Structure, Characterization and *ab Initio* Calculations of $[Mn(4,4'\text{-bipy})_2(H_2O)_4][HOOCC_6H_4SSC_6H_4COO]_2$

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The title compound was obtained by reaction of $MnCl_2 \cdot 4H_2O$, $NH_3 \cdot H_2O$, 4,4′-bipyridine, and 2,2′-dithio-bis(benzoic acid) (H_2-DTBB) in aqueous solution. It was characterized by single crystal X-ray crystallography, elemental analysis and IR spectroscopy. The compound is composed of one $[Mn(bipy)_2(H_2O)_4]^{2+}$ cation and two H-TDBB^{1-} anions, where Mn^{2+} adopts an octahedral geometry and is coordinated by four water oxygen atoms and two N atoms of 4,4′-bipyridine ligands. The $[Mn(bipy)_2(H_2O)_4]^{2+}$ cations are linked into one-dimensional chains by O–H$\cdots$N hydrogen bonds. These cationic chains are further organized into a two-dimensional network with the H-TDBB^{1-} anions through hydrogen bonds.

Key words: Crystal Structure, *ab Initio* Calculation, Hydrogen Bonds, Supramolecule