Support information

Novel single-site manganese(II) complex of pyridine derivative as catalase mimetic for disproportionation of H_2O_2 in water.

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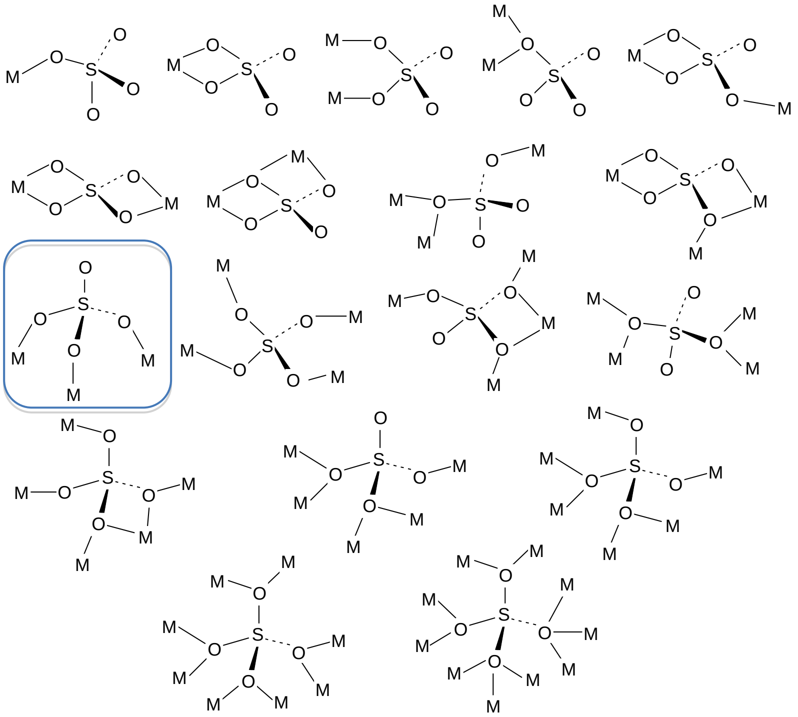

Figure S1. Possible coordination modes of sulfate ligand (μ_3, presented work).

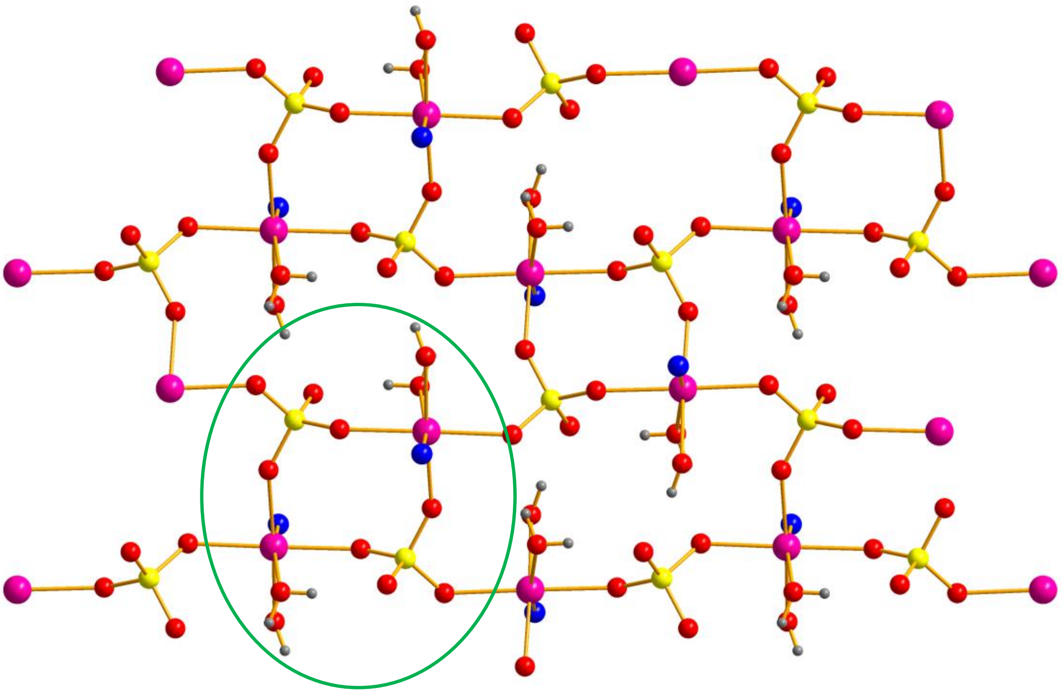

Figure S2. The fragment of 2D network with marked mimic system of catalase viewed along [1 0 0] direction. For clarity ring of ligands are omitted.

Table S1 Hydrogen bonds for Mn(II) complexes (Å) and (°).

D-H···A	*d*(D-H)	*d*(H···A)	*d*(D···A)	<(DHA)
O(11)-H(11A)···O(13)[x,-y+1/2,z-1/2]	0.817(2)	1.921(2)	2.716(3)	164(3)
O(11)-H(11B)···O(10)[-x+2,y+1/2,-z+1/2]	0.830(2)	2.02(2)	2.837(2)	169(4)
O(11)-H(11B)···O(12)[-x+2,y+1/2,-z+1/2]	0.830(2)	2.53(4)	2.939(3)	112(3)
O(8)-H(8)···O(13)[-x+2,y+1/2,-z+1/2]	0.84(4)	1.84(4)	2.671(3)	174(4)

The most important spectra bands of [Mn(2-CH_2OHpy)(SO_4)(H_2O)]$_n$ complex and free ligand, and their assignments are listed in Table 4 and the IR spectrum is depicted in Fig. S4. The free ligand, 2-CH_2OHpy exhibits broad absorption bands at 3300-3500 cm^{-1}, which are assigned to inter- and intramolecular hydrogen bond ν(O-H···N) vibration.[i] The complex formation leads to hampering this proton exchange, which results in one absorption band at 3213 cm^{-1}. In comparison to the 2-CH_2OHpy, in the spectrum of [Mn(2-CH_2OHpy)(SO_4)(H_2O)]$_n$ the ν_{OH} band is shifted by 9 cm^{-1} and the $\delta_{C\text{-}O}$ vibrations of heteroaromatic ring are shifted strongly to higher wavenumbers (Δ = 43). Additionally, the IR absorption of C=N bond appears at higher wavenumbers $\nu_{C=N}$ = 1491 cm^{-1}, compared to the 2-CH_2OHpy (Δ = 12). The degree of shifts seems to correlate with the binding mode of this ligand, being sensitive to manganese coordination not only through the nitrogen atom of the pyridine ring but also via the oxygen atom of the hydroxymethyl group, forming a five-membered chelate ring with the central ion. The new bands in the complex at 3342 cm^{-1} and 1059 cm^{-1} can be assigned to ν_{OH} stretching vibration of the coordinated water molecule and sulphate ion, respectively.[ii]

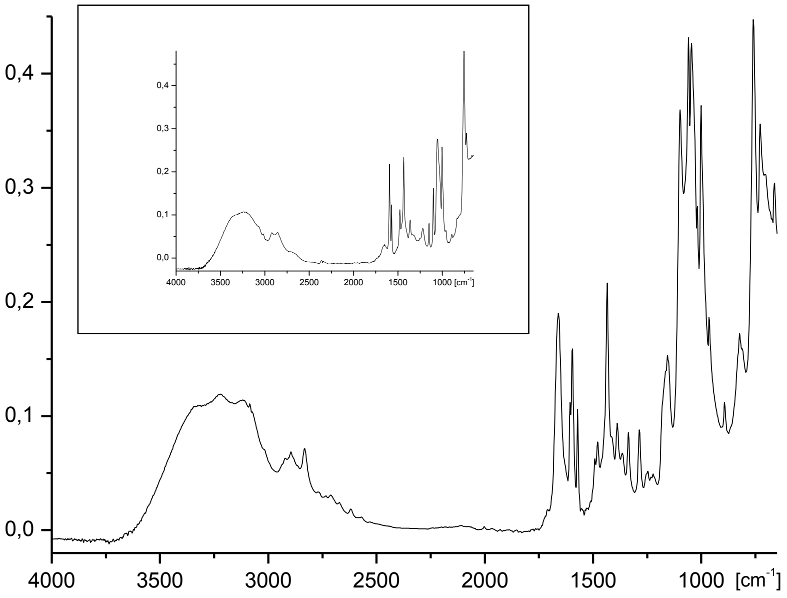

Figure S3: The FTIR spectrum of the manganese(II) complex; in inset the FTIR spectrum of 2-CH_2OHpy is presented.

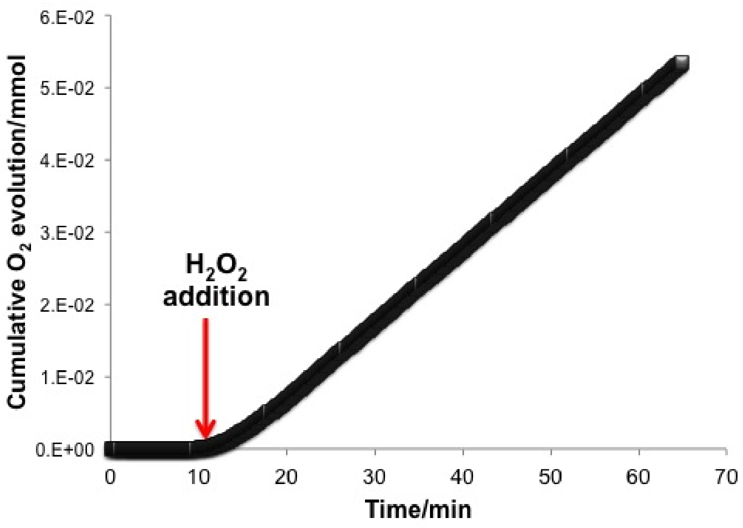

Figure S4: Cumulative oxygen liberation for the first 60 min of reaction.

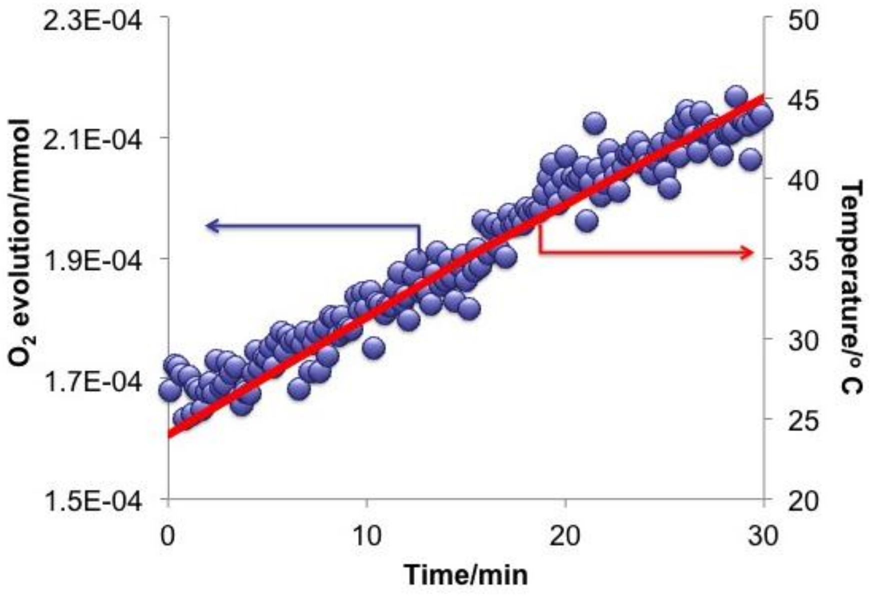

Figure S5: Oxygen liberation as a function of reaction temperature.

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i K. Nakamoto, Infrared Spectra of Inorganic and Coordination Compounds. sixth ed. New Jersey: Wiley & Sons; 2009.

ii Ch. Hong-Yan, Z. Tong-Lai, Z. Jian-Guo, Y. Kai-Bei, *Struct. Chem.*, 2005, **16**, 657-663.