

Chemistry Department, Facultad de Farmacia, Vitoria (Spain). E-mail: roberto.cortes@ehu.es

An hybrid organic-inorganic chain compound of the family Mn(II)-bpa-(NCO) is presented: $[\text{Mn}_4(\text{NCO})_8(\mu\text{-bpa})_4(\text{bpa})_4(\text{H}_2\text{O})_4]_n \cdot 2n(\text{bpa}) \cdot n\text{H}_2\text{O}$ (**1**). It contains, unusually, five different dispositions for the bpa [1,2-bis(4-pyridyl)ethane] ligand. Water molecules and free bpa ligands occupy the voids of the structure. Single-crystal X-ray diffraction reveals **1** to crystallize in the P21/n monoclinic space group. It consists of infinite chains of Mn(II) cations extending along the [100] direction and bridged by single N,N'-bpa bridges [Mn-N(3): 2.336(2) Å; Mn-N(4): 2.344(2) Å], that are in anti conformation with a torsion angle of 177.03° (Mn...Mn intrachain distance: 13.9 Å, Fig. 1). The distorted octahedral coordination of the cation is completed by a terminal bpa ligand [Mn-N(5): 2.296(2) Å], two N-terminal cyanate ligands [Mn-N(1): 2.189(2) Å; Mn-N(2): 2.163(2) Å], and a water molecule [Mn-O(3): 2.000(2) Å]. These chains are connected through intermolecular hydrogen bonding involving the atoms O(3) (water molecule) and N6 (non coordinating N-atom of the terminal bpa) [O(3)...N(6): 2.789(3) Å] or C(8) (ethane group of the bridging bpa) [O(3)...C(8): 3.414(4) Å]. Besides, the C(11) (bridging bpa) establish intermolecular connection with the O(2) (cyanate oxygen) [C(11)...O(2): 3.324(3) Å]. Interchain Mn...Mn distances are 8.6 Å and 9.0 Å and the packing is on the plane (110). The disposition of these sheets gives raise to hollows that are occupied by free molecules (water and bpa). Thus, a free bpa ligand acts as a solvate molecule occupying the voids in the lattice, in the same way as a water molecule acts.

The compound shows moderate antiferromagnetic type interactions through single bpa bridges, together with other exchange pathways. Electron spin resonance spectrum for **1** has been recorded at room temperature. The signal can be described as isotropic and is centred at 3300 Gauss.

