Synthesis, crystal structure and Hirshfeld surface analysis of Mn(II) coordination compounds with ONO-donor ligands derived from ampyrone

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Streszczenie

Four manganese(II) coordination compounds, $[Mn_2(L1)_2(NCS)_2(MeOH)_2]$ (**1**) $[Mn(HL2)_2(NCS)_2(MeOH)_2]$ (**2**) $[Mn_2(L3)_2(NCS)_2(MeOH)_2]$ (**3**) and $[Mn(HL3)_2(NCS)_2(MeOH)_2]$ (**4**) have been synthesized from the reaction of $MnCl_2{\cdot}4H_2O$, KSCN and Schiff base ligands derived from 4-aminoantipyrine (HL1= (*E*)-4-((2-hydroxybenzylidene)amino)-1,5-dimethyl-2-phenyl-1,2-dihydro-*3H*-pyrazol-3-one; HL2 = (*E*)-4-((2-hydroxy-3-methoxybenzylidene)amino)-1,5-dimethyl-2-phenyl-1,2-dihydro-*3H*-pyrazol-3-one and HL3 = (*E*)-4-((5-bromo-2-hydroxybenzylidene)amino)-1,5-dimethyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one) in methanol and the products have been characterized with single crystal X-ray diffraction (SC-XRD). The detailed studies involve the synthesis, crystal structure, FT-IR spectroscopy, UV–Vis spectroscopy, bond sum valence calculations, elemental and Hirshfeld surface analyses. In the case of **1** and **3**, the phenolate bridged dinuclear Mn^{II} complexes are formed by chelating two Schiff base ligands, two thiocyanates and two methanol molecules and two crystallographically equivalent Mn^{II} ions are connected together by phenolate oxygen with the Mn···Mn distance of 3.1618(4) (in **1**) and 3.1910(6) Å (in **3**). In the case of **2** and **4**, the octahedral coordination geometry of the Mn^{II} center in these mononuclear species is formed by chelating two Schiff base ligands, two thiocyanates and two methanol molecules. The presence of intermolecular hydrogen bond in **2** leads to the formation of molecular chains within the layers. Also, the presence of efficient π···π interactions between pyrazolone and phenyl rings and intermolecular hydrogen bonding in **4** lead to the formation of molecular chains within the layers. All of the intermolecular and intramolecular interactions have been studied by Hirshfeld surface analyses.

Słowa kluczowe

Mn(II) coordination compounds, 4-aminoantipyrine, Schiff base, Crystal structure, Hirshfeld surface analysis

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