

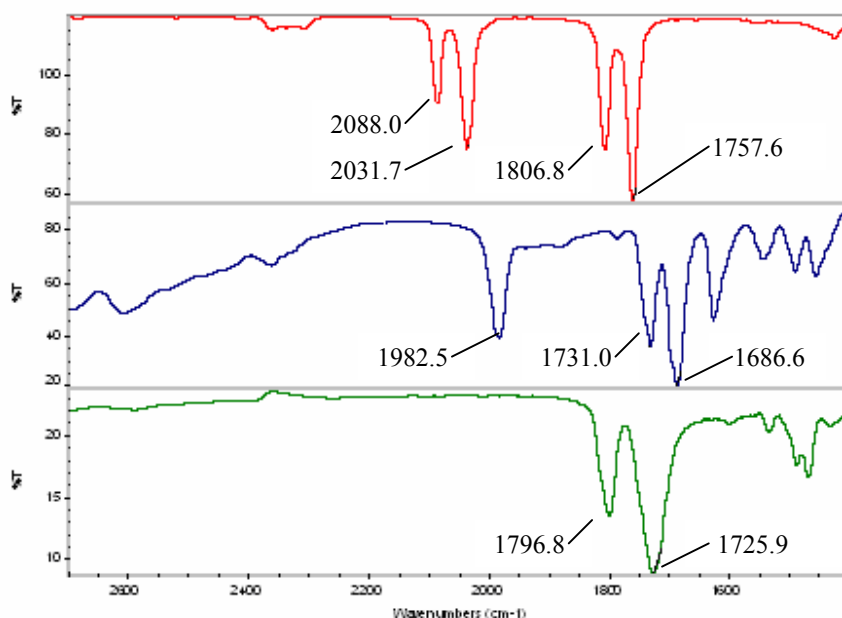
Supplementary Material (ESI) for Chemical Communications
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Electronic Supplementary Information:

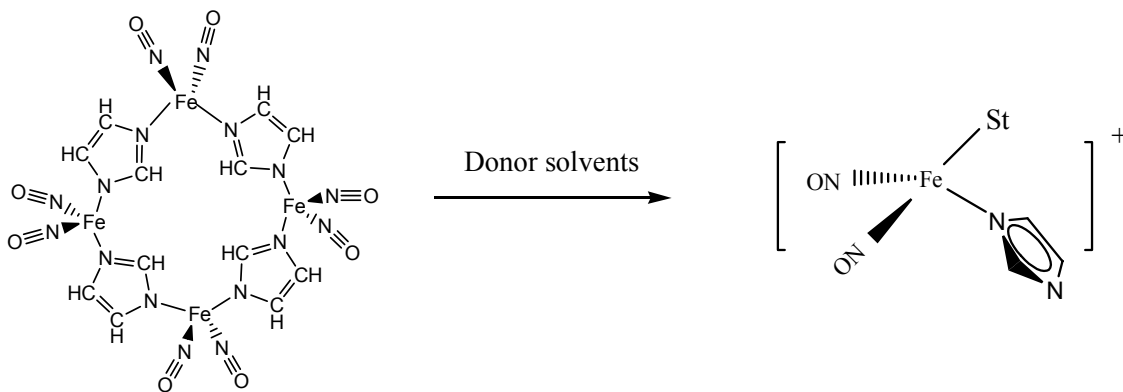
(1) Crystal data table

Chemical formula	C ₁₂ H ₁₂ Fe ₄ N ₁₆ O ₈ , C ₃ H ₆ O ₁
Formula weight	789.85
Temperature, K	243
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	
a	21.30 (3)
b	6.709 (9)
c	22.73 (3)
α	90
β	103.93 (4)
χ	90
Volume	3153 (7)
Z	4
Density (calculated), mg/m ³	1.664
Absorption coefficient, mm ⁻¹	1.871
Crystal size [mm]	0.4 x 0.10 x 0.07
Diffractometer/scan	Bruker SMART/CCD
Scan	ω scan
θ range for data collection, deg	1.85 to 28.26
Reflections measured	13412
Independent. observed reflections	3678
Independent reflections [$ I > 2s(I)$]	3085
R _{int}	0.086
Data/restraints/parameters	3678/0/201
Goodness of fit on F ²	1.196
Final R indices [$ I > 2s(I)$]	R ₁ =0.0597, wR ₂ =0.1475
R indices (all data)	R ₁ =0.0706, wR ₂ =0.1535

(2) **FT-IR spectra of the nitrosyl and carbonyl regions of** (a) $\text{Fe}(\text{CO})_2(\text{NO})_2$ in CH_2Cl_2 , (b) $\text{Fe}(\text{NO})_2(\text{CO})(\text{Imidazole})$, **2**, in CH_2Cl_2 and (c) $[\text{Fe}(\text{NO})_2(\text{Im-H})]_4$, **1**, in a KBr pellet.



(3) A scheme showing the fragmentation of $[\text{Fe}(\text{NO})_2(\text{Im-H})]_4$ in coordinating solvents, which give rise to the species responsible for the EPR spectrum shown in Figure 2(a).



(4) **Conditions for the TGA experiment.**

The TGA was performed on a Mettler TGA/sDTA 851e. The conditions were 9.62 mg starting mass, starting at 25°C to 1000°C with a ramp of $10^\circ\text{C}/\text{min}$. An isothermal run was performed prior to heating for 20 min at 25°C to purge the system with N_2 .