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Synthesis and structural characterization of dinuclear zinc complex of N,N'-bis(2-pyrazolyl-4-methylphenyl)formamidinate

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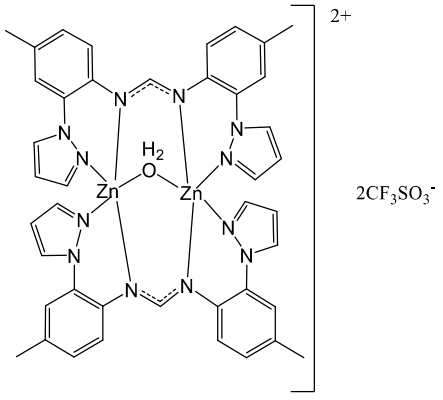
A new tetra-dentate N,N'-bis(2-pyrazolyl-4-methylphenyl)formamidine ligand (H(NNNN)) was synthesized by introducing two flanking pyrazole groups to an ortho position of each aryl group of known N,N'-bis(4-methylphenyl)formamidinate ligand. It was achieved step wise by substituting deprotonated pyrazole to the ortho position of 2-bromo-*p*-toluidine and then coupled with another same unit by half equivalents of triethyl orthoformate using acetic acid as the catalyst at the refluxing temperature of the neat reaction. The treatment of deprotonated H(NNNN) with two equivalents of zinc trifluoromethane sulfonate yielded dinuclear zinc complex, which has $Zn_2C_{44}H_{40}F_6N_{12}O_7S_2$ empirical formula. Single crystals suitable for X-ray crystallographic analysis were grown by layering pentane on the dichloromethane solution of the complex. X-ray crystal structure revealed that two ligands are bridged by two Zn atoms which bridged by a H_2O molecule. The overall charge of the complex is balanced bytwo triflate counter ions. Each Zn atom has five coordinations, with two amidinate nitrogens, two pyrazolyl nitrogens of two ligands and an O atom of bridging H_2O molecule giving distorted square-pyramidal geometry. The interatomic distance of two Zn atoms is 3.0802 Å. It was further observed that only this complex is yielded with different stoichiometric ratios of ligand to the metal ion.



Key words: *Tetra dentate, bimetallic complexes, dinuclear, flanking pyrazole*

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