

**Synthesis, structures and magnetic properties of two iron(II)  
tris(pyridyl)phosphine sulfide complexes**

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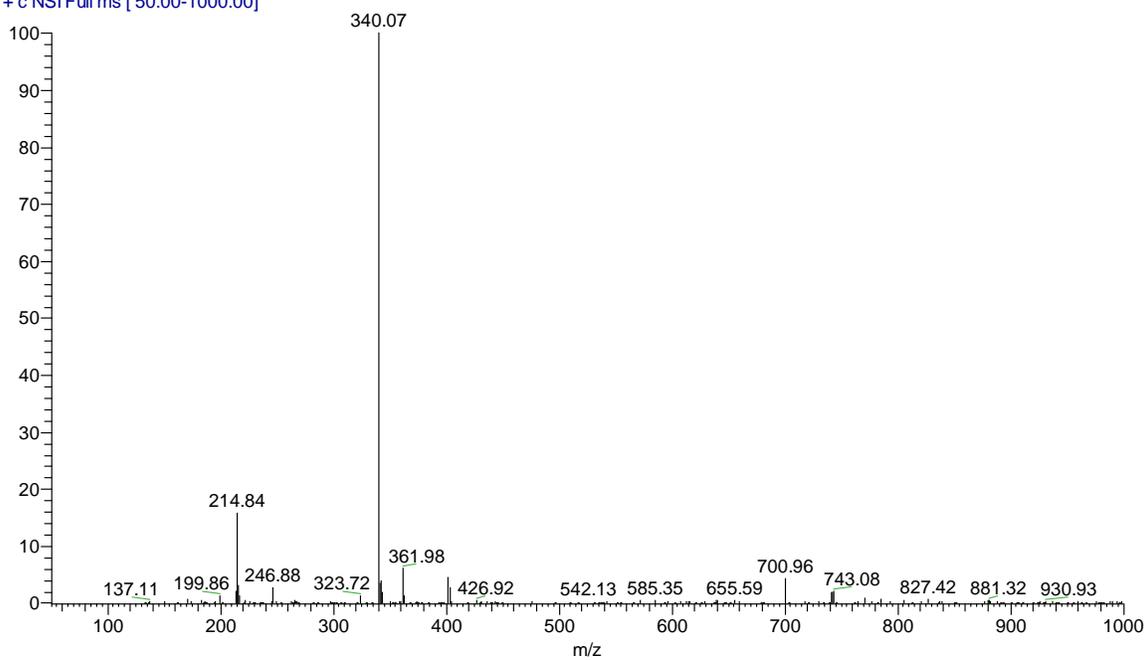
**Materials and methods**

All chemicals were commercial and purified according to standard procedures. All organic solvents were dried and freshly distilled before use. The  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and  $^{31}\text{P}$  NMR spectra were recorded on Bruker AV 300 MHz using  $\text{CDCl}_3$  as the solvent. Chemical shifts are given with respect to tetramethylsilane ( $^1\text{H}$ ,  $^{13}\text{C}$ ) and chemical shifts are expressed in  $\delta$  (ppm). Mass spectra were measured on a LCQ Advantage MAX (ESI). The melting points of the synthesized compounds were recorded on a WRX-4 monocular microscope and were not corrected. Magnetic susceptibility measurement was carried out on a Quantum Design MPMS SQUID-VSM magnetometer in the temperature range of 2–300 K with a magnetic field of 2000 Oe and the magnetic susceptibilities of the two complexes were measured at a sweep rate of 3 K  $\text{min}^{-1}$ . Magnetic data were calibrated with the sample holder and diamagnetic contributions.

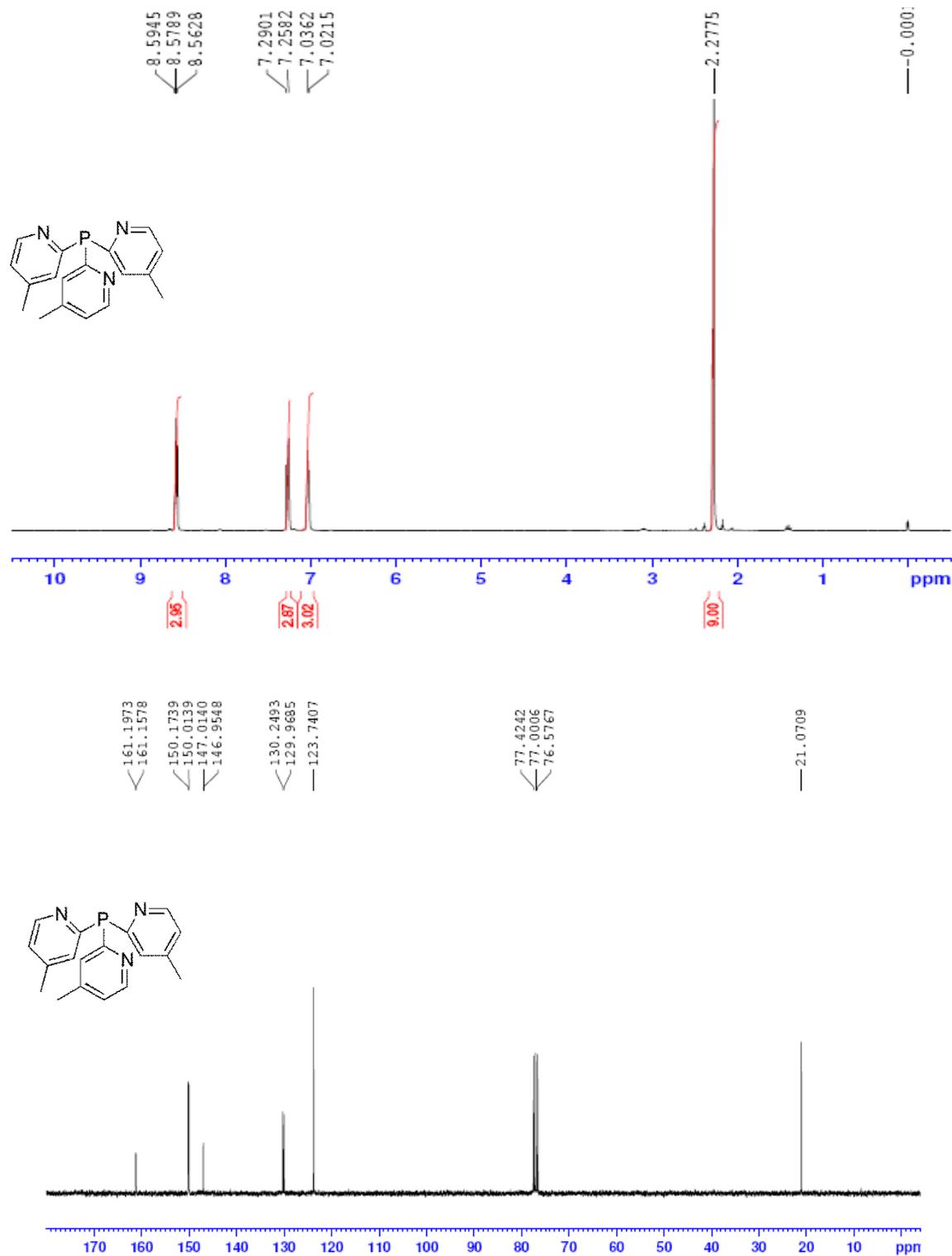
Single crystal structural data for **MeTpp**, **MeTppS**, **1** and **2** were collected on a Bruker Apex-II CCD diffractometer using graphite-collimated Mo  $K\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ). The structures were solved by direct methods (SHELXL97) and completed by difference Fourier methods (SHELXL97). Refinement was performed against  $F^2$  by weighted full-matrix least-squares (SHELXL97) and empirical absorption corrections (SADABS) were applied. Hydrogen atoms were found in difference maps and subsequently placed at calculated positions using suitable riding models with isotropic displacement parameters derived from their carrier atoms. Non-hydrogen atoms were refined with anisotropic displacement parameters.

CCDC 1568321, 1568322, 1568324 and 1568325 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via <http://www.ccdc.cam.ac.uk>.

1\_141104143511 #52 RT: 0.88 AV: 1 SB: 10 0.12-0.27 , 0.35 NL: 2.85E6  
T: + c NSI Full ms [ 50.00-1000.00]



**Figure S1** ESI-MS spectrum for **MeTppS** in MeOH.



**Figure S2** <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) and <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of MeTpp.

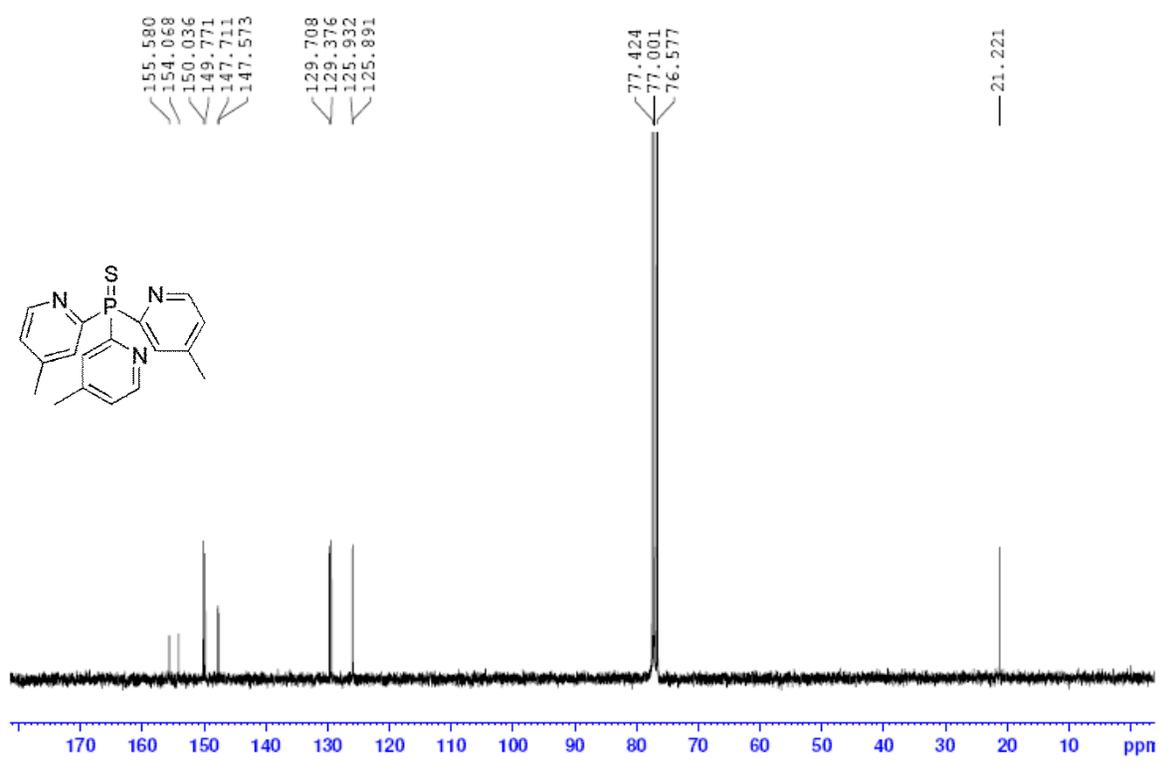
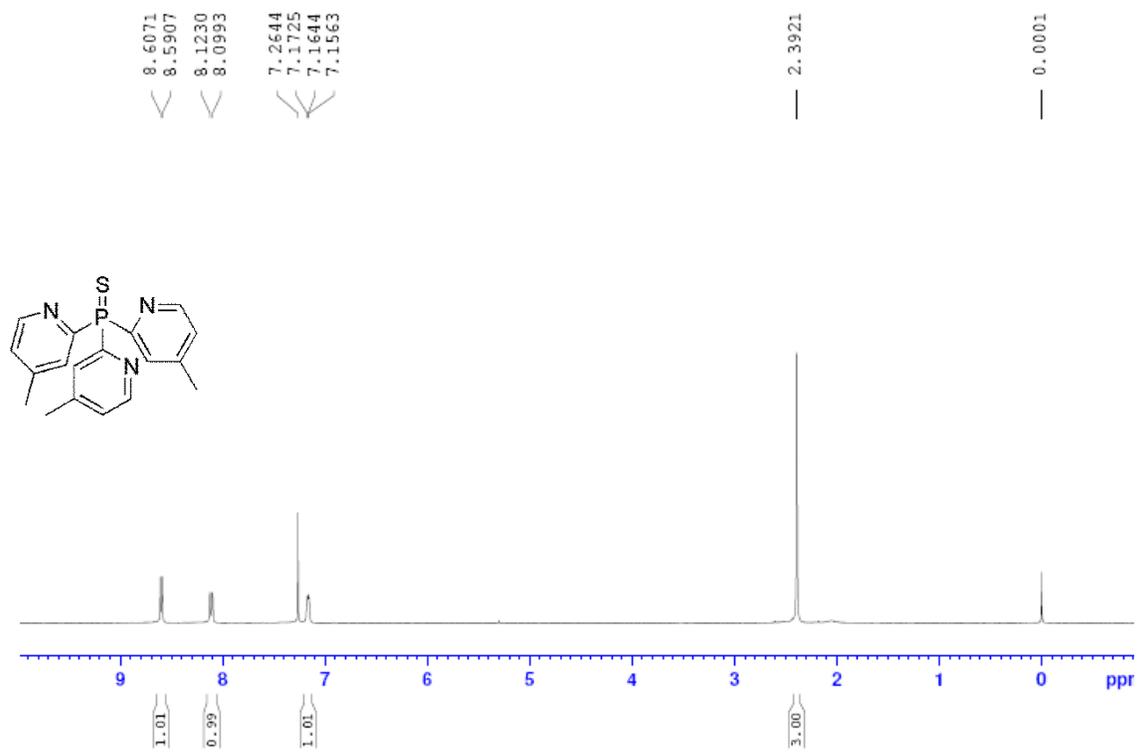
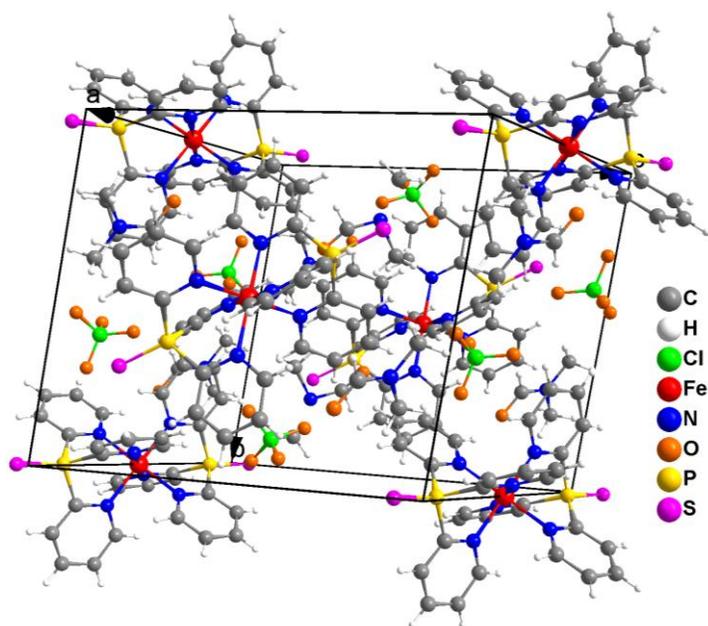


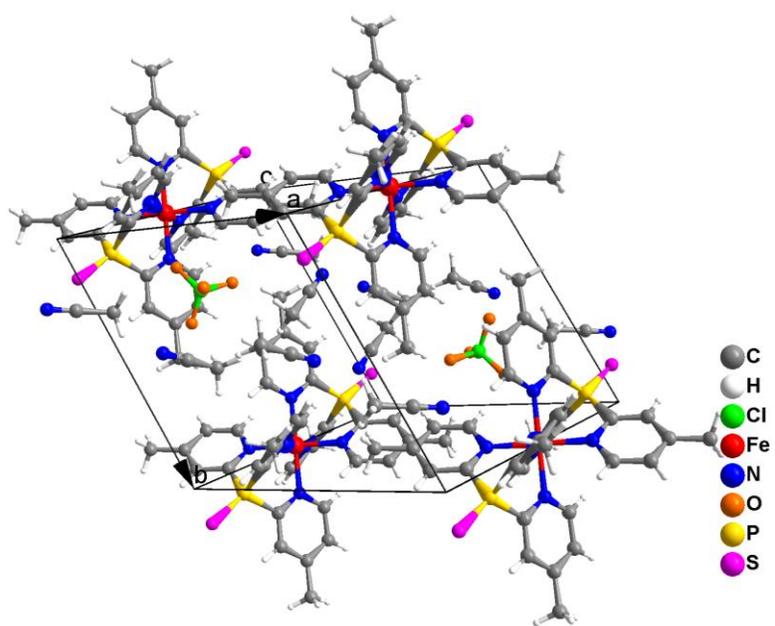
Figure S3 <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) and <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of MeTppS.

**Table S1** Selected bond distances ( $\text{\AA}$ ) in **1** and **2**.

compound	<b>1</b>	<b>2</b>
Temperature/K	298	100
Fe1–N1	2.014(3)	2.0211(14)
Fe1–N2	1.993(3)	2.0114(13)
Fe1–N3	2.019(3)	2.0126(14)
<b>Fe1–N(Av)</b>	<b>2.009(3)</b>	<b>2.0150(14)</b>
Fe2–N4	2.010(3)	
Fe2–N5	2.019(3)	
Fe2–N6	2.023(3)	
<b>Fe2–N(Av)</b>	<b>2.017(3)</b>	



**Figure S4** Partial packing diagram of the complex **1** with solvent molecules.



**Figure S5** Partial packing diagram of the complex **2** with solvent molecules.