

## Supplementary material

### A. Electron UV-VIS and infra-red spectra for $\mathbf{1} = [\{\text{Fe}^{\text{II}}(\text{CN})_6\}\{\text{Fe}^{\text{III}}(\text{salpet})_6\}]_6\text{Cl}_2$ .

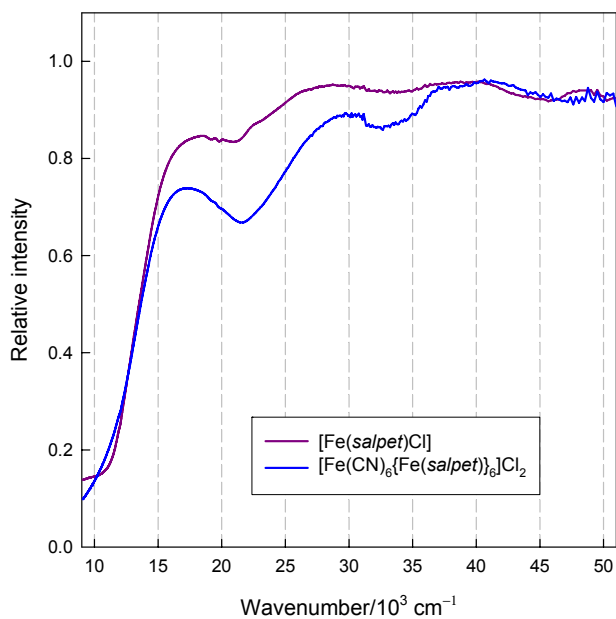


Fig. S1. Electron spectra of *salpet*-containing complexes [Nujol mull (Analytical Jena, Specord 200), 10000 – 50000 cm<sup>-1</sup>]

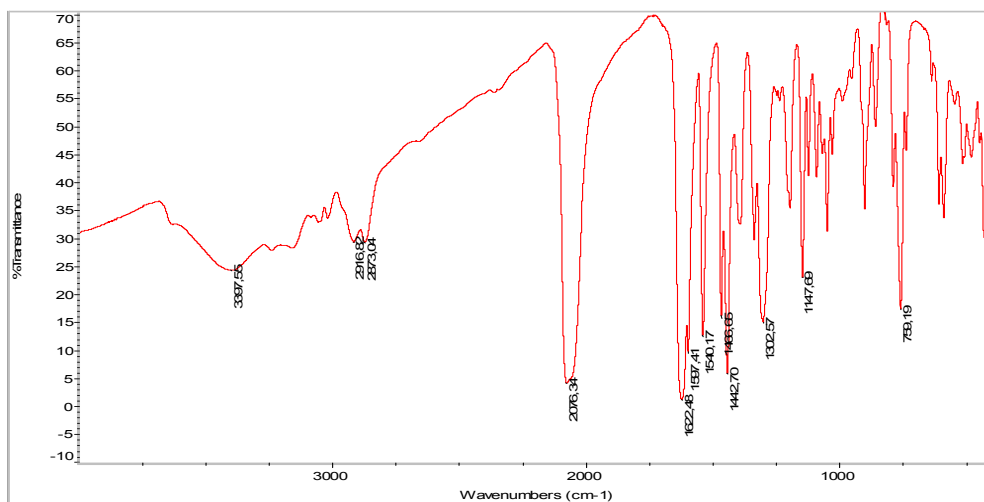


Fig. S2. MID-IR spectrum of  $\mathbf{1}$  [KBr pellets (Nicolet, Magna FTIR 750), 4000 – 400 cm<sup>-1</sup>]

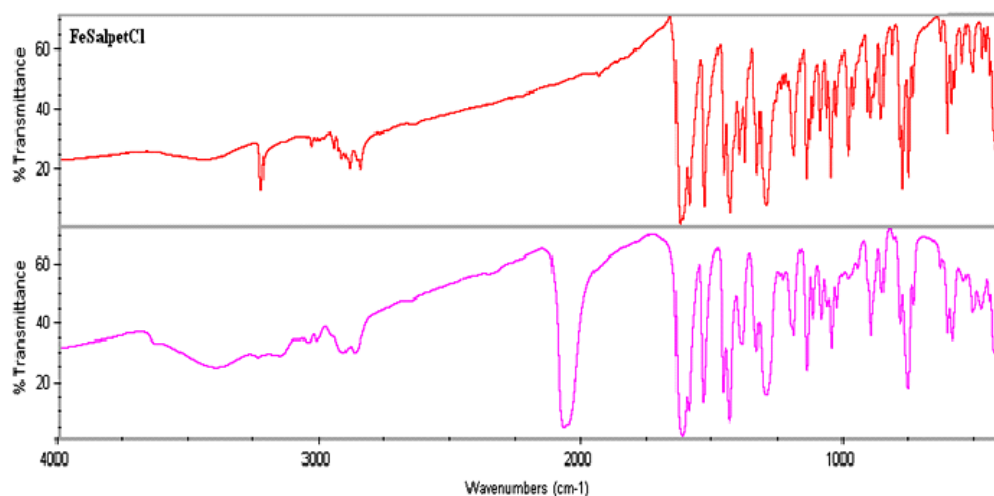


Fig. S3. MID-IR spectrum of **1** and its comparison with the mononuclear precursor [Fe(Salpet)Cl]

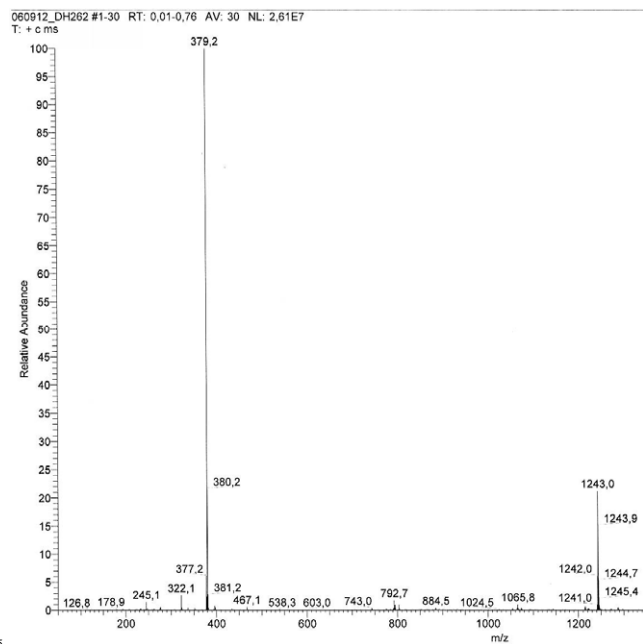
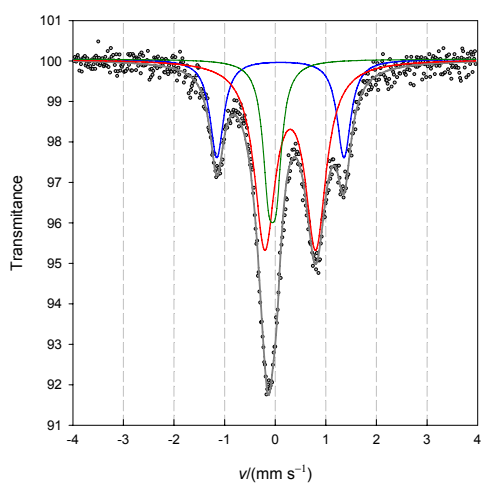
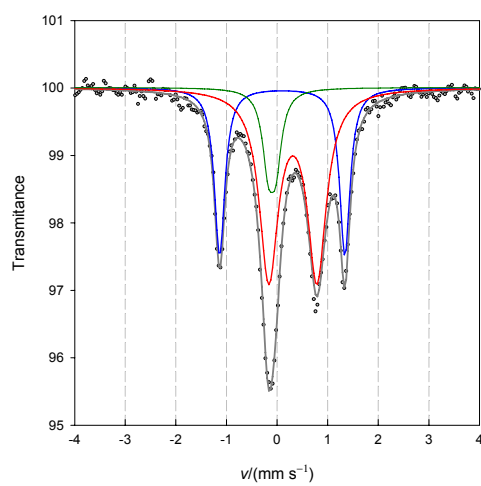


Fig. S4. ESI-mass spectra. The heptanuclear complex shows the molpeak in:  $m/z (=K^{2+}/2)$ :  $1244 \text{ g mol}^{-1}$  which matches the composition  $[K]Cl_2$ ; the molar mass of  $[K^{2+}]$  is  $2488 \text{ g mol}^{-1}$ ;  $K^{2+}$  is the heptanuclear molecular dication  $[\{Fe^{II}(CN)_6\} \{Fe^{III}(salpet)\}_6]^{2+}$ . Molpeak  $m/z (=L^+/1)$ :  $379.2 \text{ g mol}^{-1}$  is exactly the  $L = [Fe^{III}(salpet)]^+$  fragment.

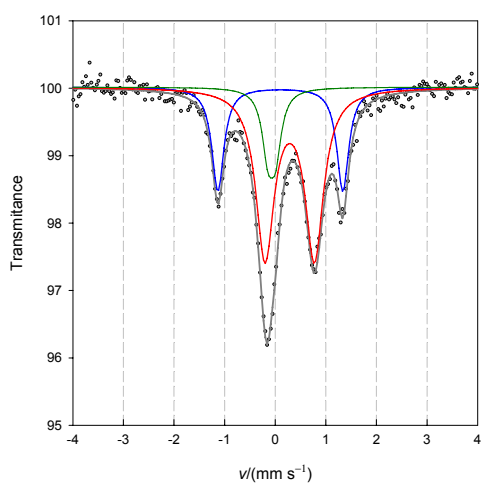
**B. Deconvolution of the Mössbauer spectra for 1**



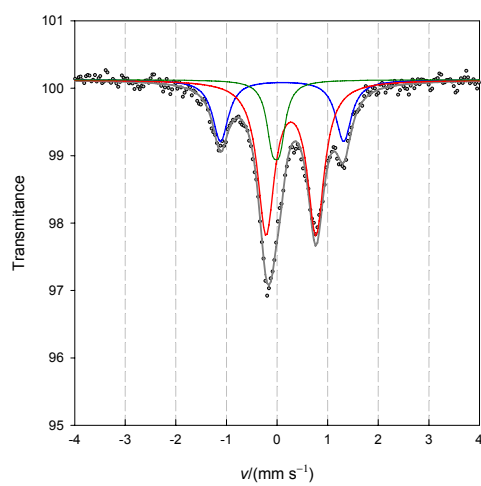
$T = 20 \text{ K}$



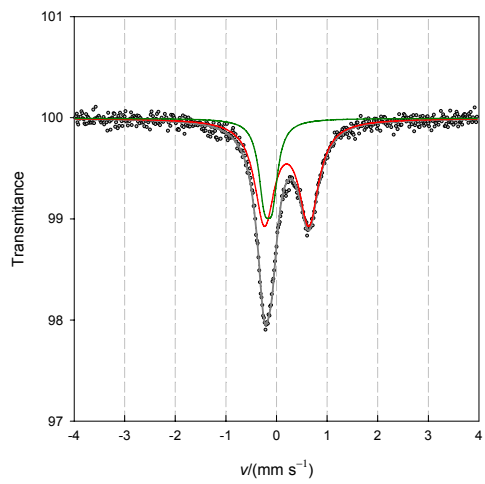
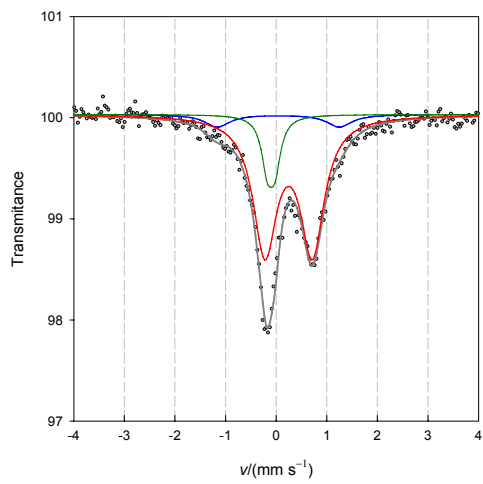
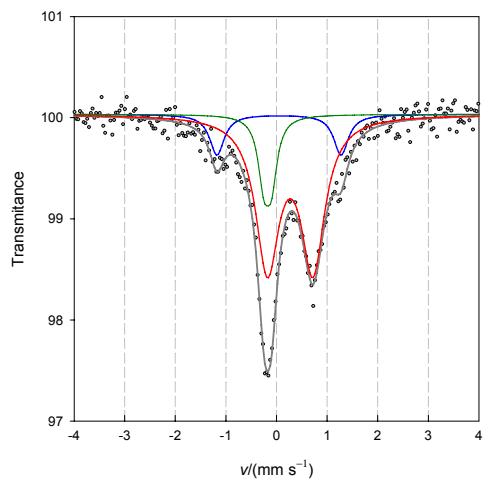
$T = 78 \text{ K}$



$T = 120 \text{ K}$



$T = 150 \text{ K}$



**C. Selected interatomic distances**

	Fe2	Fe3	Fe4
Fe <sup>II</sup> -C(cyanide)	1.879(9)	1.888(8)	1.932(10)
Fe <sup>III</sup> -N(cyanide)	2.058(9)	2.033(7)	2.013(10)
Fe <sup>III</sup> -O(phenolate)	1.897(7)	1.960(6)	1.823(10)
	1.947(7)	1.960(5)	1.863(10)
Fe <sup>III</sup> -N(amine) -NH-	2.161(9)	2.157(7)	2.020(13)
Fe <sup>III</sup> -N(imine) -N=C-	2.028(12)	2.086(9)	1.832(15)
	2.034(10)	2.110(8)	1.924(15)

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