

Table 1: Crystallographic Data of

Identification code		11	26	19	31	32
<i>Empirical formula</i>		C ₁₉ H ₁₅ N O ₃	C ₁₄ H ₁₂ N ₂ O ₃	C ₁₉ H ₁₅ N O ₄	C ₂₂ H ₂₆ N ₂ O ₆	C ₂₄ H ₂₄ N ₂ O ₄ , C Cl ₃ D
<i>Formula weight</i>		305.32	256.26	321.32	414.45	524.82
<i>Temperature (K)</i>		193(2)	193(2)	293(2)	293(2)	293(2)
<i>Diffractometer</i>		Rapid II mm007HF – CMF optics				
<i>Wavelength (Å)</i>		1.54187				
<i>Crystal system</i>		Orthorhombic	Monoclinic	Monoclinic	Orthorhombic	Monoclinic
<i>Space group</i>		P c a 2 ₁	P 2 ₁ /c	P 2 ₁ /c	P b c a	C 2/c
<i>Unit cell</i> <i>Dimensions</i>	<i>a</i> (Å)	12.0964(8)	8.1942(2)	9.6682(3)	11.2819(3)	32.2117(18)
	<i>b</i> (Å)	12.2829(4)	14.4078(5)	7.7791(3)	16.3676(4)	9.1944(4)
	<i>c</i> (Å)	10.3170(2)	10.1791(7)	21.5345(15)	23.2672(16)	23.1388(16)
	α (°)	90	90	90	90	90
	β (°)	90	96.390(7)	98.014(7)	90	132.200(9)
	γ (°)	90	90	90	90	90
<i>Volume (Å³)</i>		1532.89(12)	1194.28(10)	1603.79(14)	4296.5(3)	5076.7(9)
<i>Z, Z'</i>		4, 1	4, 1	4, 1	8, 1	8, 1
<i>Calcd density (Mg/m³)</i>		1.323	1.425	1.331	1.281	1.373
<i>Abs. coefficient (mm⁻¹)</i>		0.731	0.846	0.775	0.775	3.553
<i>F(000)</i>		640	536	672	1760	2176
<i>Crystal size (mm)</i>		0.59 x 0.25 x 0.10	0.20 x 0.16 x 0.13	0.30 x 0.22 x 0.15	0.32 x 0.25 x 0.16	0.35 x 0.15 x 0.10
<i>θ_{range} for data collect° (°)</i>		3.60 to 68.24	5.34 to 68.23	4.15 to 64.98	3.80 to 68.22	3.70 to 68.14
<i>Limiting indices</i>		-14 ≤ h ≤ 12,	-9 ≤ h ≤ 9,	-6 ≤ h ≤ 11,	-9 ≤ h ≤ 13,	-38 ≤ h ≤ 31,
		-14 ≤ k ≤ 14,	-15 ≤ k ≤ 17,	-9 ≤ k ≤ 5,	-18 ≤ k ≤ 19,	-8 ≤ k ≤ 11,
		-12 ≤ l ≤ 8	-12 ≤ l ≤ 12	-25 ≤ l ≤ 23	-21 ≤ l ≤ 28	-27 ≤ l ≤ 24
<i>Reflect° collected / unique</i>		6169 / 2368	11248 / 2175	6552 / 2616	16212 / 3825	10748 / 4462
<i>R(int)</i>		0.0483	0.0627	0.0291	0.0532	0.0360
<i>Completeness to θ_{max} (%)</i>		99.6	99.7	95.5 %	97.1	96.1
<i>Absorption correction</i>		Semi-empirical from equivalents				
<i>Max. and min. Transmission</i>		0.929 and 0.710	0.921 and 0.668	0.890 and 0.689	0.883 and 0.585	0.641 and 0.410
<i>Refinement method</i>		Full-matrix least-squares on F^2				
<i>Data / restraints / parameters</i>		2365 / 1 / 209	2175 / 0 / 174	2610 / 0 / 219	4461 / 42 / 349	2442 / 2 / 240
<i>Goodness-of-fit on F^2</i>		1.061	1.209	1.098	1.040	1.149
<i>Final R indices</i> <i>RI</i>		0.0345	0.0551	0.0506	0.0661	0.0570
<i>[I > 2σ(I)]</i> <i>wR2</i>		0.0866	0.1457	0.1425	0.1670	0.1530
<i>R indices</i> <i>RI</i>		0.0366	0.0736	0.0814	0.0888	0.0944

(all data) $wR2$	0.0896	0.1825	0.1824	0.1877	0.1881
Flack ^l parameter	0.0(2)	-		-	-
Extinction coefficient	-	0.0051(12)	0.0024(6)	0.00040(11)	0.00053(8)
Δ_{max} peak and hole (e. Å ³)	0.166 and -0.221	0.220 and -0.262	0.221 and -0.204	0.242 and -0.229	0.344 and -0.354

Computing Software for :

Data Collection, Cell Refinement and Data Reduction: CrystalClear-SM Expert 2.0 r4/Fs_Process (Rigaku, 2009).

Structure_Solution: SHELXS97 (Sheldrick, 2008).

Structure Refinement: SHELXL97 (Sheldrick, 2008) ; CRYSTALBUILDER (Welter, 2006)

Molecular_Graphics : ORTEP-III (Burnett and Johnson, 1996) ; PLATON (Spek, 2009).

References :

Burnett M N. and Johnson, C. K. ORTEP-III: Oak Ridge Thermal Ellipsoid Plot Program for Crystal Structure Illustrations, Oak Ridge National Laboratory Report ORNL-6895, 1996.

Sheldrick, G.M. (2008) *Acta Cryst.*, **A64**, 112-122.

Spek, A. L. (2009). *Acta Cryst.* 2009, **D65**, 148-155.

Welter, R. (2006), *Acta Cryst.* **A62**, s252.