

m42.p04

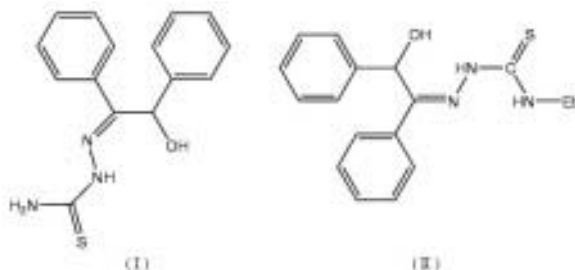
## Benzoin thiosemicarbazone and benzoin 4-ethylthiosemicarbazone

Muharrem Dincer<sup>a</sup>, Namik Özdemir<sup>a</sup>,  
Alaaddin Çukurovalı<sup>b</sup>, Ibrahim Yılmaz<sup>b</sup>

<sup>a</sup>Department of Physics, Arts and Sciences Faculty, Ondokuz Mayıs University, Samsun, Turkey. <sup>b</sup>Department of Chemistry, Arts and Sciences Faculty, Firat University, Elazığ, Turkey. E-mail: mdincer@omu.edu.tr

**Keywords:** X-ray crystallography, small organic molecules, structure comparison

In the title compounds, C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>OS (I) and C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>OS (II), the thiosemicarbazone moieties are planar and have an E configuration. In (I), the planar phenyl rings make dihedral angles of 26.56 (9) and 81.20 (5)° with the plane of the thiosemicarbazone moiety, while these rings make dihedral angles of 8.07 (17) and 82.34 (8)° in (II). The two compounds crystallize in same crystal system, but have different space groups, P2<sub>1</sub>/c and P2<sub>1</sub>, respectively. Although, the centrosymmetry of the space group of (I) does not allow the compound to exhibit any SHG efficiency, the noncentrosymmetry of the space group of (II) can allow the compound to exhibit SHG efficiency [1, 2]. There are two intramolecular interactions of types N–H...O and N–H...N for both compounds. In the crystal structure of (I), there are two intermolecular interactions of types O–H...S and N–H...S, leading to the formation of dimers. However, the crystal structure of (II) contains one intermolecular interaction (O–H...S), as well as two C–H...π(benzene) interactions. For (II), molecules are stacked in columns running along the a axis. Molecules in each column connected to each other by means of linear O–H...S hydrogen bonds and C–H...π interactions. In addition, there are also C–H...π(benzene) interactions between the columns.



[1] Tian Y.-P., Duan C.-Y., Chao C.-Y., You X.-Z., Zhang Z.-Y., Mak T.C.W., *Inorg. Chem.*, 1997, 36, 1247-1251.

[2] Liu Z.-H., Duan C.-Y., Hu J., You X.-Z., *Inorg. Chem.*, 1999, 38, 1719-1724.

m42.p05

## Structure and Magnetic Properties of a Manganese (III) Schiff-Base Complex

Emine Donmez<sup>a</sup>, Hulya Kara<sup>a</sup>, Yasemin Yahsi<sup>a</sup>

<sup>a</sup>Department of Physics, Faculty of Arts and Sciences, University of Balıkesir. E-mail: edonmez@balikesir.edu.tr

**Keywords:** crystal structure, magnetic properties, manganese compounds

A novel manganese (III) schiff-base complex, [Mn(III)(L)(H<sub>2</sub>O)]<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub> has been synthesized and characterized by elemental analysis, i.r. spectroscopy, t.g.a., by an X-ray single crystal study and magnetic susceptibility measurements. Two nitrogen atoms and two oxygen atoms from Schiff base ligands, and two oxygen atoms from capping water molecules occupy the coordination sites about each manganese. The structure has a centrosymmetric dimer in which the manganese(III) atoms are linked by μ-phenoxo bridges from one of the phenolic oxygen atoms of each ligand to the opposite metal center, thus resulting in μ-phenoxo Mn–O(1) and Mn'–O(1) bond distances of 2.403 Å. The equatorial atoms about the two manganese atoms are coplanar; consequently, the environment around each manganese atom can be described as a distorted N<sub>2</sub>O<sub>4</sub> octahedron as a result of Jahn-Teller effects [1]. In the equatorial plane, the bond distances of Mn–N1, Mn–N2, Mn–O1, Mn–O2 are 1.974, 1.989, 1.906 and 1.883 Å, respectively. The non-bonding interatomic Mn..Mn distance is 3.325 Å. The presence of lattice and coordinate water molecules were also confirmed by the t.g.a study and the i.r. spectra. Magnetic properties of the title compound have been also investigated.

[1] Shyu H.L., Wei H.H., Wang Y., *Inorganica Chimica Acta*, 1999, 290, 8.