

SUPP-Table 1. Crystal data and structure refinement for Compound 6.

Identification code	jmwbp70
Empirical formula	C11 H10 O2
Formula weight	174.19
Temperature	130.0(1) K
Radiation	CuK α
Wavelength	1.54180 Å
Crystal system	orthorhombic
Space group	Pbca
Unit cell dimensions:	
a	11.7130(10) Å
b	12.4643(10) Å
c	11.9420(10) Å
α	
β	
γ	
Volume	1743.5(3) Å ³
Z	8
Density (calculated)	1.327 Mg/m ³
μ	0.736 mm ⁻¹
F(000)	736
Crystal size	1.0 x 0.22 x 0.03 mm ³
θ range for data collection	6.37 to 74.77 °
Index ranges	-14 \leq h \leq 14 -1 \leq k \leq 15 -14 \leq l \leq 1
No. Intensity Control Reflections	3
Measurement interval	160
Decomposition	< 2%, corrections applied to data
Reflections collected	2686
Independent reflections	1777

R_{int}	0.0346
No. of Observed Reflections	1425
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1777 / 0 / 159
Goodness-of-fit on F^2	1.023
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0406$
	$wR_2 = 0.1022$
R indices (all data)	$R_1 = 0.0538$
	$wR_2 = 0.1117$
Weighting Scheme:	
calc $w = 1/[\sigma^2(Fo^2) + (0.0610P)^2 + 0.4532P]$	$A = 0.0610$
where $P = (Fo^2 + 2Fc^2)/3$	$B = 0.4532$
Extinction method	SHELXL
Extinction coefficient	0.0010(4)
Absorption Method	Analytical
Max. min Trans.	0.98 0.83.
Maximum shift/e.s.d.	0.001
Largest diff. peak and hole	0.239, -0.241 e.Å ⁻³

SUPP- Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x/a	y/b	z/c	U(eq)
O(1)	1939(1)	5783(1)	2433(1)	36(1)
O(2)	1772(1)	2282(1)	-158(1)	42(1)
C(1)	1426(1)	3941(1)	2422(1)	24(1)
C(2)	1957(1)	4931(1)	1927(1)	24(1)
C(3)	2509(1)	4876(1)	820(1)	29(1)
C(4)	2462(1)	4008(1)	169(1)	30(1)
C(5)	1857(1)	3024(1)	506(1)	28(1)
C(6)	1357(1)	2935(1)	1660(1)	25(1)
C(7)	37(1)	2694(1)	1631(2)	33(1)
C(8)	-508(1)	3621(2)	1023(2)	38(1)
C(9)	-450(1)	4472(1)	1688(2)	37(1)
C(10)	144(1)	4131(1)	2753(1)	32(1)
C(11)	-264(1)	2964(1)	2843(2)	38(1)

SUPP-Table 3. Bond lengths [Å], angles [°], and Torsion Angles for Compound 6.

Distances [Å]

O(1)-C(2)	1.2220(18)	O(2)-C(5)	1.2214(19)
C(1)-C(2)	1.503(2)	C(1)-C(6)	1.5509(19)
C(1)-C(10)	1.571(2)	C(1)-H(1)	0.950(18)
C(2)-C(3)	1.473(2)	C(3)-C(4)	1.334(2)
C(3)-H(3)	0.96(2)	C(4)-C(5)	1.473(2)
C(4)-H(4)	1.011(19)	C(5)-C(6)	1.501(2)
C(6)-C(7)	1.575(2)	C(6)-H(6)	0.972(19)
C(7)-C(8)	1.507(2)	C(7)-C(11)	1.527(3)
C(7)-H(7)	0.953(19)	C(8)-C(9)	1.327(3)
C(8)-H(8)	0.96(2)	C(9)-C(10)	1.512(2)
C(9)-H(9)	0.97(2)	C(10)-C(11)	1.535(2)
C(10)-H(10)	0.99(2)	C(11)-H(11A)	1.00(2)
C(11)-H(11B)	1.01(2)		

Angles [°]

C(2)-C(1)-C(6)	117.03(12)	C(2)-C(1)-C(10)	111.76(12)
C(6)-C(1)-C(10)	102.69(11)	C(2)-C(1)-H(1)	106.2(11)
C(6)-C(1)-H(1)	108.6(11)	C(10)-C(1)-H(1)	110.5(11)
O(1)-C(2)-C(3)	119.42(13)	O(1)-C(2)-C(1)	120.82(13)
C(3)-C(2)-C(1)	119.76(13)	C(4)-C(3)-C(2)	122.85(14)
C(4)-C(3)-H(3)	123.2(11)	C(2)-C(3)-H(3)	113.9(11)
C(3)-C(4)-C(5)	122.43(14)	C(3)-C(4)-H(4)	120.9(10)
C(5)-C(4)-H(4)	116.6(10)	O(2)-C(5)-C(4)	119.46(14)
O(2)-C(5)-C(6)	120.56(14)	C(4)-C(5)-C(6)	119.99(13)
C(5)-C(6)-C(1)	117.32(12)	C(5)-C(6)-C(7)	112.12(12)
C(1)-C(6)-C(7)	102.61(11)	C(5)-C(6)-H(6)	105.8(11)
C(1)-C(6)-H(6)	110.5(11)	C(7)-C(6)-H(6)	108.3(11)
C(8)-C(7)-C(11)	100.95(14)	C(8)-C(7)-C(6)	106.26(12)

C(11)-C(7)-C(6)	99.45(13)	C(8)-C(7)-H(7)	118.3(12)
C(11)-C(7)-H(7)	117.2(12)	C(6)-C(7)-H(7)	112.4(12)
C(9)-C(8)-C(7)	107.62(16)	C(9)-C(8)-H(8)	127.8(13)
C(7)-C(8)-H(8)	124.4(13)	C(8)-C(9)-C(10)	107.60(15)
C(8)-C(9)-H(9)	129.5(13)	C(10)-C(9)-H(9)	122.6(13)
C(9)-C(10)-C(11)	100.50(14)	C(9)-C(10)-C(1)	105.68(12)
C(11)-C(10)-C(1)	99.94(12)	C(9)-C(10)-H(10)	116.6(11)
C(11)-C(10)-H(10)	116.8(11)	C(1)-C(10)-H(10)	115.0(12)
C(7)-C(11)-C(10)	94.05(13)	C(7)-C(11)-H(11A)	112.0(12)
C(10)-C(11)-H(11A)	113.4(11)	C(7)-C(11)-H(11B)	113.3(11)
C(10)-C(11)-H(11B)	113.5(11)	H(11A)-C(11)-H(11B)	109.9(16)

Torsion angles [°]

C(6)-C(1)-C(2)-O(1)	172.60(12)	C(10)-C(1)-C(2)-O(1)	54.61(18)
C(6)-C(1)-C(2)-C(3)	-7.56(18)	C(10)-C(1)-C(2)-C(3)	-125.54(14)
O(1)-C(2)-C(3)-C(4)	-172.94(15)	C(1)-C(2)-C(3)-C(4)	7.2(2)
C(2)-C(3)-C(4)-C(5)	-0.4(2)	C(3)-C(4)-C(5)-O(2)	174.73(14)
C(3)-C(4)-C(5)-C(6)	-5.7(2)	O(2)-C(5)-C(6)-C(1)	-175.78(13)
C(4)-C(5)-C(6)-C(1)	4.65(18)	O(2)-C(5)-C(6)-C(7)	-57.41(18)
C(4)-C(5)-C(6)-C(7)	123.02(14)	C(2)-C(1)-C(6)-C(5)	1.79(18)
C(10)-C(1)-C(6)-C(5)	124.58(13)	C(2)-C(1)-C(6)-C(7)	-121.56(13)
C(10)-C(1)-C(6)-C(7)	1.23(14)	C(5)-C(6)-C(7)-C(8)	-60.42(17)
C(1)-C(6)-C(7)-C(8)	66.35(16)	C(5)-C(6)-C(7)-C(11)	-164.84(12)
C(1)-C(6)-C(7)-C(11)	-38.08(14)	C(11)-C(7)-C(8)-C(9)	32.55(16)
C(6)-C(7)-C(8)-C(9)	-70.79(17)	C(7)-C(8)-C(9)-C(10)	0.35(17)
C(8)-C(9)-C(10)-C(11)	-32.88(16)	C(8)-C(9)-C(10)-C(1)	70.67(16)
C(2)-C(1)-C(10)-C(9)	58.13(16)	C(6)-C(1)-C(10)-C(9)	-68.14(14)
C(2)-C(1)-C(10)-C(11)	162.09(13)	C(6)-C(1)-C(10)-C(11)	35.83(15)
C(8)-C(7)-C(11)-C(10)	-49.07(14)	C(6)-C(7)-C(11)-C(10)	59.67(13)
C(9)-C(10)-C(11)-C(7)	49.09(14)	C(1)-C(10)-C(11)-C(7)	-59.06(14)

SUPP-Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 6. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
O(1)	43(1)	26(1)	38(1)	-5(1)	0(1)	-4(1)
O(2)	54(1)	35(1)	37(1)	-12(1)	-2(1)	5(1)
C(1)	22(1)	26(1)	23(1)	1(1)	-1(1)	0(1)
C(2)	22(1)	23(1)	29(1)	1(1)	-4(1)	1(1)
C(3)	28(1)	28(1)	32(1)	6(1)	1(1)	-1(1)
C(4)	29(1)	36(1)	26(1)	3(1)	2(1)	5(1)
C(5)	27(1)	26(1)	31(1)	-3(1)	-5(1)	8(1)
C(6)	22(1)	20(1)	32(1)	2(1)	-3(1)	2(1)
C(7)	25(1)	29(1)	46(1)	-3(1)	-2(1)	-5(1)
C(8)	21(1)	47(1)	47(1)	1(1)	-7(1)	2(1)
C(9)	21(1)	35(1)	55(1)	4(1)	2(1)	6(1)
C(10)	26(1)	32(1)	38(1)	-4(1)	8(1)	-1(1)
C(11)	29(1)	38(1)	45(1)	3(1)	8(1)	-7(1)

SUPP-Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 6.

	x/a	y/b	z/c	U(eq)
H(1)	1867(15)	3767(14)	3064(15)	31(4)
H(3)	2881(17)	5531(16)	599(16)	38(5)
H(4)	2818(16)	4008(14)	-603(16)	36(5)
H(6)	1740(16)	2331(15)	2010(16)	32(4)
H(7)	-127(17)	1985(15)	1379(16)	42(5)
H(8)	-788(19)	3590(17)	267(18)	48(6)
H(9)	-657(17)	5211(17)	1537(17)	46(5)
H(10)	26(17)	4592(15)	3417(17)	43(5)
H(11A)	-1099(18)	2898(15)	2988(17)	42(5)
H(11B)	177(17)	2525(16)	3408(17)	39(5)

SUPP- Table 7. Crystal data and structure refinement for Compound 7.

Identification code	jmwbp91
Empirical formula	C11 H12 O2
Formula weight	176.21
Temperature	200.0(1) K
Radiation	MoK α
Wavelength	0.71069 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions:	
a	10.863(3) Å
b	10.452(2) Å
c	15.973(5) Å
α	
β	
γ	
Volume	1813.6(8) Å ³
Z	8
Density (calculated)	1.291 Mg/m ³
μ	0.088 mm ⁻¹
F(000)	752
Crystal size	0.5 x 0.2 x 0.25 mm ³
θ range for data collection	2.55 to 27.47 °
Index ranges	-1 \leq h \leq 14 -11 \leq k \leq 13 -1 \leq l \leq 20
No. Intensity Control Reflections	3
Measurement interval	160
Decomposition	< 2%, corrections applied to data
Reflections collected	2854

Independent reflections	2074
R_{int}	0.0227
No. of Observed Reflections	1655
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2074 / 0 / 175
Goodness-of-fit on F^2	1.033
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0396$ $wR_2 = 0.0938$
R indices (all data)	$R_1 = 0.0538$ $wR_2 = 0.1017$
Weighting Scheme:	
calc $w = 1/[\sigma^2(\text{Fo}^2) + (0.0520\text{P})^2 + 0.3967\text{P}]$	$A = 0.0520$
where $\text{P} = (\text{Fo}^2 + 2\text{Fc}^2)/3$	$B = 0.3967$
Extinction method	SHELXL
Extinction coefficient	0.028(2)
Maximum shift/e.s.d.	0.001
Largest diff. peak and hole	0.268, -0.186 e.Å ⁻³

SUPP-Table 8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 7. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x/a	y/b	z/c	U(eq)
O(1)	5752(1)	372(1)	2836(1)	39(1)
O(2)	1536(1)	3017(1)	3085(1)	45(1)
C(1)	4157(1)	938(1)	3781(1)	26(1)
C(2)	4692(1)	723(1)	2920(1)	27(1)
C(3)	3844(1)	938(1)	2194(1)	33(1)
C(4)	3211(1)	2243(1)	2268(1)	33(1)
C(5)	2472(1)	2377(1)	3058(1)	30(1)
C(6)	2940(1)	1731(1)	3846(1)	28(1)
C(7)	3241(1)	2711(1)	4548(1)	32(1)
C(8)	4127(1)	3725(1)	4201(1)	31(1)
C(9)	5336(1)	2959(1)	4070(1)	33(1)
C(10)	5012(1)	1616(1)	4406(1)	32(1)
C(11)	4110(2)	1933(2)	5110(1)	41(1)

SUPP-Table 9. Bond lengths [Å], angles [°], and Torsion Angles for Compound 7.

Distances [Å]

O(1)-C(2)	1.2160(16)	O(2)-C(5)	1.2172(16)
C(1)-C(2)	1.5100(19)	C(1)-C(10)	1.5370(18)
C(1)-C(6)	1.5634(17)	C(1)-H(1)	0.985(16)
C(2)-C(3)	1.4977(19)	C(3)-C(4)	1.5315(19)
C(3)-H(3A)	0.964(17)	C(3)-H(3B)	0.966(17)
C(4)-C(5)	1.502(2)	C(4)-H(4A)	0.977(18)
C(4)-H(4B)	0.959(17)	C(5)-C(6)	1.5157(19)
C(6)-C(7)	1.5534(18)	C(6)-H(6)	0.956(16)
C(7)-C(8)	1.5342(19)	C(7)-C(11)	1.535(2)
C(7)-H(7)	0.977(17)	C(8)-C(9)	1.5529(19)
C(8)-H(8A)	0.989(17)	C(8)-H(8B)	0.993(17)
C(9)-C(10)	1.5436(19)	C(9)-H(9A)	0.981(18)
C(9)-H(9B)	0.964(18)	C(10)-C(11)	1.529(2)
C(10)-H(10)	0.976(16)	C(11)-H(11A)	1.001(19)
C(11)-H(11B)	0.988(18)		

Angles [°].

C(2)-C(1)-C(10)	115.27(11)	C(2)-C(1)-C(6)	117.68(11)
C(10)-C(1)-C(6)	102.93(10)	C(2)-C(1)-H(1)	103.3(9)
C(10)-C(1)-H(1)	110.1(9)	C(6)-C(1)-H(1)	107.4(9)
O(1)-C(2)-C(3)	122.85(13)	O(1)-C(2)-C(1)	120.66(12)
C(3)-C(2)-C(1)	116.47(11)	C(2)-C(3)-C(4)	110.49(11)
C(2)-C(3)-H(3A)	110.2(10)	C(4)-C(3)-H(3A)	111.4(10)
C(2)-C(3)-H(3B)	107.7(10)	C(4)-C(3)-H(3B)	109.4(10)
H(3A)-C(3)-H(3B)	107.6(13)	C(5)-C(4)-C(3)	112.82(11)
C(5)-C(4)-H(4A)	105.3(10)	C(3)-C(4)-H(4A)	110.5(10)
C(5)-C(4)-H(4B)	109.0(10)	C(3)-C(4)-H(4B)	112.4(10)
H(4A)-C(4)-H(4B)	106.3(14)	O(2)-C(5)-C(4)	121.81(13)
O(2)-C(5)-C(6)	119.71(13)	C(4)-C(5)-C(6)	118.43(11)

C(5)-C(6)-C(7)	112.11(10)	C(5)-C(6)-C(1)	117.71(11)
C(7)-C(6)-C(1)	102.67(10)	C(5)-C(6)-H(6)	105.9(9)
C(7)-C(6)-H(6)	109.1(9)	C(1)-C(6)-H(6)	109.2(9)
C(8)-C(7)-C(11)	101.06(12)	C(8)-C(7)-C(6)	109.06(11)
C(11)-C(7)-C(6)	101.67(11)	C(8)-C(7)-H(7)	113.2(9)
C(11)-C(7)-H(7)	117.7(10)	C(6)-C(7)-H(7)	112.9(10)
C(7)-C(8)-C(9)	102.90(11)	C(7)-C(8)-H(8A)	107.9(9)
C(9)-C(8)-H(8A)	110.6(9)	C(7)-C(8)-H(8B)	112.6(9)
C(9)-C(8)-H(8B)	113.3(9)	H(8A)-C(8)-H(8B)	109.4(13)
C(10)-C(9)-C(8)	103.23(11)	C(10)-C(9)-H(9A)	110.3(10)
C(8)-C(9)-H(9A)	112.0(10)	C(10)-C(9)-H(9B)	112.2(10)
C(8)-C(9)-H(9B)	112.3(10)	H(9A)-C(9)-H(9B)	106.8(14)
C(11)-C(10)-C(1)	100.93(12)	C(11)-C(10)-C(9)	101.82(11)
C(1)-C(10)-C(9)	109.35(11)	C(11)-C(10)-H(10)	116.8(10)
C(1)-C(10)-H(10)	112.4(9)	C(9)-C(10)-H(10)	114.3(9)
C(10)-C(11)-C(7)	94.51(11)	C(10)-C(11)-H(11A)	111.3(11)
C(7)-C(11)-H(11A)	111.7(10)	C(10)-C(11)-H(11B)	114.4(10)
C(7)-C(11)-H(11B)	112.1(10)	H(11A)-C(11)-H(11B)	111.8(15)

Torsion angles [°].

C(10)-C(1)-C(2)-O(1)	41.83(16)	C(6)-C(1)-C(2)-O(1)	163.65(11)
C(10)-C(1)-C(2)-C(3)	-139.46(12)	C(6)-C(1)-C(2)-C(3)	-17.65(16)
O(1)-C(2)-C(3)-C(4)	-130.65(13)	C(1)-C(2)-C(3)-C(4)	50.68(15)
C(2)-C(3)-C(4)-C(5)	-59.13(16)	C(3)-C(4)-C(5)-O(2)	-147.73(13)
C(3)-C(4)-C(5)-C(6)	34.53(17)	O(2)-C(5)-C(6)-C(7)	-60.30(16)
C(4)-C(5)-C(6)-C(7)	117.48(13)	O(2)-C(5)-C(6)-C(1)	-179.05(11)
C(4)-C(5)-C(6)-C(1)	-1.26(17)	C(2)-C(1)-C(6)-C(5)	-7.85(16)
C(10)-C(1)-C(6)-C(5)	120.10(12)	C(2)-C(1)-C(6)-C(7)	-131.49(11)
C(10)-C(1)-C(6)-C(7)	-3.53(12)	C(5)-C(6)-C(7)-C(8)	-53.60(14)
C(1)-C(6)-C(7)-C(8)	73.68(13)	C(5)-C(6)-C(7)-C(11)	-159.79(11)
C(1)-C(6)-C(7)-C(11)	-32.50(13)	C(11)-C(7)-C(8)-C(9)	37.71(13)

C(6)-C(7)-C(8)-C(9)	-68.89(13)	C(7)-C(8)-C(9)-C(10)	-3.07(14)
C(2)-C(1)-C(10)-C(11)	168.01(10)	C(6)-C(1)-C(10)-C(11)	38.55(12)
C(2)-C(1)-C(10)-C(9)	61.22(14)	C(6)-C(1)-C(10)-C(9)	-68.24(13)
C(8)-C(9)-C(10)-C(11)	-32.80(14)	C(8)-C(9)-C(10)-C(1)	73.38(13)
C(1)-C(10)-C(11)-C(7)	-57.77(12)	C(9)-C(10)-C(11)-C(7)	54.89(13)
C(8)-C(7)-C(11)-C(10)	-56.98(12)	C(6)-C(7)-C(11)-C(10)	55.37(12)

SUPP-Table 10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for JMWBP91. 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)	29(1)	35(1)	52(1)	-5(1)	4(1)	8(1)
O(2)	34(1)	42(1)	58(1)	-12(1)	-8(1)	16(1)
C(1)	29(1)	18(1)	32(1)	3(1)	0(1)	1(1)
C(2)	29(1)	16(1)	36(1)	-2(1)	2(1)	1(1)
C(3)	36(1)	32(1)	30(1)	-4(1)	1(1)	4(1)
C(4)	34(1)	31(1)	35(1)	5(1)	-5(1)	4(1)
C(5)	25(1)	22(1)	43(1)	-5(1)	-5(1)	0(1)
C(6)	24(1)	22(1)	36(1)	0(1)	6(1)	-3(1)
C(7)	34(1)	30(1)	31(1)	-4(1)	8(1)	3(1)
C(8)	34(1)	21(1)	37(1)	-6(1)	-2(1)	1(1)
C(9)	27(1)	27(1)	43(1)	-6(1)	-4(1)	-1(1)
C(10)	36(1)	26(1)	33(1)	-1(1)	-8(1)	6(1)
C(11)	59(1)	35(1)	29(1)	2(1)	0(1)	2(1)

SUPP-Table 11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Compound 7.

	x/a	y/b	z/c	U(eq)
H(1)	3973(14)	65(16)	3977(10)	35(4)
H(3A)	4289(15)	862(16)	1675(11)	39(4)
H(3B)	3229(15)	270(16)	2205(10)	37(4)
H(4A)	3822(16)	2928(17)	2290(11)	41(4)
H(4B)	2692(15)	2426(15)	1797(10)	37(4)
H(6)	2289(14)	1185(15)	4030(10)	34(4)
H(7)	2506(16)	3078(15)	4805(10)	39(4)
H(8A)	4239(14)	4387(16)	4636(11)	40(4)
H(8B)	3815(14)	4131(15)	3680(11)	36(4)
H(9A)	6025(16)	3324(16)	4388(11)	43(4)
H(9B)	5587(15)	2939(15)	3491(12)	36(4)
H(10)	5725(14)	1096(15)	4555(10)	34(4)
H(11A)	4505(17)	2481(17)	5548(12)	49(5)
H(11B)	3696(16)	1180(17)	5357(12)	48(5)

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