Solvent-Induced Unsymmetric Salamo-Like Trinuclear Ni^{II} Complexes: Syntheses, Crystal Structures, Fluorescent and Magnetic Properties

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Table S1 Crystal data and structure refinements for Ni^{II} complexes **2**, **3** and **4**.

Compound	**2**	**3**	**4**
Molecular formula	$C_{40}H_{46}Ni_3N_4O_{20}$	$C_{44}H_{58}Ni_3N_4O_{18}$	$C_{44}H_{50}Ni_3N_4O_{16}$
Molecular weight	1078.94	1107.07	1067.01
Temperature (K)	294.29(10)	293(2)	294.29(10)
Crystal size, mm^3	0.33×0.27×0.25	0.20×0.13× 0.12	0.33×0.31×0.27
Crystal system	triclinic	monoclinic	monoclinic
Space group	*P*-1	*C*2/c	$P2_1/n$
Unit cell dimensions			
a(Å)	11.1760(11)	19.2947(6)	12.3164(7)
b(Å)	11.9520(10)	15.1426(6)	13.3441(6)
c(Å)	12.0854(14)	20.4291(6)	15.2621(8)
α(º)	68.606(9)	90	90
β(º)	66.295(10)	103.384(3)	111.426(7)
γ(º)	77.351(8)	90	90
V ($Å^3$)	1371.3(3)	5806.7(3)	2335.0(2)
Z	1	4	2
D_{calc}(Mg/m^3)	1.307	1.266	1.518
μ(mm^{-1})	1.089	1.683	1.272
F(000)	558	2312	1108
hkl range	-14 ≤ h ≤ 15,	-19 ≤ *h* ≤ 23,	-15≤ *h* ≤ 15,
	-12 ≤ k ≤ 15,	-18 ≤ *k* ≤ 15,	-15 ≤ *k* ≤ 16,
	-16≤ l ≤ 16	-21 ≤ *l* ≤ 24	-13≤ *l* ≤ 18
Θ range(º)	3.3–26.0	3.8– 69.6	3.4–26.0
Reflections collected / unique	10747/5386	11733 / 5377	10245/ 4595
*R*int	0.0306	0.0227	0.0423
Data / restraints / parameters	5386/5/313	5377 /35/338	4595/0/ 308
R_1 / wR_2 [$I \geq 2\sigma(I)$][a]	0.0618 /0.1752	0.0557 / 0.1646	0.0607 / 0.1396
R_1 / wR_2 (all data)	0.0843/0.1934	0.0692 /0.1768	0.0996 /0.1662

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Goodness off it(GOF)	1.104	1.090	1.037
$\Delta\rho_{max,min}$ (e Å^{-3})	1.12 / -0.47	1.04 / -0.40	0.63 / -0.34

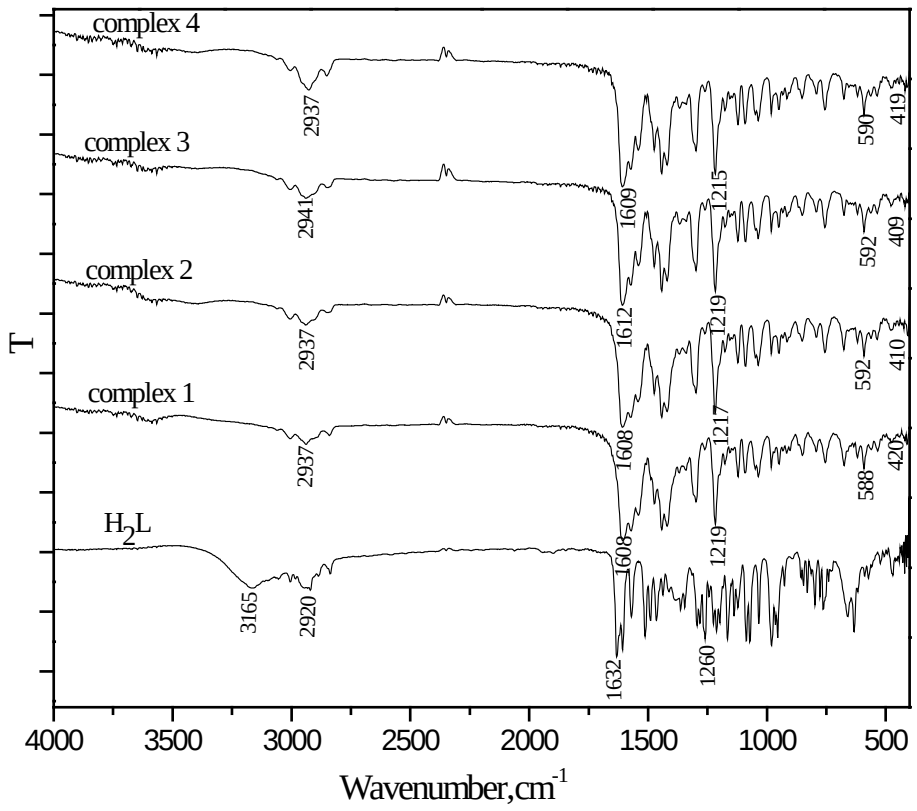

Fig. S1 The IR spectra of H_2L and its corresponding Ni^{II} complexes **1**, **2**, **3** and **4**.