Structure, Characterization and ab Initio Calculations of
[Mn(4,4′-bipy)$_2$(H$_2$O)$_4$][HOOC$_6$H$_4$SSC$_6$H$_4$COO]$_2$

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The title compound was obtained by reaction of MnCl$_2$·4H$_2$O, NH$_3$·H$_2$O, 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$_2$O)$_4$]$^{2+}$ 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$_2$O)$_4$]$^{2+}$ cations are linked into one-dimensional chains by O–H···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