

## A.1 – DATA TABLES FOR CRYSTAL STRUCTURES

**Table A.1** - Crystal data and structure refinement for **2.9**

Chemical formula	<chem>C25H22ClPPdS</chem>		
Formula weight	527.31		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	monoclinic, P2 <sub>1</sub>		
Unit cell parameters	$a = 9.7424(5)$ Å	$\alpha = 90^\circ$	
	$b = 9.1554(4)$ Å	$\beta = 96.487(2)^\circ$	
	$c = 25.4974(12)$ Å	$\gamma = 90^\circ$	
Cell volume	2259.69(19) Å <sup>3</sup>		
Z	4		
Calculated density	1.550 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	1.112 mm <sup>-1</sup>		
F(000)	1064		
Crystal colour and size	colourless, 0.56 × 0.29 × 0.12 mm <sup>3</sup>		
Reflections for cell refinement	11085 ( $\theta$ range 2.34 to 28.86°)		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
$\theta$ range for data collection	1.61 to 28.94°		
Index ranges	h –12 to 13, k –12 to 12, l –33 to 29		
Completeness to $\theta = 26.00^\circ$	98.1 %		
Intensity decay	0%		
Reflections collected	13428		
Independent reflections	9385 ( $R_{\text{int}} = 0.0113$ )		
Reflections with $F^2 > 2\sigma$	8975		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.575 and 0.878		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0210, 0.0000		
Data / restraints / parameters	9385 / 1 / 525		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0181$ , $wR_2 = 0.0438$		
R indices (all data)	$R_1 = 0.0198$ , $wR_2 = 0.0445$		
Goodness-of-fit on $F^2$	1.042		
Absolute structure parameter	–0.007(11)		
Largest and mean shift/su	0.002 and 0.000		
Largest diff. peak and hole	0.298 and –0.300 e Å <sup>–3</sup>		

**Table A.2** - Crystal data and structure refinement for **2.10**

Chemical formula	$C_{24}H_{19}Cl_2PPtS$		
Formula weight	636.41		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	monoclinic, C2/c		
Unit cell parameters	$a = 37.4809(13)$ Å	$\alpha = 90^\circ$	
	$b = 9.2237(3)$ Å		$\beta = 109.232(2)^\circ$
	$c = 27.5025(10)$ Å		$\gamma = 90^\circ$
Cell volume	$8977.3(5)$ Å <sup>3</sup>		
Z	16		
Calculated density	1.883 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	6.663 mm <sup>-1</sup>		
F(000)	4896		
Crystal colour and size	colourless, $0.36 \times 0.08 \times 0.04$ mm <sup>3</sup>		
Reflections for cell refinement	15351 ( $\theta$ range $2.28$ to $28.88^\circ$ )		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
$\theta$ range for data collection	$1.57$ to $29.06^\circ$		
Index ranges	$h -50$ to $48, k -12$ to $11, l -35$ to $35$		
Completeness to $\theta = 26.00^\circ$	99.8 %		
Intensity decay	0%		
Reflections collected	38858		
Independent reflections	10806 ( $R_{int} = 0.0347$ )		
Reflections with $F^2 > 2\sigma$	8522		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.198 and 0.791		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0256, 18.3598		
Data / restraints / parameters	10806 / 0 / 523		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0272, wR_2 = 0.0570$		
R indices (all data)	$R_1 = 0.0440, wR_2 = 0.0641$		
Goodness-of-fit on $F^2$	1.042		
Largest and mean shift/su	0.002 and 0.000		
Largest diff. peak and hole	1.437 and $-1.673$ e Å <sup>-3</sup>		

**Table A.3** - Crystal data and structure refinement for **2.18**

Chemical formula	<chem>C24H19Cl2PPdSe</chem>		
Formula weight	594.62		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	a	b	c
Unit cell parameters	11.2636(17)	13.487(2)	14.743(2)
	Å	Å	Å
	$\alpha = 90^\circ$	$\beta = 100.823(2)^\circ$	$\gamma = 90^\circ$
Cell volume	2199.9(6) Å <sup>3</sup>		
Z	4		
Calculated density	1.795 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	2.823 mm <sup>-1</sup>		
F(000)	1168		
Crystal colour and size	orange, 0.29 × 0.25 × 0.16 mm <sup>3</sup>		
Reflections for cell refinement	12002 ( $\theta$ range 2.38 to 29.03°)		
Data collection method	Bruker SMART 1000 CCD diffractometer ω rotation with narrow frames		
θ range for data collection	2.06 to 29.06°		
Index ranges	h –14 to 14, k –17 to 17, l –19 to 19		
Completeness to $\theta = 26.00^\circ$	99.7 %		
Intensity decay	0%		
Reflections collected	19227		
Independent reflections	5218 ( $R_{\text{int}} = 0.0150$ )		
Reflections with $F^2 > 2\sigma$	4704		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.495 and 0.661		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0304, 3.0778		
Data / restraints / parameters	5218 / 0 / 262		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0245$ , $wR_2 = 0.0630$		
R indices (all data)	$R_1 = 0.0289$ , $wR_2 = 0.0656$		
Goodness-of-fit on $F^2$	1.050		
Largest and mean shift/su	0.002 and 0.000		
Largest diff. peak and hole	0.718 and –0.987 e Å <sup>–3</sup>		

**Table A.4** - Crystal data and structure refinement for **2.19**

Chemical formula	$C_{24}H_{19}Cl_2PPtSe$		
Formula weight	683.31		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	monoclinic	P2 <sub>1</sub> /n	
Unit cell parameters	$a = 11.2539(7)$ Å	$\alpha = 90^\circ$	
	$b = 13.4809(8)$ Å	$\beta = 101.008(2)^\circ$	
	$c = 14.7665(9)$ Å	$\gamma = 90^\circ$	
Cell volume	$2199.0(2)$ Å <sup>3</sup>		
Z	4		
Calculated density	2.064 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	$8.361$ mm <sup>-1</sup>		
F(000)	1296		
Crystal colour and size	colourless, $0.12 \times 0.07 \times 0.05$ mm <sup>3</sup>		
Reflections for cell refinement	6473 ( $\theta$ range 2.38 to 28.79°)		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
θ range for data collection	2.06 to 29.03°		
Index ranges	h –15 to 15, k –18 to 18, l –18 to 19		
Completeness to $\theta = 29.03^\circ$	91.2 %		
Intensity decay	0%		
Reflections collected	19234		
Independent reflections	5350 ( $R_{\text{int}} = 0.0354$ )		
Reflections with $F^2 > 2\sigma$	4130		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.434 and 0.680		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0203, 5.7851		
Data / restraints / parameters	5350 / 0 / 262		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0277$ , $wR_2 = 0.0507$		
R indices (all data)	$R_1 = 0.0481$ , $wR_2 = 0.0578$		
Goodness-of-fit on $F^2$	0.986		
Largest and mean shift/su	0.001 and 0.000		
Largest diff. peak and hole	1.044 and –1.250 e Å <sup>–3</sup>		

**Table A.5** - Crystal data and structure refinement for **2.28**.

Chemical formula	<chem>C21H22ClPPdSe</chem>	
Formula weight	526.17	
Temperature	150(2) K	
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å	
Crystal system, space group	monoclinic, P2 <sub>1</sub> /n	
Unit cell parameters	a = 9.0570(3) Å	$\alpha$ = 90°
	b = 20.7000(7) Å	$\beta$ = 104.148(2)°
	c = 10.8821(4) Å	$\gamma$ = 90°
Cell volume	1978.29(12) Å <sup>3</sup>	
Z	4	
Calculated density	1.767 g/cm <sup>3</sup>	
Absorption coefficient $\mu$	2.995 mm <sup>-1</sup>	
F(000)	1040	
Crystal colour and size	orange, 0.62 × 0.26 × 0.07 mm <sup>3</sup>	
Reflections for cell refinement	9726 ( $\theta$ range 2.17 to 28.96°)	
Data collection method	Bruker SMART 1000 CCD diffractometer ω rotation with narrow frames	
θ range for data collection	1.97 to 28.98°	
Index ranges	h –11 to 12, k –27 to 27, l –12 to 14	
Completeness to $\theta$ = 26.00°	99.6 %	
Intensity decay	0%	
Reflections collected	13803	
Independent reflections	4694 ( $R_{\text{int}} = 0.0200$ )	
Reflections with $F^2 > 2\sigma$	4316	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.258 and 0.818	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on $F^2$	
Weighting parameters a, b	0.0255, 1.4905	
Data / restraints / parameters	4694 / 0 / 226	
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0209$ , $wR_2 = 0.0527$	
R indices (all data)	$R_1 = 0.0236$ , $wR_2 = 0.0542$	
Goodness-of-fit on $F^2$	1.041	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.593 and –0.557 e Å <sup>–3</sup>	

**Table A.6** - Crystal data and structure refinement for **2.31**.

Chemical formula	$C_{24}H_{21}Cl_2PPdS$		
Formula weight	549.74		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	a	b	c
Unit cell parameters	11.9228(5) Å	14.0125(6) Å	15.7851(7) Å
Cell volume	2246.21(17) Å <sup>3</sup>		
Z	4		
Calculated density	1.626 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	1.237 mm <sup>-1</sup>		
F(000)	1104		
Crystal colour and size	yellow, 0.38 × 0.22 × 0.19 mm <sup>3</sup>		
Reflections for cell refinement	10436 ( $\theta$ range 2.39 to 28.87°)		
Data collection method	Bruker SMART 1000 CCD diffractometer		
	ω rotation with narrow frames		
θ range for data collection	1.50 to 29.09°		
Index ranges	h –15 to 15, k –18 to 18, l –20 to 21		
Completeness to $\theta = 26.00^\circ$	99.3 %		
Intensity decay	0%		
Reflections collected	20128		
Independent reflections	10436 ( $R_{int} = 0.0166$ )		
Reflections with $F^2 > 2\sigma$	8536		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.651 and 0.799		
Structure solution	Patterson synthesis		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0248, 1.3679		
Data / restraints / parameters	10436 / 0 / 523		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0259$ , $wR_2 = 0.0582$		
R indices (all data)	$R_1 = 0.0356$ , $wR_2 = 0.0630$		
Goodness-of-fit on $F^2$	1.039		
Largest and mean shift/su	0.001 and 0.000		
Largest diff. peak and hole	0.846 and –0.557 e Å <sup>–3</sup>		

**Table A.7** - Crystal data and structure refinement for **2.42**.

Chemical formula	<chem>C21H21Cl2OPPdS</chem>		
Formula weight	529.71		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	monoclinic	P2 <sub>1</sub> /n	
Unit cell parameters	$a = 11.5266(6)$ Å	$\alpha = 90^\circ$	
	$b = 16.1846(8)$ Å	$\beta = 99.536(2)^\circ$	
	$c = 13.7747(7)$ Å	$\gamma = 90^\circ$	
Cell volume	2534.2(2) Å <sup>3</sup>		
Z	4		
Calculated density	1.388 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	1.096 mm <sup>-1</sup>		
F(000)	1064		
Crystal colour and size	yellow, 0.31 × 0.23 × 0.20 mm <sup>3</sup>		
Reflections for cell refinement	7505 ( $\theta$ range 2.19 to 28.83°)		
Data collection method	Bruker SMART 1000 CCD diffractometer ω rotation with narrow frames		
θ range for data collection	1.96 to 29.13°		
Index ranges	h –15 to 15, k –20 to 21, l –18 to 18		
Completeness to $\theta = 26.00^\circ$	99.9 %		
Intensity decay	0%		
Reflections collected	22337		
Independent reflections	6186 ( $R_{\text{int}} = 0.0234$ )		
Reflections with $F^2 > 2\sigma$	4267		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.728 and 0.811		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0195, 8.5914		
Data / restraints / parameters	6186 / 339 / 291		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0559$ , $wR_2 = 0.1079$		
R indices (all data)	$R_1 = 0.0772$ , $wR_2 = 0.1149$		
Goodness-of-fit on $F^2$	1.097		
Largest and mean shift/su	0.001 and 0.000		
Largest diff. peak and hole	0.890 and –1.454 e Å <sup>–3</sup>		

**Table A.8** - Crystal data and structure refinement for **2.43**.

Chemical formula	<chem>C21H21Cl2OPPdS</chem>		
Formula weight	529.71		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	monoclinic	P2 <sub>1</sub> /c	
Unit cell parameters	$a = 11.8661(5)$ Å	$\alpha = 90^\circ$	
	$b = 10.5209(4)$ Å	$\beta = 90.745(2)^\circ$	
	$c = 16.4201(7)$ Å	$\gamma = 90^\circ$	
Cell volume	2049.75(15) Å <sup>3</sup>		
Z	4		
Calculated density	1.717 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	1.355 mm <sup>-1</sup>		
F(000)	1064		
Crystal colour and size	yellow, 0.37 × 0.22 × 0.15 mm <sup>3</sup>		
Reflections for cell refinement	9781 ( $\theta$ range 2.30 to 29.17°)		
Data collection method	Bruker SMART 1000 CCD diffractometer ω rotation with narrow frames		
θ range for data collection	1.72 to 29.17°		
Index ranges	h –15 to 16, k –14 to 14, l –21 to 22		
Completeness to $\theta = 26.00^\circ$	99.9 %		
Intensity decay	0%		
Reflections collected	17917		
Independent reflections	5027 ( $R_{\text{int}} = 0.0200$ )		
Reflections with $F^2 > 2\sigma$	4252		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.634 and 0.823		
Structure solution	Patterson synthesis		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0201, 1.5435		
Data / restraints / parameters	5027 / 0 / 244		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0231$ , $wR_2 = 0.0506$		
R indices (all data)	$R_1 = 0.0315$ , $wR_2 = 0.0545$		
Goodness-of-fit on $F^2$	1.076		
Largest and mean shift/su	0.001 and 0.000		
Largest diff. peak and hole	0.441 and –0.370 e Å <sup>–3</sup>		

**Table A.9** - Crystal data and structure refinement for **2.46**.

Chemical formula	$C_{22}H_{26}NPPtS$		
Formula weight	562.56		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	triclinic	P	$\bar{1}$
Unit cell parameters	$a = 8.9196(4)$ Å	$\alpha = 84.311(2)^\circ$	
	$b = 10.8791(5)$ Å	$\beta = 87.635(2)^\circ$	
	$c = 21.8178(9)$ Å	$\gamma = 80.932(2)^\circ$	
Cell volume	2079.67(16) Å <sup>3</sup>		
Z	4		
Calculated density	1.797 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	6.930 mm <sup>-1</sup>		
F(000)	1096		
Crystal colour and size	colourless, 0.25 × 0.16 × 0.11 mm <sup>3</sup>		
Reflections for cell refinement	9794 ( $\theta$ range 2.474 to 29.043°)		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
θ range for data collection	1.88 to 29.07°		
Index ranges	h –11 to 12, k –14 to 14, l –29 to 28		
Completeness to $\theta = 26.00^\circ$	99.4 %		
Intensity decay	0%		
Reflections collected	18589		
Independent reflections	9656 ( $R_{\text{int}} = 0.0216$ )		
Reflections with $F^2 > 2\sigma$	7777		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.276 and 0.516		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0213, 0.8951		
Data / restraints / parameters	9656 / 5 / 485		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0243$ , $wR_2 = 0.0489$		
R indices (all data)	$R_1 = 0.0375$ , $wR_2 = 0.0540$		
Goodness-of-fit on $F^2$	1.034		
Largest and mean shift/su	0.002 and 0.000		
Largest diff. peak and hole	1.348 and –0.636 e Å <sup>–3</sup>		

**Table A.10** - Crystal data and structure refinement for **2.47**.

Chemical formula	$C_{24}H_{19}Cl_5NPPdS$		
Formula weight	668.08		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	orthorhombic	Pna2 <sub>1</sub>	
Unit cell parameters	$a = 18.5066(9)$ Å	$\alpha = 90^\circ$	
	$b = 9.1076(4)$ Å	$\beta = 90^\circ$	
	$c = 15.4085(7)$ Å	$\gamma = 90^\circ$	
Cell volume	2597.1(2) Å <sup>3</sup>		
Z	4		
Calculated density	1.709 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	1.386 mm <sup>-1</sup>		
F(000)	1328		
Crystal colour and size	yellow, 0.24 × 0.12 × 0.10 mm <sup>3</sup>		
Reflections for cell refinement	8650 ( $\theta$ range 2.49 to 28.72°)		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
θ range for data collection	2.20 to 29.12°		
Index ranges	h –24 to 24, k –11 to 12, l –20 to 20		
Completeness to $\theta = 26.00^\circ$	100.0 %		
Intensity decay	0%		
Reflections collected	22146		
Independent reflections	6309 ( $R_{\text{int}} = 0.0344$ )		
Reflections with $F^2 > 2\sigma$	5417		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.732 and 0.874		
Structure solution	Patterson synthesis		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0338, 1.9980		
Data / restraints / parameters	6309 / 1 / 298		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0344$ , $wR_2 = 0.0718$		
R indices (all data)	$R_1 = 0.0472$ , $wR_2 = 0.0782$		
Goodness-of-fit on $F^2$	1.076		
Absolute structure parameter	0.00(3)		
Largest and mean shift/su	0.001 and 0.000		
Largest diff. peak and hole	1.424 and –0.479 e Å <sup>–3</sup>		

**Table A.11** - Crystal data and structure refinement for **3.1**.

Chemical formula	$C_{16}H_{20}BrO_3P$		
Formula weight	371.20		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	monoclinic, P2 <sub>1</sub> /n		
Unit cell parameters	$a = 10.7207(6)$ Å	$\alpha = 90^\circ$	
	$b = 14.3856(8)$ Å	$\beta = 111.980(2)^\circ$	
	$c = 11.1856(7)$ Å	$\gamma = 90^\circ$	
Cell volume	1599.70(16) Å <sup>3</sup>		
Z	4		
Calculated density	1.541 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	2.677 mm <sup>-1</sup>		
F(000)	760		
Crystal colour and size	colourless, 0.31 × 0.19 × 0.17 mm <sup>3</sup>		
Reflections for cell refinement	6888 ( $\theta$ range 2.49 to 28.806°)		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
θ range for data collection	2.25 to 28.95°		
Index ranges	h –13 to 13, k –18 to 18, l –14 to 15		
Completeness to $\theta = 26.00^\circ$	99.8 %		
Intensity decay	0%		
Reflections collected	14002		
Independent reflections	3832 ( $R_{\text{int}} = 0.0211$ )		
Reflections with $F^2 > 2\sigma$	3243		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.491 and 0.659		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0375, 0.8448		
Data / restraints / parameters	3832 / 0 / 194		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0258$ , $wR_2 = 0.0680$		
R indices (all data)	$R_1 = 0.0346$ , $wR_2 = 0.0720$		
Goodness-of-fit on $F^2$	1.049		
Largest and mean shift/su	0.001 and 0.000		
Largest diff. peak and hole	0.452 and –0.331 e Å <sup>–3</sup>		

**Table A.12** - Crystal data and structure refinement for **3.5**.

Chemical formula	<chem>C22H26O3PSe</chem>		
Formula weight	448.36		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	orthorhombic	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	
Unit cell parameters	a = 8.1752(5) Å	$\alpha$ = 90°	
	b = 10.1189(6) Å	$\beta$ = 90°	
	c = 24.5004(14) Å	$\gamma$ = 90°	
Cell volume	2026.8(2) Å <sup>3</sup>		
Z	4		
Calculated density	1.469 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	1.951 mm <sup>-1</sup>		
F(000)	924		
Crystal colour and size	colourless, 0.52 × 0.26 × 0.10 mm <sup>3</sup>		
Reflections for cell refinement	17858 ( $\theta$ range 2.18 to 27.21°)		
Data collection method	Bruker SMART 1000 CCD diffractometer		
	$\omega$ rotation with narrow frames		
θ range for data collection	1.66 to 28.95°		
Index ranges	h –10 to 11, k –13 to 13, l –32 to 31		
Completeness to $\theta$ = 26.00°	100.0 %		
Intensity decay	0%		
Reflections collected	17792		
Independent reflections	4890 ( $R_{\text{int}} = 0.0366$ )		
Reflections with $F^2 > 2\sigma$	4049		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.430 and 0.829		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0184, 1.8456		
Data / restraints / parameters	4890 / 0 / 248		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0393$ , $wR_2 = 0.0805$		
R indices (all data)	$R_1 = 0.0573$ , $wR_2 = 0.0880$		
Goodness-of-fit on $F^2$	1.064		
Absolute structure parameter	0.018(9)		
Largest and mean shift/su	0.000 and 0.000		
Largest diff. peak and hole	1.502 and –1.220 e Å <sup>–3</sup>		

**Table A.13** - Crystal data and structure refinement for **3.6**.

Chemical formula	$C_{32}H_{40}Br_2Cl_4O_6P_2Pd_2$		
Formula weight	1097.00		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	triclinic	P $\bar{1}$	
Unit cell parameters	$a = 8.1657(16)$ Å	$\alpha = 103.794(3)^\circ$	
	$b = 10.769(2)$ Å	$\beta = 92.840(3)^\circ$	
	$c = 11.171(2)$ Å	$\gamma = 103.659(3)^\circ$	
Cell volume	921.2(3) Å <sup>3</sup>		
Z	1		
Calculated density	1.977 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	3.565 mm <sup>-1</sup>		
F(000)	540		
Crystal colour and size	yellow, 0.18 × 0.14 × 0.06 mm <sup>3</sup>		
Reflections for cell refinement	2832 ( $\theta$ range 2.38 to 28.31°)		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
θ range for data collection	1.89 to 28.65°		
Index ranges	h –10 to 10, k –14 to 14, l –14 to 14		
Completeness to $\theta = 26.00^\circ$	98.5 %		
Intensity decay	0%		
Reflections collected	7313		
Independent reflections	4121 ( $R_{\text{int}} = 0.0271$ )		
Reflections with $F^2 > 2\sigma$	2974		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.566 and 0.815		
Structure solution	Patterson synthesis		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0448, 0.3719		
Data / restraints / parameters	4121 / 0 / 221		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0359$ , $wR_2 = 0.0781$		
R indices (all data)	$R_1 = 0.0677$ , $wR_2 = 0.0894$		
Goodness-of-fit on $F^2$	1.024		
Largest and mean shift/su	0.001 and 0.000		
Largest diff. peak and hole	0.850 and –0.768 e Å <sup>–3</sup>		

**Table A.14** - Crystal data and structure refinement for **3.8**.

Chemical formula	<chem>C23H27Cl4O3PPdS</chem>		
Formula weight	662.68		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	orthorhombic	Pna2 <sub>1</sub>	
Unit cell parameters	$a = 15.2772(7)$ Å	$\alpha = 90^\circ$	
	$b = 19.9039(10)$ Å	$\beta = 90^\circ$	
	$c = 8.7801(4)$ Å	$\gamma = 90^\circ$	
Cell volume	2669.8(2) Å <sup>3</sup>		
Z	4		
Calculated density	1.649 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	1.257 mm <sup>-1</sup>		
F(000)	1336		
Crystal colour and size	yellow, 0.35 × 0.28 × 0.08 mm <sup>3</sup>		
Reflections for cell refinement	10906 ( $\theta$ range 2.44 to 28.70°)		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
θ range for data collection	1.68 to 29.01°		
Index ranges	h –20 to 20, k –26 to 26, l –11 to 11		
Completeness to $\theta = 26.00^\circ$	100.0 %		
Intensity decay	0%		
Reflections collected	22990		
Independent reflections	6424 ( $R_{\text{int}} = 0.0275$ )		
Reflections with $F^2 > 2\sigma$	5712		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.667 and 0.906		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0373, 2.1442		
Data / restraints / parameters	6424 / 1 / 302		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0320$ , $wR_2 = 0.0740$		
R indices (all data)	$R_1 = 0.0399$ , $wR_2 = 0.0782$		
Goodness-of-fit on $F^2$	1.048		
Absolute structure parameter	0.00		
Largest and mean shift/su	0.003 and 0.000		
Largest diff. peak and hole	0.790 and –0.684 e Å <sup>–3</sup>		

**Table A.15** - Crystal data and structure refinement for **3.9**.

Chemical formula	$C_{23}H_{27}Cl_4O_3PPdSe$	
Formula weight	709.58	
Temperature	150(2) K	
Radiation, wavelength	MoKa, 0.71073 Å	
Crystal system, space group	triclinic, P $\bar{1}$	
Unit cell parameters	$a = 11.0639(5)$ Å	$a = 89.742(2)^\circ$
	$b = 11.0640(5)$ Å	$b = 76.379(2)^\circ$
	$c = 11.7858(5)$ Å	$g = 68.405(2)^\circ$
Cell volume	1298.32(10) Å <sup>3</sup>	
Z	2	
Calculated density	1.815 g/cm <sup>3</sup>	
Absorption coefficient m	2.614 mm <sup>-1</sup>	
F(000)	704	
Crystal colour and size	yellow, 0.37 × 0.30 × 0.18 mm <sup>3</sup>	
Reflections for cell refinement	11577 (q range 2.251 to 28.987°)	
Data collection method	Bruker SMART 1K CCD diffractometer w rotation with narrow frames	
q range for data collection	1.79 to 28.99°	
Index ranges	h –14 to 14, k –14 to 14, l –16 to 15	
Completeness to q = 26.00°	99.3 %	
Intensity decay	0%	
Reflections collected	11577	
Independent reflections	6012 ( $R_{int} = 0.0110$ )	
Reflections with F <sup>2</sup> >2s	5490	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.445 and 0.650	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Weighting parameters a, b	0.0202, 0.8520	
Data / restraints / parameters	6012 / 0 / 302	
Final R indices [F <sup>2</sup> >2s]	$R_1 = 0.0188$ , $wR_2 = 0.0448$	
R indices (all data)	$R_1 = 0.0221$ , $wR_2 = 0.0464$	
Goodness-of-fit on F <sup>2</sup>	1.023	
Largest and mean shift/su	0.003 and 0.000	
Largest diff. peak and hole	0.495 and –0.498 e Å <sup>–3</sup>	

**Table A.16** - Crystal data and structure refinement for **3.11**.

Chemical formula	$C_{36}H_{50}Cl_6O_8P_2Pd$				
Formula weight	991.80				
Temperature	150(2) K				
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å				
Crystal system, space group	monoclinic, C2/c				
Unit cell parameters	$a = 11.7631(10)$ Å	$\alpha = 90^\circ$			
	$b = 18.7793(16)$ Å	$\beta = 92.652(2)^\circ$			
	$c = 19.5578(16)$ Å	$\gamma = 90^\circ$			
Cell volume	$4315.7(6)$ Å <sup>3</sup>				
Z	4				
Calculated density	1.526 g/cm <sup>3</sup>				
Absorption coefficient $\mu$	0.923 mm <sup>-1</sup>				
F(000)	2032				
Crystal colour and size	yellow, $0.21 \times 0.16 \times 0.11$ mm <sup>3</sup>				
Reflections for cell refinement	18846 ( $\theta$ range 2.26 to 28.79°)				
Data collection method	Bruker SMART 1000 CCD diffractometer				
	$\omega$ rotation with narrow frames				
θ range for data collection	2.04 to 25.00°				
Index ranges	h –13 to 13, k –22 to 22, l –23 to 23				
Completeness to $\theta = 25.00^\circ$	99.8 %				
Intensity decay	0%				
Reflections collected	15196				
Independent reflections	3793 ( $R_{int} = 0.0448$ )				
Reflections with $F^2 > 2\sigma$	3131				
Absorption correction	semi-empirical from equivalents				
Min. and max. transmission	0.830 and 0.905				
Structure solution	direct methods				
Refinement method	Full-matrix least-squares on $F^2$				
Weighting parameters a, b	0.0442, 125.9204				
Data / restraints / parameters	3793 / 0 / 246				
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0798$ , $wR_2 = 0.1911$				
R indices (all data)	$R_1 = 0.0918$ , $wR_2 = 0.1977$				
Goodness-of-fit on $F^2$	1.226				
Largest and mean shift/su	0.000 and 0.000				
Largest diff. peak and hole	2.874 and –0.959 e Å <sup>–3</sup>				

**Table A.17** - Crystal data and structure refinement for **3.14**.

Chemical formula	$C_{27}H_{37}Cl_3O_3P_2Pt$		
Formula weight	772.95		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	monoclinic, P2 <sub>1</sub> /c		
Unit cell parameters	$a = 11.5096(7)$ Å	$\alpha = 90^\circ$	
	$b = 11.4565(7)$ Å	$\beta = 98.545(2)^\circ$	
	$c = 23.1932(14)$ Å	$\gamma = 90^\circ$	
Cell volume	3024.3(3) Å <sup>3</sup>		
Z	4		
Calculated density	1.698 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	5.037 mm <sup>-1</sup>		
F(000)	1528		
Crystal colour and size	colourless, 0.26 × 0.21 × 0.10 mm <sup>3</sup>		
Reflections for cell refinement	11351 ( $\theta$ range 2.33 to 28.31°)		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
θ range for data collection	1.78 to 29.07°		
Index ranges	h –15 to 14, k –15 to 15, l –30 to 31		
Completeness to $\theta = 26.00^\circ$	99.9 %		
Intensity decay	0%		
Reflections collected	25066		
Independent reflections	7322 ( $R_{\text{int}} = 0.0575$ )		
Reflections with $F^2 > 2\sigma$	5537		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.354 and 0.633		
Structure solution	Patterson synthesis		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0000, 27.9824		
Data / restraints / parameters	7322 / 0 / 331		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0472$ , $wR_2 = 0.1057$		
R indices (all data)	$R_1 = 0.0661$ , $wR_2 = 0.1131$		
Goodness-of-fit on $F^2$	1.095		
Largest and mean shift/su	0.002 and 0.000		
Largest diff. peak and hole	1.591 and –1.426 e Å <sup>–3</sup>		

**Table A.18** - Crystal data and structure refinement for **3.17**.

Chemical formula	$C_{34}H_{44}Cl_2O_3P_2Ru$		
Formula weight	734.60		
Temperature	149(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	a	b	c
Unit cell parameters	$a = 7.4877(2)$ Å	$\alpha = 90^\circ$	$\beta = 92.33^\circ$
	$b = 13.4870(4)$ Å	$\gamma = 90^\circ$	
	$c = 33.2358(9)$ Å		
Cell volume	3353.60(16) Å <sup>3</sup>		
Z	4		
Calculated density	1.455 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	0.755 mm <sup>-1</sup>		
F(000)	1520		
Crystal colour and size	dark red, 0.49 × 0.32 × 0.23 mm <sup>3</sup>		
Reflections for cell refinement	18591 ( $\theta$ range 2.38 to 30.54°)		
Data collection method	Bruker APEX 2 CCD diffractometer $\omega$ rotation with narrow frames		
θ range for data collection	1.63 to 30.55°		
Index ranges	h –10 to 10, k –19 to 19, l –47 to 47		
Completeness to $\theta = 30.55^\circ$	99.6 %		
Intensity decay	0%		
Reflections collected	38615		
Independent reflections	10239 ( $R_{int} = 0.0414$ )		
Reflections with $F^2 > 2\sigma$	9053		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.709 and 0.846		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0265, 5.6732		
Data / restraints / parameters	10239 / 0 / 386		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0426$ , $wR_2 = 0.0975$		
R indices (all data)	$R_1 = 0.0487$ , $wR_2 = 0.1003$		
Goodness-of-fit on $F^2$	1.061		
Largest and mean shift/su	0.002 and 0.000		
Largest diff. peak and hole	0.796 and –1.316 e Å <sup>–3</sup>		

**Table A.19** - Crystal data and structure refinement for **3.18**.

Chemical formula	$C_{37}H_{51}AuCl_5O_3P_2Ru$		
Formula weight	1081.00		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	a	b	c
Unit cell parameters	12.2147(12) Å	12.2872(12) Å	14.1978(14) Å
	$\alpha = 84.631(2)^\circ$	$\beta = 80.527(2)^\circ$	$\gamma = 88.192(2)^\circ$
Cell volume	2092.3(4) Å <sup>3</sup>		
Z	2		
Calculated density	1.716 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	4.292 mm <sup>-1</sup>		
F(000)	1070		
Crystal colour and size	orange, 0.34 × 0.25 × 0.02 mm <sup>3</sup>		
Reflections for cell refinement	4763 ( $\theta$ range 2.31 to 26.98°)		
Data collection method	Bruker SMART 1000 CCD diffractometer ω rotation with narrow frames		
θ range for data collection	1.66 to 25.00°		
Index ranges	h –14 to 14, k –14 to 14, l –16 to 16		
Completeness to $\theta = 25.00^\circ$	99.5 %		
Intensity decay	0%		
Reflections collected	15122		
Independent reflections	7338 ( $R_{\text{int}} = 0.0379$ )		
Reflections with $F^2 > 2\sigma$	5201		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.323 and 0.919		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0601, 0.0000		
Data / restraints / parameters	7338 / 0 / 404		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0480$ , $wR_2 = 0.1133$		
R indices (all data)	$R_1 = 0.0723$ , $wR_2 = 0.1205$		
Goodness-of-fit on $F^2$	1.054		
Largest and mean shift/su	0.001 and 0.000		
Largest diff. peak and hole	2.340 and –1.499 e Å <sup>–3</sup>		

**Table A.20** - Crystal data and structure refinement for **3.19**.

Chemical formula	$C_{70}H_{92}Cl_{10}O_6P_4PdRu_2$				
Formula weight	1816.36				
Temperature	150(2) K				
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å				
Crystal system, space group	monoclinic, C2/c				
Unit cell parameters	$a = 29.148(2)$ Å	$\alpha = 90^\circ$			
	$b = 11.8624(9)$ Å	$\beta = 98.431(2)^\circ$			
	$c = 22.5109(16)$ Å	$\gamma = 90^\circ$			
Cell volume	$7699.4(10)$ Å <sup>3</sup>				
Z	4				
Calculated density	1.567 g/cm <sup>3</sup>				
Absorption coefficient $\mu$	1.097 mm <sup>-1</sup>				
F(000)	3696				
Crystal colour and size	orange, $0.49 \times 0.08 \times 0.06$ mm <sup>3</sup>				
Reflections for cell refinement	34311 ( $\theta$ range 2.466 to 24.997°)				
Data collection method	Bruker SMART 1000 CCD diffractometer				
	$\omega$ rotation with narrow frames				
θ range for data collection	1.83 to 29.02°				
Index ranges	h –39 to 38, k –15 to 16, l –30 to 29				
Completeness to $\theta = 26.00^\circ$	99.9 %				
Intensity decay	0%				
Reflections collected	33403				
Independent reflections	9320 ( $R_{\text{int}} = 0.0723$ )				
Reflections with $F^2 > 2\sigma$	5205				
Absorption correction	semi-empirical from equivalents				
Min. and max. transmission	0.616 and 0.937				
Structure solution	direct methods				
Refinement method	Full-matrix least-squares on $F^2$				
Weighting parameters a, b	0.0439, 49.2318				
Data / restraints / parameters	9320 / 5 / 438				
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0521$ , $wR_2 = 0.1070$				
R indices (all data)	$R_1 = 0.1235$ , $wR_2 = 0.1373$				
Goodness-of-fit on $F^2$	0.996				
Largest and mean shift/su	0.001 and 0.000				
Largest diff. peak and hole	0.724 and –0.911 e Å <sup>–3</sup>				

**Table A.21** - Crystal data and structure refinement for **3.22**.

Chemical formula	$C_{35}H_{46}Cl_5IrO_3P_2$		
Formula weight	946.11		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	monoclinic, P2 <sub>1</sub> /c		
Unit cell parameters	$a = 14.437(3)$ Å	$\alpha = 90^\circ$	
	$b = 12.105(2)$ Å	$\beta = 98.023(3)^\circ$	
	$c = 22.147(4)$ Å	$\gamma = 90^\circ$	
Cell volume	3832.6(11) Å <sup>3</sup>		
Z	4		
Calculated density	1.640 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	3.949 mm <sup>-1</sup>		
F(000)	1888		
Crystal colour and size	yellow, 0.34 × 0.22 × 0.05 mm <sup>3</sup>		
Reflections for cell refinement	7184 ( $\theta$ range 2.18 to 26.75°)		
Data collection method	Bruker SMART 1000 CCD diffractometer ω rotation with narrow frames		
θ range for data collection	1.86 to 25.00°		
Index ranges	h –16 to 17, k –14 to 14, l –26 to 26		
Completeness to $\theta = 25.00^\circ$	99.9 %		
Intensity decay	0%		
Reflections collected	27462		
Independent reflections	6755 ( $R_{\text{int}} = 0.0378$ )		
Reflections with $F^2 > 2\sigma$	4488		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.347 and 0.827		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.0529, 21.4119		
Data / restraints / parameters	6755 / 393 / 424		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0491$ , $wR_2 = 0.1172$		
R indices (all data)	$R_1 = 0.0815$ , $wR_2 = 0.1442$		
Goodness-of-fit on $F^2$	1.066		
Largest and mean shift/su	0.001 and 0.000		
Largest diff. peak and hole	1.061 and –1.614 e Å <sup>–3</sup>		

**Table A.22** - Crystal data and structure refinement for **4.7**

Chemical formula	$C_{33}H_{32}NO_4PS_2$	
Formula weight	601.69	
Temperature	150(2) K	
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å	
Crystal system, space group	monoclinic, P2 <sub>1</sub> /n	
Unit cell parameters	$a = 8.4226(9)$ Å	$\alpha = 90^\circ$
	$b = 18.9535(19)$ Å	$\beta = 95.978(2)^\circ$
	$c = 18.8511(19)$ Å	$\gamma = 90^\circ$
Cell volume	2993.0(5) Å <sup>3</sup>	
Z	4	
Calculated density	1.335 g/cm <sup>3</sup>	
Absorption coefficient $\mu$	0.270 mm <sup>-1</sup>	
F(000)	1264	
Crystal colour and size	colourless, 0.36 × 0.19 × 0.12 mm <sup>3</sup>	
Reflections for cell refinement	7955 ( $\theta$ range 2.41 to 28.05°)	
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames	
θ range for data collection	2.15 to 25.00°	
Index ranges	h –10 to 10, k –22 to 22, l –22 to 22	
Completeness to $\theta = 25.00^\circ$	99.8 %	
Intensity decay	0%	
Reflections collected	20863	
Independent reflections	5249 ( $R_{\text{int}} = 0.0444$ )	
Reflections with $F^2 > 2\sigma$	4091	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.909 and 0.968	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on $F^2$	
Weighting parameters a, b	0.0504, 7.0451	
Data / restraints / parameters	5249 / 1 / 379	
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0559$ , $wR_2 = 0.1451$	
R indices (all data)	$R_1 = 0.0726$ , $wR_2 = 0.1537$	
Goodness-of-fit on $F^2$	1.083	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.364 and –0.392 e Å <sup>–3</sup>	

**Table A.23** - Crystal data and structure refinement for **4.12**

Chemical formula	$C_{27}H_{37}Cl_3NO_7PS$		
Formula weight	656.96		
Temperature	150(2) K		
Radiation, wavelength	MoK $\alpha$ , 0.71073 Å		
Crystal system, space group	monoclinic, C2/c		
Unit cell parameters	$a = 18.2709(14)$ Å	$\alpha = 90^\circ$	
	$b = 12.8550(10)$ Å	$\beta = 104.835(2)^\circ$	
	$c = 26.542(2)$ Å	$\gamma = 90^\circ$	
Cell volume	6026.3(8) Å <sup>3</sup>		
Z	8		
Calculated density	1.448 g/cm <sup>3</sup>		
Absorption coefficient $\mu$	0.472 mm <sup>-1</sup>		
F(000)	2752		
Crystal colour and size	colourless, 0.50 × 0.40 × 0.27 mm <sup>3</sup>		
Reflections for cell refinement	22301 ( $\theta$ range 2.22 to 28.54°)		
Data collection method	Bruker SMART 1000 CCD diffractometer $\omega$ rotation with narrow frames		
θ range for data collection	1.96 to 28.98°		
Index ranges	h –23 to 20, k –16 to 16, l –35 to 35		
Completeness to $\theta = 26.00^\circ$	99.5 %		
Intensity decay	0%		
Reflections collected	21848		
Independent reflections	7122 ( $R_{\text{int}} = 0.0249$ )		
Reflections with $F^2 > 2\sigma$	5362		
Absorption correction	semi-empirical from equivalents		
Min. and max. transmission	0.798 and 0.883		
Structure solution	direct methods		
Refinement method	Full-matrix least-squares on $F^2$		
Weighting parameters a, b	0.1001, 23.8207		
Data / restraints / parameters	7122 / 0 / 366		
Final R indices [ $F^2 > 2\sigma$ ]	$R_1 = 0.0588$ , $wR_2 = 0.1740$		
R indices (all data)	$R_1 = 0.0797$ , $wR_2 = 0.1942$		
Goodness-of-fit on $F^2$	1.082		
Largest and mean shift/su	0.000 and 0.000		
Largest diff. peak and hole	1.140 and –1.067 e Å <sup>–3</sup>		