

Electronic Supplementary Material

Synthesis of iron(II) complexes with asymmetric N₂O₂ coordinating Schiff base-like ligands and their spin crossover properties

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Table S1 Crystallographic data of the X-ray structures discussed in this work

compound	Ligand H ₂ L2a mn260	Ligand H ₂ L2c no124	[FeL2b(py) ₂] oo080
Sum formula	C ₁₉ H ₂₂ N ₂ O ₅	C ₂₀ H ₂₄ N ₂ O ₆	C ₃₁ H ₃₄ FeN ₄ O ₇
M/gmol ⁻¹	358.39	388.41	630.47
Temperature/K	200(2)	200(3)	123(3)
Crystal size /mm	0.24 × 0.12 × 0.07	0.32 × 0.13 × 0.06	0.34 × 0.26 × 0.05
Crystal system	triclinic	triclinic	monoclinic
Space group	<i>P</i> -1	<i>P</i> -1	<i>P</i> 21/ <i>c</i>
λ/Å	0.71073	0.71073	0.71073
a/Å	7.5061(2)	7.67(1)	12.7563(8)
b/Å	11.5182(3)	11.517(4)	29.705(3)
c/Å	21.9706(6)	11.95(2)	8.1222(11)
α/°	87.9623(14)	102.87(6)	90
β/°	89.0686(18)	106.7(1)	97.942(8)
γ/°	87.7438(19)	91.26(6)	90
V/Å ³	1896.62(9)	982(2)	3084.2(6)
Z	4	2	4
ρ _{calc} /(g·cm ⁻³)	1.255	1.314	1.374
μ/mm ⁻¹	0.092	0.098	0.548
F(000)	760	412	1320
θ range/°	3.134–25.028	4.3618–24.4971	4.1969–26.2489
Index range	-8 ≤ h ≤ 8 -13 ≤ k ≤ 13 -25 ≤ l ≤ 25	-8 ≤ h ≤ 8 -13 ≤ k ≤ 13 -13 ≤ l ≤ 13	-9 ≤ h ≤ 10 -37 ≤ k ≤ 35 -15 ≤ l ≤ 15
Reflexes measured/independent	12012/6491	6092/3236	24590/6142

Number of parameters	477	257	392
R _{int}	0.0322	0.1059	0.0579
R _σ	0.0401	0.1570	0.0879
R1(all)	0.0765 (0.0963)	0.0635 (0.1434)	0.0411 (0.0822)
wR2	0.2473	0.2046	0.0896
Goof	1.138	0.825	0.865

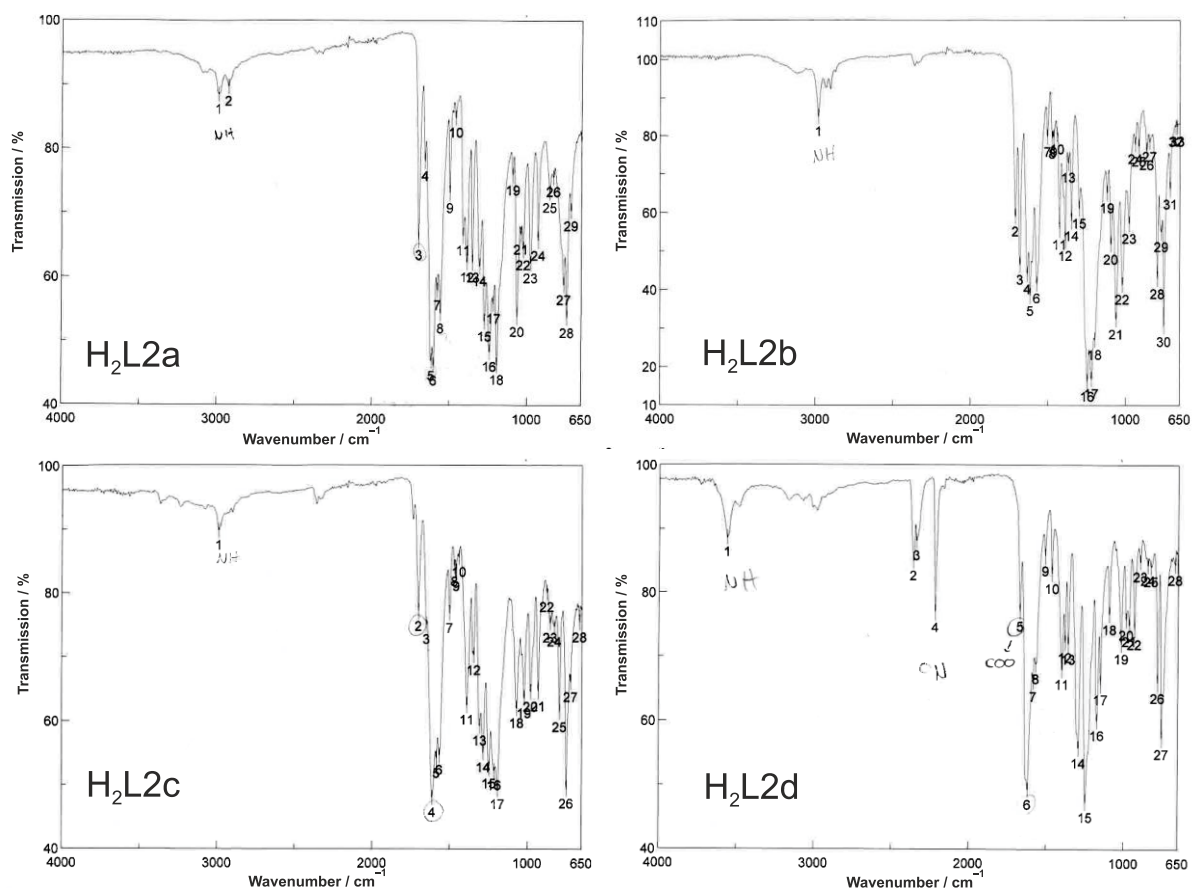


Fig. S1 IR spectra of the ligands discussed in this work

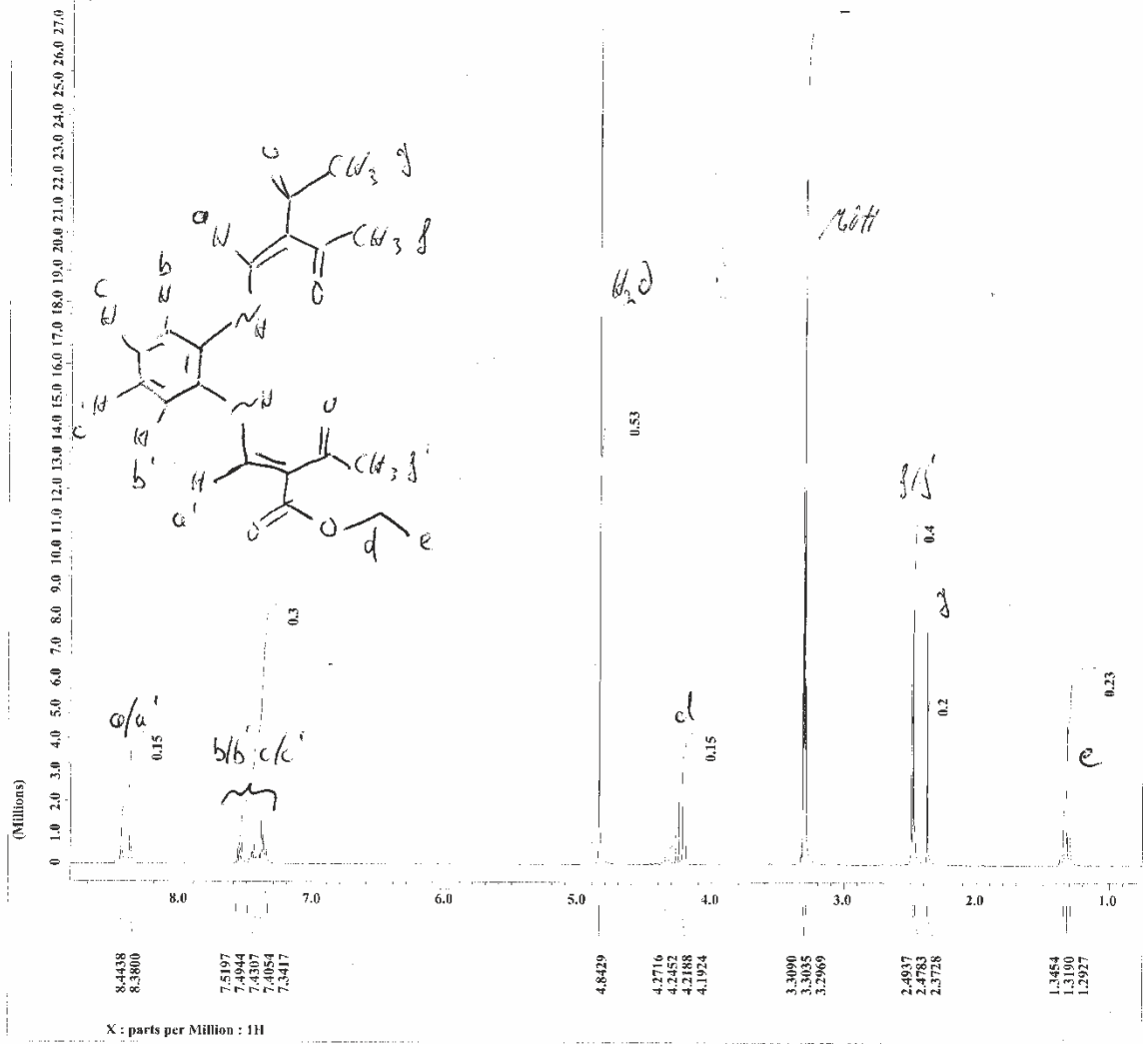


Fig. S2 ¹H NMR spectrum of H₂L₂a

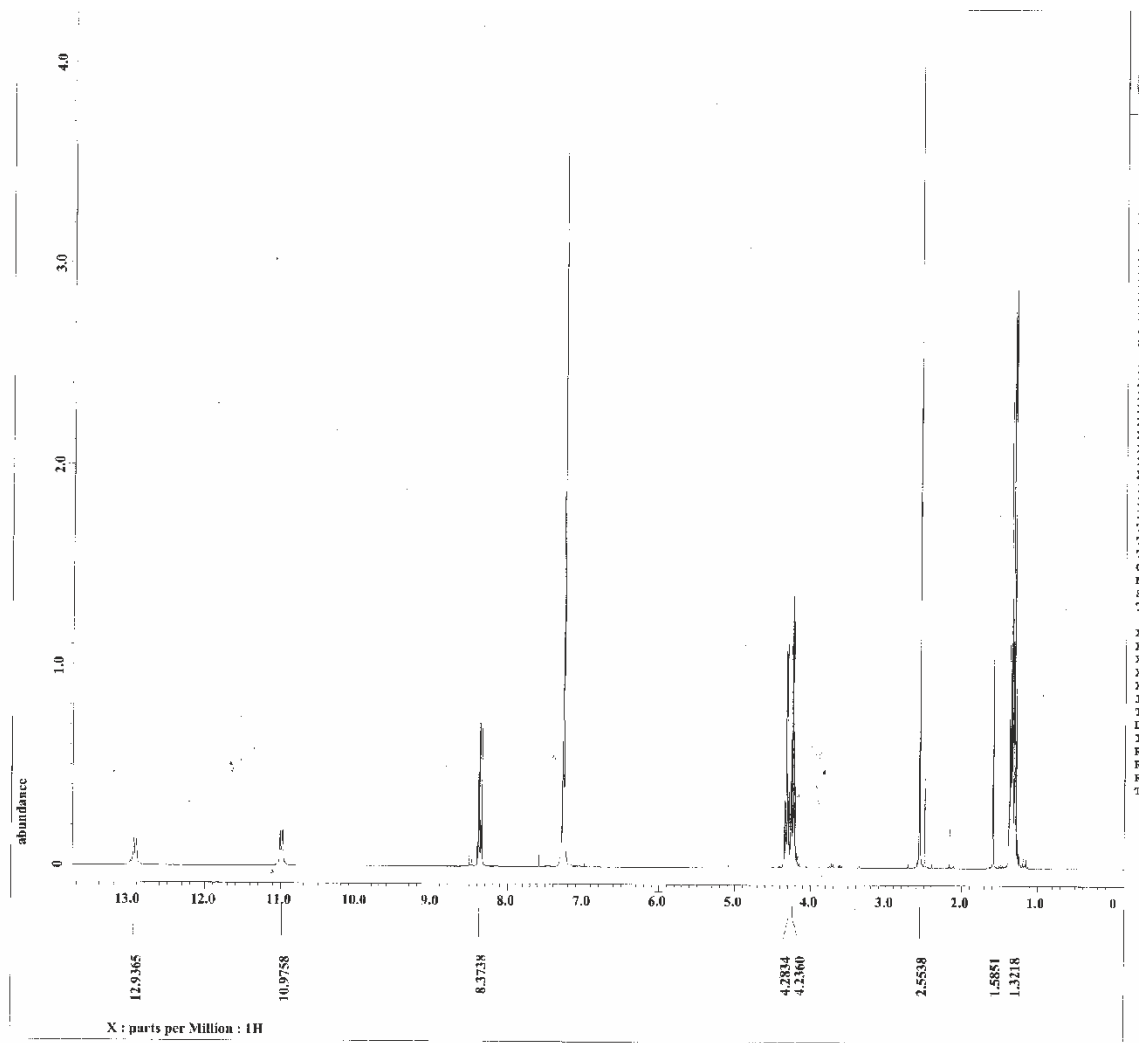


Fig. S3 ^1H NMR spectrum of $\text{H}_2\text{L}2\text{b}$

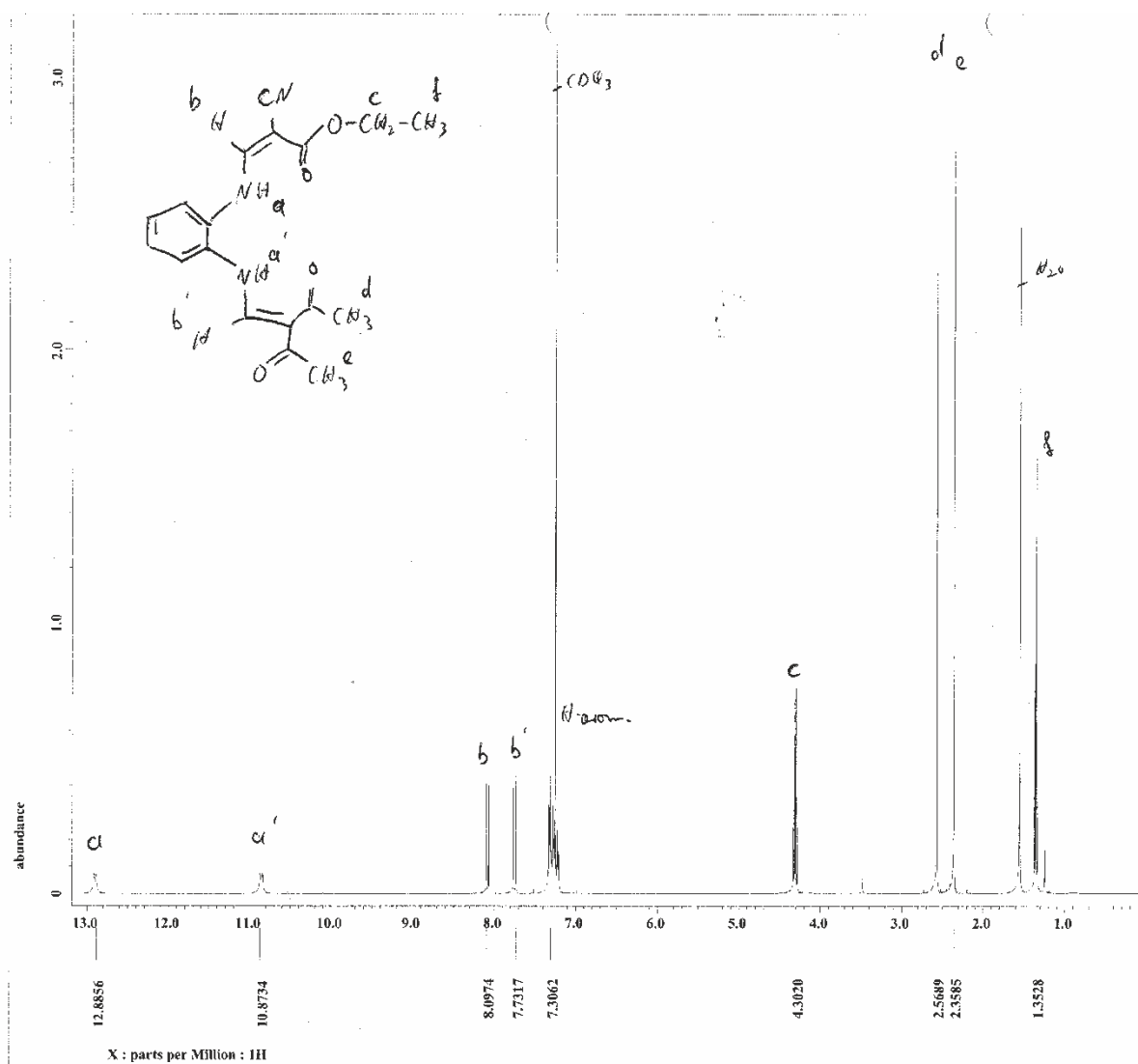


Fig. S4 ¹H NMR spectrum of H₂L₂d