A.1 – DATA TABLES FOR CRYSTAL STRUCUTRES

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

Chemical formula	$C_{25}H_{22}ClPPdS$	
Formula weight	527.31	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1$	
Unit cell parameters	a = 9.7424(5) Å	α = 90°
	b = 9.1554(4) Å	β = 96.487(2)°
	c = 25.4974(12) Å	γ = 90°
Cell volume	2259.69(19) $Å^3$	
Z	4	
Calculated density	1.550 g/cm^3	
Absorption coefficient μ	1.112 mm^{-1}	
F(000)	1064	
Crystal colour and size	colourless, 0.56 × 0.29 × 0.12 mm^3	
Reflections for cell refinement	11085 (θ range 2.34 to 28.86°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω rotation with narrow frames	
θ 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 θ = 26.00°	98.1 %	
Intensity decay	0%	
Reflections collected	13428	
Independent reflections	9385 (R_{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 [$F^2>2\sigma$]	R1 = 0.0181, wR2 = 0.0438	
R indices (all data)	R1 = 0.0198, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, C2/c	
Unit cell parameters	a = 37.4809(13) Å	α = 90°
	b = 9.2237(3) Å	β = 109.232(2)°
	c = 27.5025(10) Å	γ = 90°
Cell volume	8977.3(5) $Å^3$	
Z	16	
Calculated density	1.883 g/cm^3	
Absorption coefficient μ	6.663 mm^{-1}	
F(000)	4896	
Crystal colour and size	colourless, 0.36 × 0.08 × 0.04 mm^3	
Reflections for cell refinement	15351 (θ range 2.28 to 28.88°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω rotation with narrow frames	
θ range for data collection	1.57 to 29.06°	
Index ranges	h –50 to 48, k –12 to 11, l –35 to 35	
Completeness to θ = 26.00°	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 [$F^2>2\sigma$]	R1 = 0.0272, wR2 = 0.0570	
R indices (all data)	R1 = 0.0440, wR2 = 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 $Å^{-3}$	

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

Chemical formula	$C_{24}H_{19}Cl_2PPdSe$	
Formula weight	594.62	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/n$	
Unit cell parameters	a = 11.2636(17) Å	α = 90°
	b = 13.487(2) Å	β = 100.823(2)°
	c = 14.743(2) Å	γ = 90°
Cell volume	2199.9(6) $Å^3$	
Z	4	
Calculated density	1.795 g/cm^3	
Absorption coefficient μ	2.823 mm^{-1}	
F(000)	1168	
Crystal colour and size	orange, 0.29 × 0.25 × 0.16 mm^3	
Reflections for cell refinement	12002 (θ 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 θ = 26.00°	99.7 %	
Intensity decay	0%	
Reflections collected	19227	
Independent reflections	5218 (R_{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 [$F^2>2\sigma$]	R1 = 0.0245, wR2 = 0.0630	
R indices (all data)	R1 = 0.0289, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/n$	
Unit cell parameters	a = 11.2539(7) Å	α = 90°
	b = 13.4809(8) Å	β = 101.008(2)°
	c = 14.7665(9) Å	γ = 90°
Cell volume	2199.0(2) $Å^3$	
Z	4	
Calculated density	2.064 g/cm^3	
Absorption coefficient μ	8.361 mm^{-1}	
F(000)	1296	
Crystal colour and size	colourless, 0.12 × 0.07 × 0.05 mm^3	
Reflections for cell refinement	6473 (θ range 2.38 to 28.79°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 29.03°	91.2 %	
Intensity decay	0%	
Reflections collected	19234	
Independent reflections	5350 (R_{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 [$F^2>2\sigma$]	R1 = 0.0277, wR2 = 0.0507	
R indices (all data)	R1 = 0.0481, wR2 = 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 $Å^{-3}$	

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

Chemical formula	$C_{21}H_{22}ClPPdSe$	
Formula weight	526.17	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/n$	
Unit cell parameters	a = 9.0570(3) Å	α = 90°
	b = 20.7000(7) Å	β = 104.148(2)°
	c = 10.8821(4) Å	γ = 90°
Cell volume	1978.29(12) $Å^3$	
Z	4	
Calculated density	1.767 g/cm^3	
Absorption coefficient μ	2.995 mm^{-1}	
F(000)	1040	
Crystal colour and size	orange, 0.62 × 0.26 × 0.07 mm^3	
Reflections for cell refinement	9726 (θ 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 θ = 26.00°	99.6 %	
Intensity decay	0%	
Reflections collected	13803	
Independent reflections	4694 (R_{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 [$F^2>2\sigma$]	R1 = 0.0209, wR2 = 0.0527	
R indices (all data)	R1 = 0.0236, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 11.9228(5) Å	α = 64.871(2)°
	b = 14.0125(6) Å	β = 70.252(2)°
	c = 15.7851(7) Å	γ = 83.189(2)°
Cell volume	2246.21(17) $Å^3$	
Z	4	
Calculated density	1.626 g/cm^3	
Absorption coefficient μ	1.237 mm^{-1}	
F(000)	1104	
Crystal colour and size	yellow, 0.38 × 0.22 × 0.19 mm^3	
Reflections for cell refinement	10436 (θ 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 θ = 26.00°	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 [$F^2>2\sigma$]	R1 = 0.0259, wR2 = 0.0582	
R indices (all data)	R1 = 0.0356, wR2 = 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 $Å^{-3}$	

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

Chemical formula	$C_{21}H_{21}Cl_2OPPdS$	
Formula weight	529.71	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/n$	
Unit cell parameters	a = 11.5266(6) Å	α = 90°
	b = 16.1846(8) Å	β = 99.536(2)°
	c = 13.7747(7) Å	γ = 90°
Cell volume	2534.2(2) $Å^3$	
Z	4	
Calculated density	1.388 g/cm^3	
Absorption coefficient μ	1.096 mm^{-1}	
F(000)	1064	
Crystal colour and size	yellow, 0.31 × 0.23 × 0.20 mm^3	
Reflections for cell refinement	7505 (θ 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 θ = 26.00°	99.9 %	
Intensity decay	0%	
Reflections collected	22337	
Independent reflections	6186 (R_{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 [$F^2>2\sigma$]	R1 = 0.0559, wR2 = 0.1079	
R indices (all data)	R1 = 0.0772, wR2 = 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 $Å^{-3}$	

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

Chemical formula	$C_{21}H_{21}Cl_2OPPdS$	
Formula weight	529.71	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/c$	
Unit cell parameters	a = 11.8661(5) Å	α = 90°
	b = 10.5209(4) Å	β = 90.745(2)°
	c = 16.4201(7) Å	γ = 90°
Cell volume	2049.75(15) $Å^3$	
Z	4	
Calculated density	1.717 g/cm^3	
Absorption coefficient μ	1.355 mm^{-1}	
F(000)	1064	
Crystal colour and size	yellow, 0.37 × 0.22 × 0.15 mm^3	
Reflections for cell refinement	9781 (θ 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 θ = 26.00°	99.9 %	
Intensity decay	0%	
Reflections collected	17917	
Independent reflections	5027 (R_{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 [$F^2>2\sigma$]	R1 = 0.0231, wR2 = 0.0506	
R indices (all data)	R1 = 0.0315, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 8.9196(4) Å	α = 84.311(2)°
	b = 10.8791(5) Å	β = 87.635(2)°
	c = 21.8178(9) Å	γ = 80.932(2)°
Cell volume	2079.67(16) $Å^3$	
Z	4	
Calculated density	1.797 g/cm^3	
Absorption coefficient μ	6.930 mm^{-1}	
F(000)	1096	
Crystal colour and size	colourless, 0.25 × 0.16 × 0.11 mm^3	
Reflections for cell refinement	9794 (θ range 2.474 to 29.043°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 26.00°	99.4 %	
Intensity decay	0%	
Reflections collected	18589	
Independent reflections	9656 (R_{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 [$F^2>2\sigma$]	R1 = 0.0243, wR2 = 0.0489	
R indices (all data)	R1 = 0.0375, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	orthorhombic, $Pna2_1$	
Unit cell parameters	a = 18.5066(9) Å	α = 90°
	b = 9.1076(4) Å	β = 90°
	c = 15.4085(7) Å	γ = 90°
Cell volume	2597.1(2) $Å^3$	
Z	4	
Calculated density	1.709 g/cm^3	
Absorption coefficient μ	1.386 mm^{-1}	
F(000)	1328	
Crystal colour and size	yellow, 0.24 × 0.12 × 0.10 mm^3	
Reflections for cell refinement	8650 (θ range 2.49 to 28.72°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 26.00°	100.0 %	
Intensity decay	0%	
Reflections collected	22146	
Independent reflections	6309 (R_{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 [$F^2>2\sigma$]	R1 = 0.0344, wR2 = 0.0718	
R indices (all data)	R1 = 0.0472, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/n$	
Unit cell parameters	a = 10.7207(6) Å	α = 90°
	b = 14.3856(8) Å	β = 111.980(2)°
	c = 11.1856(7) Å	γ = 90°
Cell volume	1599.70(16) $Å^3$	
Z	4	
Calculated density	1.541 g/cm^3	
Absorption coefficient μ	2.677 mm^{-1}	
F(000)	760	
Crystal colour and size	colourless, 0.31 × 0.19 × 0.17 mm^3	
Reflections for cell refinement	6888 (θ range 2.49 to 28.806°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 26.00°	99.8 %	
Intensity decay	0%	
Reflections collected	14002	
Independent reflections	3832 (R_{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 [$F^2>2\sigma$]	R1 = 0.0258, wR2 = 0.0680	
R indices (all data)	R1 = 0.0346, wR2 = 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 $Å^{-3}$	

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

Chemical formula	$C_{22}H_{26}O_3PSe$	
Formula weight	448.36	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	orthorhombic, $P2_12_12_1$	
Unit cell parameters	a = 8.1752(5) Å	α = 90°
	b = 10.1189(6) Å	β = 90°
	c = 24.5004(14) Å	γ = 90°
Cell volume	2026.8(2) $Å^3$	
Z	4	
Calculated density	1.469 g/cm^3	
Absorption coefficient μ	1.951 mm^{-1}	
F(000)	924	
Crystal colour and size	colourless, 0.52 × 0.26 × 0.10 mm^3	
Reflections for cell refinement	17858 (θ range 2.18 to 27.21°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 26.00°	100.0 %	
Intensity decay	0%	
Reflections collected	17792	
Independent reflections	4890 (R_{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 [$F^2>2\sigma$]	R1 = 0.0393, wR2 = 0.0805	
R indices (all data)	R1 = 0.0573, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 8.1657(16) Å	α = 103.794(3)°
	b = 10.769(2) Å	β = 92.840(3)°
	c = 11.171(2) Å	γ = 103.659(3)°
Cell volume	921.2(3) $Å^3$	
Z	1	
Calculated density	1.977 g/cm^3	
Absorption coefficient μ	3.565 mm^{-1}	
F(000)	540	
Crystal colour and size	yellow, 0.18 × 0.14 × 0.06 mm^3	
Reflections for cell refinement	2832 (θ range 2.38 to 28.31°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 26.00°	98.5 %	
Intensity decay	0%	
Reflections collected	7313	
Independent reflections	4121 (R_{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 [$F^2>2\sigma$]	R1 = 0.0359, wR2 = 0.0781	
R indices (all data)	R1 = 0.0677, wR2 = 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 $Å^{-3}$	

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

Chemical formula	$C_{23}H_{27}Cl_4O_3PPdS$	
Formula weight	662.68	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	orthorhombic, $Pna2_1$	
Unit cell parameters	a = 15.2772(7) Å	α = 90°
	b = 19.9039(10) Å	β = 90°
	c = 8.7801(4) Å	γ = 90°
Cell volume	2669.8(2) $Å^3$	
Z	4	
Calculated density	1.649 g/cm^3	
Absorption coefficient μ	1.257 mm^{-1}	
F(000)	1336	
Crystal colour and size	yellow, 0.35 × 0.28 × 0.08 mm^3	
Reflections for cell refinement	10906 (θ range 2.44 to 28.70°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 26.00°	100.0 %	
Intensity decay	0%	
Reflections collected	22990	
Independent reflections	6424 (R_{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 [$F^2>2\sigma$]	R1 = 0.0320, wR2 = 0.0740	
R indices (all data)	R1 = 0.0399, wR2 = 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 $Å^{-3}$	

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)°
	b = 11.0640(5) Å	b = 76.379(2)°
	c = 11.7858(5) Å	g = 68.405(2)°
Cell volume	1298.32(10) $Å^3$	
Z	2	
Calculated density	1.815 g/cm^3	
Absorption coefficient m	2.614 mm^{-1}	
F(000)	704	
Crystal colour and size	yellow, 0.37 × 0.30 × 0.18 mm^3	
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^2>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^2	
Weighting parameters a, b	0.0202, 0.8520	
Data / restraints / parameters	6012 / 0 / 302	
Final R indices [F^2>2s]	R1 = 0.0188, wR2 = 0.0448	
R indices (all data)	R1 = 0.0221, wR2 = 0.0464	
Goodness-of-fit on F^2	1.023	
Largest and mean shift/su	0.003 and 0.000	
Largest diff. peak and hole	0.495 and –0.498 e $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, C2/c	
Unit cell parameters	a = 11.7631(10) Å	α = 90°
	b = 18.7793(16) Å	β = 92.652(2)°
	c = 19.5578(16) Å	γ = 90°
Cell volume	4315.7(6) $Å^3$	
Z	4	
Calculated density	1.526 g/cm^3	
Absorption coefficient μ	0.923 mm^{-1}	
F(000)	2032	
Crystal colour and size	yellow, 0.21 × 0.16 × 0.11 mm^3	
Reflections for cell refinement	18846 (θ range 2.26 to 28.79°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 25.00°	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 [$F^2>2\sigma$]	R1 = 0.0798, wR2 = 0.1911	
R indices (all data)	R1 = 0.0918, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/c$	
Unit cell parameters	a = 11.5096(7) Å	α = 90°
	b = 11.4565(7) Å	β = 98.545(2)°
	c = 23.1932(14) Å	γ = 90°
Cell volume	3024.3(3) $Å^3$	
Z	4	
Calculated density	1.698 g/cm^3	
Absorption coefficient μ	5.037 mm^{-1}	
F(000)	1528	
Crystal colour and size	colourless, 0.26 × 0.21 × 0.10 mm^3	
Reflections for cell refinement	11351 (θ range 2.33 to 28.31°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 26.00°	99.9 %	
Intensity decay	0%	
Reflections collected	25066	
Independent reflections	7322 (R_{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 [$F^2>2\sigma$]	R1 = 0.0472, wR2 = 0.1057	
R indices (all data)	R1 = 0.0661, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/c$	
Unit cell parameters	a = 7.4877(2) Å	α = 90°
	b = 13.4870(4) Å	β = 92.33°
	c = 33.2358(9) Å	γ = 90°
Cell volume	3353.60(16) $Å^3$	
Z	4	
Calculated density	1.455 g/cm^3	
Absorption coefficient μ	0.755 mm^{-1}	
F(000)	1520	
Crystal colour and size	dark red, 0.49 × 0.32 × 0.23 mm^3	
Reflections for cell refinement	18591 (θ range 2.38 to 30.54°)	
Data collection method	Bruker APEX 2 CCD diffractometer	
	ω 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 θ = 30.55°	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 [$F^2>2\sigma$]	R1 = 0.0426, wR2 = 0.0975	
R indices (all data)	R1 = 0.0487, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 12.2147(12) Å	α = 84.631(2)°
	b = 12.2872(12) Å	β = 80.527(2)°
	c = 14.1978(14) Å	γ = 88.192(2)°
Cell volume	2092.3(4) $Å^3$	
Z	2	
Calculated density	1.716 g/cm^3	
Absorption coefficient μ	4.292 mm^{-1}	
F(000)	1070	
Crystal colour and size	orange, 0.34 × 0.25 × 0.02 mm^3	
Reflections for cell refinement	4763 (θ 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 θ = 25.00°	99.5 %	
Intensity decay	0%	
Reflections collected	15122	
Independent reflections	7338 (R_{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 [$F^2>2\sigma$]	R1 = 0.0480, wR2 = 0.1133	
R indices (all data)	R1 = 0.0723, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, C2/c	
Unit cell parameters	a = 29.148(2) Å	α = 90°
	b = 11.8624(9) Å	β = 98.431(2)°
	c = 22.5109(16) Å	γ = 90°
Cell volume	7699.4(10) $Å^3$	
Z	4	
Calculated density	1.567 g/cm^3	
Absorption coefficient μ	1.097 mm^{-1}	
F(000)	3696	
Crystal colour and size	orange, 0.49 × 0.08 × 0.06 mm^3	
Reflections for cell refinement	34311 (θ range 2.466 to 24.997°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 26.00°	99.9 %	
Intensity decay	0%	
Reflections collected	33403	
Independent reflections	9320 (R_{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 [$F^2>2\sigma$]	R1 = 0.0521, wR2 = 0.1070	
R indices (all data)	R1 = 0.1235, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/c$	
Unit cell parameters	a = 14.437(3) Å	α = 90°
	b = 12.105(2) Å	β = 98.023(3)°
	c = 22.147(4) Å	γ = 90°
Cell volume	3832.6(11) $Å^3$	
Z	4	
Calculated density	1.640 g/cm^3	
Absorption coefficient μ	3.949 mm^{-1}	
F(000)	1888	
Crystal colour and size	yellow, 0.34 × 0.22 × 0.05 mm^3	
Reflections for cell refinement	7184 (θ 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 θ = 25.00°	99.9 %	
Intensity decay	0%	
Reflections collected	27462	
Independent reflections	6755 (R_{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 [$F^2>2\sigma$]	R1 = 0.0491, wR2 = 0.1172	
R indices (all data)	R1 = 0.0815, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/n$	
Unit cell parameters	a = 8.4226(9) Å	α = 90°
	b = 18.9535(19) Å	β = 95.978(2)°
	c = 18.8511(19) Å	γ = 90°
Cell volume	2993.0(5) $Å^3$	
Z	4	
Calculated density	1.335 g/cm^3	
Absorption coefficient μ	0.270 mm^{-1}	
F(000)	1264	
Crystal colour and size	colourless, 0.36 × 0.19 × 0.12 mm^3	
Reflections for cell refinement	7955 (θ range 2.41 to 28.05°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 25.00°	99.8 %	
Intensity decay	0%	
Reflections collected	20863	
Independent reflections	5249 (R_{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 [$F^2>2\sigma$]	R1 = 0.0559, wR2 = 0.1451	
R indices (all data)	R1 = 0.0726, wR2 = 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 $Å^{-3}$	

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	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, C2/c	
Unit cell parameters	a = 18.2709(14) Å	α = 90°
	b = 12.8550(10) Å	β = 104.835(2)°
	c = 26.542(2) Å	γ = 90°
Cell volume	6026.3(8) $Å^3$	
Z	8	
Calculated density	1.448 g/cm^3	
Absorption coefficient μ	0.472 mm^{-1}	
F(000)	2752	
Crystal colour and size	colourless, 0.50 × 0.40 × 0.27 mm^3	
Reflections for cell refinement	22301 (θ range 2.22 to 28.54°)	
Data collection method	Bruker SMART 1000 CCD diffractometer	
	ω 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 θ = 26.00°	99.5 %	
Intensity decay	0%	
Reflections collected	21848	
Independent reflections	7122 (R_{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 [$F^2>2\sigma$]	R1 = 0.0588, wR2 = 0.1740	
R indices (all data)	R1 = 0.0797, wR2 = 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 $Å^{-3}$	