(000)	568
Crystal size	0.12 x 0.10 x 0.03 mm
Theta range for data collection	1.79 to 24.99 deg.
Limiting indices	0<=h<=10, -13<=k<=13, -13<=l<=14
Reflections collected / unique	4210 / 3920 [R(int) = 0.0266]
Absorption correction	Ellipsoidal
Max. and min. transmission	0.8983 and 0.5748
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3851 / 0 / 280
Goodness-of-fit on F^2	0.981
Final R indices [I>2σ(I)]	R1 = 0.0279, wR2 = 0.0662
R indices (all data)	R1 = 0.0331, wR2 = 0.0676
Largest diff. peak and hole	0.870 and -0.755 e.$Å^{-3}$

Table 10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1e**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
W	1244(1)	3010(1)	2711(1)	34(1)
C(1)	2119(6)	2557(4)	1380(4)	37(1)
C(2)	2928(6)	2110(4)	402(4)	36(1)
C(3)	1999(7)	1738(5)	-340(5)	48(1)
C(4)	2757(7)	1298(5)	-1278(5)	51(1)
C(5)	4381(7)	1250(5)	-1530(5)	53(1)
C(6)	5257(6)	1632(5)	-797(5)	48(1)
C(7)	4601(6)	2065(5)	156(5)	42(1)
C(8)	227(7)	1805(7)	-132(6)	64(2)
C(9)	5152(10)	785(7)	-2555(7)	84(2)
C(10)	5611(7)	2501(6)	897(6)	62(2)
N(11)	506(5)	3339(3)	4551(4)	36(1)
N(12)	-974(5)	3146(4)	5078(4)	39(1)
C(13)	-1059(7)	3277(5)	6169(5)	47(1)
C(14)	374(8)	3561(5)	6397(5)	56(2)
C(15)	1293(7)	3588(4)	5369(5)	47(1)
N(16)	-1140(5)	3946(3)	2397(4)	36(1)
N(17)	-2378(5)	3748(3)	3239(4)	35(1)
C(18)	-3633(6)	4495(5)	2880(5)	48(1)
C(19)	-3245(7)	5194(5)	1811(6)	56(2)
C(20)	-1695(7)	4823(5)	1532(5)	46(1)
N(21)	-201(5)	1499(4)	3404(4)	37(1)
N(22)	-1577(5)	1598(3)	4075(3)	35(1)
C(23)	-2200(6)	546(4)	4358(5)	41(1)
C(24)	-1212(7)	-254(5)	3869(5)	46(1)
C(25)	5(7)	373(4)	3283(5)	43(1)
B	-2209(7)	2793(5)	4392(5)	37(1)
C(26)	2273(6)	4507(5)	2101(5)	46(1)
O(26)	2836(5)	5388(4)	1717(4)	68(1)
C(27)	3192(6)	2195(5)	3426(5)	44(1)
O(27)	4276(5)	1707(4)	3897(4)	68(1)

Table 11. Bond lengths [Å] and angles [deg] for **1e**.

W-C(1)	1.826(5)
W-C(27)	1.978(5)
W-C(26)	1.989(6)
W-N(21)	2.212(4)
W-N(16)	2.214(4)
W-N(11)	2.298(4)
C(1)-C(2)	1.449(7)
C(2)-C(3)	1.412(8)
C(2)-C(7)	1.424(7)
C(3)-C(4)	1.390(8)
C(3)-C(8)	1.503(8)
C(4)-C(5)	1.384(8)
C(5)-C(6)	1.380(8)
C(5)-C(9)	1.496(8)
C(6)-C(7)	1.375(7)
C(7)-C(10)	1.497(8)
N(11)-C(15)	1.336(7)
N(11)-N(12)	1.366(6)
N(12)-C(13)	1.323(7)
N(12)-B	1.543(7)
C(13)-C(14)	1.376(9)
C(14)-C(15)	1.366(8)
N(16)-C(20)	1.339(6)
N(16)-N(17)	1.371(5)
N(17)-C(18)	1.334(6)
N(17)-B	1.544(7)
C(18)-C(19)	1.357(8)
C(19)-C(20)	1.372(8)
N(21)-C(25)	1.336(6)
N(21)-N(22)	1.352(6)
N(22)-C(23)	1.347(6)
N(22)-B	1.541(7)
C(23)-C(24)	1.366(8)
C(24)-C(25)	1.370(8)
C(26)-O(26)	1.155(7)
C(27)-O(27)	1.149(7)
C(1)-W-C(27)	85.9(2)
C(1)-W-C(26)	86.7(2)
C(27)-W-C(26)	91.1(2)
C(1)-W-N(21)	97.6(2)
C(27)-W-N(21)	95.5(2)
C(26)-W-N(21)	172.3(2)
C(1)-W-N(16)	109.2(2)
C(27)-W-N(16)	164.8(2)
C(26)-W-N(16)	92.2(2)
N(21)-W-N(16)	80.43(14)
C(1)-W-N(11)	169.5(2)
C(27)-W-N(11)	83.9(2)
C(26)-W-N(11)	95.7(2)
N(21)-W-N(11)	81.18(14)
N(16)-W-N(11)	81.02(15)
C(2)-C(1)-W	173.9(4)
C(3)-C(2)-C(7)	119.8(5)
C(3)-C(2)-C(1)	117.8(4)
C(7)-C(2)-C(1)	122.4(5)
C(4)-C(3)-C(2)	118.6(5)

C(4)-C(3)-C(8)	119.9(5)
C(2)-C(3)-C(8)	121.5(5)
C(5)-C(4)-C(3)	122.3(5)
C(6)-C(5)-C(4)	117.8(5)
C(6)-C(5)-C(9)	121.4(6)
C(4)-C(5)-C(9)	120.8(6)
C(7)-C(6)-C(5)	123.5(5)
C(6)-C(7)-C(2)	118.0(5)
C(6)-C(7)-C(10)	121.0(5)
C(2)-C(7)-C(10)	121.0(5)
C(15)-N(11)-N(12)	105.1(4)
C(15)-N(11)-W	133.5(4)
N(12)-N(11)-W	121.0(3)
C(13)-N(12)-N(11)	109.6(4)
C(13)-N(12)-B	130.8(5)
N(11)-N(12)-B	119.5(4)
N(12)-C(13)-C(14)	109.4(5)
C(15)-C(14)-C(13)	103.9(5)
N(11)-C(15)-C(14)	111.9(5)
C(20)-N(16)-N(17)	105.8(4)
C(20)-N(16)-W	133.1(4)
N(17)-N(16)-W	120.8(3)
C(18)-N(17)-N(16)	109.0(4)
C(18)-N(17)-B	129.3(4)
N(16)-N(17)-B	121.8(4)
N(17)-C(18)-C(19)	109.3(5)
C(18)-C(19)-C(20)	105.3(5)
N(16)-C(20)-C(19)	110.6(5)
C(25)-N(21)-N(22)	105.9(4)
C(25)-N(21)-W	131.5(4)
N(22)-N(21)-W	122.6(3)
C(23)-N(22)-N(21)	109.5(4)
C(23)-N(22)-B	129.9(4)
N(21)-N(22)-B	120.6(4)
N(22)-C(23)-C(24)	108.5(5)
C(23)-C(24)-C(25)	104.9(5)
N(21)-C(25)-C(24)	111.1(5)
N(22)-B-N(12)	108.4(4)
N(22)-B-N(17)	107.9(4)
N(12)-B-N(17)	108.3(4)
O(26)-C(26)-W	177.7(5)
O(27)-C(27)-W	176.4(5)

Table 12. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1e**.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
W	31(1)	36(1)	36(1)	-12(1)	0(1)	-2(1)
C(1)	33(2)	36(3)	43(3)	-9(2)	-2(2)	-7(2)
C(2)	39(3)	33(3)	33(3)	-2(2)	0(2)	-5(2)
C(3)	47(3)	52(3)	44(3)	-12(3)	-4(2)	-5(3)
C(4)	64(4)	53(3)	41(3)	-21(3)	-3(3)	-10(3)
C(5)	64(4)	49(3)	43(3)	-14(3)	5(3)	4(3)
C(6)	41(3)	48(3)	51(3)	-10(3)	10(2)	1(2)
C(7)	36(3)	44(3)	41(3)	-7(2)	2(2)	1(2)
C(8)	46(3)	90(5)	66(4)	-32(4)	-4(3)	-14(3)
C(9)	98(6)	89(6)	67(5)	-35(4)	17(4)	0(5)
C(10)	40(3)	87(5)	65(4)	-29(4)	7(3)	-13(3)
N(11)	39(2)	33(2)	40(2)	-12(2)	-3(2)	-6(2)
N(12)	46(2)	33(2)	37(2)	-13(2)	-1(2)	0(2)
C(13)	71(4)	37(3)	34(3)	-13(2)	-1(3)	0(3)
C(14)	93(5)	40(3)	42(3)	-22(3)	-18(3)	2(3)
C(15)	58(3)	31(3)	56(3)	-13(2)	-18(3)	-5(2)
N(16)	38(2)	30(2)	37(2)	-5(2)	0(2)	-1(2)
N(17)	33(2)	32(2)	39(2)	-7(2)	0(2)	-2(2)
C(18)	38(3)	37(3)	65(4)	-7(3)	-8(3)	5(2)
C(19)	46(3)	41(3)	71(4)	6(3)	-18(3)	7(3)
C(20)	57(3)	38(3)	39(3)	-1(2)	-5(2)	-4(2)
N(21)	37(2)	34(2)	40(2)	-13(2)	-6(2)	2(2)
N(22)	35(2)	32(2)	36(2)	-3(2)	-4(2)	-5(2)
C(23)	39(3)	34(3)	49(3)	1(2)	-14(2)	-8(2)
C(24)	56(3)	29(3)	57(3)	-10(2)	-20(3)	-6(2)
C(25)	54(3)	35(3)	45(3)	-19(2)	-11(2)	5(2)
B	38(3)	34(3)	39(3)	-6(2)	0(2)	-4(2)
C(26)	38(3)	47(3)	55(3)	-21(3)	5(2)	-4(2)
O(26)	61(3)	52(3)	90(4)	-12(2)	13(2)	-21(2)
C(27)	37(3)	43(3)	50(3)	-10(2)	1(2)	-3(2)
O(27)	42(2)	80(3)	79(3)	-13(3)	-18(2)	10(2)