Supplementary Material (ESI) for Chemical Communications

Tricarbonylmanganese(I)-lysozyme complex: a structurally characterized organometallic protein

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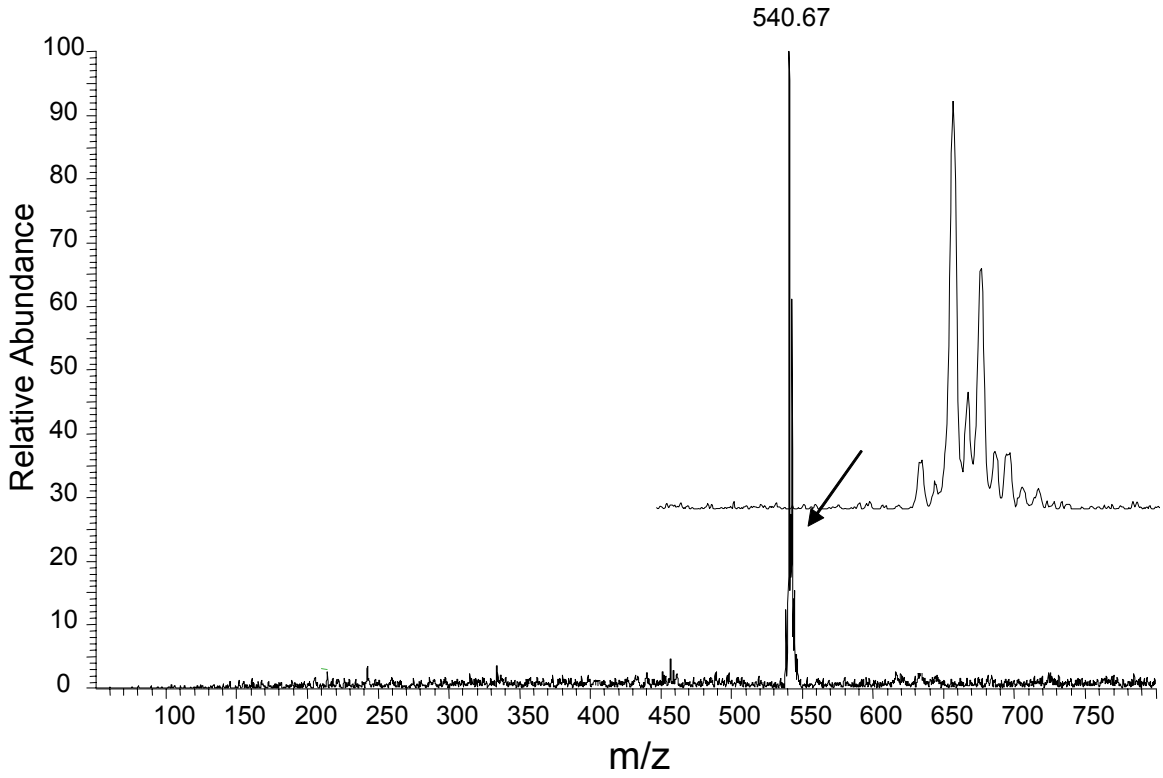
Experimental:

[(lysozyme)–$Mn(CO)_3(OH_2)_2$] (**3**): Lysozyme crystals were grown at room temperature within one day from a 0.05 mol.L^{-1} acetate buffer pH 4.4 solution (1 mL) containing 50 mg of hen egg white lysozyme (Euromedex) added with 53 mg of NaCl. The flask is then protected from ambient light and about 10 mg of oily $[Mn(CO)_3(acetone)_3](CF_3SO_3)$ is dissolved. After two days, the reaction mixture is filtered in the dark on a sinked frit and washed twice with a 0.05 mol.L^{-1} acetate buffer pH 4.4 solution containing 2 mol.L^{-1} NaCl. The yellow powder of **3** is partially dried under vacuum yielding 615 mg corresponding from Bradford Analysis using Bio-Rad protein assay to 320–400 mg of lyophilized lysozyme.

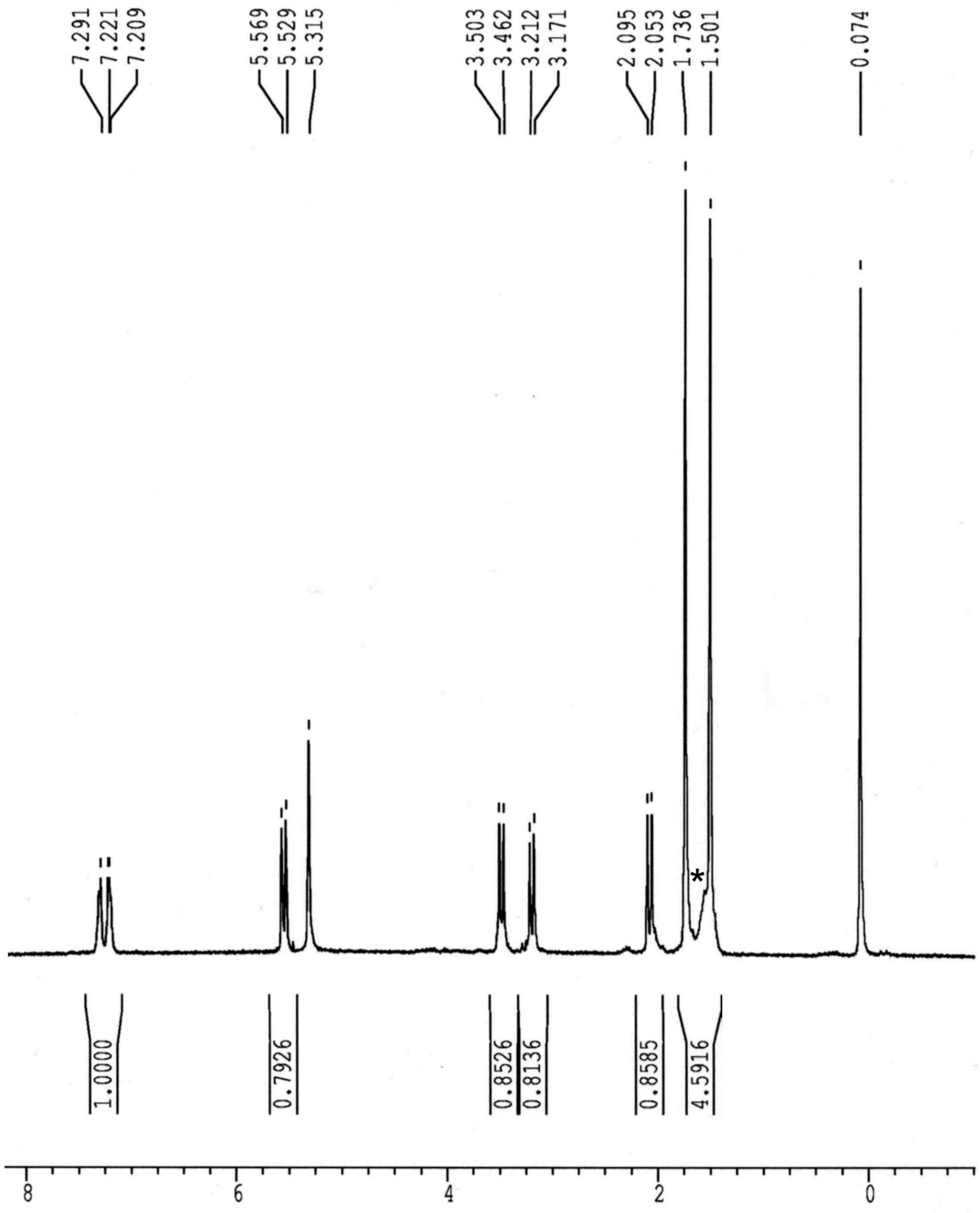
[Ni(xbsms)Mn(CO)$_3$(OH)$_2$]Cl (4): A solution of [Ni(xbsms)] (4 mg, 0.01 mmol) in CH_2Cl_2 (1 mL) is added to a solution of **3** (300 mg) in 0.05 mol.L^{-1} ammonium acetate buffer pH 4.4 solution (2 mL) under inert atmosphere in the dark. The reaction mixture is stirred for two hours. The organic phase is decanted and the aqueous layer extracted twice with CH_2Cl_2 (1 mL). The organic fractions are combined, dried on anhydrous $MgSO_4$ and evaporated to dryness to yield a salt of **4** as a red solid (5 mg, 83%).

IR (CH_2Cl_2) : $\bar{\nu}_{CO}$ = 2018 (s), 1929 (m), 1910 (m) cm^{-1}.

300 MHz ^{1}H NMR (ppm, CD_2Cl_2): 7.91 (d, 2H, H_{arom}), 7.21(d, 2H, H_{arom}), 5.55 (d, 2H, 12.3 Hz, H_{benz}), 3.48 (d, 2H, 12.3 Hz, H_{benz}), 3.19 (d, 2H, 12.6Hz, -CMe$_2$-CH_2-S), 2.07 (d, 2H, 12.6 Hz, -CMe$_2$-CH_2-S), 1.74 (s, 6H, -CH_3), 1.50 (s, 6H, -CH_3).



ESI-MS spectrum of the crude sample of **4** (methanol solution).



300 MHz ^{1}H NMR spectrum of the crude sample of **4** at 298 K in CD_2Cl_2 (* indicates the position of the peak of water)