

## Eight- and six-coordinated Mn(II) complexes of heteroaromatic alcohol and aldehyde: Crystal structure, spectral, magnetic, thermal and antibacterial activity studies.

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### Streszczenie

Crystal, molecular and electronic structure of new manganese(II) compounds:  $[\text{Mn}(\text{2-CH}_2\text{OHpy})_2(\text{NO}_3)_2]$  (**1**),  $[\text{Mn}(\text{4-CHO-5-Melm})_2(\text{NO}_3)_2]$  (**2**) and  $[\text{Mn}(\text{4-CHO-5-Melm})_2\text{Cl}_2]$  (**3**), where 2-hydroxymethylpyridine (2-CH<sub>2</sub>OHpy) and 5(4)-carbaldehyde-4(5)-methylimidazole (5(4)-CHO-4(5)-Melm), have been characterised using X-ray, spectroscopic, magnetic and TG/DTG data. In compounds **1** and **2**, the Mn(II) ion is eight-coordinated forming distorted pseudo-dodecahedron, that is rather unusual for the manganese(II) complexes, whereas in **3** the Mn(II) ion environment is a distorted octahedron. The high coordination number (CN = 8) of **1** and **2** results from bidentate character of the nitrate ligands. The X-band EPR spectra of compounds **2** and **3** exhibit fine structure signals resulting from zero-field splitting (ZFS) of the spin states for high spin d<sup>5</sup> Mn(II), whereas for **1** the broad isotropic signals were observed. The estimation of ZFS for individual Mn(II) ions was carried out for all compounds using DFT calculations. The free ligands and their manganese(II) complexes have been tested *in vitro* against gram-positive and gram-negative bacteria in order to assess their antimicrobial properties.

### Słowa kluczowe

manganese complex, crystal structure, magnetic properties, EPR spectroscopy, N.O-donor ligand, anyibacterial activity

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