

Appendix 3 - crystallographic data tables

Compound	1
Empirical Formula	C ₃₀ H ₂₃ BrSn
Formula Weight	582.11
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.31 X 0.18 X 0.08
Crystal System	orthorhombic
Lattice Parameters	a = 16.7705(12) Å b = 17.506(2) Å c = 16.2008(4) Å - - -
Volume (Å ³)	V = 4756.2(7)
Space Group	Pbca
Z value	8
D _{calc} (g/cm ³)	1.626
F ₀₀₀	2304
μ(MoKα) (cm ⁻¹)	27.751
No. of Reflections Measured	39031
R _{int}	0.0703
Min and Max Transmissions	0.623 - 0.801
Observed Reflection (No. Variables)	4181(289)
Reflection/Parameter Ratio	14.47
Residuals: R ₁ (I>2.00σ(I))	0.0359
Residuals: R (All reflections)	0.0478
Residuals: wR ₂ (All reflections)	0.0783
Goodness of Fit Indicator	1.125
Flack Parameter	-
Maximum peak in Final Diff. Map	1.26 e-/Å ³
Minimum peak in Final Diff. Map	-0.54 e-/Å ³

Compound	2
Empirical Formula	C ₂₄ H ₁₈ BrClSn
Formula Weight	540.45
Temperature (°C)	-148
Crystal Colour, Habit	colourless, prism
Crystal Dimensions (mm ³)	0.16 X 0.13 X 0.04
Crystal System	monoclinic
Lattice Parameters	a = 9.127(2) Å b = 16.587(4) Å c = 14.900(3) Å - β = 93.060(13)° -
Volume (Å ³)	V = 2252.5(9)
Space Group	P 2 ₁ /n
Z value	4
D _{calc} (g/cm ³)	1.594
F ₀₀₀	1056
μ(MoKα) (cm ⁻¹)	30.373
No. of Reflections Measured	19184
R _{int}	0.1044
Min and Max Transmissions	0.531 - 0.886
Observed Reflection (No. Variables)	3963(244)
Reflection/Parameter Ratio	16.24
Residuals: R ₁ (I>2.00σ(I))	0.0753
Residuals: R (All reflections)	0.0976
Residuals: wR ₂ (All reflections)	0.2530
Goodness of Fit Indicator	1.104
Flack Parameter	-
Maximum peak in Final Diff. Map	3.56 e-/Å ³
Minimum peak in Final Diff. Map	-1.27 e-/Å ³

Compound	3
Empirical Formula	C ₂₈ H ₂₄ Br ₂ Cl ₂ OSn
Formula Weight	725.90
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.19 X 0.10 X 0.05
Crystal System	triclinic
Lattice Parameters	a = 7.198(6) Å b = 10.31(7) Å c = 18.69(2) Å α = 81.51(3)° β = 87.91(2)° γ = 74.41(2)°
Volume (Å ³)	V = 1322(2)
Space Group	P -1
Z value	2
D _{calc} (g/cm ³)	1.824
F ₀₀₀	708
μ(MoKα) (cm ⁻¹)	42.209
No. of Reflections Measured	11197
R _{int}	0.0554
Min and Max Transmissions	0.609 - 0.81
Observed Reflection (No. Variables)	4648(307)
Reflection/Parameter Ratio	15.14
Residuals: R ₁ (I>2.00σ(I))	0.0498
Residuals: R (All reflections)	0.076
Residuals: wR ₂ (All reflections)	0.1443
Goodness of Fit Indicator	1.127
Flack Parameter	-
Maximum peak in Final Diff. Map	1.16 e-/Å ³
Minimum peak in Final Diff. Map	-1.40 e-/Å ³

Compound	4
Empirical Formula	C ₄₄ H ₄₃ Br ₃ Sn
Formula Weight	930.23
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.1 X 0.1 X 0.01
Crystal System	triclinic
Lattice Parameters	a = 7.601(3) Å b = 15.347(7) Å c = 16.066(7) Å α = 102.200(11)° β = 92.613(10)° γ = 100.486(10)°
Volume (Å ³)	V = 1794.2(12)
Space Group	P -1
Z value	2
D _{calc} (g/cm ³)	1.722
F ₀₀₀	924
μ(MoKα) (cm ⁻¹)	40.946
No. of Reflections Measured	11439
R _{int}	0.0421
Min and Max Transmissions	0.683 - 0.96
Observed Reflection (No. Variables)	6329(433)
Reflection/Parameter Ratio	14.62
Residuals: R ₁ (I>2.00σ(I))	0.0633
Residuals: R (All reflections)	0.0800
Residuals: wR ₂ (All reflections)	0.1564
Goodness of Fit Indicator	1.225
Flack Parameter	-
Maximum peak in Final Diff. Map	2.50 e-/Å ³
Minimum peak in Final Diff. Map	-1.26 e-/Å ³

Compound	5
Empirical Formula	C ₃₆ H ₂₆ Br ₂ Sn
Formula Weight	737.10
Temperature (°C)	-148
Crystal Colour, Habit	colourless, prism
Crystal Dimensions (mm ³)	0.05 X 0.05 X 0.05
Crystal System	triclinic
Lattice Parameters	a = 10.073(5) Å b = 11.839(4) Å c = 12.381(6) Å α = 90.697(10)° β = 109.926(12)° γ = 95.247(9)°
Volume (Å ³)	V = 1380.7(10)
Space Group	P -1
Z value	2
D _{calc} (g/cm ³)	1.773
F ₀₀₀	724
μ(MoKα) (cm ⁻¹)	38.529
No. of Reflections Measured	8596
R _{int}	0.0438
Min and Max Transmissions	0.631 - 0.825
Observed Reflection (No. Variables)	4719(352)
Reflection/Parameter Ratio	13.41
Residuals: R ₁ (I>2.00σ(I))	0.0512
Residuals: R (All reflections)	0.0711
Residuals: wR ₂ (All reflections)	0.1396
Goodness of Fit Indicator	1.087
Flack Parameter	-
Maximum peak in Final Diff. Map	1.01 e-/Å ³
Minimum peak in Final Diff. Map	-1.31 e-/Å ³

Compound	6
Empirical Formula	C ₃₈ H ₃₀ Br ₂ Sn
Formula Weight	765.15
Temperature (°C)	-148
Crystal Colour, Habit	colourless, chunk
Crystal Dimensions (mm ³)	0.21 X 0.15 X 0.05
Crystal System	monoclinic
Lattice Parameters	a = 12.467(3) Å b = 9.296(2) Å c = 26.334(6) Å - β = 91.447(6)° -
Volume (Å ³)	V = 3051.0(11)
Space Group	P2 ₁ /c
Z value	4
D _{calc} (g/cm ³)	1.667
F ₀₀₀	1512
μ(MoKα) (cm ⁻¹)	34.907
No. of Reflections Measured	22065
R _{int}	0.0476
Min and Max Transmissions	0.58 - 0.84
Observed Reflection (No. Variables)	5335(370)
Reflection/Parameter Ratio	14.42
Residuals: R ₁ (I>2.00σ(I))	0.0504
Residuals: R (All reflections)	0.0615
Residuals: wR ₂ (All reflections)	0.1635
Goodness of Fit Indicator	1.152
Flack Parameter	-
Maximum peak in Final Diff. Map	2.52 e-/Å ³
Minimum peak in Final Diff. Map	-1.18 e-/Å ³

Compound	7
Empirical Formula	C ₃₆ H ₂₈ SSn
Formula Weight	611.37
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.18 X 0.16 X 0.020
Crystal System	monoclinic
Lattice Parameters	a = 9.179(6) Å b = 16.871(11) Å c = 18.287(11) Å A = 90° B = 92.120(8)° γ = 90°
Volume (Å ³)	V = 2830(3)
Space Group	P21/n
Z value	4
D _{calc} (g/cm ³)	1.435
F ₀₀₀	1240
μ(MoKα) (cm ⁻¹)	9.996
No. of Reflections Measured	24170
R _{int}	0.0811
Min and Max Transmissions	0.821 - 0.980
Observed Reflection (No. Variables)	4979(343)
Reflection/Parameter Ratio	14.52
Residuals: R ₁ (I>2.00σ(I))	0.0469
Residuals: R (All reflections)	0.0710
Residuals: wR ₂ (All reflections)	0.0948
Goodness of Fit Indicator	1.172
Flack Parameter	-
Maximum peak in Final Diff. Map	0.70 e-/Å ³
Minimum peak in Final Diff. Map	-0.72 e-/Å ³

Compound	8
Empirical Formula	C ₃₆ H ₂₈ SeSn
Formula Weight	658.27
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.130 X 0.120 X 0.030
Crystal System	monoclinic
Lattice Parameters	a = 9.223(5) Å b = 16.740(8) Å c = 18.435(8) Å α = 90° β = 91.963(6)° γ = 90°
Volume (Å ³)	V = 2844(3)
Space Group	P 21/n
Z value	4
D _{calc} (g/cm ³)	1.537
F ₀₀₀	1312
μ(MoKα) (cm ⁻¹)	22.011
No. of Reflections Measured	24262
R _{int}	0.0917
Min and Max Transmissions	0.707 - 0.936
Observed Reflection (No. Variables)	5006(343)
Reflection/Parameter Ratio	14.59
Residuals: R ₁ (I>2.00σ(I))	0.0547
Residuals: R (All reflections)	0.0760
Residuals: wR ₂ (All reflections)	0.0885
Goodness of Fit Indicator	1.156
Flack Parameter	-
Maximum peak in Final Diff. Map	0.99 e-/Å ³
Minimum peak in Final Diff. Map	-0.74 e-/Å ³

Compound	9
Empirical Formula	C ₃₆ H ₂₈ TeSn
Formula Weight	706.91
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.090 X 0.060 X 0.030
Crystal System	monoclinic
Lattice Parameters	a = 14.016(2) Å b = 14.825(2) Å c = 14.364(2) Å α = 90° β = 103.616(4)° γ = 90°
Volume (Å ³)	V = 2900.7(7)
Space Group	P 21/n
Z value	4
D _{calc} (g/cm ³)	1.619
F ₀₀₀	1384
μ(MoKα) (cm ⁻¹)	18.894
No. of Reflections Measured	21582
R _{int}	0.0433
Min and Max Transmissions	0.753 - 0.945
Observed Reflection (No. Variables)	5057(343)
Reflection/Parameter Ratio	14.74
Residuals: R ₁ (I>2.00σ(I))	0.0454
Residuals: R (All reflections)	0.0577
Residuals: wR ₂ (All reflections)	0.1415
Goodness of Fit Indicator	1.111
Flack Parameter	-
Maximum peak in Final Diff. Map	0.68 e-/Å ³
Minimum peak in Final Diff. Map	-0.91 e-/Å ³

Compound	10
Empirical Formula	C ₃₀ H ₂₃ ClSSn
Formula Weight	569.71
Temperature (°C)	-148
Crystal Colour, Habit	colourless, chunk
Crystal Dimensions (mm ³)	0.180 X 0.120 X 0.030
Crystal System	triclinic
Lattice Parameters	a = 10.8028(12) Å b = 12.202(2) Å c = 19.344(3) Å α = 86.738(8)° β = 79.174(6)° γ = 82.691(8)°
Volume (Å ³)	V = 2482.7(5)
Space Group	P -1
Z value	4
D _{calc} (g/cm ³)	1.524
F ₀₀₀	1144
μ(MoKα) (cm ⁻¹)	12.369
No. of Reflections Measured	19129
R _{int}	0.0495
Min and Max Transmissions	0.748 - 0.964
Observed Reflection (No. Variables)	8636(595)
Reflection/Parameter Ratio	14.51
Residuals: R ₁ (I>2.00σ(I))	0.0566
Residuals: R (All reflections)	0.0733
Residuals: wR ₂ (All reflections)	0.2028
Goodness of Fit Indicator	1.067
Flack Parameter	-
Maximum peak in Final Diff. Map	1.58 e-/Å ³
Minimum peak in Final Diff. Map	-1.14 e-/Å ³

Compound	11
Empirical Formula	C ₃₀ H ₂₃ ClSeSn
Formula Weight	616.61
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.150 X 0.120 X 0.030
Crystal System	triclinic
Lattice Parameters	a = 10.922(1) Å b = 11.015(1) Å c = 12.402(2) Å α = 103.324(7)° β = 96.476(7)° γ = 117.990(8)°
Volume (Å ³)	V = 1238.8(3)
Space Group	P -1
Z value	2
D _{calc} (g/cm ³)	1.653
F ₀₀₀	608
μ(MoKα) (cm ⁻¹)	26.246
No. of Reflections Measured	10495
R _{int}	0.0725
Min and Max Transmissions	0.642 - 0.924
Observed Reflection (No. Variables)	4346(298)
Reflection/Parameter Ratio	14.58
Residuals: R ₁ (I>2.00σ(I))	0.0676
Residuals: R (All reflections)	0.1010
Residuals: wR ₂ (All reflections)	0.1552
Goodness of Fit Indicator	1.045
Flack Parameter	-
Maximum peak in Final Diff. Map	1.92 e-/Å ³
Minimum peak in Final Diff. Map	-0.62 e-/Å ³

Compound	12
Empirical Formula	C ₄₀ H ₃₄ Cl ₂ OS ₂ Sn
Formula Weight	784.42
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.21 X 0.13 X 0.02
Crystal System	monoclinic
Lattice Parameters	a = 10.164(2) Å b = 17.454(4) Å c = 21.111(5) Å - β = 101.876(10)° -
Volume (Å ³)	V = 3664.9(14)
Space Group	P2 ₁ /c
Z value	4
D _{calc} (g/cm ³)	1.422
F ₀₀₀	1592
μ(MoKα) (cm ⁻¹)	9.866
No. of Reflections Measured	31253
R _{int}	0.1377
Min and Max Transmissions	0.658 - 0.980
Observed Reflection (No. Variables)	6444(415)
Reflection/Parameter Ratio	15.53
Residuals: R ₁ (I>2.00σ(I))	0.1032
Residuals: R (All reflections)	0.1400
Residuals: wR ₂ (All reflections)	0.2946
Goodness of Fit Indicator	1.094
Flack Parameter	-
Maximum peak in Final Diff. Map	4.43 e-/Å ³
Minimum peak in Final Diff. Map	-0.90 e-/Å ³

Compound	13
Empirical Formula	C ₄₈ H ₃₆ S ₂ Sn
Formula Weight	795.62
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.300 X 0.150 X 0.060
Crystal System	monoclinic
Lattice Parameters	a = 12.407(5) Å b = 12.099(4) Å c = 24.697(9) Å α = 90° β = 102.376(4)° γ = 90°
Volume (Å ³)	V = 3621(3)
Space Group	P 21/n
Z value	4
D _{calc} (g/cm ³)	1.459
F ₀₀₀	1624
μ(MoKα) (cm ⁻¹)	8.557
No. of Reflections Measured	30652
R _{int}	0.0537
Min and Max Transmissions	0.815 - 0.950
Observed Reflection (No. Variables)	6379(460)
Reflection/Parameter Ratio	13.87
Residuals: R ₁ (I>2.00σ(I))	0.0333
Residuals: R (All reflections)	0.0454
Residuals: wR ₂ (All reflections)	0.0775
Goodness of Fit Indicator	1.112
Flack Parameter	-
Maximum peak in Final Diff. Map	0.54 e-/Å ³
Minimum peak in Final Diff. Map	-0.58 e-/Å ³

Compound	14
Empirical Formula	C ₂₆ H ₃₁ ClSSn
Formula Weight	529.73
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.320 X 0.240 X 0.060
Crystal System	monoclinic
Lattice Parameters	a = 10.931(4) Å b = 11.186(4) Å c = 19.577(8) Å α = 90° β = 95.331(5)° γ = 90°
Volume (Å ³)	V = 2383(2)
Space Group	P 21/n
Z value	4
D _{calc} (g/cm ³)	1.476
F ₀₀₀	1080
μ(MoKα) (cm ⁻¹)	12.816
No. of Reflections Measured	20059
R _{int}	0.0438
Min and Max Transmissions	0.688 - 0.926
Observed Reflection (No. Variables)	4186(262)
Reflection/Parameter Ratio	15.98
Residuals: R ₁ (I>2.00σ(I))	0.0330
Residuals: R (All reflections)	0.0401
Residuals: wR ₂ (All reflections)	0.0757
Goodness of Fit Indicator	1.121
Flack Parameter	-
Maximum peak in Final Diff. Map	0.58 e-/Å ³
Minimum peak in Final Diff. Map	-0.66 e-/Å ³

Compounds	15
Empirical Formula	C ₂₆ H ₃₁ ClSeSn
Formula Weight	576.63
Temperature (°C)	-148
Crystal Colour, Habit	yellow, chunk
Crystal Dimensions (mm ³)	0.210 X 0.080 X 0.020
Crystal System	monoclinic
Lattice Parameters	a = 11.126(3) Å b = 11.304(3) Å c = 19.508(4) Å α = 90° β = 96.212(9)° γ = 90°
Volume (Å ³)	V = 2439.1(9)
Space Group	P 2/1 n
Z value	4
D _{calc} (g/cm ³)	1.570
F ₀₀₀	1152
μ(MoKα) (cm ⁻¹)	26.594
No. of Reflections Measured	20591
R _{int}	0.1006
Min and Max Transmissions	0.712 - 0.948
Observed Reflection (No. Variables)	4287(262)
Reflection/Parameter Ratio	16.36
Residuals: R ₁ (I>2.00σ(I))	0.0557
Residuals: R (All reflections)	0.0906
Residuals: wR ₂ (All reflections)	0.1092
Goodness of Fit Indicator	1.052
Flack Parameter	-
Maximum peak in Final Diff. Map	0.78 e-/Å ³
Minimum peak in Final Diff. Map	-0.70 e-/Å ³

Compound	16
Empirical Formula	C ₁₄ H ₁₃ BrS
Formula Weight	293.22
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.18 X 0.06 X 0.02
Crystal System	monoclinic
Lattice Parameters	a = 15.932(10) Å b = 7.746(5) Å c = 18.895(11) Å
	-
	β = 99.01(2)°
	-
Volume (Å ³)	V = 2303(3)
Space Group	C2/c
Z value	8
D _{calc} (g/cm ³)	1.691
F ₀₀₀	1184
μ(MoKα) (cm ⁻¹)	37.277
No. of Reflections Measured	8750
R _{int}	0.1005
Min and Max Transmissions	0.667 - 0.928
Observed Reflection (No. Variables)	2315(145)
Reflection/Parameter Ratio	15.97
Residuals: R ₁ (I>2.00σ(I))	0.0656
Residuals: R (All reflections)	0.0777
Residuals: wR ₂ (All reflections)	0.1962
Goodness of Fit Indicator	1.215
Flack Parameter	-
Maximum peak in Final Diff. Map	0.82 e-/Å ³
Minimum peak in Final Diff. Map	-0.97 e-/Å ³

Compound	17
Empirical Formula	C ₂₂ H ₃₁ ClSSn
Formula Weight	481.69
Temperature (°C)	-148
Crystal Colour, Habit	colourless, prism
Crystal Dimensions (mm ³)	0.16 X 0.13 X 0.07
Crystal System	triclinic
Lattice Parameters	a = 9.627(2) Å b = 10.451(3) Å c = 11.881(3) Å α = 94.473(7)° β = 111.675(8)° γ = 95.075(7)°
Volume (Å ³)	V = 1098.6(5)
Space Group	P-1
Z value	2
D _{calc} (g/cm ³)	1.456
F ₀₀₀	492
μ(MoKα) (cm ⁻¹)	13.818
No. of Reflections Measured	8326
R _{int}	0.0438
Min and Max Transmissions	0.720 - 0.908
Observed Reflection (No. Variables)	3852(237)
Reflection/Parameter Ratio	16.25
Residuals: R ₁ (I>2.00σ(I))	0.0402
Residuals: R (All reflections)	0.0521
Residuals: wR ₂ (All reflections)	0.1030
Goodness of Fit Indicator	0.899
Flack Parameter	-
Maximum peak in Final Diff. Map	0.50 e-/Å ³
Minimum peak in Final Diff. Map	-0.66 e-/Å ³

Compound	18
Empirical Formula	C ₃₂ H ₂₈ SSn
Formula Weight	563.32
Temperature (°C)	-148
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.18 X 0.12 X 0.02
Crystal System	orthorhombic
Lattice Parameters	a = 31.415(4) Å b = 9.6005(11) Å c = 17.971(2) Å - - -
Volume (Å ³)	V = 5420.0(11)
Space Group	Pbcn
Z value	8
D _{calc} (g/cm ³)	1.381
F ₀₀₀	2288
μ(MoKα) (cm ⁻¹)	10.371
No. of Reflections Measured	37365
R _{int}	0.0652
Min and Max Transmissions	0.781 - 0.979
Observed Reflection (No. Variables)	4760(318)
Reflection/Parameter Ratio	14.97
Residuals: R ₁ (I>2.00σ(I))	0.0593
Residuals: R (All reflections)	0.0774
Residuals: wR ₂ (All reflections)	0.1886
Goodness of Fit Indicator	1.276
Flack Parameter	-
Maximum peak in Final Diff. Map	0.45 e-/Å ³
Minimum peak in Final Diff. Map	-0.66 e-/Å ³

Compound	19
Empirical Formula	C ₃₆ H ₃₇ PSn
Formula Weight	619.35
Temperature (°C)	-148(1)
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.150 X 0.150 X 0.020
Crystal System	monoclinic
Lattice Parameters	a = 11.655(4) Å b = 13.276(5) Å c = 19.392(7) Å - β = 100.548(9)° -
Volume (Å ³)	V = 2949.7(18)
Space Group	P2 ₁ /c
Z value	4
D _{calc} (g/cm ³)	1.395
F ₀₀₀	1272
μ(MoKα) (cm ⁻¹)	9.433
No. of Reflections Measured	22035
R _{int}	0.0876
Min and Max Transmissions	0.706 - 0.981
Observed Reflection (No. Variables)	5164(343)
Reflection/Parameter Ratio	15.06
Residuals: R ₁ (I>2.00σ(I))	0.0667
Residuals: R (All reflections)	0.0907
Residuals: wR ₂ (All reflections)	0.2271
Goodness of Fit Indicator	1.293
Flack Parameter	-
Maximum peak in Final Diff. Map	1.10 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-1.13 e ⁻ /Å ³

Compound	20
Empirical Formula	C ₃₀ H ₃₂ ClPSn
Formula Weight	577.70
Temperature (°C)	-148(1)
Crystal Colour, Habit	colourless, chip
Crystal Dimensions (mm ³)	0.090 X 0.090 X 0.030
Crystal System	monoclinic
Lattice Parameters	a = 10.118(5) Å b = 18.035(8) Å c = 14.906(7) Å - β = 93.905(12)° -
Volume (Å ³)	V = 2714(2)
Space Group	P2 ₁ /n
Z value	4
D _{calc} (g/cm ³)	1.414
F ₀₀₀	1176
μ(MoKα) (cm ⁻¹)	11.144
No. of Reflections Measured	20422
R _{int}	0.1413
Min and Max Transmissions	0.371 - 0.967
Observed Reflection (No. Variables)	4757(298)
Reflection/Parameter Ratio	15.96
Residuals: R ₁ (I>2.00σ(I))	0.1016
Residuals: R (All reflections)	0.1437
Residuals: wR ₂ (All reflections)	0.2898
Goodness of Fit Indicator	1.200
Flack Parameter	-
Maximum peak in Final Diff. Map	1.31 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-1.52 e ⁻ /Å ³

Compound	21
Empirical Formula	C ₂₀ H ₂₈ ClPSn
Formula Weight	453.56
Temperature (°C)	-180(1)
Crystal Colour, Habit	colourless, chunk
Crystal Dimensions (mm ³)	0.120 X 0.090 X 0.030
Crystal System	monoclinic
Lattice Parameters	a = 10.041(3) Å b = 11.762(4) Å c = 18.064(6) Å - β = 93.926(10)° -
Volume (Å ³)	V = 2128.5(11)
Space Group	P2 ₁ /n
Z value	4
D _{calc} (g/cm ³)	1.415
F ₀₀₀	920
μ(MoKα) (cm ⁻¹)	13.988
No. of Reflections Measured	11801
R _{int}	0.1050
Min and Max Transmissions	0.425 - 0.959
Observed Reflection (No. Variables)	3701(208)
Reflection/Parameter Ratio	17.79
Residuals: R ₁ (I>2.00σ(I))	0.0889
Residuals: R (All reflections)	0.1744
Residuals: wR ₂ (All reflections)	0.2857
Goodness of Fit Indicator	1.062
Flack Parameter	-
Maximum peak in Final Diff. Map	1.85 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-0.69 e ⁻ /Å ³

Compound	22
Empirical Formula	C ₂₆ H ₄₀ ClPSn
Formula Weight	537.72
Temperature (°C)	-180(1)
Crystal Colour, Habit	colourless, prism
Crystal Dimensions (mm ³)	0.090 X 0.060 X 0.030
Crystal System	Orthorhombic
Lattice Parameters	a = 14.086(3) Å b = 18.692(4) Å c = 20.000(4) Å
	-
	-
	-
Volume (Å ³)	V = 5266(2)
Space Group	Pbca
Z value	8
D _{calc} (g/cm ³)	1.356
F ₀₀₀	2224
μ(MoKα) (cm ⁻¹)	11.425
No. of Reflections Measured	32034
R _{int}	0.1882
Min and Max Transmissions	0.551 - 0.966
Observed Reflection (No. Variables)	4599(262)
Reflection/Parameter Ratio	17.55
Residuals: R ₁ (I>2.00σ(I))	0.0558
Residuals: R (All reflections)	0.0959
Residuals: wR ₂ (All reflections)	0.1782
Goodness of Fit Indicator	1.024
Flack Parameter	-
Maximum peak in Final Diff. Map	0.83 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-1.04 e ⁻ /Å ³

Compound	23
Empirical Formula	C ₃₆ H ₄₄ Cl ₂ P ₂ Sn
Formula Weight	728.29
Temperature (°C)	-180(1)
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.090 X 0.060 X 0.020
Crystal System	monoclinic
Lattice Parameters	a = 18.192(7) Å b = 13.185(5) Å c = 15.021(5) Å - β = 111.193(8)° -
Volume (Å ³)	V = 3359(2)
Space Group	P2/c
Z value	4
D _{calc} (g/cm ³)	1.440
F ₀₀₀	1496
μ(MoKα) (cm ⁻¹)	10.388
No. of Reflections Measured	18205
R _{int}	0.1556
Min and Max Transmissions	0.437 - 0.979
Observed Reflection (No. Variables)	5830(370)
Reflection/Parameter Ratio	15.76
Residuals: R ₁ (I>2.00σ(I))	0.1173
Residuals: R (All reflections)	0.2633
Residuals: wR ₂ (All reflections)	0.3738
Goodness of Fit Indicator	1.027
Flack Parameter	-
Maximum peak in Final Diff. Map	3.50 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-1.16 e ⁻ /Å ³

Compound	24
Empirical Formula	C ₁₈ H ₂₆ Sn ₂
Formula Weight	479.78
Temperature (°C)	-148(1)
Crystal Colour, Habit	colourless, platelet
Crystal Dimensions (mm ³)	0.210 X 0.060 X 0.040
Crystal System	monoclinic
Lattice Parameters	a = 7.773(2) Å b = 13.833(4) Å c = 16.708(5) Å - β = 92.443(10)° -
Volume (Å ³)	V = 1794.8(9)
Space Group	P2 ₁ /n
Z value	4
D _{calc} (g/cm ³)	1.775
F ₀₀₀	936
μ(MoKα) (cm ⁻¹)	27.728
No. of Reflections Measured	11465
R _{int}	0.0900
Min and Max Transmissions	-
Observed Reflection (No. Variables)	3051(181)
Reflection/Parameter Ratio	16.86
Residuals: R ₁ (I>2.00σ(I))	0.0659
Residuals: R (All reflections)	0.0918
Residuals: wR ₂ (All reflections)	0.1184
Goodness of Fit Indicator	1.254
Flack Parameter	-
Maximum peak in Final Diff. Map	0.94 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-0.96 e ⁻ /Å ³

Compound	25
Empirical Formula	C ₄₈ H ₃₈ Sn ₂
Formula Weight	852.21
Temperature (°C)	-100(1)
Crystal Colour, Habit	colourless, prism
Crystal Dimensions (mm ³)	0.200 X 0.200 X 0.200
Crystal System	triclinic
Lattice Parameters	a = 9.7934(17) Å b = 10.2626(15) Å c = 19.442(3) Å α = 75.210(14)° β = 78.183(16)° γ = 85.544(15)°
Volume (Å ³)	V = 1848.6(6)
Space Group	P-1
Z value	2
D _{calc} (g/cm ³)	1.531
F ₀₀₀	852
μ(MoKα) (cm ⁻¹)	13.842
No. of Reflections Measured	19769
R _{int}	0.0675
Min and Max Transmissions	0.414 - 0.758
Observed Reflection (No. Variables)	6469(451)
Reflection/Parameter Ratio	14.34
Residuals: R ₁ (I>2.00σ(I))	0.0324
Residuals: R (All reflections)	0.0346
Residuals: wR ₂ (All reflections)	0.0920
Goodness of Fit Indicator	0.998
Flack Parameter	-
Maximum peak in Final Diff. Map	1.13 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-1.05 e ⁻ /Å ³

Compound	26
Empirical Formula	C ₂₈ H ₂₈ Sn ₂
Formula Weight	601.91
Temperature (°C)	-148(1)
Crystal Colour, Habit	colourless, prism
Crystal Dimensions (mm ³)	0.200 X 0.050 X 0.040
Crystal System	triclinic
Lattice Parameters	a = 7.419(1) Å b = 8.172(1) Å c = 10.625(2) Å α = 108.784(8)° β = 108.004(8)° γ = 90.700(6)°
Volume (Å ³)	V = 575.6(2)
Space Group	P-1
Z value	1
D _{calc} (g/cm ³)	1.736
F ₀₀₀	296
μ(MoKα) (cm ⁻¹)	21.818
No. of Reflections Measured	4963
R _{int}	0.0415
Min and Max Transmissions	0.713 - 0.916
Observed Reflection (No. Variables)	2021(136)
Reflection/Parameter Ratio	14.86
Residuals: R ₁ (I>2.00σ(I))	0.0310
Residuals: R (All reflections)	0.0363
Residuals: wR ₂ (All reflections)	0.0737
Goodness of Fit Indicator	1.190
Flack Parameter	-
Maximum peak in Final Diff. Map	0.56 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-0.69 e ⁻ /Å ³

