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Zinc complexes of 3-pyrimidinyl-benzo-1,2,4-thiadiazine[§]

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§ Dedicated to Prof. Spyros P. Perlepes on the occasion of his 65th birthday

ABSTRACT

The synthesis of the novel redox active ligand 3-(2',6'-pyrimidine)-benzo-1,2,4-thiadiazine (pmbtdaH) is reported. The radical pmbtda[•] can be prepared by *in situ* 1e⁻ oxidation and its radical character confirmed by EPR spectroscopy, along with DFT calculations of the spin density distribution. Reaction of pmbtdaH with ZnCl₂·2H₂O in a 1:1 mole ratio afforded the dinuclear complex Zn₂Cl₄(pmbtdaH)₂ (**1**) in which the two trigonal bipyramidal metal centres are linked *via* μ₂-bridging Cl⁻ ligands while the pmbtdaH ligand binds in an N,N'-chelate fashion *via* N(4) and the pyrimidinyl N(1) atom. The outcome of the reaction of pmbtdaH with Zn(hfac)₂ (hfac = hexafluoroacetylacetonate) proved sensitive to the crystallization method; the mononuclear octahedral complex Zn(hfac)₂(pmbtdaH) (**2**) in which the ligand coordinates in a similar N,N'-chelate fashion to that observed in **1** was isolated by layering a concentrated CH₂Cl₂ solution with hexane. Conversely the same reaction mixture afforded the tetranuclear complex Zn₄(hfac)₆(pmbtda_{ox})₂ (**3**) when left undisturbed in a sealed vial. In **3** the ligand is both deprotonated and oxidized forming an anionic ligand in which there are two potential N,N'-chelate pockets and an additional S-oxide donor. The pmbtda_{ox}⁻ ligand bridges between a Zn(hfac)₂ and a Zn(hfac) unit to form Zn₂(hfac)₃(pmbtda_{ox}). Two such Zn₂(hfac)₃(pmbtda_{ox}) units dimerise through the S-oxide oxygen atom to form a centrosymmetric tetranuclear Zn₄(hfac)₆(pmbtda_{ox})₂ cluster. The structures of **1** - **3** have been determined by X-ray diffraction, elemental analysis, IR and UV/vis spectroscopies as well as ¹H NMR spectroscopy for complex **2**.

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