Inorganic Chemistry
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Table 1. Crystal data and structure refinement for 3a.

Identification code	roe437
Empirical formula	$C_{14}H_{24}Cl_2MoN$
Formula weight	373.18
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 8.6040(10) Å alpha = 90° b = 12.0490(10) Å beta = 90° c = 17.020(2) Å gamma = 90°
Volume, Z	1764.5(3) $Å^3$, 4
Density (calculated)	1.405 Mg/m^3
Absorption coefficient	1.032 mm^{-1}
F(000)	764
Crystal size	0.40 x 0.40 x 0.30 mm
θ range for data collection	3.59 to 22.51°
Limiting indices	$-9 \le h \le 9$, $-12 \le k \le 12$, $-18 \le l \le 18$
Reflections collected	8121
Independent reflections	2294 (R_{int} = 0.0394)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2293 / 0 / 171
Goodness-of-fit on F^2	1.057
Final R indices [I>2σ(I)]	R1 = 0.0213, wR2 = 0.0561
R indices (all data)	R1 = 0.0217, wR2 = 0.0570
Absolute structure parameter	-0.02(6)
Largest diff. peak and hole	0.247 and -0.414 $eÅ^{-3}$

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Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 3Å·U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	1769(1)	5088(1)	8732(1)	33(1)
Cl(1)	3337(1)	5328(1)	9863(1)	66(1)
Cl(2)	3280(2)	3570(1)	8287(1)	66(1)
N(1)	126(3)	4441(2)	9080(2)	38(1)
C(11)	-1254(4)	3854(3)	9345(2)	49(1)
C(12)	-671(6)	2787(4)	9736(4)	99(2)
C(13)	-2276(6)	3592(5)	8655(3)	101(2)
C(14)	-2098(6)	4572(5)	9933(3)	105(2)
C(1)	2796(6)	6058(4)	7570(2)	68(1)
C(2)	3061(5)	6754(3)	8202(2)	55(1)
C(3)	1623(4)	7015(2)	8560(2)	45(1)
C(4)	437(4)	6511(3)	8118(2)	50(1)
C(5)	1152(6)	5855(3)	7523(2)	64(1)
C(6)	4051(10)	5618(6)	7020(4)	147(3)
C(7)	4620(6)	7182(5)	8471(4)	110(2)
C(8)	1385(8)	7798(3)	9232(3)	88(2)
C(9)	-1268(5)	6697(5)	8217(4)	101(2)
C(10)	332(9)	5196(5)	6893(3)	129(3)

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Table 3. Bond lengths [Å] and angles [°] for 3a.

Mo(1)-N(1)	1.719(3)	Mo(1)-C(4)	2.312(3)
Mo(1)-C(5)	2.317(4)	Mo(1)-C(3)	2.344(3)
Mo(1)-Cl(1)	2.3674(9)	Mo(1)-Cl(2)	2.3695(10)
Mo(1)-C(1)	2.462(4)	Mo(1)-C(2)	2.466(4)
N(1)-C(11)	1.454(4)	C(11)-C(13)	1.500(6)
C(11)-C(14)	1.508(6)	C(11)-C(12)	1.532(6)
C(1)-C(2)	1.383(6)	C(1)-C(5)	1.437(7)
C(1)-C(6)	1.525(6)	C(2)-C(3)	1.414(6)
C(2)-C(7)	1.508(7)	C(3)-C(4)	1.407(5)
C(3)-C(8)	1.497(5)	C(4)-C(5)	1.423(6)
C(4)-C(9)	1.494(6)	C(5)-C(10)	1.510(6)

N(1)-Mo(1)-C(4)	94.86(12)	N(1)-Mo(1)-C(5)	107.3(2)
C(4)-Mo(1)-C(5)	35.8(2)	N(1)-Mo(1)-C(3)	116.66(12)
C(4)-Mo(1)-C(3)	35.16(13)	C(5)-Mo(1)-C(3)	58.77(13)
N(1)-Mo(1)-Cl(1)	104.17(9)	C(4)-Mo(1)-Cl(1)	124.01(11)
C(5)-Mo(1)-Cl(1)	143.43(11)	C(3)-Mo(1)-Cl(1)	90.61(9)
N(1)-Mo(1)-Cl(2)	102.19(9)	C(4)-Mo(1)-Cl(2)	134.41(11)
C(5)-Mo(1)-Cl(2)	98.61(12)	C(3)-Mo(1)-Cl(2)	138.96(9)
Cl(1)-Mo(1)-Cl(2)	92.38(4)	N(1)-Mo(1)-C(1)	141.9(2)
C(4)-Mo(1)-C(1)	57.46(14)	C(5)-Mo(1)-C(1)	34.8(2)
C(3)-Mo(1)-C(1)	56.52(13)	Cl(1)-Mo(1)-C(1)	112.97(14)
Cl(2)-Mo(1)-C(1)	84.98(10)	N(1)-Mo(1)-C(2)	149.98(13)
C(4)-Mo(1)-C(2)	56.92(13)	C(5)-Mo(1)-C(2)	56.9(2)
C(3)-Mo(1)-C(2)	34.08(14)	Cl(1)-Mo(1)-C(2)	86.60(11)
Cl(2)-Mo(1)-C(2)	105.31(11)	C(1)-Mo(1)-C(2)	32.6(2)
C(11)-N(1)-Mo(1)	177.3(2)	N(1)-C(11)-C(13)	109.7(3)
N(1)-C(11)-C(14)	108.7(3)	C(13)-C(11)-C(14)	110.9(4)
N(1)-C(11)-C(12)	106.0(3)	C(13)-C(11)-C(12)	110.8(4)
C(14)-C(11)-C(12)	110.5(4)	C(2)-C(1)-C(5)	108.0(4)
C(2)-C(1)-C(6)	124.9(6)	C(5)-C(1)-C(6)	127.2(6)
C(2)-C(1)-Mo(1)	73.9(2)	C(5)-C(1)-Mo(1)	67.1(2)
C(6)-C(1)-Mo(1)	125.6(3)	C(1)-C(2)-C(3)	109.0(4)
C(1)-C(2)-C(7)	126.1(5)	C(3)-C(2)-C(7)	124.8(4)
C(1)-C(2)-Mo(1)	73.5(2)	C(3)-C(2)-Mo(1)	68.2(2)
C(7)-C(2)-Mo(1)	124.6(3)	C(4)-C(3)-C(2)	107.9(3)
C(4)-C(3)-C(8)	125.6(4)	C(2)-C(3)-C(8)	126.1(4)
C(4)-C(3)-Mo(1)	71.2(2)	C(2)-C(3)-Mo(1)	77.7(2)
C(8)-C(3)-Mo(1)	122.4(2)	C(3)-C(4)-C(5)	107.9(3)
C(3)-C(4)-C(9)	125.9(4)	C(5)-C(4)-C(9)	126.1(4)
C(3)-C(4)-Mo(1)	73.7(2)	C(5)-C(4)-Mo(1)	72.3(2)
C(9)-C(4)-Mo(1)	123.1(3)	C(4)-C(5)-C(1)	106.9(4)
C(4)-C(5)-C(10)	126.5(5)	C(1)-C(5)-C(10)	126.0(5)
C(4)-C(5)-Mo(1)	71.9(2)	C(1)-C(5)-Mo(1)	78.1(2)
C(10)-C(5)-Mo(1)	121.9(3)		

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 3a.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mo(1)	36(1)	33(1)	30(1)	2(1)	-2(1)	1(1)
Cl(1)	82(1)	68(1)	50(1)	11(1)	-29(1)	-14(1)
Cl(2)	74(1)	53(1)	71(1)	-4(1)	8(1)	24(1)
N(1)	40(2)	34(1)	41(1)	2(1)	-1(1)	0(1)
C(11)	43(2)	42(2)	61(2)	2(2)	7(2)	-6(2)
C(12)	87(4)	71(3)	138(5)	50(3)	23(3)	-6(3)
C(13)	86(4)	110(4)	107(4)	8(4)	-23(3)	-55(3)
C(14)	87(3)	104(4)	125(4)	-14(4)	54(3)	-13(3)
C(1)	91(3)	60(2)	51(2)	24(2)	36(2)	25(2)
C(2)	48(2)	52(2)	65(3)	25(2)	1(2)	-5(2)
C(3)	52(2)	35(2)	46(2)	4(1)	-3(2)	1(2)
C(4)	40(2)	53(2)	58(2)	24(2)	-7(2)	4(2)
C(5)	111(4)	49(2)	33(2)	8(2)	-18(2)	-9(2)
C(6)	215(8)	122(5)	106(4)	42(4)	111(5)	70(5)
C(7)	56(3)	119(4)	155(5)	63(4)	-14(3)	-32(3)
C(8)	141(5)	49(2)	74(3)	-16(2)	-2(3)	14(3)
C(9)	51(3)	89(3)	162(5)	59(4)	-14(3)	12(3)
C(10)	230(8)	102(4)	56(3)	11(3)	-64(4)	-37(5)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 3a.

	x	y	z	U(eq)
H(12A)	-56(43)	2366(18)	9363(9)	148
H(12B)	-1552(6)	2345(18)	9905(23)	148
H(12C)	-36(42)	2974(4)	10188(16)	148
H(13A)	-2673(39)	4277(6)	8433(15)	151
H(13B)	-3138(27)	3133(29)	8826(6)	151
H(13C)	-1678(14)	3198(30)	8261(11)	151
H(14A)	-2214(45)	5315(11)	9722(11)	158
H(14B)	-1506(26)	4603(29)	10417(9)	158
H(14C)	-3116(21)	4259(20)	10037(20)	158
H(6A)	4497(56)	6230(9)	6726(29)	221
H(6B)	3597(18)	5087(42)	6659(25)	221
H(6C)	4858(39)	5258(49)	7326(4)	221
H(7A)	4819(25)	7898(19)	8230(23)	165
H(7B)	5425(8)	6662(21)	8317(24)	165
H(7C)	4617(18)	7260(36)	9038(5)	165
H(8A)	1613(45)	8549(6)	9063(7)	132
H(8B)	2072(35)	7597(21)	9661(10)	132
H(8C)	314(15)	7756(24)	9408(15)	132
H(9A)	-1588(11)	7327(23)	7902(20)	151
H(9B)	-1493(8)	6844(34)	8766(6)	151
H(9C)	-1830(6)	6041(15)	8049(24)	151
H(10A)	340(58)	5612(22)	6405(9)	194
H(10B)	-733(21)	5058(40)	7051(15)	194
H(10C)	864(40)	4494(22)	6817(23)	194

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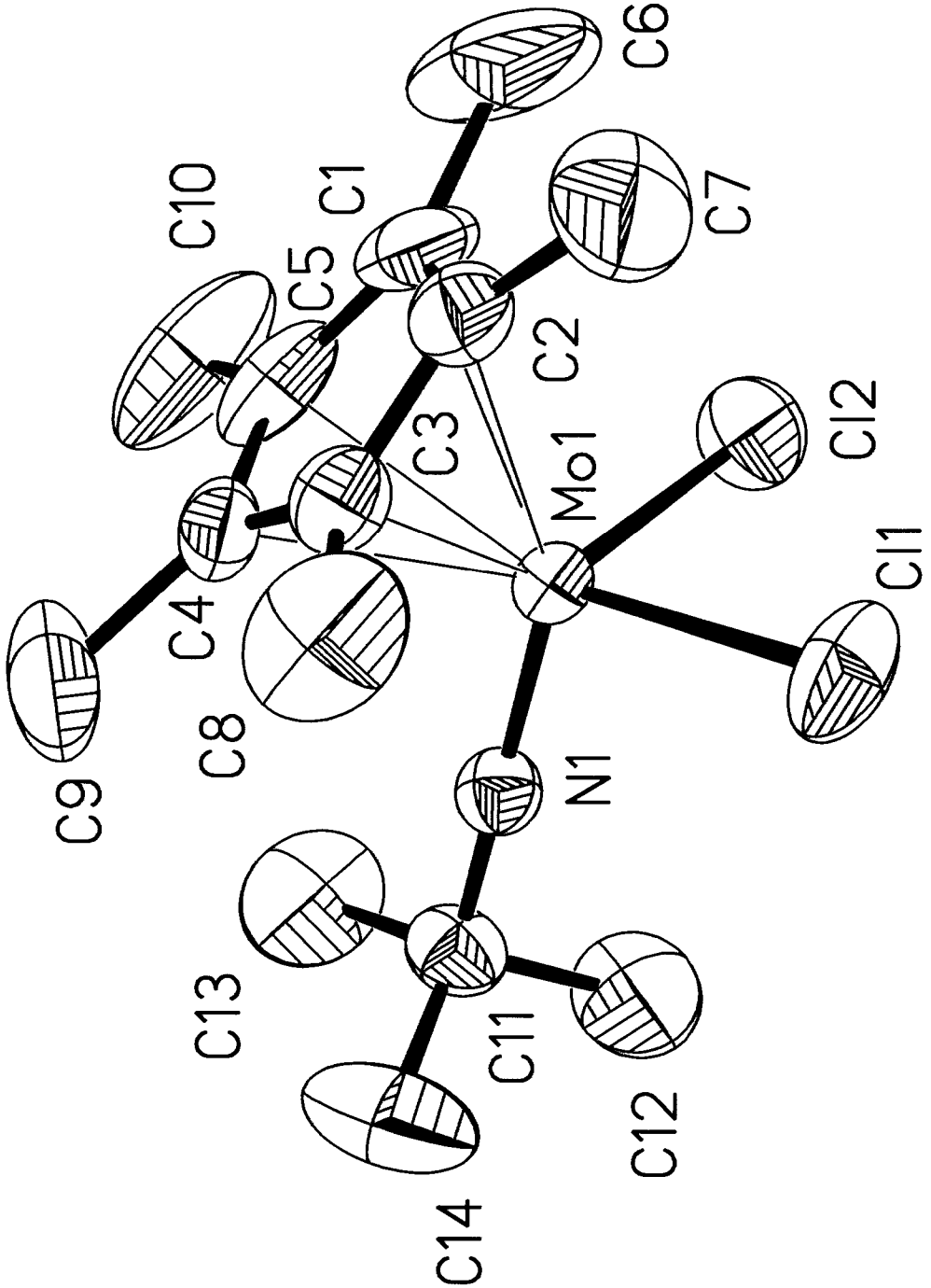

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Table 1. Crystal data and structure refinement for 3c.

Identification code	k6/koeler1
Empirical formula	$C_{16}H_{15}Cl_2F_5MoN$
Formula weight	483.13
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 10.4502(7) Å alpha = 90° b = 10.6897(11) Å beta = 94.342(8)° c = 15.915(2) Å gamma = 90°
Volume, Z	1772.7(3) $Å^3$, 4
Density (calculated)	1.810 Mg/m^3
Absorption coefficient	1.089 mm^{-1}
F(000)	956
Crystal size	0.25 x 0.25 x 0.25 mm
θ range for data collection	2.57 to 22.55°
Limiting indices	$-11 \le h \le 11$, $-10 \le k \le 11$, $-16 \le l \le 17$
Reflections collected	3067
Independent reflections	2341 (R_{int} = 0.0116)
Absorption correction	Psi-scans 36 ref,30 deg,285 accesible
Max. and min. transmission	0.934 and 0.872
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2339 / 0 / 231
Goodness-of-fit on F^2	1.052
Final R indices [I>2σ(I)]	R1 = 0.0194, wR2 = 0.0440
R indices (all data)	R1 = 0.0239, wR2 = 0.0753
Largest diff. peak and hole	.249 and -.230 $eÅ^{-3}$

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Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 3c. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2741(1)	2170(1)	724(1)	17(1)
Cl(1)	1422(1)	2844(1)	1766(1)	29(1)
Cl(2)	3801(1)	697(1)	1623(1)	27(1)
N(1)	1699(2)	1351(2)	11(1)	22(1)
C(1)	897(2)	1021(2)	-686(2)	19(1)
C(2)	1224(2)	115(2)	-1257(2)	22(1)
C(3)	436(2)	-161(3)	-1959(2)	23(1)
C(4)	-702(2)	462(3)	-2113(2)	23(1)
C(5)	-1061(2)	1349(3)	-1557(2)	22(1)
C(6)	-278(2)	1612(2)	-852(2)	23(1)
F(2)	2354(1)	-471(2)	-1139(1)	39(1)
F(3)	790(2)	-1011(2)	-2513(1)	38(1)
F(4)	-1442(2)	234(2)	-2816(1)	37(1)
F(5)	-2169(1)	1973(2)	-1706(1)	37(1)
F(6)	-639(2)	2485(2)	-315(1)	41(1)
C(11)	2942(2)	4127(2)	123(2)	22(1)
C(12)	3721(2)	4218(2)	906(2)	22(1)
C(13)	4725(2)	3359(3)	891(2)	22(1)
C(14)	4604(2)	2716(2)	97(2)	22(1)
C(15)	3529(2)	3232(2)	-385(2)	20(1)
C(21)	1799(3)	4922(3)	-118(2)	35(1)
C(22)	3508(3)	5129(3)	1594(2)	34(1)
C(23)	5778(3)	3161(3)	1573(2)	34(1)
C(24)	5526(3)	1773(3)	-192(2)	32(1)
C(25)	3137(3)	2931(3)	-1287(2)	31(1)

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Table 3. Bond lengths [Å] and angles [°] for 3c.

Mo(1)-N(1)	1.748(2)	Mo(1)-C(15)	2.303(2)
Mo(1)-C(11)	2.317(3)	Mo(1)-C(14)	2.329(2)
Mo(1)-Cl(2)	2.3480(7)	Mo(1)-Cl(1)	2.3482(7)
Mo(1)-C(12)	2.426(3)	Mo(1)-C(13)	2.430(3)
N(1)-C(1)	1.384(3)	C(1)-C(2)	1.389(4)
C(1)-C(6)	1.389(4)	C(2)-F(2)	1.338(3)
C(2)-C(3)	1.369(4)	C(3)-F(3)	1.338(3)
C(3)-C(4)	1.370(4)	C(4)-F(4)	1.332(3)
C(4)-C(5)	1.369(4)	C(5)-F(5)	1.342(3)
C(5)-C(6)	1.366(4)	C(6)-F(6)	1.339(3)
C(11)-C(15)	1.421(4)	C(11)-C(12)	1.439(4)
C(11)-C(21)	1.493(4)	C(12)-C(13)	1.396(4)
C(12)-C(22)	1.495(4)	C(13)-C(14)	1.436(4)
C(13)-C(23)	1.500(4)	C(14)-C(15)	1.423(4)
C(14)-C(24)	1.492(4)	C(15)-C(25)	1.498(4)

N(1)-Mo(1)-C(15)	89.44(9)	N(1)-Mo(1)-C(11)	104.80(10)
C(15)-Mo(1)-C(11)	35.82(9)	N(1)-Mo(1)-C(14)	110.31(9)
C(15)-Mo(1)-C(14)	35.78(9)	C(11)-Mo(1)-C(14)	59.43(9)
N(1)-Mo(1)-Cl(2)	107.57(7)	C(15)-Mo(1)-Cl(2)	128.20(7)
C(11)-Mo(1)-Cl(2)	143.51(7)	C(14)-Mo(1)-Cl(2)	93.35(7)
N(1)-Mo(1)-Cl(1)	104.03(7)	C(15)-Mo(1)-Cl(1)	130.75(7)
C(11)-Mo(1)-Cl(1)	95.22(7)	C(14)-Mo(1)-Cl(1)	141.27(7)
Cl(2)-Mo(1)-Cl(1)	92.90(3)	N(1)-Mo(1)-C(12)	140.02(9)
C(15)-Mo(1)-C(12)	58.26(9)	C(11)-Mo(1)-C(12)	35.23(9)
C(14)-Mo(1)-C(12)	57.68(9)	Cl(2)-Mo(1)-C(12)	110.95(7)
Cl(1)-Mo(1)-C(12)	84.48(6)	N(1)-Mo(1)-C(13)	144.86(9)
C(15)-Mo(1)-C(13)	58.27(9)	C(11)-Mo(1)-C(13)	57.94(9)
C(14)-Mo(1)-C(13)	35.05(9)	Cl(2)-Mo(1)-C(13)	85.71(7)
Cl(1)-Mo(1)-C(13)	107.68(6)	C(12)-Mo(1)-C(13)	33.42(9)
C(1)-N(1)-Mo(1)	163.3(2)	N(1)-C(1)-C(2)	122.5(2)
N(1)-C(1)-C(6)	120.7(2)	C(2)-C(1)-C(6)	116.7(2)
F(2)-C(2)-C(3)	118.9(2)	F(2)-C(2)-C(1)	119.5(2)
C(3)-C(2)-C(1)	121.5(2)	F(3)-C(3)-C(2)	120.4(2)
F(3)-C(3)-C(4)	119.5(2)	C(2)-C(3)-C(4)	120.1(2)
F(4)-C(4)-C(5)	120.0(2)	F(4)-C(4)-C(3)	120.1(2)
C(5)-C(4)-C(3)	119.8(2)	F(5)-C(5)-C(6)	119.9(2)
F(5)-C(5)-C(4)	120.3(2)	C(6)-C(5)-C(4)	119.8(2)
F(6)-C(6)-C(5)	119.2(2)	F(6)-C(6)-C(1)	118.8(2)
C(5)-C(6)-C(1)	121.9(2)	C(15)-C(11)-C(12)	107.4(2)
C(15)-C(11)-C(21)	127.5(2)	C(12)-C(11)-C(21)	125.0(2)
C(15)-C(11)-Mo(1)	71.56(14)	C(12)-C(11)-Mo(1)	76.5(2)
C(21)-C(11)-Mo(1)	121.6(2)	C(13)-C(12)-C(11)	108.5(2)
C(13)-C(12)-C(22)	126.5(2)	C(11)-C(12)-C(22)	125.0(2)
C(13)-C(12)-Mo(1)	73.4(2)	C(11)-C(12)-Mo(1)	68.25(14)
C(22)-C(12)-Mo(1)	126.2(2)	C(12)-C(13)-C(14)	108.3(2)
C(12)-C(13)-C(23)	126.3(2)	C(14)-C(13)-C(23)	125.4(2)
C(12)-C(13)-Mo(1)	73.13(14)	C(14)-C(13)-Mo(1)	68.63(14)
C(23)-C(13)-Mo(1)	125.3(2)	C(15)-C(14)-C(13)	107.6(2)
C(15)-C(14)-C(24)	126.7(2)	C(13)-C(14)-C(24)	125.4(2)
C(15)-C(14)-Mo(1)	71.13(14)	C(13)-C(14)-Mo(1)	76.32(14)
C(24)-C(14)-Mo(1)	122.9(2)	C(11)-C(15)-C(14)	108.1(2)
C(11)-C(15)-C(25)	126.2(2)	C(14)-C(15)-C(25)	125.5(2)
C(11)-C(15)-Mo(1)	72.62(14)	C(14)-C(15)-Mo(1)	73.09(14)
C(25)-C(15)-Mo(1)	122.8(2)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 3¢.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Mo(1)	18(1)	19(1)	12(1)	-1(1)	-2(1)	-1(1)
Cl(1)	30(1)	32(1)	25(1)	-2(1)	10(1)	0(1)
Cl(2)	36(1)	24(1)	20(1)	3(1)	-2(1)	6(1)
N(1)	25(1)	24(1)	18(1)	0(1)	-2(1)	-4(1)
C(1)	21(1)	20(1)	16(1)	1(1)	-1(1)	-3(1)
C(2)	17(1)	21(2)	28(2)	0(1)	0(1)	2(1)
C(3)	25(2)	24(2)	20(1)	-8(1)	8(1)	-6(1)
C(4)	21(2)	29(2)	17(1)	2(1)	-3(1)	-11(1)
C(5)	13(1)	23(2)	29(2)	4(1)	-3(1)	1(1)
C(6)	24(2)	19(2)	26(2)	-6(1)	3(1)	0(1)
F(2)	25(1)	40(1)	52(1)	-11(1)	-7(1)	14(1)
F(3)	35(1)	43(1)	38(1)	-24(1)	12(1)	-7(1)
F(4)	33(1)	55(1)	22(1)	-5(1)	-11(1)	-12(1)
F(5)	22(1)	33(1)	55(1)	2(1)	-9(1)	5(1)
F(6)	35(1)	38(1)	49(1)	-25(1)	2(1)	7(1)
C(11)	22(1)	20(1)	25(2)	6(1)	3(1)	1(1)
C(12)	23(1)	18(1)	24(2)	-3(1)	5(1)	-5(1)
C(13)	21(1)	23(2)	23(1)	0(1)	0(1)	-5(1)
C(14)	21(1)	23(2)	22(1)	2(1)	5(1)	-1(1)
C(15)	21(1)	23(2)	17(1)	5(1)	2(1)	-2(1)
C(21)	35(2)	31(2)	39(2)	12(1)	3(1)	12(1)
C(22)	37(2)	27(2)	39(2)	-12(1)	9(1)	-7(1)
C(23)	26(2)	40(2)	33(2)	-4(1)	-9(1)	-5(1)
C(24)	31(2)	32(2)	35(2)	-3(1)	7(1)	7(1)
C(25)	37(2)	38(2)	17(1)	6(1)	2(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 3c.

	x	y	z	U(eq)
H(21A)	2082(3)	5742(7)	-306(12)	53
H(21B)	1290(10)	5027(15)	370(4)	53
H(21C)	1273(10)	4517(9)	-577(8)	53
H(22A)	2589(3)	5313(14)	1596(8)	51
H(22B)	3978(15)	5903(7)	1500(7)	51
H(22C)	3816(17)	4767(8)	2138(2)	51
H(23A)	6512(7)	3693(13)	1466(7)	50
H(23B)	6043(12)	2282(5)	1579(8)	50
H(23C)	5466(6)	3380(17)	2120(2)	50
H(24A)	5679(14)	1127(10)	241(5)	48
H(24B)	6338(7)	2185(4)	-292(11)	48
H(24C)	5166(8)	1386(13)	-717(7)	48
H(25A)	3370(16)	2065(6)	-1406(3)	46
H(25B)	3577(14)	3497(11)	-1655(2)	46
H(25C)	2206(4)	3036(17)	-1391(3)	46

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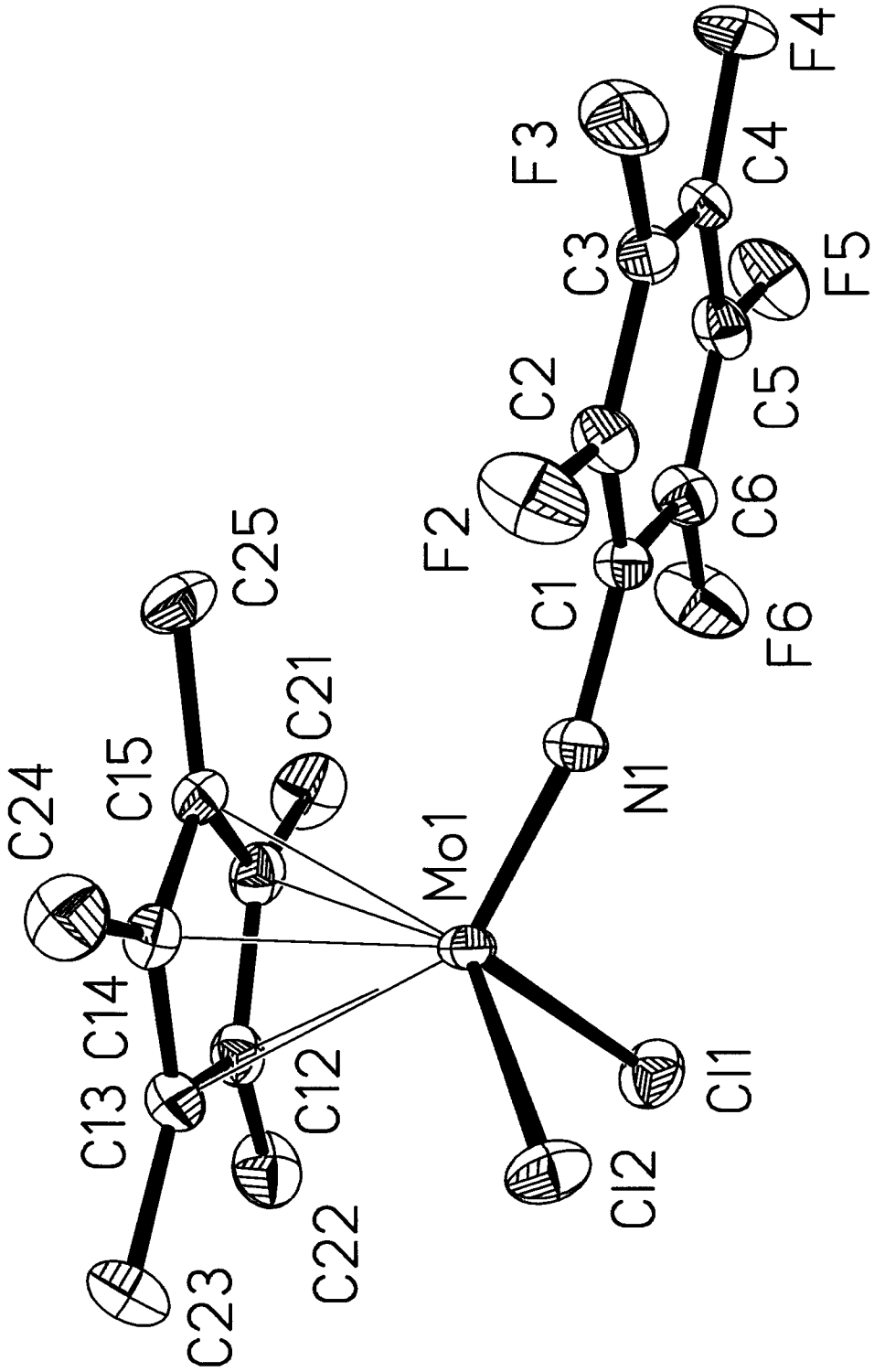

ORTEP 3c

 P-1777-m13

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Table 1. Crystal data and structure refinement for 3c.

Identification code	a
Empirical formula	$C_{14}H_{24}Cl_2NW$
Formula weight	461.09
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 15.171(3) Å alpha = 90° b = 7.615(2) Å beta = 90.29(3)° c = 14.758(3) Å gamma = 90°
Volume, Z	1704.9(7) $Å^3$, 4
Density (calculated)	1.796 Mg/m^3
Absorption coefficient	7.074 mm^{-1}
F(000)	892
Crystal size	0.7 x 0.5 x 0.2 mm
θ range for data collection	3.79 to 22.50°
Limiting indices	$-16 \le h \le 16$, $-8 \le k \le 8$, $-15 \le l \le 15$
Reflections collected	6587
Independent reflections	2210 (R_{int} = 0.1021)
Absorption correction	Semi-empirical with 184 psi-scans
Max. and min. transmission	0.270 and 0.096
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2210 / 0 / 172
Goodness-of-fit on F^2	1.050
Final R indices [I>2σ(I)]	R1 = 0.0522, wR2 = 0.1388
R indices (all data)	R1 = 0.0534, wR2 = 0.1395
Largest diff. peak and hole	2.528 and -2.783 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 3e. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1)	2752(1)	7783(1)	7964(1)	21(1)
Cl(1)	3561(2)	5680(4)	8777(2)	33(1)
Cl(2)	2607(2)	5844(4)	6714(2)	34(1)
N(1)	1743(9)	7689(12)	8481(9)	28(3)
C(1)	4174(7)	9372(15)	7895(8)	27(3)
C(2)	3536(7)	10149(18)	8514(8)	30(3)
C(3)	2820(7)	10788(16)	7955(7)	29(3)
C(4)	2950(7)	10242(16)	7045(7)	26(2)
C(5)	3810(7)	9401(15)	7004(7)	29(3)
C(6)	5060(8)	8642(17)	8170(9)	34(3)
C(7)	3696(9)	10544(17)	9480(8)	37(3)
C(8)	2073(10)	11928(18)	8279(12)	42(4)
C(9)	2407(9)	10662(18)	6221(9)	43(3)
C(10)	4254(8)	8729(20)	6161(8)	37(3)
C(11)	851(11)	7535(18)	8898(12)	33(4)
C(12)	918(9)	8292(21)	9845(9)	37(3)
C(13)	640(8)	5564(17)	8932(9)	36(3)
C(14)	174(8)	8540(21)	8306(9)	43(4)

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Table 3. Bond lengths [Å] and angles [°] for 3c.

W(1)-N(1)	1.716(12)	W(1)-C(3)	2.291(12)
W(1)-C(2)	2.304(13)	W(1)-C(4)	2.333(11)
W(1)-Cl(1)	2.345(3)	W(1)-Cl(2)	2.372(3)
W(1)-C(5)	2.475(12)	W(1)-C(1)	2.477(11)
N(1)-C(11)	1.49(2)	C(1)-C(5)	1.42(2)
C(1)-C(2)	1.46(2)	C(1)-C(6)	1.51(2)
C(2)-C(3)	1.44(2)	C(2)-C(7)	1.48(2)
C(3)-C(4)	1.42(2)	C(3)-C(8)	1.51(2)
C(4)-C(5)	1.46(2)	C(4)-C(9)	1.50(2)
C(5)-C(10)	1.51(2)	C(11)-C(12)	1.51(2)
C(11)-C(13)	1.54(2)	C(11)-C(14)	1.55(2)

N(1)-W(1)-C(3)	94.8(4)	N(1)-W(1)-C(2)	109.6(5)
C(3)-W(1)-C(2)	36.6(4)	N(1)-W(1)-C(4)	114.2(5)
C(3)-W(1)-C(4)	35.8(4)	C(2)-W(1)-C(4)	60.6(4)
N(1)-W(1)-Cl(1)	102.1(4)	C(3)-W(1)-Cl(1)	131.4(3)
C(2)-W(1)-Cl(1)	94.9(3)	C(4)-W(1)-Cl(1)	141.0(3)
N(1)-W(1)-Cl(2)	103.9(4)	C(3)-W(1)-Cl(2)	128.4(3)
C(2)-W(1)-Cl(2)	143.7(3)	C(4)-W(1)-Cl(2)	93.4(3)
Cl(1)-W(1)-Cl(2)	91.11(11)	N(1)-W(1)-C(5)	149.1(4)
C(3)-W(1)-C(5)	58.0(4)	C(2)-W(1)-C(5)	58.5(4)
C(4)-W(1)-C(5)	35.1(4)	Cl(1)-W(1)-C(5)	107.0(3)
Cl(2)-W(1)-C(5)	85.6(3)	N(1)-W(1)-C(1)	144.9(5)
C(3)-W(1)-C(1)	58.1(4)	C(2)-W(1)-C(1)	35.3(4)
C(4)-W(1)-C(1)	57.9(4)	Cl(1)-W(1)-C(1)	84.3(3)
Cl(2)-W(1)-C(1)	110.4(3)	C(5)-W(1)-C(1)	33.4(4)
C(11)-N(1)-W(1)	177.1(10)	C(5)-C(1)-C(2)	108.4(10)
C(5)-C(1)-C(6)	126.5(11)	C(2)-C(1)-C(6)	125.0(10)
C(5)-C(1)-W(1)	73.2(6)	C(2)-C(1)-W(1)	65.9(6)
C(6)-C(1)-W(1)	125.8(8)	C(3)-C(2)-C(1)	106.2(10)
C(3)-C(2)-C(7)	127.0(11)	C(1)-C(2)-C(7)	125.5(11)
C(3)-C(2)-W(1)	71.2(7)	C(1)-C(2)-W(1)	78.8(7)
C(7)-C(2)-W(1)	125.6(9)	C(4)-C(3)-C(2)	109.5(10)
C(4)-C(3)-C(8)	125.2(11)	C(2)-C(3)-C(8)	125.2(12)
C(4)-C(3)-W(1)	73.7(7)	C(2)-C(3)-W(1)	72.2(7)
C(8)-C(3)-W(1)	122.6(8)	C(3)-C(4)-C(5)	107.2(9)
C(3)-C(4)-C(9)	128.8(11)	C(5)-C(4)-C(9)	123.3(11)
C(3)-C(4)-W(1)	70.5(6)	C(5)-C(4)-W(1)	77.8(6)
C(9)-C(4)-W(1)	124.8(8)	C(1)-C(5)-C(4)	108.2(10)
C(1)-C(5)-C(10)	125.8(10)	C(4)-C(5)-C(10)	126.0(10)
C(1)-C(5)-W(1)	73.3(6)	C(4)-C(5)-W(1)	67.1(6)
C(10)-C(5)-W(1)	126.7(8)	N(1)-C(11)-C(12)	107.1(12)
N(1)-C(11)-C(13)	106.2(11)	C(12)-C(11)-C(13)	110.8(13)
N(1)-C(11)-C(14)	109.1(12)	C(12)-C(11)-C(14)	112.0(13)
C(13)-C(11)-C(14)	111.3(13)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 3c.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
W(1)	21(1)	19(1)	24(1)	-1(1)	1(1)	-2(1)
Cl(1)	30(1)	31(2)	37(2)	0(1)	-2(1)	0(1)
Cl(2)	37(2)	33(2)	33(1)	-5(1)	0(1)	-7(1)
N(1)	41(8)	16(5)	27(7)	-1(4)	30(6)	-4(4)
C(1)	27(6)	20(6)	33(6)	8(6)	-2(5)	-6(5)
C(2)	19(5)	30(7)	40(6)	-4(6)	8(5)	-5(6)
C(3)	28(6)	21(7)	38(6)	8(6)	5(6)	-6(5)
C(4)	27(5)	16(5)	34(6)	14(5)	-5(4)	-4(5)
C(5)	36(6)	25(6)	27(5)	-2(6)	-5(5)	-7(5)
C(6)	30(6)	29(7)	45(7)	5(6)	-1(5)	-1(6)
C(7)	49(8)	22(6)	40(6)	0(6)	3(5)	-11(6)
C(8)	38(8)	22(6)	65(10)	-1(7)	-1(7)	-3(6)
C(9)	50(8)	29(7)	49(7)	8(7)	-12(6)	-8(6)
C(10)	41(7)	44(8)	26(6)	-3(7)	8(5)	-20(7)
C(11)	39(9)	25(6)	35(9)	3(6)	5(7)	-4(6)
C(12)	31(7)	38(6)	42(7)	-4(8)	-5(6)	-3(7)
C(13)	31(6)	34(7)	44(7)	-4(7)	12(5)	-10(6)
C(14)	23(7)	50(9)	56(8)	13(8)	-2(5)	11(7)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 3e.

	x	y	z	U(eq)
H(6A)	5023(18)	8151(113)	8782(27)	52
H(6B)	5501(15)	9583(32)	8161(63)	52
H(6C)	5233(30)	7716(90)	7745(39)	52
H(7A)	3924(58)	11742(46)	9540(10)	55
H(7B)	4128(47)	9712(78)	9726(18)	55
H(7C)	3142(15)	10439(119)	9815(14)	55
H(8A)	1547(22)	11703(100)	7909(44)	62
H(8B)	2240(28)	13167(18)	8225(68)	62
H(8C)	1946(45)	11656(95)	8915(22)	62
H(9A)	2506(55)	9764(81)	5756(29)	64
H(9B)	2579(51)	11814(67)	5984(44)	64
H(9C)	1782(10)	10681(140)	6383(18)	64
H(10A)	4593(53)	9680(40)	5882(37)	56
H(10B)	3806(9)	8309(121)	5732(29)	56
H(10C)	4651(50)	7761(89)	6321(13)	56
H(12A)	348(20)	8176(118)	10149(25)	55
H(12B)	1079(63)	9536(39)	9809(10)	55
H(12C)	1369(47)	7654(87)	10190(23)	55
H(13A)	41(20)	5396(18)	9163(51)	55
H(13B)	1062(33)	4973(24)	9334(43)	55
H(13C)	682(52)	5066(27)	8322(12)	55
H(14A)	-424(8)	8283(108)	8517(46)	65
H(14B)	232(47)	8169(99)	7673(15)	65
H(14C)	285(43)	9805(22)	8352(54)	65

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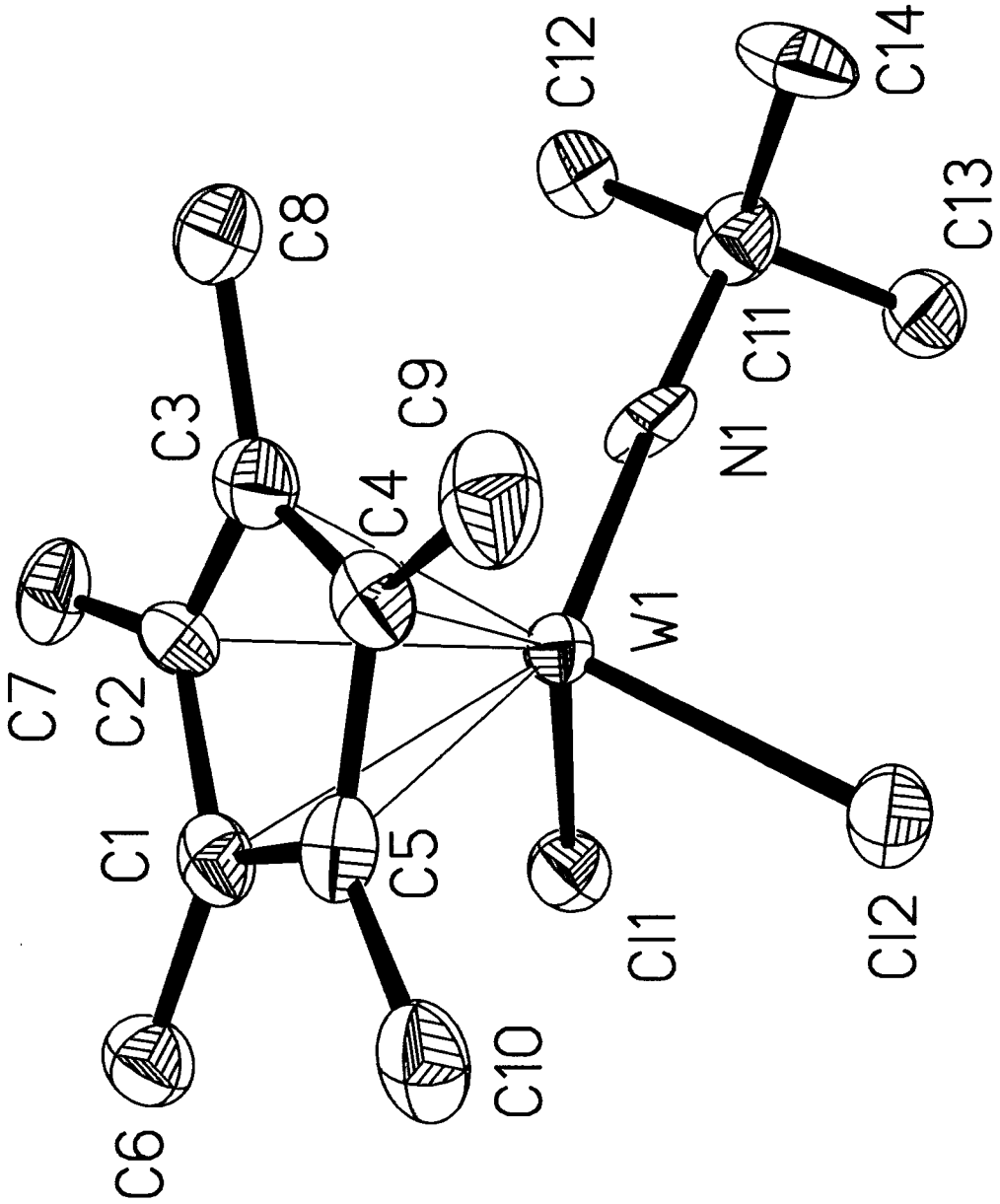

ORTEP 3e

P-1773-m19

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Table 1. Crystal data and structure refinement for 4.

Identification code	k
Empirical formula	$C_{16}H_{15}Cl_3F_5NW$
Formula weight	606.49
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 7.3843(10) Å alpha = 77.38(2)°
	b = 11.529(2) Å beta = 80.15(2)°
	c = 11.558(2) Å gamma = 79.88(2)°
Volume, Z	936.2(3) $Å^3$, 2
Density (calculated)	2.151 Mg/m^3
Absorption coefficient	6.645 mm^{-1}
F(000)	576
Crystal size	0.70 x 0.25 x 0.25 mm
θ range for data collection	2.82 to 25.01°
Limiting indices	$-7 \le h \le 3$, $-12 \le k \le 13$, $-13 \le l \le 12$
Reflections collected	4718
Independent reflections	2548 (R_{int} = 0.0468)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9922 and 0.7167
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2548 / 0 / 240
Goodness-of-fit on F^2	1.063
Final R indices [I>2σ(I)]	R1 = 0.0206, wR2 = 0.0542
R indices (all data)	R1 = 0.0211, wR2 = 0.0548
Largest diff. peak and hole	.717 and -.814 $eÅ^{-3}$

P-1777-M20

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

	x	y	z	U(eq)
W(1)	972(1)	7908(1)	3049(1)	19(1)
Cl(1)	-543(2)	9903(1)	3227(1)	33(1)
Cl(2)	587(2)	5838(1)	3261(1)	32(1)
Cl(3)	-1369(2)	8123(1)	1779(1)	29(1)
N(1)	754(5)	7590(3)	4617(3)	25(1)
C(1)	283(6)	7267(4)	5825(4)	22(1)
C(2)	1587(6)	6877(4)	6631(4)	25(1)
C(3)	1061(7)	6515(4)	7833(4)	27(1)
C(4)	-791(7)	6546(4)	8291(4)	28(1)
C(5)	-2126(6)	6949(4)	7527(4)	26(1)
C(6)	-1592(6)	7288(4)	6325(4)	24(1)
F(2)	3405(4)	6840(3)	6228(2)	37(1)
F(3)	2350(4)	6114(3)	8585(2)	40(1)
F(4)	-1325(4)	6208(3)	9470(2)	42(1)
F(5)	-3939(4)	6986(3)	7975(2)	37(1)
F(6)	-2893(4)	7648(3)	5594(2)	35(1)
C(11)	3132(6)	9190(4)	1649(4)	23(1)
C(12)	3806(6)	8587(4)	2754(4)	24(1)
C(13)	4160(6)	7319(4)	2733(4)	24(1)
C(14)	3639(6)	7175(4)	1652(4)	22(1)
C(15)	2975(6)	8311(4)	985(4)	21(1)
C(21)	2785(7)	10509(4)	1213(5)	31(1)
C(22)	4298(7)	9201(5)	3652(5)	31(1)
C(23)	5135(6)	6332(4)	3596(4)	29(1)
C(24)	3921(8)	6023(5)	1193(5)	35(1)
C(25)	2355(7)	8536(5)	-219(4)	29(1)

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Table 3. Bond lengths [Å] and angles [°] for 4.

W(1)-N(1)	1.754(4)	W(1)-C(12)	2.308(4)
W(1)-C(13)	2.321(4)	W(1)-Cl(3)	2.4004(12)
W(1)-Cl(2)	2.4067(13)	W(1)-Cl(1)	2.4101(13)
W(1)-C(14)	2.474(4)	W(1)-C(11)	2.500(4)
W(1)-C(15)	2.578(4)	N(1)-C(1)	1.364(6)
C(1)-C(2)	1.404(7)	C(1)-C(6)	1.404(7)
C(2)-F(2)	1.340(5)	C(2)-C(3)	1.368(7)
C(3)-F(3)	1.353(5)	C(3)-C(4)	1.376(7)
C(4)-F(4)	1.342(5)	C(4)-C(5)	1.388(7)
C(5)-F(5)	1.347(5)	C(5)-C(6)	1.366(7)
C(6)-F(6)	1.339(5)	C(11)-C(15)	1.428(7)
C(11)-C(12)	1.439(7)	C(11)-C(21)	1.484(7)
C(12)-C(13)	1.444(7)	C(12)-C(22)	1.500(7)
C(13)-C(14)	1.419(7)	C(13)-C(23)	1.506(7)
C(14)-C(15)	1.418(6)	C(14)-C(24)	1.505(7)
C(15)-C(25)	1.495(6)		

N(1)-W(1)-C(12)	95.7(2)	N(1)-W(1)-C(13)	96.0(2)
C(12)-W(1)-C(13)	36.4(2)	N(1)-W(1)-Cl(3)	129.00(12)
C(12)-W(1)-Cl(3)	132.80(12)	C(13)-W(1)-Cl(3)	131.30(12)
N(1)-W(1)-Cl(2)	84.73(13)	C(12)-W(1)-Cl(2)	124.43(12)
C(13)-W(1)-Cl(2)	88.17(12)	Cl(3)-W(1)-Cl(2)	79.73(4)
N(1)-W(1)-Cl(1)	86.49(13)	C(12)-W(1)-Cl(1)	89.11(12)
C(13)-W(1)-Cl(1)	125.46(12)	Cl(3)-W(1)-Cl(1)	80.55(5)
Cl(2)-W(1)-Cl(1)	145.97(4)	N(1)-W(1)-C(14)	126.6(2)
C(12)-W(1)-C(14)	57.5(2)	C(13)-W(1)-C(14)	34.2(2)
Cl(3)-W(1)-C(14)	97.11(12)	Cl(2)-W(1)-C(14)	78.04(11)
Cl(1)-W(1)-C(14)	131.94(11)	N(1)-W(1)-C(11)	126.7(2)
C(12)-W(1)-C(11)	34.5(2)	C(13)-W(1)-C(11)	57.3(2)
Cl(3)-W(1)-C(11)	98.41(11)	Cl(2)-W(1)-C(11)	132.32(11)
Cl(1)-W(1)-C(11)	77.95(11)	C(14)-W(1)-C(11)	54.7(2)
N(1)-W(1)-C(15)	150.7(2)	C(12)-W(1)-C(15)	56.7(2)
C(13)-W(1)-C(15)	56.3(2)	Cl(3)-W(1)-C(15)	80.33(10)
Cl(2)-W(1)-C(15)	102.19(11)	Cl(1)-W(1)-C(15)	101.49(11)
C(14)-W(1)-C(15)	32.53(14)	C(11)-W(1)-C(15)	32.6(2)
C(1)-N(1)-W(1)	169.2(3)	N(1)-C(1)-C(2)	123.6(4)
N(1)-C(1)-C(6)	120.2(4)	C(2)-C(1)-C(6)	116.2(4)
F(2)-C(2)-C(3)	118.3(4)	F(2)-C(2)-C(1)	119.9(4)
C(3)-C(2)-C(1)	121.8(4)	F(3)-C(3)-C(2)	120.6(4)
F(3)-C(3)-C(4)	119.1(4)	C(2)-C(3)-C(4)	120.4(4)
F(4)-C(4)-C(3)	120.9(4)	F(4)-C(4)-C(5)	119.5(4)
C(3)-C(4)-C(5)	119.6(4)	F(5)-C(5)-C(6)	120.5(4)
F(5)-C(5)-C(4)	119.6(4)	C(6)-C(5)-C(4)	119.8(4)
F(6)-C(6)-C(5)	119.2(4)	F(6)-C(6)-C(1)	118.6(4)
C(5)-C(6)-C(1)	122.2(4)	C(15)-C(11)-C(12)	108.9(4)
C(15)-C(11)-C(21)	124.8(4)	C(12)-C(11)-C(21)	126.2(4)
C(15)-C(11)-W(1)	76.7(2)	C(12)-C(11)-W(1)	65.4(2)
C(21)-C(11)-W(1)	127.3(3)	C(11)-C(12)-C(13)	106.9(4)
C(11)-C(12)-C(22)	125.0(4)	C(13)-C(12)-C(22)	127.4(4)
C(11)-C(12)-W(1)	80.1(3)	C(13)-C(12)-W(1)	72.3(3)
C(22)-C(12)-W(1)	120.3(3)	C(14)-C(13)-C(12)	107.3(4)
C(14)-C(13)-C(23)	124.9(4)	C(12)-C(13)-C(23)	127.3(4)
C(14)-C(13)-W(1)	78.8(3)	C(12)-C(13)-W(1)	71.3(2)
C(23)-C(13)-W(1)	121.9(3)	C(15)-C(14)-C(13)	109.9(4)
C(15)-C(14)-C(24)	123.6(4)	C(13)-C(14)-C(24)	126.2(4)
C(15)-C(14)-W(1)	77.7(3)	C(13)-C(14)-W(1)	67.0(2)
C(24)-C(14)-W(1)	126.8(3)	C(14)-C(15)-C(11)	106.9(4)
C(14)-C(15)-C(25)	126.0(4)	C(11)-C(15)-C(25)	127.1(4)
C(14)-C(15)-W(1)	69.7(2)	C(11)-C(15)-W(1)	70.7(2)

C(25)-C(15)-W(1)	127.6(3)

Symmetry transformations used to generate equivalent atoms:

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

	U11	U22	U33	U23	U13	U12
W(1)	11(1)	24(1)	22(1)	-3(1)	-4(1)	0(1)
Cl(1)	21(1)	30(1)	45(1)	-12(1)	-2(1)	4(1)
Cl(2)	27(1)	25(1)	43(1)	-2(1)	-5(1)	-5(1)
Cl(3)	18(1)	41(1)	28(1)	-2(1)	-9(1)	-5(1)
N(1)	13(2)	28(2)	33(2)	-8(2)	-3(2)	-1(2)
C(1)	20(3)	24(3)	21(2)	-4(2)	-7(2)	-1(2)
C(2)	17(3)	29(3)	29(3)	-8(2)	-2(2)	1(2)
C(3)	27(3)	28(3)	26(3)	-3(2)	-13(2)	2(2)
C(4)	33(3)	26(3)	23(2)	-3(2)	-3(2)	-4(2)
C(5)	13(3)	30(3)	34(3)	-12(2)	2(2)	-1(2)
C(6)	14(3)	27(3)	30(3)	-5(2)	-7(2)	2(2)
F(2)	14(2)	59(2)	34(2)	-6(1)	-6(1)	-1(1)
F(3)	32(2)	54(2)	31(2)	-1(1)	-16(1)	2(1)
F(4)	42(2)	56(2)	24(2)	-4(1)	0(1)	-7(2)
F(5)	24(2)	49(2)	35(2)	-10(1)	5(1)	-8(1)
F(6)	16(2)	53(2)	35(2)	-5(1)	-10(1)	-1(1)
C(11)	10(2)	25(3)	28(2)	1(2)	0(2)	-3(2)
C(12)	8(2)	33(3)	31(3)	-5(2)	-3(2)	0(2)
C(13)	11(2)	27(3)	31(3)	-5(2)	-2(2)	4(2)
C(14)	11(2)	25(3)	26(2)	2(2)	3(2)	-5(2)
C(15)	13(2)	25(3)	24(2)	-4(2)	-1(2)	-2(2)
C(21)	21(3)	31(3)	40(3)	-2(2)	-9(2)	-4(2)
C(22)	19(3)	37(3)	39(3)	-10(2)	-7(2)	-3(2)
C(23)	15(2)	29(3)	38(3)	0(2)	-3(2)	3(2)
C(24)	33(3)	31(3)	35(3)	-6(2)	4(2)	1(2)
C(25)	22(3)	36(3)	28(3)	-4(2)	-3(2)	-2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 4.

	x	y	z	U(eq)
H(21A)	3792(24)	10752(6)	583(21)	46
H(21B)	2734(45)	10920(4)	1878(8)	46
H(21C)	1602(23)	10724(6)	890(27)	46
H(22A)	5510(22)	9472(27)	3364(14)	47
H(22B)	4352(45)	8638(10)	4418(9)	47
H(22C)	3352(25)	9895(18)	3759(22)	47
H(23A)	5185(40)	6623(10)	4324(12)	44
H(23B)	6401(16)	6089(20)	3223(11)	44
H(23C)	4455(26)	5641(12)	3801(23)	44
H(24A)	5014(29)	6006(15)	579(23)	52
H(24B)	2822(21)	5973(15)	846(28)	52
H(24C)	4109(48)	5339(5)	1855(8)	52
H(25A)	1884(43)	9390(7)	-455(13)	44
H(25B)	1367(32)	8057(23)	-185(8)	44
H(25C)	3407(13)	8308(28)	-807(7)	44

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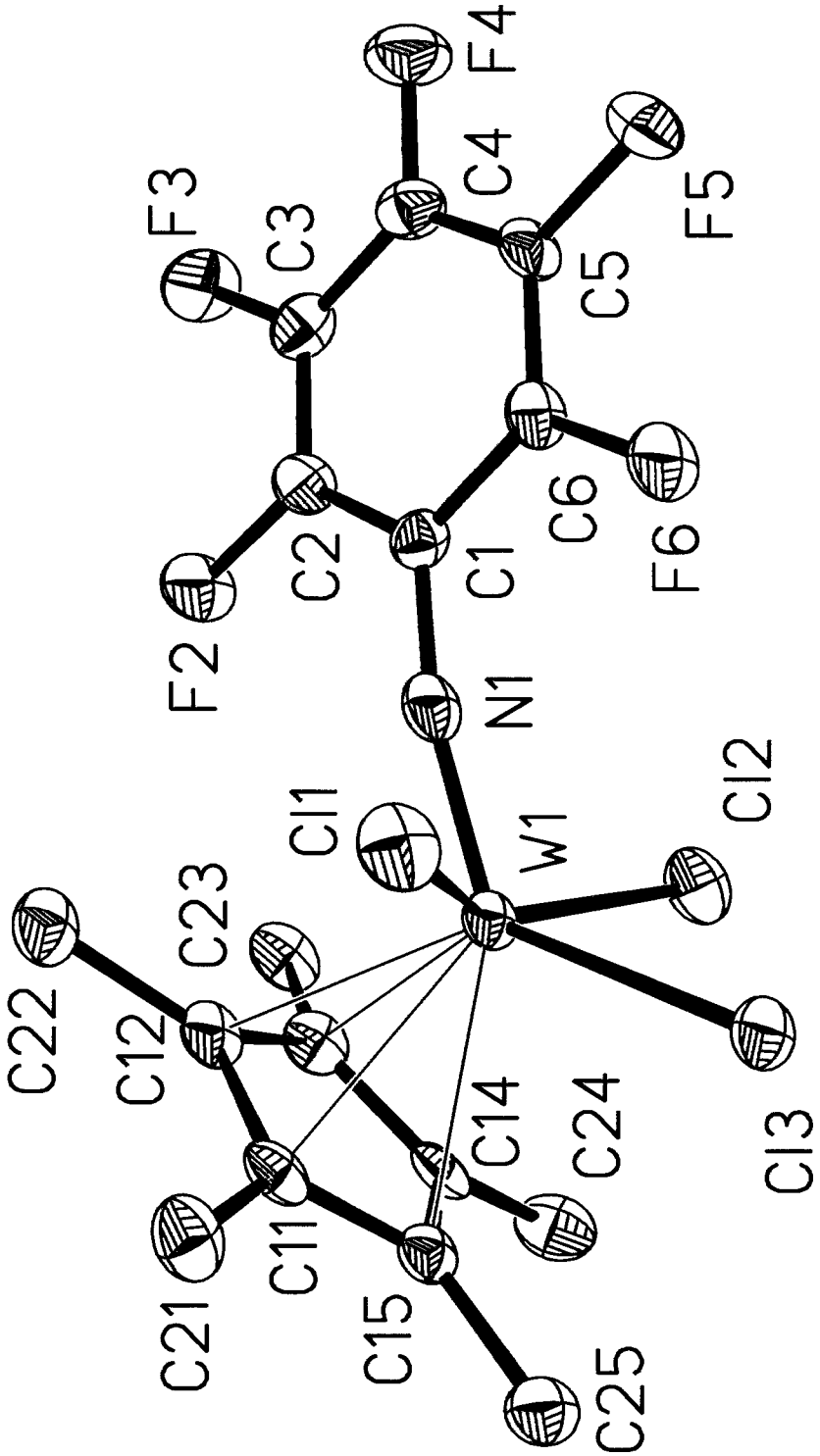

ORTEP 4

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Table 1. Crystal data and structure refinement for 5.

Identification code	hallo2
Empirical formula	$C_{16}H_{17}F_5NO_{2.50}W$
Formula weight	542.16
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 13.246(3) Å alpha = 90° b = 10.043(2) Å beta = 104.37(3)° c = 14.102(3) Å gamma = 90°
Volume, Z	1817.3(6) $Å^3$, 4
Density (calculated)	1.982 Mg/m^3
Absorption coefficient	6.417 mm^{-1}
F(000)	1036
Crystal size	0.40 x 0.30 x 0.30 mm
θ range for data collection	4.06 to 22.48°
Limiting indices	$-14 \le h \le 14$, $-10 \le k \le 10$, $-15 \le l \le 15$
Reflections collected	3977
Independent reflections	2349 (R_{int} = 0.0326)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9690 and 0.4015
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2345 / 218 / 237
Goodness-of-fit on F^2	1.055
Final R indices [I>2σ(I)]	R1 = 0.0295, wR2 = 0.0735
R indices (all data)	R1 = 0.0316, wR2 = 0.0765
Largest diff. peak and hole	1.037 and -1.227 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 5. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1)	-1318(1)	-336(1)	4159(1)	29(1)
O(1)	0	0	5000	39(1)
O(2)	-1901(3)	1204(4)	3952(3)	49(1)
O(3)	-1069(4)	-756(5)	3055(3)	51(1)
C(1)	-2671(5)	-891(6)	4947(5)	41(1)
C(2)	-2805(5)	-1607(7)	4052(5)	46(1)
C(3)	-1979(5)	-2571(6)	4171(4)	39(1)
C(4)	-1333(4)	-2388(5)	5116(4)	31(1)
C(5)	-1765(4)	-1353(6)	5591(4)	33(1)
C(11)	-3388(6)	179(8)	5149(8)	70(2)
C(12)	-3701(6)	-1488(9)	3149(6)	77(3)
C(13)	-1819(7)	-3568(7)	3436(5)	69(2)
C(14)	-343(5)	-3138(6)	5558(5)	44(2)
C(15)	-1300(5)	-849(7)	6611(4)	48(2)
N(1)	-1809(5)	-1469(6)	966(4)	59(2)
C(22)	-1825(7)	-594(7)	223(6)	56(2)
C(23)	-1084(7)	470(7)	332(7)	62(2)
F(1)	-395(4)	582(4)	1175(4)	78(1)
C(24)	-1107(9)	1340(8)	-426(8)	81(2)
F(2)	-377(5)	2304(5)	-285(5)	115(2)
C(25)	-1824(10)	1224(10)	-1296(8)	88(2)
F(3)	-1846(7)	2065(6)	-2051(5)	142(3)
C(26)	-2560(9)	237(10)	-1418(7)	82(2)
F(4)	-3299(6)	113(7)	-2256(4)	117(2)
C(27)	-2544(7)	-674(9)	-684(6)	65(2)
F(5)	-3287(4)	-1645(6)	-812(3)	81(1)

Table 3. Bond lengths [Å] and angles [°] for 5.

W(1)-O(2)	1.722(4)	W(1)-O(3)	1.721(5)
W(1)-O(1)	1.8817(7)	W(1)-C(2)	2.320(6)
W(1)-C(1)	2.397(6)	W(1)-C(3)	2.411(6)
W(1)-C(5)	2.463(6)	W(1)-C(4)	2.466(5)
O(1)-W(1)#1	1.8817(7)	C(1)-C(5)	1.392(8)
C(1)-C(2)	1.426(10)	C(1)-C(11)	1.508(10)
C(2)-C(3)	1.438(9)	C(2)-C(12)	1.515(8)
C(3)-C(4)	1.406(8)	C(3)-C(13)	1.493(9)
C(4)-C(5)	1.431(8)	C(4)-C(14)	1.507(8)
C(5)-C(15)	1.505(8)	N(1)-C(22)	1.363(9)
C(22)-C(27)	1.394(12)	C(22)-C(23)	1.433(11)
C(23)-F(1)	1.312(10)	C(23)-C(24)	1.376(12)
C(24)-F(2)	1.347(11)	C(24)-C(25)	1.36(2)
C(25)-F(3)	1.354(10)	C(25)-C(26)	1.37(2)
C(26)-F(4)	1.340(12)	C(26)-C(27)	1.378(13)
C(27)-F(5)	1.366(10)		

O(2)-W(1)-O(3)	104.2(2)	O(2)-W(1)-O(1)	104.62(14)
O(3)-W(1)-O(1)	105.0(2)	O(2)-W(1)-C(2)	98.3(2)
O(3)-W(1)-C(2)	99.0(2)	O(1)-W(1)-C(2)	141.2(2)
O(2)-W(1)-C(1)	86.1(2)	O(3)-W(1)-C(1)	134.1(2)
O(1)-W(1)-C(1)	115.6(2)	C(2)-W(1)-C(1)	35.1(2)
O(2)-W(1)-C(3)	133.5(2)	O(3)-W(1)-C(3)	86.0(2)
O(1)-W(1)-C(3)	116.40(14)	C(2)-W(1)-C(3)	35.3(2)
C(1)-W(1)-C(3)	57.7(2)	O(2)-W(1)-C(5)	108.8(2)
O(3)-W(1)-C(5)	141.2(2)	O(1)-W(1)-C(5)	86.06(13)
C(2)-W(1)-C(5)	56.8(2)	C(1)-W(1)-C(5)	33.3(2)
C(3)-W(1)-C(5)	56.4(2)	O(2)-W(1)-C(4)	141.2(2)
O(3)-W(1)-C(4)	108.6(2)	O(1)-W(1)-C(4)	86.40(12)
C(2)-W(1)-C(4)	56.9(2)	C(1)-W(1)-C(4)	56.2(2)
C(3)-W(1)-C(4)	33.5(2)	C(5)-W(1)-C(4)	33.8(2)
W(1)-O(1)-W(1)#1	180.0	C(5)-C(1)-C(2)	107.9(6)
C(5)-C(1)-C(11)	126.6(7)	C(2)-C(1)-C(11)	125.5(6)
C(5)-C(1)-W(1)	76.0(3)	C(2)-C(1)-W(1)	69.5(3)
C(11)-C(1)-W(1)	120.1(5)	C(1)-C(2)-C(3)	108.2(5)
C(1)-C(2)-C(12)	127.1(7)	C(3)-C(2)-C(12)	124.5(7)
C(1)-C(2)-W(1)	75.4(3)	C(3)-C(2)-W(1)	75.8(3)
C(12)-C(2)-W(1)	119.2(4)	C(4)-C(3)-C(2)	106.8(5)
C(4)-C(3)-C(13)	125.9(6)	C(2)-C(3)-C(13)	127.2(6)
C(4)-C(3)-W(1)	75.4(3)	C(2)-C(3)-W(1)	68.9(3)
C(13)-C(3)-W(1)	120.3(4)	C(3)-C(4)-C(5)	108.6(5)
C(3)-C(4)-C(14)	126.2(5)	C(5)-C(4)-C(14)	125.3(5)
C(3)-C(4)-W(1)	71.1(3)	C(5)-C(4)-W(1)	73.0(3)
C(14)-C(4)-W(1)	121.3(4)	C(1)-C(5)-C(4)	108.5(5)
C(1)-C(5)-C(15)	126.4(6)	C(4)-C(5)-C(15)	125.2(5)
C(1)-C(5)-W(1)	70.8(3)	C(4)-C(5)-W(1)	73.2(3)
C(15)-C(5)-W(1)	121.3(4)	N(1)-C(22)-C(27)	123.0(8)
N(1)-C(22)-C(23)	121.2(8)	C(27)-C(22)-C(23)	115.7(8)
F(1)-C(23)-C(24)	121.7(9)	F(1)-C(23)-C(22)	117.7(7)
C(24)-C(23)-C(22)	120.6(9)	F(2)-C(24)-C(25)	120.8(9)
F(2)-C(24)-C(23)	117.7(10)	C(25)-C(24)-C(23)	121.5(10)
F(3)-C(25)-C(24)	122.1(11)	F(3)-C(25)-C(26)	118.4(11)
C(24)-C(25)-C(26)	119.5(8)	F(4)-C(26)-C(25)	121.3(10)
F(4)-C(26)-C(27)	118.2(11)	C(25)-C(26)-C(27)	120.5(10)
F(5)-C(27)-C(26)	119.9(9)	F(5)-C(27)-C(22)	117.9(7)
C(26)-C(27)-C(22)	122.1(10)		

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

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Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 5.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
W(1)	25(1)	34(1)	23(1)	4(1)	0(1)	-6(1)
O(1)	29(3)	44(3)	36(3)	9(3)	-7(3)	-11(3)
O(2)	33(2)	49(2)	60(3)	22(2)	2(2)	1(2)
O(3)	56(3)	64(3)	34(2)	-9(2)	13(2)	-27(2)
C(1)	35(3)	42(3)	50(3)	11(3)	18(3)	-3(3)
C(2)	33(3)	58(4)	40(3)	18(3)	-5(2)	-22(3)
C(3)	47(3)	41(3)	26(3)	-2(2)	6(2)	-25(3)
C(4)	33(3)	31(3)	28(3)	1(2)	9(2)	-5(2)
C(5)	31(3)	38(3)	29(3)	5(2)	9(2)	-7(2)
C(11)	44(4)	66(5)	109(8)	30(4)	36(5)	16(4)
C(12)	50(4)	101(6)	61(5)	39(5)	-24(4)	-40(4)
C(13)	109(6)	54(4)	46(4)	-22(3)	24(4)	-38(4)
C(14)	45(3)	35(3)	53(4)	8(3)	13(3)	2(3)
C(15)	55(4)	60(4)	32(3)	-10(3)	16(3)	-20(4)
N(1)	87(5)	55(3)	40(3)	-2(3)	24(3)	-2(3)
C(22)	80(5)	51(4)	48(4)	-2(3)	35(3)	16(3)
C(23)	85(5)	52(4)	66(5)	-3(3)	51(4)	12(3)
F(1)	89(4)	65(3)	91(4)	-21(3)	43(3)	-18(3)
C(24)	114(7)	55(5)	105(5)	13(4)	84(5)	20(4)
F(2)	141(4)	62(3)	184(6)	18(3)	121(4)	8(3)
C(25)	132(7)	76(5)	86(5)	34(4)	84(4)	60(4)
F(3)	226(7)	113(4)	133(5)	74(4)	134(5)	94(5)
C(26)	115(7)	95(6)	49(5)	11(4)	43(4)	51(4)
F(4)	141(5)	164(5)	53(3)	25(3)	37(3)	83(4)
C(27)	82(5)	67(4)	53(4)	-1(4)	33(4)	24(4)
F(5)	91(3)	100(3)	50(3)	-5(3)	15(2)	20(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 5.

	x	y	z	U(eq)
H(11A)	-3985(26)	-235(8)	5328(47)	105
H(11B)	-3636(39)	725(40)	4561(16)	105
H(11C)	-3011(16)	742(39)	5689(31)	105
H(12A)	-3990(33)	-585(23)	3111(26)	116
H(12B)	-4244(24)	-2133(47)	3189(24)	116
H(12C)	-3450(13)	-1668(64)	2564(7)	116
H(13A)	-2362(28)	-3459(40)	2827(16)	103
H(13B)	-1856(47)	-4468(7)	3693(19)	103
H(13C)	-1133(20)	-3430(39)	3307(33)	103
H(14A)	-27(18)	-3440(37)	5037(6)	66
H(14B)	-502(7)	-3911(25)	5920(26)	66
H(14C)	145(14)	-2552(14)	6006(24)	66
H(15A)	-539(6)	-836(45)	6735(13)	72
H(15B)	-1505(30)	-1437(27)	7086(5)	72
H(15C)	-1554(29)	55(19)	6677(11)	72

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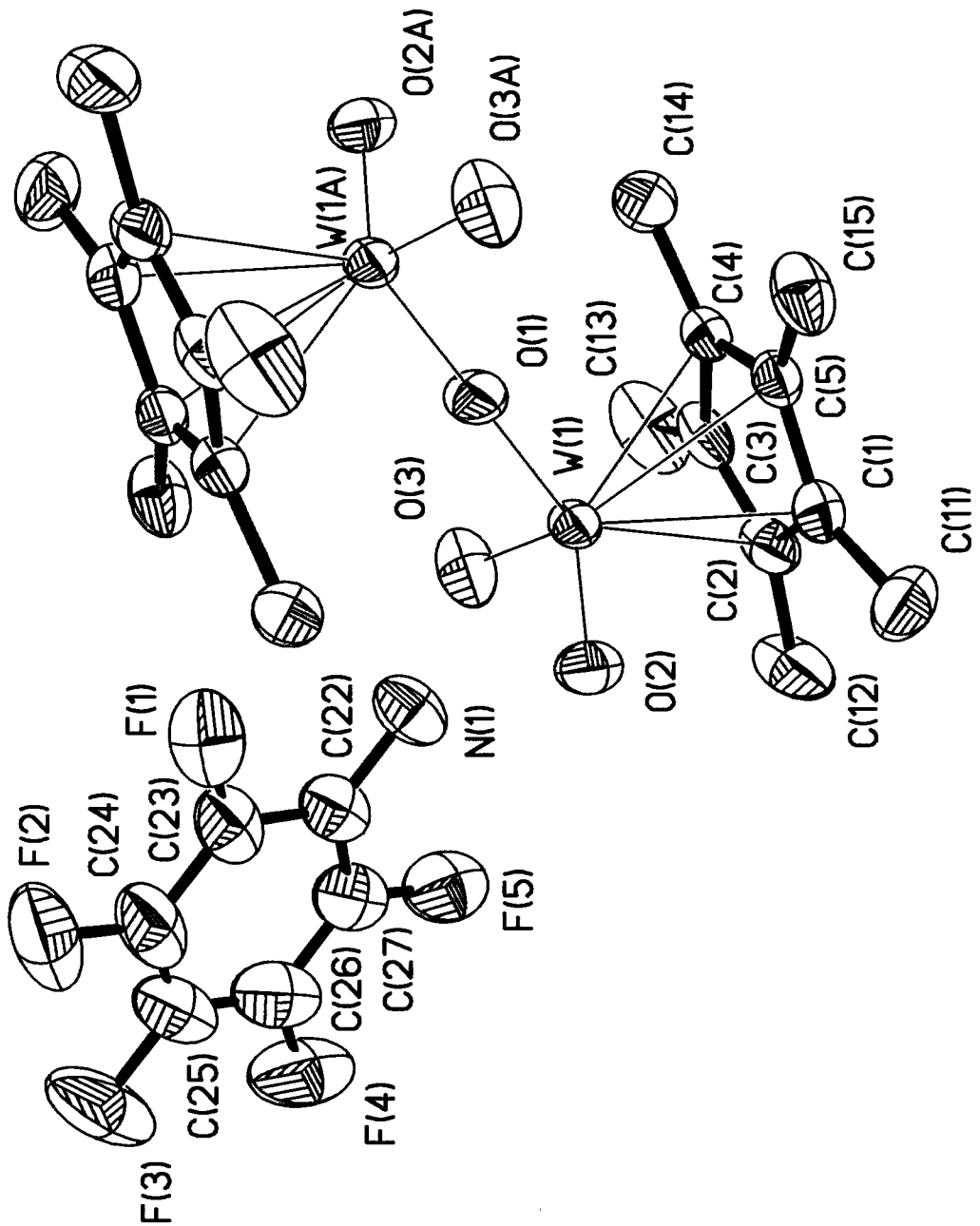

ORTEP for 5