

An Octahedral Aluminium(III) Complex as a Three-Fold node for Supramolecular Heterometallic Self-Assemblies: Solution and Solid State Chemistry

Damien Simond,^[a] Sarah E. Clifford,^[a,b] Andreia F. Vieira,^[a] Céline Besnard^[c] and Alan F. Williams*^[a]

Supplementary material

Figure S1. Change in spectrum of $[\text{AlL}_3]$ 10^{-2}M titrated with Cu(II) $5 \cdot 10^{-2}\text{M}$ in acetonitrile.

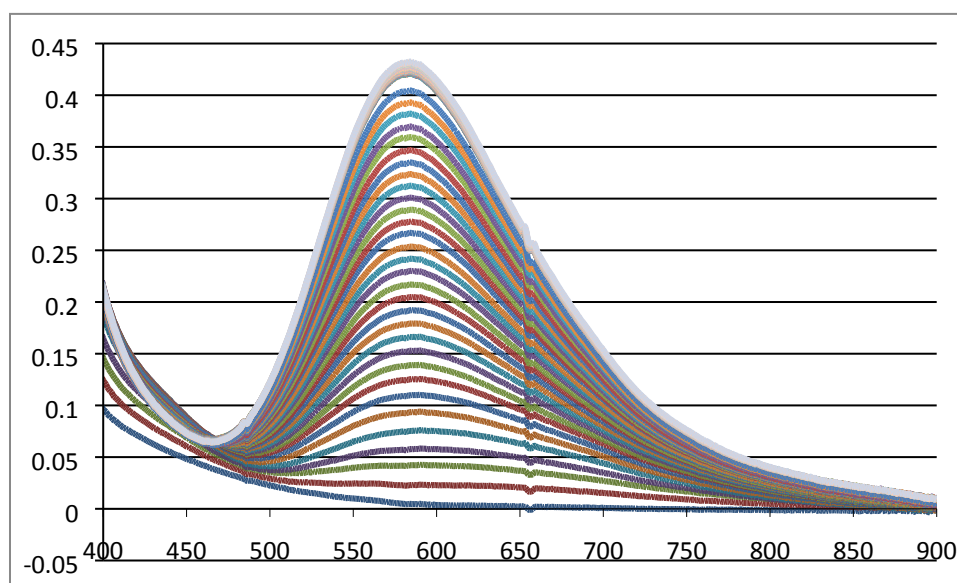


Table S1. Diffusion coefficients measured by DOSY for different protons.

	α -py	β -py	CH_2	mean [$\text{m}^2 \cdot \text{s}^{-1}$]	r_h [\AA]
AlL_3	2.30E-10	2.24E-10	2.24E-10	2.26E-10	4.86
$[\text{Pd}_6(\text{AlL}_3)_8]^{12+}$	7.64E-11	7.45E-11	7.72E-11	7.60E-11	14.46

Table S2. Hydrogen-bond geometries (\AA , $^\circ$) for $\text{AlL}_3 \cdot \text{H}_2\text{O}$ and $[(\text{AlL}_3)\{\text{Co}(\text{NCS})_2(\text{H}_2\text{O})\}]_n$

D-H .. A	D-H (\AA)	H .. A (\AA)	D ... A (\AA)	D-H .. A ($^\circ$)	symop
$\text{AlL}_3 \cdot \text{H}_2\text{O}$					
O44 -- H44A .. N37	0.8500	1.9900	2.788(10)	158.00	1-x,y,-z
O44 -- H44B .. N23	0.8500	2.4800	3.084(12)	129.00	1/2-x,1/2+y,-z
$[(\text{AlL}_3)\{\text{Co}(\text{NCS})_2(\text{H}_2\text{O})\}]_n$					
OW1 -- HW1A .. O10B	0.8500	1.9200	2.735(7)	160.00	1+x,y,z
OW1 -- HW1B .. O13C	0.8500	2.2900	2.864(7)	125.00	1+x,y,z