

The synthesis and characterization of mono and dinuclear group 13 Schiff base complexes

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Supplementary Information

S1: Crystal Data for Compounds **1 - 7:**

Compound Name	1	2	3	4
	[L{Al(Me) ₂ } ₂]	[{(NO)Al(thf) ₂ }I]	[H ₂ L{GaCl(Me) ₂ } ₂]	[{LGaCl} ₂ (μLi)]GaCl ₄
Chemical Formula	C ₁₆ H ₃₀ Al ₂ N ₂ O ₂	C ₂₀ H ₃₄ AlIN ₂ O ₄	C ₁₆ H ₃₂ Ga ₂ Cl ₂ N ₂ O ₂	C ₂₄ H ₃₆ Ga ₃ Cl ₆ LiN ₄ O ₄
Formula Weight	336.38	520.37	494.78	873.37
Crystal System	Triclinic	Monoclinic	Triclinic	Orthorhombic
Space Group	P-1	C 2 / c	P-1	Pccn
T(K)	123(2)	123(2)	123(2)	173(2)
a (Å)	5.8360(6)	12.7840(10)	6.9600(2)	11.0058(5)
b (Å)	8.5491(10)	14.1352(9)	7.3178(3)	19.6503(9)
c (Å)	10.8312(11)	29.117(2)	11.7649(4)	16.5196(9)
α (°)	68.177(10)	90	80.036(3)	90
β (°)	80.886(8)	97.139(7)	88.925(3)	90
γ (°)	71.595(10)	90	75.353(3)	90
V (Å ³)	475.49(9)	5220.7(7)	570.79(3)	3572.6(3)

Z	1	8	1	4
Reflections collected	3757	9835	12375	35029
Independent reflections	2180	4697	2599	4602
Data/restraints/parameter ratio	2180/0/104	4697/0/266	2599/0/117	4602/0/195
R int	0.0146	0.0377	0.0362	0.0367
Dcalc (Mg/m ³)	1.175	1.324	1.439	1.624
F(000)	182	2128	254	1752
R indices (all data)	R1 = 0.0415 , wR2 = 0.1017	R1 = 0.0544, wR2 = 0.1458	R1 = 0.0338, wR2 = 0.0654	R1 = 0.0558, wR2 = 0.0894
Final R indices [I > 2σ(I)]	R1 = 0.0354, wR2 = 0.0962	R1 = 0.0483, wR2 = 0.1395	R1 = 0.0270 wR2 = 0.0617	R1 = 0.0367, wR2 = 0.0805
Largest difference in peak and hole (e Å ⁻³)	0.305 and -0.259	1.958 and -0.888	0.339 and -0.306	0.693 and - 0.344

S 1 (contd).

Compound Name	5	6	7
	[LnCl] ₂	[LnCl(thf)]	[L ₃ In ₂]
Chemical Formula	C ₃₁ H ₄₄ In ₂ Cl ₂ N ₄ O ₄	C ₁₆ H ₂₆ InClN ₂ O ₃	C ₄₄ H ₆₄ In ₂ N ₆ O ₆
Formula Weight	837.24	444.66	988.63
Crystal System	Triclinic	Monoclinic	Triclinic
Space Group	P-1	P21/n	P-1
T(K)	173(2)	173(2)	173(2)
a (Å)	9.4301(7)	8.0463(14)	8.5167(7)
b (Å)	9.6908(9)	14.8894(7)	11.0176(8)
c (Å)	11.2031(9)	15.5567(7)	12.5746(7)
α (°)	90.674(7)	90	80.165(6)
β (°)	110.084(7)	93.294(8)	80.237(5)
γ (°)	112.240(8)	90	73.433(7)
V (Å ³)	878.10(13)	1860.7(3)	1105.15(14)
Z	1	4	1
Reflections collected	5976	24793	10106

Independent reflections	3427	4740	4908
Data/restraints/parameter ratio	3427/73/213	4740/0/208	4908/7/292
R int	0.0559	0.0316	0.0286
Dcalc (Mg/m ³)	1.583	1.587	1.485
F(000)	422	904	508
R indices (all data)	R1 = 0.0505, wR2 = 0.1247	R1 = 0.0477, wR2 = 0.0934	R1 = 0.0421, wR2 = 0.0877
Final R indices [I > 2σ(I)]	R1 = 0.0442, wR2 = 0.1187	R1 = 0.0356, wR2 = 0.0854	R1 = 0.0350, wR2 = 0.0838
Largest difference in peak and hole (e Å ⁻³)	1.675 and -0.996	0.883 and -0.949	0.681 and -0.589

S2: DSC Data for 7.

