

Chemoselective stepwise demetallation of unusually stable Fischer biscarbene complexes by domino [4+2]/[2+2] cycloaddition of 2-isopropenyl-2-oxazoline to 1-alkynyl Fischer carbene complexes of chromium and tungsten

Jinzhu Chen, Zhengkun Yu*, Zhaoyan Zheng, Kaichun Gu, Sizhong Wu, Fanlong Zeng,

Weiqiang Tan, Xiaowei Wu, Wenjing Xiao*

Experimental Section (Supporting Information)

Contents:

- 1) Crystallographic data for **3a**, **5b**, **6b**, and **7** 2

1. X-Ray Crystal Structure Information for 3a.

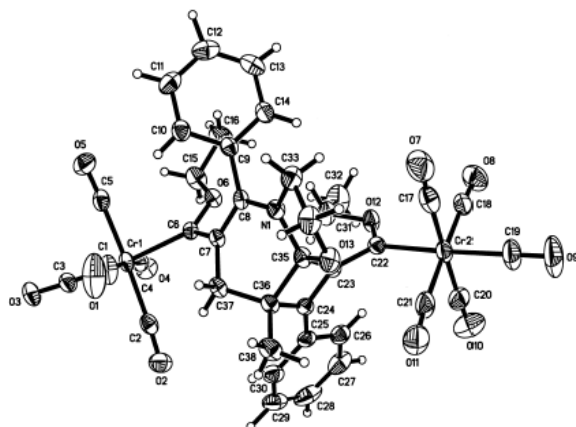


Table 1. Crystal data and structure refinement for **3a**.

Identification code	cd24161
Empirical formula	C ₃₈ H ₂₉ N O ₁₃ Cr ₂
Formula weight	811.62
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.5659(9) Å alpha = 90 deg. b = 20.5264(14) Å beta = 90.1920(10)deg. c = 14.4656(10) Å gamma = 90 deg.
Volume	3731.1(5) Å ³
Z, Calculated density	4, 1.445 Mg/m ³
Absorption coefficient	0.649 mm ⁻¹
F(000)	1664
Crystal size	0.535 x 0.489 x 0.467 mm
Theta range for data collection	1.62 to 28.29 deg.
Limiting indices	-16<=h<=16, -20<=k<=27, -16<=l<=19
Reflections collected / unique	22520 / 8666 [R(int) = 0.0458]
Completeness to theta = 28.29	93.5 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.72979
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8666 / 0 / 573
Goodness-of-fit on F ²	0.870
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.0977
R indices (all data)	R1 = 0.0856, wR2 = 0.1089
Largest diff. peak and hole	0.294 and -0.217 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3a**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Cr(1)	-518(1)	10785(1)	3159(1)	42(1)
Cr(2)	4893(1)	7832(1)	2223(1)	54(1)
O(1)	252(2)	11465(1)	1446(2)	124(1)
O(2)	1357(2)	11307(1)	4246(1)	70(1)
O(3)	-1738(2)	12010(1)	3558(2)	77(1)
O(4)	-1160(2)	10361(1)	5083(1)	61(1)
O(5)	-2476(2)	10371(1)	2083(1)	77(1)
O(6)	-158(1)	9301(1)	2910(1)	43(1)
O(7)	3953(2)	7697(1)	298(2)	106(1)
O(8)	3876(2)	6562(1)	2798(2)	93(1)
O(9)	6841(2)	7086(1)	1631(2)	140(1)
O(10)	5803(2)	7899(2)	4160(2)	108(1)
O(11)	6044(2)	9096(1)	1799(2)	107(1)
O(12)	2832(1)	7970(1)	3055(1)	54(1)
O(13)	3881(1)	9295(1)	847(1)	52(1)
N(1)	2102(2)	9222(1)	1079(1)	42(1)
C(1)	-18(3)	11188(2)	2081(2)	67(1)
C(2)	677(2)	11095(1)	3810(2)	49(1)
C(3)	-1259(2)	11546(1)	3415(2)	52(1)
C(4)	-954(2)	10478(1)	4337(2)	44(1)
C(5)	-1743(2)	10509(1)	2501(2)	53(1)
C(6)	194(2)	9903(1)	2746(2)	37(1)
C(7)	1104(2)	9838(1)	2144(2)	36(1)
C(8)	1153(2)	9354(1)	1480(2)	38(1)
C(9)	218(2)	9003(1)	1096(2)	42(1)
C(10)	-691(2)	9343(2)	838(2)	51(1)
C(11)	-1567(3)	9025(2)	516(2)	67(1)
C(12)	-1576(3)	8361(2)	438(2)	72(1)
C(13)	-682(3)	8024(2)	667(2)	67(1)
C(14)	213(3)	8336(1)	989(2)	53(1)
C(15)	-1130(2)	9154(1)	3397(2)	64(1)
C(16)	-1436(3)	8478(2)	3212(2)	78(1)
C(17)	4315(3)	7757(2)	1015(3)	72(1)

C(18)	4240(2)	7042(2)	2575(2)	62(1)
C(19)	6108(3)	7371(2)	1845(3)	85(1)
C(20)	5458(3)	7884(2)	3433(3)	71(1)
C(21)	5580(2)	8634(2)	1941(2)	72(1)
C(22)	3565(2)	8297(1)	2605(2)	42(1)
C(23)	3341(2)	8991(1)	2436(2)	37(1)
C(24)	3329(2)	9538(1)	2949(2)	38(1)
C(25)	3487(2)	9670(1)	3931(2)	44(1)
C(26)	3706(2)	9175(2)	4553(2)	56(1)
C(27)	3832(3)	9308(3)	5480(2)	74(1)
C(28)	3748(3)	9924(3)	5798(3)	85(1)
C(29)	3544(3)	10423(2)	5202(3)	77(1)
C(30)	3409(2)	10298(2)	4276(2)	58(1)
C(31)	1810(3)	8249(2)	3351(3)	62(1)
C(32)	1395(3)	7814(2)	4050(3)	97(1)
C(33)	2304(3)	8988(2)	143(2)	58(1)
C(34)	3370(3)	9288(2)	-33(2)	63(1)
C(35)	3103(2)	9358(1)	1538(2)	41(1)
C(36)	3105(2)	9997(1)	2137(2)	41(1)
C(37)	2011(2)	10319(1)	2138(2)	44(1)
C(38)	3984(3)	10472(2)	1891(3)	63(1)

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

Cr(1)-C(3)	1.857(3)
Cr(1)-C(1)	1.875(3)
Cr(1)-C(2)	1.881(3)
Cr(1)-C(5)	1.893(3)
Cr(1)-C(4)	1.900(3)
Cr(1)-C(6)	2.106(2)
Cr(2)-C(19)	1.879(3)
Cr(2)-C(18)	1.888(3)
Cr(2)-C(20)	1.889(4)
Cr(2)-C(17)	1.897(4)
Cr(2)-C(21)	1.904(3)
Cr(2)-C(22)	2.003(2)
O(1)-C(1)	1.134(3)
O(2)-C(2)	1.147(3)
O(3)-C(3)	1.146(3)
O(4)-C(4)	1.136(3)
O(5)-C(5)	1.136(3)

O(6)-C(6)	1.334(3)
O(6)-C(15)	1.445(3)
O(7)-C(17)	1.139(4)
O(8)-C(18)	1.133(3)
O(9)-C(19)	1.135(3)
O(10)-C(20)	1.136(4)
O(11)-C(21)	1.132(3)
O(12)-C(22)	1.315(3)
O(12)-C(31)	1.471(3)
O(13)-C(35)	1.406(3)
O(13)-C(34)	1.424(4)
N(1)-C(8)	1.356(3)
N(1)-C(35)	1.449(3)
N(1)-C(33)	1.459(3)
C(6)-C(7)	1.446(3)
C(7)-C(8)	1.384(3)
C(7)-C(37)	1.508(3)
C(8)-C(9)	1.484(3)
C(9)-C(14)	1.378(4)
C(9)-C(10)	1.389(4)
C(10)-C(11)	1.361(4)
C(10)-H(10)	0.92(2)
C(11)-C(12)	1.368(5)
C(11)-H(11)	0.93(3)
C(12)-C(13)	1.359(5)
C(12)-H(12)	1.04(3)
C(13)-C(14)	1.374(4)
C(13)-H(13)	0.84(3)
C(14)-H(14)	0.92(2)
C(15)-C(16)	1.464(4)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-H(35A)	0.9600
C(16)-H(35B)	0.9600
C(16)-H(35C)	0.9600
C(22)-C(23)	1.472(3)
C(23)-C(24)	1.347(3)
C(23)-C(35)	1.530(3)
C(24)-C(25)	1.458(3)
C(24)-C(36)	1.532(3)
C(25)-C(26)	1.384(4)
C(25)-C(30)	1.386(4)
C(26)-C(27)	1.376(4)
C(26)-H(26)	0.89(2)

C(27)-C(28)	1.352(5)
C(27)-H(27)	0.90(3)
C(28)-C(29)	1.361(5)
C(28)-H(28)	0.91(3)
C(29)-C(30)	1.374(4)
C(29)-H(29)	1.01(3)
C(30)-H(30)	0.84(2)
C(31)-C(32)	1.447(4)
C(31)-H(31A)	1.03(4)
C(31)-H(31B)	0.90(3)
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-C(34)	1.497(5)
C(33)-H(33A)	0.88(3)
C(33)-H(33B)	0.93(3)
C(34)-H(34A)	0.94(3)
C(34)-H(34B)	0.97(2)
C(35)-C(36)	1.572(3)
C(36)-C(38)	1.516(4)
C(36)-C(37)	1.525(3)
C(37)-H(37A)	0.98(2)
C(37)-H(37B)	0.96(2)
C(38)-H(38A)	1.05(3)
C(38)-H(38B)	0.84(3)
C(38)-H(38C)	0.96(3)

C(3)-Cr(1)-C(1)	87.97(12)
C(3)-Cr(1)-C(2)	90.85(12)
C(1)-Cr(1)-C(2)	89.86(13)
C(3)-Cr(1)-C(5)	86.85(12)
C(1)-Cr(1)-C(5)	89.34(14)
C(2)-Cr(1)-C(5)	177.59(12)
C(3)-Cr(1)-C(4)	87.33(11)
C(1)-Cr(1)-C(4)	172.17(13)
C(2)-Cr(1)-C(4)	83.96(11)
C(5)-Cr(1)-C(4)	96.65(11)
C(3)-Cr(1)-C(6)	173.49(11)
C(1)-Cr(1)-C(6)	89.97(11)
C(2)-Cr(1)-C(6)	95.32(10)
C(5)-Cr(1)-C(6)	86.95(10)
C(4)-Cr(1)-C(6)	95.37(10)
C(19)-Cr(2)-C(18)	90.02(14)
C(19)-Cr(2)-C(20)	89.73(16)

C(18)-Cr(2)-C(20)	87.77(14)
C(19)-Cr(2)-C(17)	89.98(15)
C(18)-Cr(2)-C(17)	90.72(14)
C(20)-Cr(2)-C(17)	178.45(14)
C(19)-Cr(2)-C(21)	90.23(14)
C(18)-Cr(2)-C(21)	176.68(15)
C(20)-Cr(2)-C(21)	88.92(15)
C(17)-Cr(2)-C(21)	92.60(15)
C(19)-Cr(2)-C(22)	177.82(14)
C(18)-Cr(2)-C(22)	88.35(11)
C(20)-Cr(2)-C(22)	91.65(12)
C(17)-Cr(2)-C(22)	88.60(12)
C(21)-Cr(2)-C(22)	91.48(11)
C(6)-O(6)-C(15)	124.17(19)
C(22)-O(12)-C(31)	124.0(2)
C(35)-O(13)-C(34)	108.9(2)
C(8)-N(1)-C(35)	121.96(19)
C(8)-N(1)-C(33)	128.2(2)
C(35)-N(1)-C(33)	109.6(2)
O(1)-C(1)-Cr(1)	175.7(3)
O(2)-C(2)-Cr(1)	175.1(2)
O(3)-C(3)-Cr(1)	178.1(3)
O(4)-C(4)-Cr(1)	171.8(2)
O(5)-C(5)-Cr(1)	176.7(3)
O(6)-C(6)-C(7)	106.53(19)
O(6)-C(6)-Cr(1)	127.17(16)
C(7)-C(6)-Cr(1)	126.00(17)
C(8)-C(7)-C(6)	121.4(2)
C(8)-C(7)-C(37)	115.6(2)
C(6)-C(7)-C(37)	122.8(2)
N(1)-C(8)-C(7)	118.8(2)
N(1)-C(8)-C(9)	116.1(2)
C(7)-C(8)-C(9)	124.9(2)
C(14)-C(9)-C(10)	117.8(3)
C(14)-C(9)-C(8)	121.8(2)
C(10)-C(9)-C(8)	120.4(2)
C(11)-C(10)-C(9)	120.9(3)
C(11)-C(10)-H(10)	123.7(16)
C(9)-C(10)-H(10)	115.4(16)
C(10)-C(11)-C(12)	120.9(3)
C(10)-C(11)-H(11)	117.9(19)
C(12)-C(11)-H(11)	121.2(19)
C(13)-C(12)-C(11)	118.7(3)
C(13)-C(12)-H(12)	127.8(18)

C(11)-C(12)-H(12)	113.2(18)
C(12)-C(13)-C(14)	121.4(3)
C(12)-C(13)-H(13)	126(2)
C(14)-C(13)-H(13)	113(2)
C(13)-C(14)-C(9)	120.3(3)
C(13)-C(14)-H(14)	120.9(15)
C(9)-C(14)-H(14)	118.7(15)
O(6)-C(15)-C(16)	109.3(2)
O(6)-C(15)-H(15A)	109.8
C(16)-C(15)-H(15A)	109.8
O(6)-C(15)-H(15B)	109.8
C(16)-C(15)-H(15B)	109.8
H(15A)-C(15)-H(15B)	108.3
C(15)-C(16)-H(35A)	109.5
C(15)-C(16)-H(35B)	109.5
H(35A)-C(16)-H(35B)	109.5
C(15)-C(16)-H(35C)	109.5
H(35A)-C(16)-H(35C)	109.5
H(35B)-C(16)-H(35C)	109.5
O(7)-C(17)-Cr(2)	178.2(3)
O(8)-C(18)-Cr(2)	177.9(3)
O(9)-C(19)-Cr(2)	178.7(4)
O(10)-C(20)-Cr(2)	178.3(3)
O(11)-C(21)-Cr(2)	175.7(3)
O(12)-C(22)-C(23)	116.3(2)
O(12)-C(22)-Cr(2)	118.60(18)
C(23)-C(22)-Cr(2)	125.07(18)
C(24)-C(23)-C(22)	135.8(2)
C(24)-C(23)-C(35)	93.2(2)
C(22)-C(23)-C(35)	130.8(2)
C(23)-C(24)-C(25)	133.6(2)
C(23)-C(24)-C(36)	95.26(19)
C(25)-C(24)-C(36)	131.1(2)
C(26)-C(25)-C(30)	117.5(3)
C(26)-C(25)-C(24)	121.6(2)
C(30)-C(25)-C(24)	120.9(3)
C(27)-C(26)-C(25)	120.7(3)
C(27)-C(26)-H(26)	119.6(15)
C(25)-C(26)-H(26)	119.7(15)
C(28)-C(27)-C(26)	120.6(4)
C(28)-C(27)-H(27)	122.0(19)
C(26)-C(27)-H(27)	117.3(19)
C(27)-C(28)-C(29)	120.2(4)

C(27)-C(28)-H(28)	122(2)
C(29)-C(28)-H(28)	118(2)
C(28)-C(29)-C(30)	120.0(4)
C(28)-C(29)-H(29)	124.9(15)
C(30)-C(29)-H(29)	115.0(16)
C(29)-C(30)-C(25)	121.1(4)
C(29)-C(30)-H(30)	119.9(17)
C(25)-C(30)-H(30)	118.9(17)
C(32)-C(31)-O(12)	106.3(3)
C(32)-C(31)-H(31A)	109(2)
O(12)-C(31)-H(31A)	108(2)
C(32)-C(31)-H(31B)	114(2)
O(12)-C(31)-H(31B)	108(2)
H(31A)-C(31)-H(31B)	111(3)
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
N(1)-C(33)-C(34)	100.5(3)
N(1)-C(33)-H(33A)	110.8(18)
C(34)-C(33)-H(33A)	115.3(19)
N(1)-C(33)-H(33B)	108.3(17)
C(34)-C(33)-H(33B)	110.4(18)
H(33A)-C(33)-H(33B)	111(3)
O(13)-C(34)-C(33)	104.7(2)
O(13)-C(34)-H(34A)	109.8(18)
C(33)-C(34)-H(34A)	112.7(18)
O(13)-C(34)-H(34B)	106.9(14)
C(33)-C(34)-H(34B)	113.5(14)
H(34A)-C(34)-H(34B)	109(2)
O(13)-C(35)-N(1)	105.14(19)
O(13)-C(35)-C(23)	115.1(2)
N(1)-C(35)-C(23)	117.4(2)
O(13)-C(35)-C(36)	118.0(2)
N(1)-C(35)-C(36)	114.42(19)
C(23)-C(35)-C(36)	86.73(17)
C(38)-C(36)-C(37)	112.3(2)
C(38)-C(36)-C(24)	116.3(2)
C(37)-C(36)-C(24)	115.37(19)
C(38)-C(36)-C(35)	114.0(2)
C(37)-C(36)-C(35)	111.3(2)
C(24)-C(36)-C(35)	84.81(18)

C(7)-C(37)-C(36)	113.4(2)
C(7)-C(37)-H(37A)	108.4(15)
C(36)-C(37)-H(37A)	105.2(15)
C(7)-C(37)-H(37B)	110.3(13)
C(36)-C(37)-H(37B)	110.4(13)
H(37A)-C(37)-H(37B)	108.8(19)
C(36)-C(38)-H(38A)	114.3(17)
C(36)-C(38)-H(38B)	108(2)
H(38A)-C(38)-H(38B)	112(3)
C(36)-C(38)-H(38C)	113.3(17)
H(38A)-C(38)-H(38C)	107(2)
H(38B)-C(38)-H(38C)	100(3)

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **3a**.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Cr(1)	47(1)	38(1)	43(1)	0(1)	8(1)	9(1)
Cr(2)	45(1)	43(1)	74(1)	-3(1)	13(1)	7(1)
O(1)	138(2)	132(2)	103(2)	70(2)	59(2)	59(2)
O(2)	60(1)	70(2)	79(2)	-15(1)	6(1)	-10(1)
O(3)	78(2)	50(1)	103(2)	-17(1)	1(1)	22(1)
O(4)	56(1)	82(2)	45(1)	1(1)	10(1)	-1(1)
O(5)	72(2)	87(2)	72(1)	-9(1)	-19(1)	7(1)
O(6)	44(1)	39(1)	45(1)	1(1)	11(1)	0(1)
O(7)	130(3)	108(2)	78(2)	-23(2)	-2(2)	30(2)
O(8)	101(2)	49(1)	128(2)	10(1)	5(2)	-6(1)
O(9)	99(2)	103(2)	218(3)	8(2)	68(2)	50(2)
O(10)	90(2)	133(3)	99(2)	3(2)	-23(2)	-17(2)
O(11)	62(2)	75(2)	185(3)	27(2)	19(2)	-13(1)
O(12)	45(1)	43(1)	75(1)	10(1)	17(1)	4(1)
O(13)	46(1)	66(1)	43(1)	0(1)	17(1)	9(1)
N(1)	42(1)	47(1)	36(1)	-7(1)	7(1)	6(1)
C(1)	75(2)	63(2)	63(2)	18(2)	20(2)	28(2)
C(2)	53(2)	41(2)	54(2)	-2(1)	16(1)	3(1)
C(3)	54(2)	45(2)	59(2)	-6(1)	3(1)	4(1)

C(4)	36(2)	48(2)	47(2)	-8(1)	4(1)	5(1)
C(5)	61(2)	52(2)	47(2)	-2(1)	3(1)	16(2)
C(6)	40(2)	37(1)	35(1)	1(1)	0(1)	5(1)
C(7)	39(1)	31(1)	39(1)	0(1)	7(1)	3(1)
C(8)	40(2)	35(1)	39(1)	6(1)	5(1)	6(1)
C(9)	46(2)	43(2)	36(1)	-4(1)	7(1)	3(1)
C(10)	55(2)	51(2)	48(2)	-3(1)	2(1)	9(2)
C(11)	47(2)	93(3)	61(2)	-5(2)	-7(2)	6(2)
C(12)	60(2)	94(3)	62(2)	-14(2)	3(2)	-22(2)
C(13)	89(3)	48(2)	64(2)	-10(2)	7(2)	-15(2)
C(14)	62(2)	44(2)	53(2)	-3(1)	0(2)	6(2)
C(15)	62(2)	53(2)	76(2)	5(2)	30(2)	-5(2)
C(16)	68(2)	64(2)	103(3)	-8(2)	25(2)	-20(2)
C(17)	79(3)	59(2)	76(2)	-8(2)	18(2)	16(2)
C(18)	57(2)	47(2)	82(2)	-5(2)	3(2)	8(2)
C(19)	66(2)	67(2)	121(3)	2(2)	31(2)	21(2)
C(20)	48(2)	68(2)	96(3)	2(2)	5(2)	-2(2)
C(21)	44(2)	59(2)	112(3)	7(2)	21(2)	8(2)
C(22)	42(2)	42(2)	43(1)	-4(1)	1(1)	0(1)
C(23)	30(1)	38(1)	42(1)	-1(1)	8(1)	1(1)
C(24)	28(1)	40(1)	46(2)	-3(1)	8(1)	-3(1)
C(25)	29(1)	53(2)	49(2)	-8(1)	6(1)	-6(1)
C(26)	44(2)	70(2)	53(2)	-9(2)	1(1)	0(2)
C(27)	51(2)	117(3)	53(2)	0(2)	0(2)	0(2)
C(28)	45(2)	157(5)	53(2)	-34(3)	2(2)	-16(2)
C(29)	49(2)	98(3)	84(3)	-49(3)	10(2)	-16(2)
C(30)	46(2)	63(2)	65(2)	-13(2)	6(2)	-10(2)
C(31)	44(2)	60(2)	82(2)	13(2)	23(2)	4(2)
C(32)	84(3)	100(3)	107(3)	40(2)	38(2)	6(2)
C(33)	58(2)	74(2)	43(2)	-9(2)	3(2)	14(2)
C(34)	67(2)	79(3)	45(2)	1(2)	20(2)	14(2)
C(35)	39(2)	43(2)	41(1)	-2(1)	14(1)	4(1)
C(36)	39(2)	34(1)	50(2)	-2(1)	13(1)	-4(1)
C(37)	50(2)	34(1)	46(2)	-1(1)	12(1)	2(1)
C(38)	60(2)	50(2)	78(3)	-4(2)	24(2)	-11(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for **3a**.

	x	y	z	U(eq)
--	---	---	---	-------

H(15A)	-1692	9446	3194	76
H(15B)	-1025	9216	4056	76
H(35A)	-1534	8418	2559	118
H(35B)	-2089	8381	3527	118
H(35C)	-886	8191	3429	118
H(32A)	1262	7394	3782	145
H(32B)	743	7988	4291	145
H(32C)	1905	7772	4542	145
H(10)	-646(19)	9789(12)	886(16)	48(8)
H(11)	-2160(20)	9274(14)	350(19)	75(10)
H(12)	-2270(30)	8180(16)	140(20)	96(11)
H(13)	-610(20)	7616(14)	633(18)	60(9)
H(14)	810(19)	8103(11)	1163(14)	36(7)
H(26)	3766(18)	8766(11)	4352(15)	37(7)
H(27)	4020(20)	8972(14)	5852(19)	63(10)
H(28)	3820(20)	10021(15)	6410(20)	77(10)
H(29)	3510(20)	10898(14)	5379(18)	59(8)
H(30)	3307(19)	10608(11)	3905(15)	30(7)
H(31A)	1310(30)	8244(19)	2790(30)	131(15)
H(33A)	1800(20)	9110(13)	-234(19)	60(9)
H(34A)	3320(20)	9716(15)	-267(19)	71(10)
H(37A)	1977(19)	10569(12)	1559(17)	53(8)
H(38A)	3900(20)	10683(15)	1230(20)	82(10)
H(31B)	1930(20)	8656(15)	3550(20)	75(11)
H(33B)	2360(20)	8534(15)	162(18)	66(10)
H(34B)	3816(19)	9030(11)	-442(16)	46(7)
H(37B)	1950(16)	10614(11)	2649(14)	31(6)
H(38B)	4030(20)	10752(14)	2312(19)	59(10)
H(38C)	4680(20)	10284(14)	1928(18)	69(10)

Table 6. Torsion angles [deg] for **3a**.

C(3)-Cr(1)-C(1)-O(1)	3(5)
C(2)-Cr(1)-C(1)-O(1)	-88(5)
C(5)-Cr(1)-C(1)-O(1)	90(5)
C(4)-Cr(1)-C(1)-O(1)	-50(5)
C(6)-Cr(1)-C(1)-O(1)	177(5)
C(3)-Cr(1)-C(2)-O(2)	31(3)

C(1)-Cr(1)-C(2)-O(2)	119(3)
C(5)-Cr(1)-C(2)-O(2)	48(5)
C(4)-Cr(1)-C(2)-O(2)	-57(3)
C(6)-Cr(1)-C(2)-O(2)	-151(3)
C(1)-Cr(1)-C(3)-O(3)	85(8)
C(2)-Cr(1)-C(3)-O(3)	175(100)
C(5)-Cr(1)-C(3)-O(3)	-4(8)
C(4)-Cr(1)-C(3)-O(3)	-101(8)
C(6)-Cr(1)-C(3)-O(3)	14(9)
C(3)-Cr(1)-C(4)-O(4)	-55.2(16)
C(1)-Cr(1)-C(4)-O(4)	-2(2)
C(2)-Cr(1)-C(4)-O(4)	36.0(16)
C(5)-Cr(1)-C(4)-O(4)	-141.7(16)
C(6)-Cr(1)-C(4)-O(4)	130.8(16)
C(3)-Cr(1)-C(5)-O(5)	53(5)
C(1)-Cr(1)-C(5)-O(5)	-35(5)
C(2)-Cr(1)-C(5)-O(5)	36(6)
C(4)-Cr(1)-C(5)-O(5)	140(5)
C(6)-Cr(1)-C(5)-O(5)	-125(5)
C(15)-O(6)-C(6)-C(7)	-172.7(2)
C(15)-O(6)-C(6)-Cr(1)	1.4(3)
C(3)-Cr(1)-C(6)-O(6)	-75.6(10)
C(1)-Cr(1)-C(6)-O(6)	-147.1(2)
C(2)-Cr(1)-C(6)-O(6)	123.1(2)
C(5)-Cr(1)-C(6)-O(6)	-57.7(2)
C(4)-Cr(1)-C(6)-O(6)	38.7(2)
C(3)-Cr(1)-C(6)-C(7)	97.4(10)
C(1)-Cr(1)-C(6)-C(7)	25.9(2)
C(2)-Cr(1)-C(6)-C(7)	-64.0(2)
C(5)-Cr(1)-C(6)-C(7)	115.2(2)
C(4)-Cr(1)-C(6)-C(7)	-148.4(2)
O(6)-C(6)-C(7)-C(8)	34.4(3)
Cr(1)-C(6)-C(7)-C(8)	-139.7(2)
O(6)-C(6)-C(7)-C(37)	-151.0(2)
Cr(1)-C(6)-C(7)-C(37)	34.9(3)
C(35)-N(1)-C(8)-C(7)	25.2(3)
C(33)-N(1)-C(8)-C(7)	-149.1(3)
C(35)-N(1)-C(8)-C(9)	-160.5(2)
C(33)-N(1)-C(8)-C(9)	25.2(4)
C(6)-C(7)-C(8)-N(1)	-165.4(2)
C(37)-C(7)-C(8)-N(1)	19.5(3)
C(6)-C(7)-C(8)-C(9)	20.8(4)
C(37)-C(7)-C(8)-C(9)	-154.2(2)
N(1)-C(8)-C(9)-C(14)	51.5(3)

C(7)-C(8)-C(9)-C(14)	-134.6(3)
N(1)-C(8)-C(9)-C(10)	-129.0(2)
C(7)-C(8)-C(9)-C(10)	44.9(3)
C(14)-C(9)-C(10)-C(11)	1.9(4)
C(8)-C(9)-C(10)-C(11)	-177.7(3)
C(9)-C(10)-C(11)-C(12)	0.0(5)
C(10)-C(11)-C(12)-C(13)	-1.5(5)
C(11)-C(12)-C(13)-C(14)	1.2(5)
C(12)-C(13)-C(14)-C(9)	0.7(5)
C(10)-C(9)-C(14)-C(13)	-2.2(4)
C(8)-C(9)-C(14)-C(13)	177.3(3)
C(6)-O(6)-C(15)-C(16)	163.0(2)
C(19)-Cr(2)-C(17)-O(7)	94(10)
C(18)-Cr(2)-C(17)-O(7)	4(10)
C(20)-Cr(2)-C(17)-O(7)	15(14)
C(21)-Cr(2)-C(17)-O(7)	-176(100)
C(22)-Cr(2)-C(17)-O(7)	-85(10)
C(19)-Cr(2)-C(18)-O(8)	43(8)
C(20)-Cr(2)-C(18)-O(8)	-47(8)
C(17)-Cr(2)-C(18)-O(8)	133(8)
C(21)-Cr(2)-C(18)-O(8)	-51(9)
C(22)-Cr(2)-C(18)-O(8)	-138(8)
C(18)-Cr(2)-C(19)-O(9)	-46(19)
C(20)-Cr(2)-C(19)-O(9)	41(19)
C(17)-Cr(2)-C(19)-O(9)	-137(19)
C(21)-Cr(2)-C(19)-O(9)	130(19)
C(22)-Cr(2)-C(19)-O(9)	-88(20)
C(19)-Cr(2)-C(20)-O(10)	-48(11)
C(18)-Cr(2)-C(20)-O(10)	42(11)
C(17)-Cr(2)-C(20)-O(10)	31(14)
C(21)-Cr(2)-C(20)-O(10)	-138(11)
C(22)-Cr(2)-C(20)-O(10)	130(11)
C(19)-Cr(2)-C(21)-O(11)	-44(4)
C(18)-Cr(2)-C(21)-O(11)	50(6)
C(20)-Cr(2)-C(21)-O(11)	45(4)
C(17)-Cr(2)-C(21)-O(11)	-134(4)
C(22)-Cr(2)-C(21)-O(11)	137(4)
C(31)-O(12)-C(22)-C(23)	2.8(4)
C(31)-O(12)-C(22)-Cr(2)	-178.2(2)
C(19)-Cr(2)-C(22)-O(12)	51(4)
C(18)-Cr(2)-C(22)-O(12)	9.7(2)
C(20)-Cr(2)-C(22)-O(12)	-78.0(2)
C(17)-Cr(2)-C(22)-O(12)	100.5(2)
C(21)-Cr(2)-C(22)-O(12)	-167.0(2)

C(19)-Cr(2)-C(22)-C(23)	-130(4)
C(18)-Cr(2)-C(22)-C(23)	-171.4(2)
C(20)-Cr(2)-C(22)-C(23)	100.9(2)
C(17)-Cr(2)-C(22)-C(23)	-80.7(2)
C(21)-Cr(2)-C(22)-C(23)	11.9(2)
O(12)-C(22)-C(23)-C(24)	73.8(4)
Cr(2)-C(22)-C(23)-C(24)	-105.1(3)
O(12)-C(22)-C(23)-C(35)	-111.4(3)
Cr(2)-C(22)-C(23)-C(35)	69.7(3)
C(22)-C(23)-C(24)-C(25)	-3.8(5)
C(35)-C(23)-C(24)-C(25)	-179.8(3)
C(22)-C(23)-C(24)-C(36)	175.3(3)
C(35)-C(23)-C(24)-C(36)	-0.71(18)
C(23)-C(24)-C(25)-C(26)	0.3(4)
C(36)-C(24)-C(25)-C(26)	-178.6(2)
C(23)-C(24)-C(25)-C(30)	-178.9(3)
C(36)-C(24)-C(25)-C(30)	2.3(4)
C(30)-C(25)-C(26)-C(27)	0.5(4)
C(24)-C(25)-C(26)-C(27)	-178.7(3)
C(25)-C(26)-C(27)-C(28)	-0.3(5)
C(26)-C(27)-C(28)-C(29)	-0.4(5)
C(27)-C(28)-C(29)-C(30)	0.8(5)
C(28)-C(29)-C(30)-C(25)	-0.5(5)
C(26)-C(25)-C(30)-C(29)	-0.1(4)
C(24)-C(25)-C(30)-C(29)	179.1(3)
C(22)-O(12)-C(31)-C(32)	-162.5(3)
C(8)-N(1)-C(33)-C(34)	149.8(3)
C(35)-N(1)-C(33)-C(34)	-25.1(3)
C(35)-O(13)-C(34)-C(33)	-30.3(3)
N(1)-C(33)-C(34)-O(13)	32.8(3)
C(34)-O(13)-C(35)-N(1)	14.2(3)
C(34)-O(13)-C(35)-C(23)	145.1(2)
C(34)-O(13)-C(35)-C(36)	-114.7(3)
C(8)-N(1)-C(35)-O(13)	-167.3(2)
C(33)-N(1)-C(35)-O(13)	7.9(3)
C(8)-N(1)-C(35)-C(23)	63.2(3)
C(33)-N(1)-C(35)-C(23)	-121.5(3)
C(8)-N(1)-C(35)-C(36)	-36.3(3)
C(33)-N(1)-C(35)-C(36)	139.0(2)
C(24)-C(23)-C(35)-O(13)	120.2(2)
C(22)-C(23)-C(35)-O(13)	-56.2(3)
C(24)-C(23)-C(35)-N(1)	-115.2(2)
C(22)-C(23)-C(35)-N(1)	68.4(3)
C(24)-C(23)-C(35)-C(36)	0.69(18)

C(22)-C(23)-C(35)-C(36)	-175.6(2)
C(23)-C(24)-C(36)-C(38)	-113.5(3)
C(25)-C(24)-C(36)-C(38)	65.6(3)
C(23)-C(24)-C(36)-C(37)	111.8(2)
C(25)-C(24)-C(36)-C(37)	-69.0(3)
C(23)-C(24)-C(36)-C(35)	0.70(18)
C(25)-C(24)-C(36)-C(35)	179.8(2)
O(13)-C(35)-C(36)-C(38)	-0.9(3)
N(1)-C(35)-C(36)-C(38)	-125.4(3)
C(23)-C(35)-C(36)-C(38)	115.9(3)
O(13)-C(35)-C(36)-C(37)	127.4(2)
N(1)-C(35)-C(36)-C(37)	2.9(3)
C(23)-C(35)-C(36)-C(37)	-115.9(2)
O(13)-C(35)-C(36)-C(24)	-117.4(2)
N(1)-C(35)-C(36)-C(24)	118.1(2)
C(23)-C(35)-C(36)-C(24)	-0.61(16)
C(8)-C(7)-C(37)-C(36)	-50.6(3)
C(6)-C(7)-C(37)-C(36)	134.4(2)
C(38)-C(36)-C(37)-C(7)	165.7(3)
C(24)-C(36)-C(37)-C(7)	-57.9(3)
C(35)-C(36)-C(37)-C(7)	36.5(3)

2. X-Ray Crystal Structure Information for 5b.

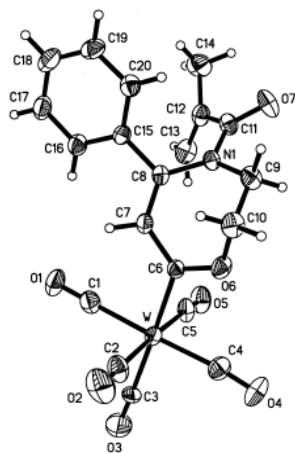


Table 7. Crystal data and structure refinement for **5b**.

Identification code	cd24277
Empirical formula	C ₂₀ H ₁₅ N O ₇ W
Formula weight	565.18
Temperature	293(2) K
Wavelength	0.71073 Å

Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 7.4353(7) Å alpha = 65.069(2) deg. b = 12.1255(11) Å beta = 82.996(2) deg. c = 12.5732(12) Å gamma = 79.906(2) deg.
Volume	1010.55(16) Å ³
Z, Calculated density	2, 1.857 Mg/m ³
Absorption coefficient	5.757 mm ⁻¹
F(000)	544
Crystal size	0.425 x 0.196 x 0.091 mm
Theta range for data collection	1.79 to 27.00 deg.
Limiting indices	-9<=h<=9, -15<=k<=15, -12<=l<=16
Reflections collected / unique	5994 / 4294 [R(int) = 0.1375]
Completeness to theta = 27.00	97.2 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.47279
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4294 / 0 / 263
Goodness-of-fit on F ²	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0719, wR2 = 0.1744
R indices (all data)	R1 = 0.0757, wR2 = 0.1776
Largest diff. peak and hole	4.217 and -3.525 e.Å ⁻³

Table 8. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **5b**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W	523(1)	2669(1)	4570(1)	41(1)
N(1)	3089(10)	950(6)	1629(7)	38(2)
O(1)	354(17)	5229(9)	2363(9)	79(3)
O(2)	3872(17)	3191(12)	5533(13)	99(4)
O(3)	-2178(17)	3971(11)	5952(10)	95(3)
O(4)	678(16)	111(9)	6769(9)	82(3)
O(5)	-2963(15)	2111(10)	3782(10)	76(3)
O(6)	3039(10)	654(6)	4063(6)	54(2)
O(7)	2741(13)	-322(7)	832(9)	71(2)
C(1)	397(19)	4303(11)	3175(11)	59(3)
C(2)	2679(19)	3054(11)	5203(13)	63(3)

C(3)	-1193(17)	3484(10)	5479(10)	52(3)
C(4)	678(19)	1008(12)	5927(11)	61(3)
C(5)	-1665(17)	2267(10)	4043(11)	56(3)
C(6)	2405(13)	1839(8)	3575(8)	39(2)
C(7)	3025(13)	2509(8)	2370(8)	42(2)
C(8)	3209(11)	2145(8)	1480(8)	37(2)
C(9)	3995(15)	-129(9)	2566(10)	52(2)
C(10)	4583(15)	180(10)	3503(10)	57(3)
C(11)	2327(13)	683(9)	822(9)	46(2)
C(12)	943(15)	1607(9)	27(9)	50(2)
C(13)	-382(14)	2185(10)	463(10)	63(3)
C(14)	1020(20)	1675(14)	-1178(12)	76(4)
C(15)	3639(12)	3033(8)	268(8)	39(2)
C(16)	2919(16)	4267(9)	-116(9)	53(2)
C(17)	3400(20)	5085(11)	-1237(10)	65(3)
C(18)	4570(20)	4691(13)	-1964(11)	71(4)
C(19)	5267(16)	3482(12)	-1586(10)	61(3)
C(20)	4827(15)	2643(10)	-483(9)	51(2)

Table 9. Bond lengths [Å] and angles [deg] for **5b**.

W-C(4)	2.013(13)
W-C(1)	2.014(13)
W-C(3)	2.017(9)
W-C(5)	2.034(11)
W-C(2)	2.075(12)
W-C(6)	2.162(9)
N(1)-C(11)	1.391(12)
N(1)-C(8)	1.398(10)
N(1)-C(9)	1.464(12)
O(1)-C(1)	1.155(16)
O(2)-C(2)	1.089(16)
O(3)-C(3)	1.130(13)
O(4)-C(4)	1.154(16)
O(5)-C(5)	1.126(15)
O(6)-C(6)	1.324(11)
O(6)-C(10)	1.434(13)
O(7)-C(11)	1.198(12)
C(6)-C(7)	1.446(12)

C(7)-C(8)	1.351(12)
C(7)-H(7)	0.9300
C(8)-C(15)	1.483(12)
C(9)-C(10)	1.509(15)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.489(14)
C(12)-C(13)	1.308(15)
C(12)-C(14)	1.477(16)
C(13)-H(13A)	0.9300
C(13)-H(13B)	0.9300
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-C(20)	1.387(13)
C(15)-C(16)	1.391(13)
C(16)-C(17)	1.384(15)
C(16)-H(16)	0.9300
C(17)-C(18)	1.362(19)
C(17)-H(17)	0.9300
C(18)-C(19)	1.360(19)
C(18)-H(18)	0.9300
C(19)-C(20)	1.372(16)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300
C(4)-W-C(1)	178.1(4)
C(4)-W-C(3)	93.2(5)
C(1)-W-C(3)	88.6(5)
C(4)-W-C(5)	88.7(5)
C(1)-W-C(5)	90.6(5)
C(3)-W-C(5)	89.6(5)
C(4)-W-C(2)	89.3(5)
C(1)-W-C(2)	91.4(5)
C(3)-W-C(2)	87.9(5)
C(5)-W-C(2)	176.7(5)
C(4)-W-C(6)	88.0(4)
C(1)-W-C(6)	90.2(4)
C(3)-W-C(6)	178.4(3)
C(5)-W-C(6)	91.6(4)
C(2)-W-C(6)	91.1(5)
C(11)-N(1)-C(8)	123.4(8)
C(11)-N(1)-C(9)	114.0(7)

C(8)-N(1)-C(9)	122.1(8)
C(6)-O(6)-C(10)	119.0(8)
O(1)-C(1)-W	178.5(13)
O(2)-C(2)-W	175.5(12)
O(3)-C(3)-W	177.5(12)
O(4)-C(4)-W	173.5(12)
O(5)-C(5)-W	174.4(12)
O(6)-C(6)-C(7)	116.5(8)
O(6)-C(6)-W	120.0(7)
C(7)-C(6)-W	123.5(6)
C(8)-C(7)-C(6)	127.7(8)
C(8)-C(7)-H(7)	116.1
C(6)-C(7)-H(7)	116.1
C(7)-C(8)-N(1)	123.9(8)
C(7)-C(8)-C(15)	119.3(8)
N(1)-C(8)-C(15)	116.7(7)
N(1)-C(9)-C(10)	112.1(8)
N(1)-C(9)-H(9A)	109.2
C(10)-C(9)-H(9A)	109.2
N(1)-C(9)-H(9B)	109.2
C(10)-C(9)-H(9B)	109.2
H(9A)-C(9)-H(9B)	107.9
O(6)-C(10)-C(9)	111.1(8)
O(6)-C(10)-H(10A)	109.4
C(9)-C(10)-H(10A)	109.4
O(6)-C(10)-H(10B)	109.4
C(9)-C(10)-H(10B)	109.4
H(10A)-C(10)-H(10B)	108.0
O(7)-C(11)-N(1)	118.3(10)
O(7)-C(11)-C(12)	121.5(9)
N(1)-C(11)-C(12)	120.0(8)
C(13)-C(12)-C(14)	123.8(11)
C(13)-C(12)-C(11)	119.1(9)
C(14)-C(12)-C(11)	116.5(10)
C(12)-C(13)-H(13A)	120.0
C(12)-C(13)-H(13B)	120.0
H(13A)-C(13)-H(13B)	120.0
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(20)-C(15)-C(16)	119.1(9)

C(20)-C(15)-C(8)	119.9(8)
C(16)-C(15)-C(8)	120.9(8)
C(17)-C(16)-C(15)	119.7(10)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(18)-C(17)-C(16)	120.6(12)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	119.5(11)
C(19)-C(18)-H(18)	120.2
C(17)-C(18)-H(18)	120.2
C(18)-C(19)-C(20)	121.7(11)
C(18)-C(19)-H(19)	119.1
C(20)-C(19)-H(19)	119.1
C(19)-C(20)-C(15)	119.3(10)
C(19)-C(20)-H(20)	120.3
C(15)-C(20)-H(20)	120.3

Table 10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5b**.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
W	41(1)	38(1)	40(1)	-11(1)	-4(1)	-9(1)
N(1)	35(4)	34(3)	46(4)	-16(3)	-8(3)	-1(3)
O(1)	96(8)	51(5)	70(6)	-1(4)	-6(5)	-20(5)
O(2)	83(7)	97(8)	136(10)	-55(8)	-46(7)	-14(6)
O(3)	105(9)	91(7)	90(7)	-45(6)	21(6)	-12(6)
O(4)	79(7)	65(6)	66(6)	10(4)	1(5)	-15(5)
O(5)	70(6)	64(5)	93(7)	-22(5)	-27(5)	-17(5)
O(6)	54(4)	42(4)	49(4)	-6(3)	-7(3)	4(3)
O(7)	72(5)	52(4)	108(7)	-49(5)	-20(5)	-1(4)
C(1)	68(7)	50(6)	62(7)	-22(5)	-20(5)	-4(5)
C(2)	64(7)	49(6)	80(8)	-24(6)	-25(6)	-6(5)
C(3)	63(7)	55(6)	47(5)	-32(5)	21(5)	-17(5)
C(4)	60(7)	57(7)	55(7)	-13(5)	-12(5)	0(5)

C(5)	58(6)	39(5)	68(7)	-14(5)	-19(5)	-9(4)
C(6)	44(5)	34(4)	36(4)	-12(3)	-7(3)	-4(3)
C(7)	47(5)	32(4)	43(5)	-11(3)	-6(4)	-8(4)
C(8)	31(4)	32(4)	47(5)	-14(4)	-4(3)	-3(3)
C(9)	47(5)	43(5)	61(6)	-19(5)	-16(5)	13(4)
C(10)	45(5)	51(6)	63(6)	-16(5)	-21(5)	13(4)
C(11)	38(5)	44(5)	63(6)	-26(4)	-3(4)	-9(4)
C(12)	51(6)	46(5)	53(5)	-15(4)	-12(4)	-14(4)
C(13)	46(6)	60(7)	68(8)	-12(6)	-17(5)	-1(5)
C(14)	83(9)	94(10)	69(8)	-43(7)	-14(7)	-25(8)
C(15)	35(4)	39(4)	40(4)	-12(4)	-3(3)	-8(3)
C(16)	61(6)	42(5)	49(5)	-12(4)	-6(4)	-6(4)
C(17)	87(9)	48(6)	56(6)	-10(5)	-8(6)	-22(6)
C(18)	80(9)	78(8)	49(6)	-12(6)	5(6)	-36(7)
C(19)	51(6)	77(8)	55(6)	-27(6)	12(5)	-20(5)
C(20)	40(5)	50(5)	62(6)	-23(5)	1(4)	-9(4)

Table 11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5b**.

	x	y	z	U(eq)
H(7)	3333	3282	2187	50
H(9A)	5060	-484	2232	63
H(9B)	3166	-739	2921	63
H(10A)	5225	-551	4087	68
H(10B)	5420	786	3153	68
H(13A)	-1351	2673	6	75
H(13B)	-354	2107	1229	75
H(14A)	1000	871	-1145	114
H(14B)	2119	1980	-1593	114
H(14C)	-24	2217	-1579	114
H(16)	2119	4543	377	63
H(17)	2911	5910	-1494	79
H(18)	4890	5244	-2715	86
H(19)	6063	3218	-2089	73
H(20)	5320	1820	-242	61

Table 12. Torsion angles [deg] for **5b**.

C(4)-W-C(1)-O(1)	-27(53)
C(3)-W-C(1)-O(1)	174(46)
C(5)-W-C(1)-O(1)	-97(46)
C(2)-W-C(1)-O(1)	86(46)
C(6)-W-C(1)-O(1)	-5(46)
C(4)-W-C(2)-O(2)	55(19)
C(1)-W-C(2)-O(2)	-124(19)
C(3)-W-C(2)-O(2)	148(19)
C(5)-W-C(2)-O(2)	108(19)
C(6)-W-C(2)-O(2)	-33(19)
C(4)-W-C(3)-O(3)	-153(25)
C(1)-W-C(3)-O(3)	26(25)
C(5)-W-C(3)-O(3)	-65(25)
C(2)-W-C(3)-O(3)	118(25)
C(6)-W-C(3)-O(3)	70(32)
C(1)-W-C(4)-O(4)	-168(12)
C(3)-W-C(4)-O(4)	-9(11)
C(5)-W-C(4)-O(4)	-98(11)
C(2)-W-C(4)-O(4)	79(11)
C(6)-W-C(4)-O(4)	170(11)
C(4)-W-C(5)-O(5)	108(12)
C(1)-W-C(5)-O(5)	-74(12)
C(3)-W-C(5)-O(5)	15(12)
C(2)-W-C(5)-O(5)	54(15)
C(6)-W-C(5)-O(5)	-164(12)
C(10)-O(6)-C(6)-C(7)	15.0(13)
C(10)-O(6)-C(6)-W	-165.7(7)
C(4)-W-C(6)-O(6)	-0.1(8)
C(1)-W-C(6)-O(6)	-179.4(8)
C(3)-W-C(6)-O(6)	137(13)
C(5)-W-C(6)-O(6)	-88.8(8)
C(2)-W-C(6)-O(6)	89.2(8)
C(4)-W-C(6)-C(7)	179.1(8)
C(1)-W-C(6)-C(7)	-0.2(8)
C(3)-W-C(6)-C(7)	-44(14)

C(5)-W-C(6)-C(7)	90.5(8)
C(2)-W-C(6)-C(7)	-91.6(8)
O(6)-C(6)-C(7)-C(8)	42.1(14)
W-C(6)-C(7)-C(8)	-137.2(9)
C(6)-C(7)-C(8)-N(1)	-10.4(15)
C(6)-C(7)-C(8)-C(15)	172.2(9)
C(11)-N(1)-C(8)-C(7)	144.6(9)
C(9)-N(1)-C(8)-C(7)	-44.5(13)
C(11)-N(1)-C(8)-C(15)	-37.9(12)
C(9)-N(1)-C(8)-C(15)	133.0(9)
C(11)-N(1)-C(9)-C(10)	-172.6(9)
C(8)-N(1)-C(9)-C(10)	15.7(13)
C(6)-O(6)-C(10)-C(9)	-85.0(11)
N(1)-C(9)-C(10)-O(6)	61.7(12)
C(8)-N(1)-C(11)-O(7)	158.6(10)
C(9)-N(1)-C(11)-O(7)	-13.0(14)
C(8)-N(1)-C(11)-C(12)	-25.3(13)
C(9)-N(1)-C(11)-C(12)	163.1(9)
O(7)-C(11)-C(12)-C(13)	130.7(12)
N(1)-C(11)-C(12)-C(13)	-45.2(13)
O(7)-C(11)-C(12)-C(14)	-40.6(15)
N(1)-C(11)-C(12)-C(14)	143.4(10)
C(7)-C(8)-C(15)-C(20)	141.8(9)
N(1)-C(8)-C(15)-C(20)	-35.8(12)
C(7)-C(8)-C(15)-C(16)	-35.8(13)
N(1)-C(8)-C(15)-C(16)	146.6(9)
C(20)-C(15)-C(16)-C(17)	-0.1(16)
C(8)-C(15)-C(16)-C(17)	177.6(10)
C(15)-C(16)-C(17)-C(18)	-0.2(18)
C(16)-C(17)-C(18)-C(19)	0(2)
C(17)-C(18)-C(19)-C(20)	0(2)
C(18)-C(19)-C(20)-C(15)	0.0(18)
C(16)-C(15)-C(20)-C(19)	0.1(15)
C(8)-C(15)-C(20)-C(19)	-177.6(10)

3. X-Ray Structure Information for 6b.

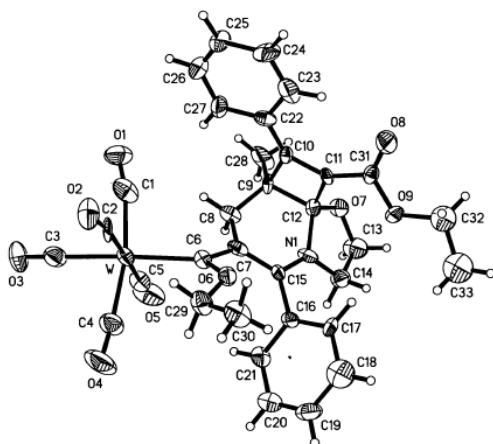


Table 13. Crystal data and structure refinement for **6b**.

Identification code	cd24220
Empirical formula	C ₃₃ H ₂₉ N O ₉ W
Formula weight	767.42
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 11.1571(9) Å alpha = 90 deg. b = 13.6990(11) Å beta = 113.103(2) deg. c = 11.3873(10) Å gamma = 90 deg.
Volume	1600.9(2) Å ³
Z, Calculated density	2, 1.592 Mg/m ³
Absorption coefficient	3.662 mm ⁻¹
F(000)	760
Crystal size	0.275 x 0.166 x 0.123 mm
Theta range for data collection	1.94 to 27.00 deg.
Limiting indices	-10 ≤ h ≤ 14, -14 ≤ k ≤ 17, -14 ≤ l ≤ 12
Reflections collected / unique	9521 / 6185 [R(int) = 0.0674]
Completeness to theta = 27.00	99.8 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.73228
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6185 / 14 / 386
Goodness-of-fit on F ²	0.912
Final R indices [I > 2σ(I)]	R1 = 0.0519, wR2 = 0.1181
R indices (all data)	R1 = 0.0804, wR2 = 0.1752
Absolute structure parameter	-4(10)
Largest diff. peak and hole	1.632 and -0.690 e.Å ⁻³

Table 14. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **6b**. U(eq) is defined as one third of the trace of the

orthogonalized Uij tensor.

	x	y	z	U(eq)
W	6218(1)	7571(1)	-589(1)	46(1)
O(1)	8634(13)	7822(14)	-1411(15)	94(7)
O(2)	6845(16)	5279(11)	-236(13)	86(4)
O(3)	4773(16)	7029(12)	-3514(14)	100(5)
O(4)	3404(14)	7196(18)	-658(18)	150(13)
O(5)	5456(16)	9816(11)	-1190(20)	113(6)
O(6)	7085(8)	7592(16)	2476(8)	49(2)
O(7)	10398(10)	11080(8)	3804(11)	53(3)
O(8)	12365(14)	8566(12)	6084(13)	88(5)
O(9)	10791(12)	9574(13)	6111(12)	75(5)
N(1)	8660(13)	10102(10)	3472(17)	57(5)
C(1)	7837(19)	7790(20)	-1015(18)	80(9)
C(2)	6690(20)	6108(16)	-215(17)	62(5)
C(3)	5277(18)	7207(15)	-2490(20)	75(7)
C(4)	4426(19)	7315(18)	-564(19)	77(9)
C(5)	5706(18)	8982(11)	-984(18)	54(4)
C(6)	7160(14)	8019(10)	1461(15)	40(4)
C(7)	7894(13)	8888(12)	1964(15)	46(4)
C(8)	8668(15)	9405(13)	1325(17)	53(4)
C(9)	9966(15)	9707(11)	2190(13)	38(3)
C(10)	10879(13)	8878(10)	3076(13)	34(3)
C(11)	10885(13)	9262(11)	4178(13)	37(3)
C(12)	9975(15)	10108(11)	3470(16)	47(4)
C(13)	9570(20)	11713(15)	4170(20)	87(7)
C(14)	8530(20)	10992(17)	4120(30)	60(8)
C(15)	7815(13)	9402(12)	2976(14)	45(4)
C(16)	6812(14)	9291(13)	3546(15)	54(5)
C(17)	7171(16)	9132(13)	4806(14)	55(5)
C(18)	6196(19)	9042(19)	5270(20)	107(8)
C(19)	4875(18)	9058(15)	4480(19)	80(7)
C(20)	4548(17)	9271(11)	3235(19)	59(5)
C(21)	5494(13)	9355(11)	2768(15)	51(4)
C(22)	11444(14)	8061(11)	2770(15)	49(4)
C(23)	12326(14)	7480(16)	3678(15)	78(7)
C(24)	12852(19)	6644(13)	3362(19)	73(6)

C(25)	12570(20)	6461(15)	2100(20)	101(10)
C(26)	11770(20)	7108(15)	1170(20)	84(7)
C(27)	11155(19)	7868(12)	1474(15)	64(7)
C(28)	10664(18)	10412(17)	1550(20)	90(8)
C(29)	6170(18)	6785(13)	2308(18)	65(5)
C(30)	6390(20)	6342(16)	3583(19)	72(6)
C(31)	11450(20)	9100(16)	5520(20)	41(5)
C(32)	11250(20)	9402(18)	7550(20)	89(7)
C(33)	10270(40)	9910(30)	7920(40)	128(17)

Table 15. Bond lengths [Å] and angles [deg] for **6b**.

W-C(5)	2.015(16)
W-C(4)	2.041(19)
W-C(3)	2.06(2)
W-C(1)	2.07(2)
W-C(2)	2.07(2)
W-C(6)	2.237(15)
O(1)-C(1)	1.14(2)
O(2)-C(2)	1.15(2)
O(3)-C(3)	1.10(2)
O(4)-C(4)	1.11(2)
O(5)-C(5)	1.18(2)
O(6)-C(6)	1.326(18)
O(6)-C(29)	1.47(2)
O(7)-C(12)	1.414(16)
O(7)-C(13)	1.44(2)
O(8)-C(31)	1.21(3)
O(9)-C(31)	1.35(2)
O(9)-C(32)	1.53(3)
N(1)-C(15)	1.307(19)
N(1)-C(14)	1.46(3)
N(1)-C(12)	1.468(19)
C(6)-C(7)	1.43(2)
C(7)-C(15)	1.38(2)
C(7)-C(8)	1.51(2)
C(8)-C(9)	1.46(2)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-C(12)	1.55(2)

C(9)-C(10)	1.59(2)
C(9)-C(28)	1.58(2)
C(10)-C(11)	1.358(19)
C(10)-C(22)	1.39(2)
C(11)-C(31)	1.42(3)
C(11)-C(12)	1.54(2)
C(13)-C(14)	1.51(3)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(16)	1.51(2)
C(16)-C(17)	1.347(16)
C(16)-C(21)	1.390(15)
C(17)-C(18)	1.391(17)
C(17)-H(17)	0.9300
C(18)-C(19)	1.394(17)
C(18)-H(18)	0.9300
C(19)-C(20)	1.349(16)
C(19)-H(19)	0.9300
C(20)-C(21)	1.361(16)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(22)-C(23)	1.368(16)
C(22)-C(27)	1.407(15)
C(23)-C(24)	1.397(17)
C(23)-H(23)	0.9300
C(24)-C(25)	1.371(17)
C(24)-H(24)	0.9300
C(25)-C(26)	1.403(17)
C(25)-H(25)	0.9300
C(26)-C(27)	1.364(16)
C(26)-H(26)	0.9300
C(27)-H(27)	0.9300
C(28)-H(28A)	0.9601
C(28)-H(28B)	0.9601
C(28)-H(28C)	0.9601
C(29)-C(30)	1.50(2)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(32)-C(33)	1.493(18)

C(32)-H(32A)	0.9700
C(32)-H(32B)	0.9700
C(33)-H(33A)	0.9657
C(33)-H(33B)	0.9662
C(33)-H(33C)	0.9660
C(5)-W-C(4)	88.6(8)
C(5)-W-C(3)	90.9(8)
C(4)-W-C(3)	82.9(8)
C(5)-W-C(1)	90.3(9)
C(4)-W-C(1)	168.2(8)
C(3)-W-C(1)	85.4(8)
C(5)-W-C(2)	178.3(8)
C(4)-W-C(2)	90.1(9)
C(3)-W-C(2)	88.0(7)
C(1)-W-C(2)	90.8(9)
C(5)-W-C(6)	86.9(6)
C(4)-W-C(6)	95.4(7)
C(3)-W-C(6)	177.2(7)
C(1)-W-C(6)	96.3(7)
C(2)-W-C(6)	94.2(6)
C(6)-O(6)-C(29)	119.8(12)
C(12)-O(7)-C(13)	117.5(13)
C(31)-O(9)-C(32)	116.3(17)
C(15)-N(1)-C(14)	129.3(16)
C(15)-N(1)-C(12)	123.7(13)
C(14)-N(1)-C(12)	106.9(14)
O(1)-C(1)-W	169(2)
O(2)-C(2)-W	168.0(16)
O(3)-C(3)-W	178.7(19)
O(4)-C(4)-W	174.0(19)
O(5)-C(5)-W	177.4(18)
O(6)-C(6)-C(7)	103.9(15)
O(6)-C(6)-W	128.6(11)
C(7)-C(6)-W	127.3(11)
C(15)-C(7)-C(6)	122.9(14)
C(15)-C(7)-C(8)	113.5(15)
C(6)-C(7)-C(8)	123.0(16)
C(9)-C(8)-C(7)	114.4(14)
C(9)-C(8)-H(8A)	108.7
C(7)-C(8)-H(8A)	108.7
C(9)-C(8)-H(8B)	108.6
C(7)-C(8)-H(8B)	108.7
H(8A)-C(8)-H(8B)	107.6
C(8)-C(9)-C(12)	111.9(14)

C(8)-C(9)-C(10)	116.4(12)
C(12)-C(9)-C(10)	83.7(11)
C(8)-C(9)-C(28)	113.6(13)
C(12)-C(9)-C(28)	113.1(14)
C(10)-C(9)-C(28)	114.7(14)
C(11)-C(10)-C(22)	134.7(14)
C(11)-C(10)-C(9)	94.5(11)
C(22)-C(10)-C(9)	130.8(13)
C(10)-C(11)-C(31)	140.3(17)
C(10)-C(11)-C(12)	92.6(12)
C(31)-C(11)-C(12)	127.1(15)
O(7)-C(12)-N(1)	103.5(12)
O(7)-C(12)-C(11)	119.0(12)
N(1)-C(12)-C(11)	116.6(13)
O(7)-C(12)-C(9)	117.6(14)
N(1)-C(12)-C(9)	111.2(12)
C(11)-C(12)-C(9)	89.1(11)
O(7)-C(13)-C(14)	99.5(15)
O(7)-C(13)-H(13A)	111.9
C(14)-C(13)-H(13A)	111.7
O(7)-C(13)-H(13B)	111.9
C(14)-C(13)-H(13B)	112.0
H(13A)-C(13)-H(13B)	109.6
N(1)-C(14)-C(13)	109.6(18)
N(1)-C(14)-H(14A)	109.6
C(13)-C(14)-H(14A)	109.6
N(1)-C(14)-H(14B)	109.9
C(13)-C(14)-H(14B)	109.9
H(14A)-C(14)-H(14B)	108.2
N(1)-C(15)-C(7)	117.5(14)
N(1)-C(15)-C(16)	114.9(14)
C(7)-C(15)-C(16)	127.5(13)
C(17)-C(16)-C(21)	119.2(16)
C(17)-C(16)-C(15)	121.0(13)
C(21)-C(16)-C(15)	119.9(15)
C(16)-C(17)-C(18)	118.1(18)
C(16)-C(17)-H(17)	121.0
C(18)-C(17)-H(17)	120.9
C(17)-C(18)-C(19)	123(2)
C(17)-C(18)-H(18)	118.8
C(19)-C(18)-H(18)	118.7
C(20)-C(19)-C(18)	117.7(19)
C(20)-C(19)-H(19)	121.1
C(18)-C(19)-H(19)	121.2

C(19)-C(20)-C(21)	119.8(17)
C(19)-C(20)-H(20)	120.1
C(21)-C(20)-H(20)	120.1
C(20)-C(21)-C(16)	122.3(16)
C(20)-C(21)-H(21)	118.9
C(16)-C(21)-H(21)	118.8
C(23)-C(22)-C(10)	122.6(16)
C(23)-C(22)-C(27)	119.0(15)
C(10)-C(22)-C(27)	118.2(14)
C(22)-C(23)-C(24)	122.1(17)
C(22)-C(23)-H(23)	119.0
C(24)-C(23)-H(23)	118.9
C(25)-C(24)-C(23)	118.4(17)
C(25)-C(24)-H(24)	120.7
C(23)-C(24)-H(24)	120.9
C(24)-C(25)-C(26)	119.4(18)
C(24)-C(25)-H(25)	120.3
C(26)-C(25)-H(25)	120.3
C(27)-C(26)-C(25)	122(2)
C(27)-C(26)-H(26)	119.1
C(25)-C(26)-H(26)	119.1
C(26)-C(27)-C(22)	118.6(17)
C(26)-C(27)-H(27)	120.7
C(22)-C(27)-H(27)	120.6
C(9)-C(28)-H(28A)	109.6
C(9)-C(28)-H(28B)	109.4
H(28A)-C(28)-H(28B)	109.5
C(9)-C(28)-H(28C)	109.4
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
O(6)-C(29)-C(30)	109.6(15)
O(6)-C(29)-H(29A)	109.8
C(30)-C(29)-H(29A)	109.8
O(6)-C(29)-H(29B)	109.7
C(30)-C(29)-H(29B)	109.8
H(29A)-C(29)-H(29B)	108.2
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.4
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
O(8)-C(31)-O(9)	122(2)
O(8)-C(31)-C(11)	127(2)

O(9)-C(31)-C(11)	111.2(19)
C(33)-C(32)-O(9)	105(2)
C(33)-C(32)-H(32A)	110.8
O(9)-C(32)-H(32A)	110.6
C(33)-C(32)-H(32B)	111.0
O(9)-C(32)-H(32B)	110.8
H(32A)-C(32)-H(32B)	108.8
C(32)-C(33)-H(33A)	109.7
C(32)-C(33)-H(33B)	110.4
H(33A)-C(33)-H(33B)	108.8
C(32)-C(33)-H(33C)	110.1
H(33A)-C(33)-H(33C)	108.9
H(33B)-C(33)-H(33C)	108.9

Table 16. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6b**.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
W	38(1)	49(1)	41(1)	2(1)	5(1)	0(1)
O(1)	71(8)	120(20)	105(11)	14(10)	51(8)	11(9)
O(2)	108(12)	72(11)	60(9)	-6(8)	12(8)	2(9)
O(3)	100(11)	125(13)	42(9)	-6(8)	-8(8)	-9(9)
O(4)	58(9)	270(40)	126(15)	-4(15)	35(9)	-56(14)
O(5)	74(11)	55(10)	192(19)	19(11)	36(12)	10(8)
O(6)	46(5)	47(5)	47(5)	-2(13)	10(4)	11(12)
O(7)	50(7)	35(6)	72(8)	-11(6)	23(6)	-11(5)
O(8)	78(10)	112(12)	58(9)	-1(8)	10(8)	36(9)
O(9)	51(8)	139(15)	41(8)	-2(8)	27(7)	16(9)
N(1)	25(7)	42(8)	97(13)	-32(8)	16(7)	-3(6)
C(1)	64(11)	100(30)	63(11)	38(13)	8(9)	0(12)
C(2)	64(12)	59(13)	46(11)	-43(10)	2(9)	-17(10)
C(3)	55(10)	110(20)	59(13)	10(11)	21(9)	1(11)
C(4)	60(11)	100(30)	74(12)	5(12)	28(9)	-17(12)
C(5)	56(11)	24(9)	72(12)	10(8)	16(10)	-2(8)
C(6)	42(8)	27(7)	44(9)	3(6)	10(7)	1(6)
C(7)	28(7)	55(10)	51(10)	20(8)	8(7)	6(7)

C(8)	38(8)	54(10)	64(12)	17(9)	17(8)	0(8)
C(9)	56(9)	32(8)	18(7)	-8(6)	7(6)	-12(7)
C(10)	40(8)	29(7)	29(8)	-5(6)	12(6)	-8(6)
C(11)	28(7)	39(8)	36(8)	-13(6)	3(6)	-12(6)
C(12)	43(9)	38(9)	59(11)	-33(8)	18(8)	-22(7)
C(13)	75(14)	59(13)	130(20)	-31(13)	40(14)	-4(11)
C(14)	52(14)	57(15)	73(18)	-16(12)	28(13)	-10(12)
C(15)	29(7)	68(11)	35(9)	-17(8)	10(6)	-18(7)
C(16)	33(9)	52(11)	77(14)	-40(10)	23(9)	-20(8)
C(17)	57(10)	81(13)	34(9)	-17(9)	25(8)	-8(10)
C(19)	61(13)	83(15)	110(20)	-19(14)	55(13)	-2(11)
C(20)	53(10)	31(9)	93(15)	4(9)	29(10)	2(8)
C(21)	48(9)	46(10)	45(10)	15(8)	3(8)	21(8)
C(22)	31(8)	53(10)	69(12)	9(8)	26(8)	-6(7)
C(23)	52(9)	134(19)	50(9)	10(20)	21(8)	-40(19)
C(24)	71(13)	40(10)	116(19)	-11(11)	47(13)	15(9)
C(25)	67(14)	93(17)	140(20)	-98(18)	32(15)	-16(13)
C(26)	79(16)	102(18)	72(16)	-36(12)	32(13)	2(13)
C(27)	68(12)	80(20)	38(10)	-6(8)	11(9)	9(10)
C(28)	47(11)	140(20)	80(16)	17(14)	23(10)	-52(13)
C(29)	63(11)	57(11)	70(13)	-1(9)	22(10)	-26(9)
C(30)	69(14)	73(15)	62(13)	40(12)	14(11)	9(12)
C(31)	52(12)	36(11)	39(11)	-6(8)	22(9)	-10(9)

Table 17. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6b**.

	x	y	z	U(eq)
H(8A)	8749	8975	683	64
H(8B)	8187	9978	890	64
H(13A)	9220	12240	3558	105
H(13B)	10027	11981	5014	105
H(14A)	8625	10836	4986	72
H(14B)	7679	11276	3675	72
H(17)	8046	9084	5348	66
H(18)	6434	8969	6147	128

H(19)	4241	8927	4798	95
H(20)	3678	9359	2698	70
H(21)	5251	9460	1898	61
H(23)	12584	7647	4534	94
H(24)	13378	6221	3993	87
H(25)	12916	5913	1860	121
H(26)	11650	7017	321	100
H(27)	10557	8251	838	76
H(28A)	10090	10941	1137	135
H(28B)	10877	10055	933	135
H(28C)	11447	10666	2197	135
H(29A)	6294	6294	1752	77
H(29B)	5282	7024	1913	77
H(30A)	6390	6847	4166	108
H(30B)	7222	6015	3909	108
H(30C)	5715	5880	3488	108
H(32A)	11281	8710	7733	107
H(32B)	12113	9678	7997	107
H(33A)	10528	9866	8825	143
H(33B)	9434	9599	7499	143
H(33C)	10208	10580	7666	143

Table 18. Torsion angles [deg] for **6b**.

C(5)-W-C(1)-O(1)	-111(12)
C(4)-W-C(1)-O(1)	-27(16)
C(3)-W-C(1)-O(1)	-20(12)
C(2)-W-C(1)-O(1)	67(12)
C(6)-W-C(1)-O(1)	162(12)
C(5)-W-C(2)-O(2)	51(29)
C(4)-W-C(2)-O(2)	86(9)
C(3)-W-C(2)-O(2)	4(9)
C(1)-W-C(2)-O(2)	-82(9)
C(6)-W-C(2)-O(2)	-178(9)
C(5)-W-C(3)-O(3)	12(82)
C(4)-W-C(3)-O(3)	101(82)
C(1)-W-C(3)-O(3)	-78(82)
C(2)-W-C(3)-O(3)	-169(82)

C(6)-W-C(3)-O(3)	49(90)
C(5)-W-C(4)-O(4)	64(23)
C(3)-W-C(4)-O(4)	-27(23)
C(1)-W-C(4)-O(4)	-20(27)
C(2)-W-C(4)-O(4)	-115(23)
C(6)-W-C(4)-O(4)	151(23)
C(4)-W-C(5)-O(5)	151(41)
C(3)-W-C(5)-O(5)	-126(41)
C(1)-W-C(5)-O(5)	-41(41)
C(2)-W-C(5)-O(5)	-174(32)
C(6)-W-C(5)-O(5)	55(41)
C(29)-O(6)-C(6)-C(7)	167.0(16)
C(29)-O(6)-C(6)-W	-8(2)
C(5)-W-C(6)-O(6)	134.0(14)
C(4)-W-C(6)-O(6)	45.7(15)
C(3)-W-C(6)-O(6)	97(14)
C(1)-W-C(6)-O(6)	-136.1(15)
C(2)-W-C(6)-O(6)	-44.7(14)
C(5)-W-C(6)-C(7)	-40.1(13)
C(4)-W-C(6)-C(7)	-128.3(14)
C(3)-W-C(6)-C(7)	-77(15)
C(1)-W-C(6)-C(7)	49.9(15)
C(2)-W-C(6)-C(7)	141.2(14)
O(6)-C(6)-C(7)-C(15)	-33.7(19)
W-C(6)-C(7)-C(15)	141.5(13)
O(6)-C(6)-C(7)-C(8)	155.5(14)
W-C(6)-C(7)-C(8)	-29(2)
C(15)-C(7)-C(8)-C(9)	53.1(19)
C(6)-C(7)-C(8)-C(9)	-135.4(16)
C(7)-C(8)-C(9)-C(12)	-40(2)
C(7)-C(8)-C(9)-C(10)	54(2)
C(7)-C(8)-C(9)-C(28)	-169.5(16)
C(8)-C(9)-C(10)-C(11)	-112.6(15)
C(12)-C(9)-C(10)-C(11)	-1.2(11)
C(28)-C(9)-C(10)-C(11)	111.3(15)
C(8)-C(9)-C(10)-C(22)	67(2)
C(12)-C(9)-C(10)-C(22)	178.8(15)
C(28)-C(9)-C(10)-C(22)	-69(2)
C(22)-C(10)-C(11)-C(31)	4(3)
C(9)-C(10)-C(11)-C(31)	-177(2)
C(22)-C(10)-C(11)-C(12)	-178.8(16)
C(9)-C(10)-C(11)-C(12)	1.2(11)
C(13)-O(7)-C(12)-N(1)	6(2)
C(13)-O(7)-C(12)-C(11)	-124.9(17)

C(13)-O(7)-C(12)-C(9)	129.4(17)
C(15)-N(1)-C(12)-O(7)	166.1(16)
C(14)-N(1)-C(12)-O(7)	-14(2)
C(15)-N(1)-C(12)-C(11)	-61(2)
C(14)-N(1)-C(12)-C(11)	118.3(17)
C(15)-N(1)-C(12)-C(9)	39(2)
C(14)-N(1)-C(12)-C(9)	-141.6(17)
C(10)-C(11)-C(12)-O(7)	-122.7(14)
C(31)-C(11)-C(12)-O(7)	55(2)
C(10)-C(11)-C(12)-N(1)	112.2(14)
C(31)-C(11)-C(12)-N(1)	-70(2)
C(10)-C(11)-C(12)-C(9)	-1.2(11)
C(31)-C(11)-C(12)-C(9)	176.9(17)
C(8)-C(9)-C(12)-O(7)	-120.3(15)
C(10)-C(9)-C(12)-O(7)	123.7(14)
C(28)-C(9)-C(12)-O(7)	9(2)
C(8)-C(9)-C(12)-N(1)	-1.3(19)
C(10)-C(9)-C(12)-N(1)	-117.3(13)
C(28)-C(9)-C(12)-N(1)	128.5(15)
C(8)-C(9)-C(12)-C(11)	117.0(13)
C(10)-C(9)-C(12)-C(11)	1.0(9)
C(28)-C(9)-C(12)-C(11)	-113.2(14)
C(12)-O(7)-C(13)-C(14)	4(2)
C(15)-N(1)-C(14)-C(13)	-163(2)
C(12)-N(1)-C(14)-C(13)	18(3)
O(7)-C(13)-C(14)-N(1)	-13(3)
C(14)-N(1)-C(15)-C(7)	152(2)
C(12)-N(1)-C(15)-C(7)	-29(3)
C(14)-N(1)-C(15)-C(16)	-25(3)
C(12)-N(1)-C(15)-C(16)	154.4(16)
C(6)-C(7)-C(15)-N(1)	170.5(15)
C(8)-C(7)-C(15)-N(1)	-18(2)
C(6)-C(7)-C(15)-C(16)	-13(3)
C(8)-C(7)-C(15)-C(16)	158.5(15)
N(1)-C(15)-C(16)-C(17)	-57(2)
C(7)-C(15)-C(16)-C(17)	126.3(19)
N(1)-C(15)-C(16)-C(21)	122.5(17)
C(7)-C(15)-C(16)-C(21)	-54(3)
C(21)-C(16)-C(17)-C(18)	0(3)
C(15)-C(16)-C(17)-C(18)	179.6(18)
C(16)-C(17)-C(18)-C(19)	4(4)
C(17)-C(18)-C(19)-C(20)	-7(4)
C(18)-C(19)-C(20)-C(21)	7(3)
C(19)-C(20)-C(21)-C(16)	-4(3)

C(17)-C(16)-C(21)-C(20)	0(3)
C(15)-C(16)-C(21)-C(20)	-179.3(15)
C(11)-C(10)-C(22)-C(23)	-8(3)
C(9)-C(10)-C(22)-C(23)	172.5(15)
C(11)-C(10)-C(22)-C(27)	176.8(17)
C(9)-C(10)-C(22)-C(27)	-3(2)
C(10)-C(22)-C(23)-C(24)	177.8(16)
C(27)-C(22)-C(23)-C(24)	-7(3)
C(22)-C(23)-C(24)-C(25)	7(3)
C(23)-C(24)-C(25)-C(26)	-1(3)
C(24)-C(25)-C(26)-C(27)	-6(3)
C(25)-C(26)-C(27)-C(22)	6(3)
C(23)-C(22)-C(27)-C(26)	0(3)
C(10)-C(22)-C(27)-C(26)	175.7(16)
C(6)-O(6)-C(29)-C(30)	172.4(17)
C(32)-O(9)-C(31)-O(8)	0(3)
C(32)-O(9)-C(31)-C(11)	176.0(16)
C(10)-C(11)-C(31)-O(8)	14(4)
C(12)-C(11)-C(31)-O(8)	-163.5(19)
C(10)-C(11)-C(31)-O(9)	-162.2(18)
C(12)-C(11)-C(31)-O(9)	21(3)
C(31)-O(9)-C(32)-C(33)	-173(2)

4. X-Ray Crystal Structure Information for 7.

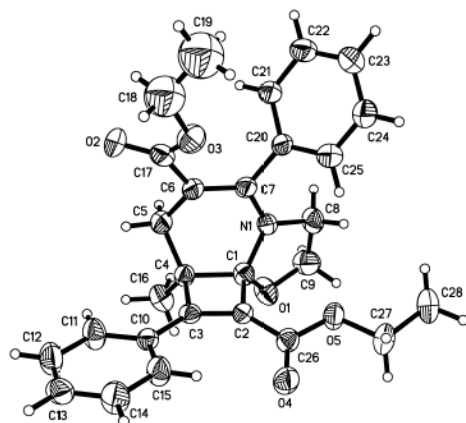


Table 19. Crystal data and structure refinement for 7.

Identification code	cd24278
Empirical formula	C ₂₈ H ₂₉ N O ₅

Formula weight	459.52
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 38.242(9) Å alpha = 90 deg. b = 7.1774(17) Å beta = 92.733(5) deg. c = 17.705(4) Å gamma = 90 deg.
Volume	4854.1(19) Å ³
Z, Calculated density	8, 1.258 Mg/m ³
Absorption coefficient	0.086 mm ⁻¹
F(000)	1952
Crystal size	0.378 x 0.153 x 0.068 mm
Theta range for data collection	2.13 to 26.00 deg.
Limiting indices	-46 ≤ h ≤ 45, -7 ≤ k ≤ 8, -18 ≤ l ≤ 21
Reflections collected / unique	12758 / 4754 [R(int) = 0.0837]
Completeness to theta = 26.00	99.8 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.76367
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4754 / 1 / 300
Goodness-of-fit on F ²	0.707
Final R indices [I > 2σ(I)]	R1 = 0.0583, wR2 = 0.1318
R indices (all data)	R1 = 0.1657, wR2 = 0.1543
Largest diff. peak and hole	0.572 and -0.276 e.Å ⁻³

Table 20. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	1021(1)	-947(4)	2276(1)	77(1)
O(2)	1731(1)	1323(5)	-719(2)	106(1)
O(3)	1722(1)	3969(5)	-56(2)	94(1)
O(4)	325(1)	3675(4)	1631(1)	82(1)
O(5)	790(1)	3371(4)	2433(1)	67(1)
N(1)	1408(1)	1071(4)	1802(2)	57(1)
C(1)	1072(1)	186(5)	1644(2)	55(1)
C(2)	768(1)	1446(5)	1389(2)	50(1)
C(3)	733(1)	675(5)	700(2)	48(1)

C(4)	1024(1)	-780(5)	856(2)	54(1)
C(5)	1349(1)	-561(6)	394(2)	69(1)
C(6)	1535(1)	1270(6)	525(2)	61(1)
C(7)	1590(1)	1890(6)	1249(2)	57(1)
C(8)	1502(1)	949(6)	2605(2)	71(1)
C(9)	1257(1)	-489(7)	2868(2)	88(1)
C(10)	516(1)	1010(5)	10(2)	51(1)
C(11)	528(1)	-186(6)	-597(2)	79(1)
C(12)	327(1)	112(7)	-1251(2)	89(1)
C(13)	109(1)	1582(7)	-1308(2)	79(1)
C(14)	96(1)	2785(7)	-717(3)	94(2)
C(15)	298(1)	2488(6)	-64(2)	77(1)
C(16)	907(1)	-2808(5)	880(2)	73(1)
C(17)	1673(1)	2128(8)	-138(3)	75(1)
C(18)	1894(2)	4922(9)	-656(3)	146(2)
C(19)	2107(2)	6350(9)	-437(4)	140(3)
C(20)	1854(1)	3309(6)	1495(2)	56(1)
C(21)	2198(1)	3103(6)	1309(2)	70(1)
C(22)	2447(1)	4414(7)	1526(2)	81(1)
C(23)	2356(1)	5907(7)	1946(3)	88(2)
C(24)	2015(1)	6119(6)	2143(2)	86(1)
C(25)	1766(1)	4822(6)	1917(2)	73(1)
C(26)	599(1)	2924(6)	1804(2)	58(1)
C(27)	652(1)	4821(6)	2908(2)	78(1)
C(28)	906(1)	5063(6)	3565(2)	96(2)

Table 21. Bond lengths [Å] and angles [deg] for **7**.

O(1)-C(9)	1.390(4)
O(1)-C(1)	1.405(4)
O(2)-C(17)	1.210(5)
O(3)-C(17)	1.341(5)
O(3)-C(18)	1.447(6)
O(4)-C(26)	1.205(4)
O(5)-C(26)	1.340(4)
O(5)-C(27)	1.454(4)
N(1)-C(7)	1.363(4)
N(1)-C(1)	1.449(4)

N(1)-C(8)	1.453(4)
C(1)-C(2)	1.522(5)
C(1)-C(4)	1.560(5)
C(2)-C(3)	1.340(4)
C(2)-C(26)	1.459(5)
C(3)-C(10)	1.463(4)
C(3)-C(4)	1.543(4)
C(4)-C(16)	1.524(5)
C(4)-C(5)	1.527(5)
C(5)-C(6)	1.507(5)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-C(7)	1.364(5)
C(6)-C(17)	1.448(5)
C(7)-C(20)	1.484(5)
C(8)-C(9)	1.484(5)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(15)	1.353(4)
C(10)-C(11)	1.378(5)
C(11)-C(12)	1.376(5)
C(11)-H(11)	0.9300
C(12)-C(13)	1.344(5)
C(12)-H(12)	0.9300
C(13)-C(14)	1.359(5)
C(13)-H(13)	0.9300
C(14)-C(15)	1.375(5)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(18)-C(19)	1.354(7)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-C(25)	1.369(5)
C(20)-C(21)	1.378(4)
C(21)-C(22)	1.380(5)
C(21)-H(21)	0.9300

C(22)-C(23)	1.359(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.374(5)
C(23)-H(23)	0.9300
C(24)-C(25)	1.377(5)
C(24)-H(24)	0.9300
C(25)-H(25)	0.9300
C(27)-C(28)	1.490(5)
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(9)-O(1)-C(1)	110.7(3)
C(17)-O(3)-C(18)	116.9(4)
C(26)-O(5)-C(27)	117.0(3)
C(7)-N(1)-C(1)	122.1(3)
C(7)-N(1)-C(8)	128.1(3)
C(1)-N(1)-C(8)	109.8(3)
O(1)-C(1)-N(1)	104.8(3)
O(1)-C(1)-C(2)	116.6(3)
N(1)-C(1)-C(2)	117.0(3)
O(1)-C(1)-C(4)	116.2(3)
N(1)-C(1)-C(4)	115.5(3)
C(2)-C(1)-C(4)	86.9(3)
C(3)-C(2)-C(26)	137.0(3)
C(3)-C(2)-C(1)	93.8(3)
C(26)-C(2)-C(1)	129.2(3)
C(2)-C(3)-C(10)	136.1(4)
C(2)-C(3)-C(4)	94.4(3)
C(10)-C(3)-C(4)	129.5(3)
C(16)-C(4)-C(5)	111.2(3)
C(16)-C(4)-C(3)	116.1(3)
C(5)-C(4)-C(3)	115.7(3)
C(16)-C(4)-C(1)	114.9(3)
C(5)-C(4)-C(1)	111.8(3)
C(3)-C(4)-C(1)	84.9(3)
C(6)-C(5)-C(4)	113.4(3)
C(6)-C(5)-H(5A)	108.9
C(4)-C(5)-H(5A)	108.9
C(6)-C(5)-H(5B)	108.9
C(4)-C(5)-H(5B)	108.9
H(5A)-C(5)-H(5B)	107.7
C(7)-C(6)-C(17)	125.2(4)

C(7)-C(6)-C(5)	118.7(4)
C(17)-C(6)-C(5)	115.8(4)
N(1)-C(7)-C(6)	118.1(4)
N(1)-C(7)-C(20)	116.7(3)
C(6)-C(7)-C(20)	125.0(4)
N(1)-C(8)-C(9)	102.6(3)
N(1)-C(8)-H(8A)	111.3
C(9)-C(8)-H(8A)	111.3
N(1)-C(8)-H(8B)	111.3
C(9)-C(8)-H(8B)	111.3
H(8A)-C(8)-H(8B)	109.2
O(1)-C(9)-C(8)	109.0(3)
O(1)-C(9)-H(9A)	109.9
C(8)-C(9)-H(9A)	109.9
O(1)-C(9)-H(9B)	109.9
C(8)-C(9)-H(9B)	109.9
H(9A)-C(9)-H(9B)	108.3
C(15)-C(10)-C(11)	117.0(3)
C(15)-C(10)-C(3)	122.2(4)
C(11)-C(10)-C(3)	120.8(4)
C(12)-C(11)-C(10)	121.5(4)
C(12)-C(11)-H(11)	119.2
C(10)-C(11)-H(11)	119.2
C(13)-C(12)-C(11)	120.2(4)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	119.2(4)
C(12)-C(13)-H(13)	120.4
C(14)-C(13)-H(13)	120.4
C(13)-C(14)-C(15)	120.5(4)
C(13)-C(14)-H(14)	119.7
C(15)-C(14)-H(14)	119.7
C(10)-C(15)-C(14)	121.5(4)
C(10)-C(15)-H(15)	119.3
C(14)-C(15)-H(15)	119.3
C(4)-C(16)-H(16A)	109.5
C(4)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(4)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(2)-C(17)-O(3)	122.2(5)
O(2)-C(17)-C(6)	125.1(5)
O(3)-C(17)-C(6)	112.7(4)

C(19)-C(18)-O(3)	115.7(6)
C(19)-C(18)-H(18A)	108.3
O(3)-C(18)-H(18A)	108.3
C(19)-C(18)-H(18B)	108.4
O(3)-C(18)-H(18B)	108.3
H(18A)-C(18)-H(18B)	107.4
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(25)-C(20)-C(21)	118.6(4)
C(25)-C(20)-C(7)	121.5(3)
C(21)-C(20)-C(7)	119.9(4)
C(20)-C(21)-C(22)	120.9(4)
C(20)-C(21)-H(21)	119.5
C(22)-C(21)-H(21)	119.5
C(23)-C(22)-C(21)	119.8(4)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(24)	119.9(4)
C(22)-C(23)-H(23)	120.1
C(24)-C(23)-H(23)	120.1
C(23)-C(24)-C(25)	120.2(4)
C(23)-C(24)-H(24)	119.9
C(25)-C(24)-H(24)	119.9
C(20)-C(25)-C(24)	120.6(4)
C(20)-C(25)-H(25)	119.7
C(24)-C(25)-H(25)	119.7
O(4)-C(26)-O(5)	122.4(4)
O(4)-C(26)-C(2)	126.7(4)
O(5)-C(26)-C(2)	110.9(3)
O(5)-C(27)-C(28)	107.1(3)
O(5)-C(27)-H(27A)	110.3
C(28)-C(27)-H(27A)	110.3
O(5)-C(27)-H(27B)	110.3
C(28)-C(27)-H(27B)	110.3
H(27A)-C(27)-H(27B)	108.5
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5

Table 22. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7**. The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
O(1)	97(2)	76(2)	56(2)	16(2)	-14(2)	-20(2)
O(2)	96(2)	169(3)	54(2)	-30(2)	20(2)	-17(2)
O(3)	101(2)	129(3)	53(2)	19(2)	17(2)	-32(2)
O(4)	73(2)	97(2)	74(2)	-15(2)	-5(2)	29(2)
O(5)	75(2)	73(2)	52(2)	-13(2)	-1(1)	10(2)
N(1)	51(2)	78(2)	41(2)	-2(2)	-3(2)	-3(2)
C(1)	63(3)	59(3)	42(2)	9(2)	0(2)	-4(2)
C(2)	48(2)	57(3)	45(2)	-1(2)	4(2)	-2(2)
C(3)	44(2)	51(3)	50(2)	6(2)	5(2)	-4(2)
C(4)	55(2)	56(3)	50(2)	-3(2)	1(2)	6(2)
C(5)	57(3)	86(3)	63(3)	-16(2)	0(2)	8(2)
C(6)	47(2)	85(3)	52(3)	-8(2)	3(2)	6(2)
C(7)	43(2)	78(3)	49(2)	-3(2)	-1(2)	9(2)
C(8)	77(3)	84(3)	49(3)	3(2)	-12(2)	6(3)
C(9)	76(3)	120(4)	67(3)	22(3)	-4(3)	-2(3)
C(10)	49(2)	57(3)	45(2)	2(2)	3(2)	1(2)
C(11)	96(3)	77(3)	63(3)	-8(3)	-19(3)	28(3)
C(12)	102(4)	105(4)	58(3)	-12(3)	-12(3)	11(3)
C(13)	63(3)	110(4)	62(3)	15(3)	-8(2)	7(3)
C(14)	96(3)	105(4)	78(3)	-5(3)	-16(3)	42(3)
C(15)	82(3)	92(4)	56(3)	-8(2)	-15(2)	31(3)
C(16)	84(3)	57(3)	76(3)	2(2)	-18(2)	4(3)
C(17)	48(3)	114(5)	60(3)	-4(3)	-6(2)	-10(3)
C(20)	47(2)	75(3)	44(2)	-2(2)	1(2)	2(2)
C(21)	49(2)	96(4)	64(3)	-12(2)	-1(2)	3(3)
C(22)	53(3)	112(4)	77(3)	-3(3)	0(2)	-5(3)
C(23)	79(4)	102(4)	83(3)	-14(3)	3(3)	-24(3)
C(24)	87(3)	82(4)	88(3)	-24(3)	15(3)	-8(3)
C(25)	58(3)	84(4)	76(3)	-5(3)	4(2)	-1(3)

C(26)	62(3)	62(3)	50(3)	2(2)	6(2)	-2(2)
C(27)	102(3)	71(3)	62(3)	-18(2)	10(3)	7(3)
C(28)	128(4)	96(4)	62(3)	-22(3)	-5(3)	-2(3)

Table 23. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7**.

	x	y	z	U(eq)
H(5A)	1511	-1567	521	82
H(5B)	1280	-671	-139	82
H(8A)	1467	2132	2856	85
H(8B)	1744	563	2691	85
H(9A)	1387	-1589	3034	106
H(9B)	1132	-15	3292	106
H(11)	674	-1219	-564	95
H(12)	341	-707	-1656	107
H(13)	-30	1774	-1745	94
H(14)	-50	3819	-755	112
H(15)	283	3321	336	93
H(16A)	869	-3267	373	110
H(16B)	693	-2893	1140	110
H(16C)	1084	-3541	1141	110
H(18A)	2031	4018	-923	147
H(18B)	1715	5399	-1013	147
H(19A)	1969	7343	-241	144
H(19B)	2229	6793	-863	144
H(19C)	2273	5927	-51	144
H(21)	2263	2067	1034	84
H(22)	2677	4276	1385	97
H(23)	2524	6783	2100	106
H(24)	1952	7140	2430	103
H(25)	1536	4975	2052	87
H(27A)	424	4461	3081	94
H(27B)	626	5977	2628	94
H(28A)	931	3906	3834	143
H(28B)	822	6002	3897	143
H(28C)	1129	5435	3388	143

Table 24. Torsion angles [deg] for 7.

C(9)-O(1)-C(1)-N(1)	13.7(4)
C(9)-O(1)-C(1)-C(2)	-117.3(4)
C(9)-O(1)-C(1)-C(4)	142.5(3)
C(7)-N(1)-C(1)-O(1)	162.6(3)
C(8)-N(1)-C(1)-O(1)	-18.2(4)
C(7)-N(1)-C(1)-C(2)	-66.6(4)
C(8)-N(1)-C(1)-C(2)	112.6(3)
C(7)-N(1)-C(1)-C(4)	33.5(5)
C(8)-N(1)-C(1)-C(4)	-147.3(3)
O(1)-C(1)-C(2)-C(3)	-119.9(3)
N(1)-C(1)-C(2)-C(3)	115.0(3)
C(4)-C(1)-C(2)-C(3)	-2.1(3)
O(1)-C(1)-C(2)-C(26)	60.1(5)
N(1)-C(1)-C(2)-C(26)	-64.9(5)
C(4)-C(1)-C(2)-C(26)	177.9(4)
C(26)-C(2)-C(3)-C(10)	3.8(7)
C(1)-C(2)-C(3)-C(10)	-176.2(4)
C(26)-C(2)-C(3)-C(4)	-177.9(4)
C(1)-C(2)-C(3)-C(4)	2.2(3)
C(2)-C(3)-C(4)-C(16)	113.2(3)
C(10)-C(3)-C(4)-C(16)	-68.3(5)
C(2)-C(3)-C(4)-C(5)	-113.8(3)
C(10)-C(3)-C(4)-C(5)	64.7(5)
C(2)-C(3)-C(4)-C(1)	-2.1(3)
C(10)-C(3)-C(4)-C(1)	176.4(3)
O(1)-C(1)-C(4)-C(16)	3.7(4)
N(1)-C(1)-C(4)-C(16)	127.0(3)
C(2)-C(1)-C(4)-C(16)	-114.5(3)
O(1)-C(1)-C(4)-C(5)	-124.3(3)
N(1)-C(1)-C(4)-C(5)	-1.0(4)
C(2)-C(1)-C(4)-C(5)	117.5(3)
O(1)-C(1)-C(4)-C(3)	120.0(3)
N(1)-C(1)-C(4)-C(3)	-116.6(3)
C(2)-C(1)-C(4)-C(3)	1.9(2)
C(16)-C(4)-C(5)-C(6)	-164.0(3)
C(3)-C(4)-C(5)-C(6)	60.8(4)

C(1)-C(4)-C(5)-C(6)	-34.1(4)
C(4)-C(5)-C(6)-C(7)	45.4(4)
C(4)-C(5)-C(6)-C(17)	-141.2(3)
C(1)-N(1)-C(7)-C(6)	-25.8(5)
C(8)-N(1)-C(7)-C(6)	155.1(3)
C(1)-N(1)-C(7)-C(20)	158.3(3)
C(8)-N(1)-C(7)-C(20)	-20.8(5)
C(17)-C(6)-C(7)-N(1)	172.1(3)
C(5)-C(6)-C(7)-N(1)	-15.1(5)
C(17)-C(6)-C(7)-C(20)	-12.4(6)
C(5)-C(6)-C(7)-C(20)	160.4(3)
C(7)-N(1)-C(8)-C(9)	-165.6(4)
C(1)-N(1)-C(8)-C(9)	15.2(4)
C(1)-O(1)-C(9)-C(8)	-4.5(4)
N(1)-C(8)-C(9)-O(1)	-6.6(4)
C(2)-C(3)-C(10)-C(15)	5.6(6)
C(4)-C(3)-C(10)-C(15)	-172.2(3)
C(2)-C(3)-C(10)-C(11)	-174.4(4)
C(4)-C(3)-C(10)-C(11)	7.8(6)
C(15)-C(10)-C(11)-C(12)	0.2(6)
C(3)-C(10)-C(11)-C(12)	-179.8(4)
C(10)-C(11)-C(12)-C(13)	-0.8(7)
C(11)-C(12)-C(13)-C(14)	1.2(7)
C(12)-C(13)-C(14)-C(15)	-1.1(7)
C(11)-C(10)-C(15)-C(14)	-0.1(6)
C(3)-C(10)-C(15)-C(14)	179.9(4)
C(13)-C(14)-C(15)-C(10)	0.6(7)
C(18)-O(3)-C(17)-O(2)	-8.2(6)
C(18)-O(3)-C(17)-C(6)	173.8(3)
C(7)-C(6)-C(17)-O(2)	153.1(4)
C(5)-C(6)-C(17)-O(2)	-19.9(6)
C(7)-C(6)-C(17)-O(3)	-28.9(5)
C(5)-C(6)-C(17)-O(3)	158.1(3)
C(17)-O(3)-C(18)-C(19)	-145.2(5)
N(1)-C(7)-C(20)-C(25)	-55.4(5)
C(6)-C(7)-C(20)-C(25)	129.0(4)
N(1)-C(7)-C(20)-C(21)	123.6(4)
C(6)-C(7)-C(20)-C(21)	-51.9(5)
C(25)-C(20)-C(21)-C(22)	-1.6(6)
C(7)-C(20)-C(21)-C(22)	179.4(3)
C(20)-C(21)-C(22)-C(23)	1.8(6)
C(21)-C(22)-C(23)-C(24)	-1.0(7)
C(22)-C(23)-C(24)-C(25)	0.1(7)
C(21)-C(20)-C(25)-C(24)	0.7(6)

C(7)-C(20)-C(25)-C(24)	179.7(4)
C(23)-C(24)-C(25)-C(20)	0.1(6)
C(27)-O(5)-C(26)-O(4)	0.1(5)
C(27)-O(5)-C(26)-C(2)	-179.6(3)
C(3)-C(2)-C(26)-O(4)	13.4(7)
C(1)-C(2)-C(26)-O(4)	-166.7(4)
C(3)-C(2)-C(26)-O(5)	-167.0(4)
C(1)-C(2)-C(26)-O(5)	12.9(5)
C(26)-O(5)-C(27)-C(28)	179.8(3)
