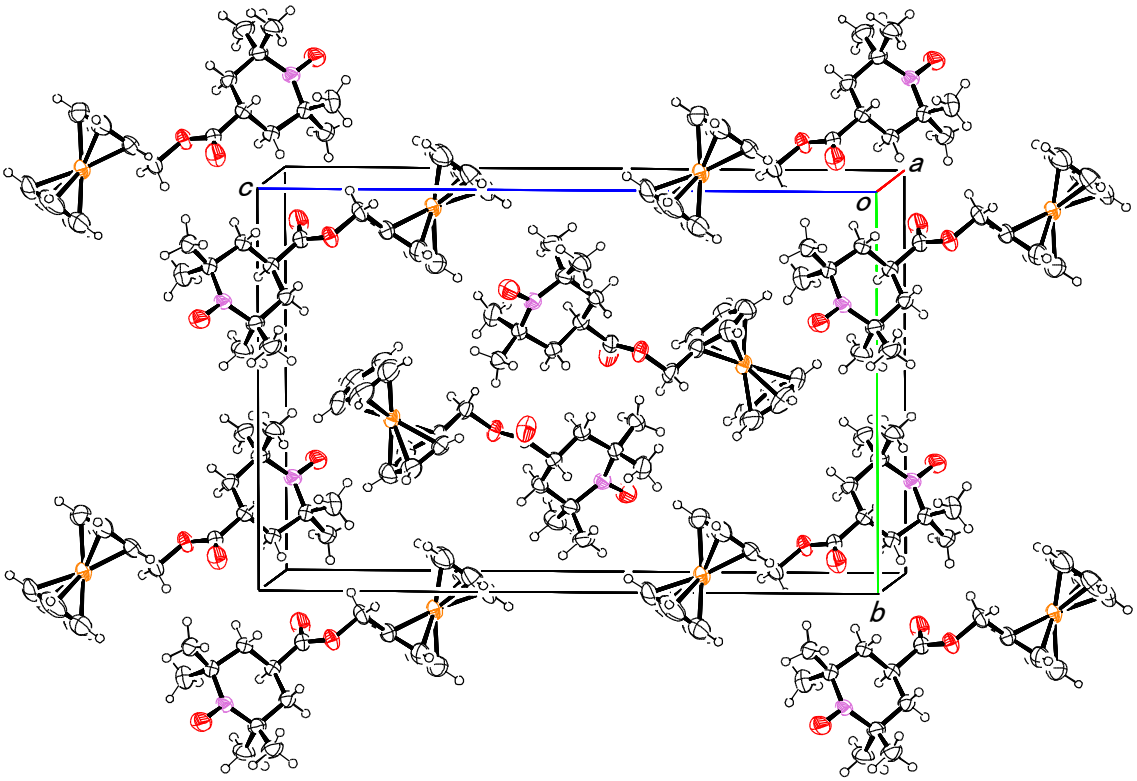
Supporting Information

SI-1. Summary of Crystal Data for **1 - 3**[a]

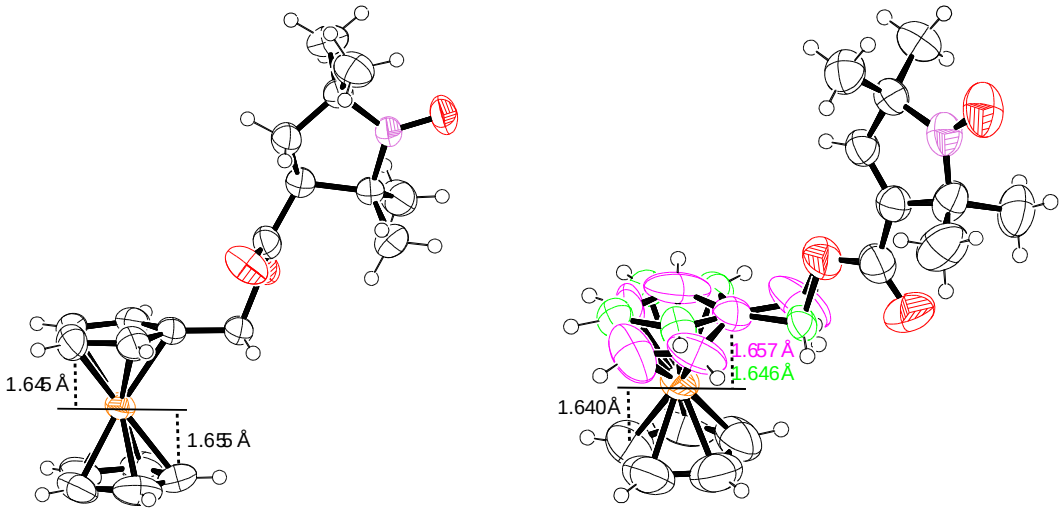
	1	**2**	**3**
Formula	$C_{21}H_{28}NO_3Fe$	$C_{20}H_{26}NO_3Fe$	$C_{20}H_{24}NO_3Fe$
Formula weight	398.30	384.28	382.26
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/c$
a/ Å	6.0132(13)	10.7610(7)	21.162(6)
b/ Å	14.588(4)	11.9388(15)	8.427(3)
c/ Å	22.279(5)	15.1774(3)	10.717(3)
α/degrees	90	90	90
β/degrees	95.358(5)	105.6595(5)	91.718(7)
γ/degrees	90	90	90
V/ Å^3	1945.7(8)	1877.5(3)	1910.4(9)
Z	4	4	4
D (calc)/gcm^{-3}	1.360	1.359	1.329
No. of total processed reflections	14855	15079	8163
No. of unique reflections in refinement F>2σ	4336	4162	4213
R_1	0.0636	0.0639	0.0548
R_W	0.0976	0.1715	0.1857

[a]X-ray data were collected with Mo Kα radiation at room temperature.

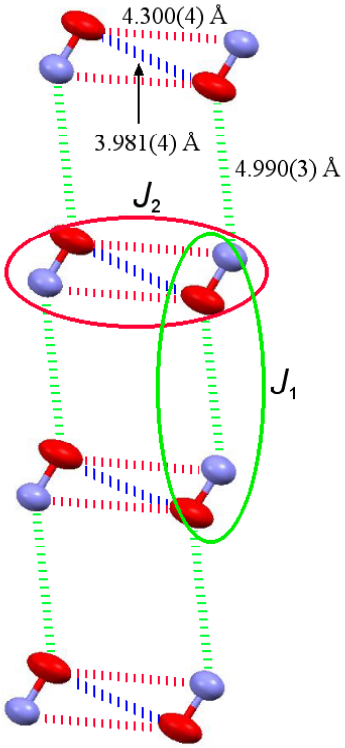
Electronic Supplementary Material (ESI) for New Journal of Chemistry



SI-2. Packing feature of **1** viewed almost along the a-axis.



SI-3. Molecular structures of **2** (left) and **3** (right) obtained by the X-ray analysis.

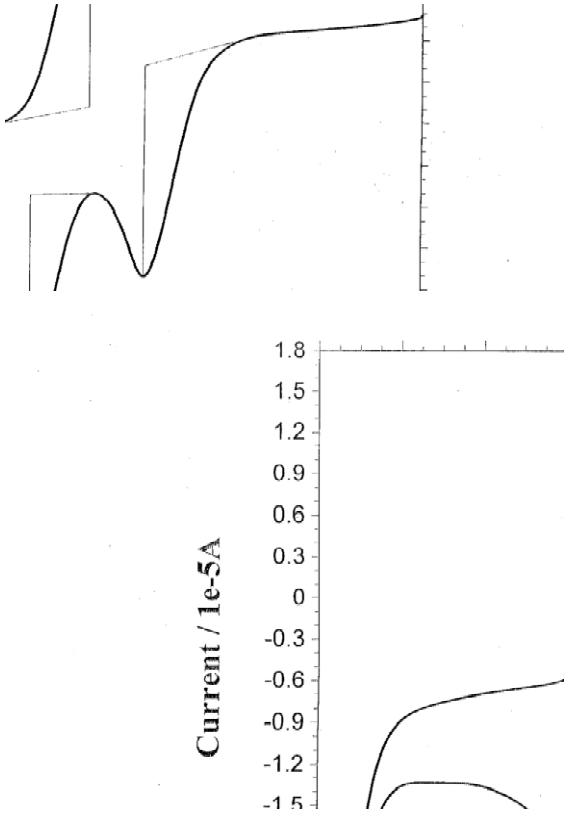


SI-4. Schematic drawing of spin-spin interactions between spin centres in **3**, where J_1 denotes the magnitude of inter-dimer interactions and J_2 denotes those of intra-dimer ones respectively.

SI-5. Summary of ESR data for **1** - **3**

Compound	g	a_N / G
1 (solid)	2.0080	–
1 (solution [a])	2.0066	15.67
2 (solid)	2.0081	–
2 (solution [a])	2.0065	14.32
3 (solid)	2.0077	–
3 (solution [a])	2.0064	14.61

[a]Solvent: benzene.



SI-6. CV plots for **2** as a representative.