

Cyclam-based Iron(III) and Copper(II) Complexes: Synthesis, Characterization and Application as Antifungal Agents

Stephanie Almada, Luísa B. Maia, João C. Waerenborgh, Bruno J. C. Vieira, Nuno P. Mira, Elisabete R. Silva, Fátima Cerqueira, Eugénia Pinto, Luis G. Alves

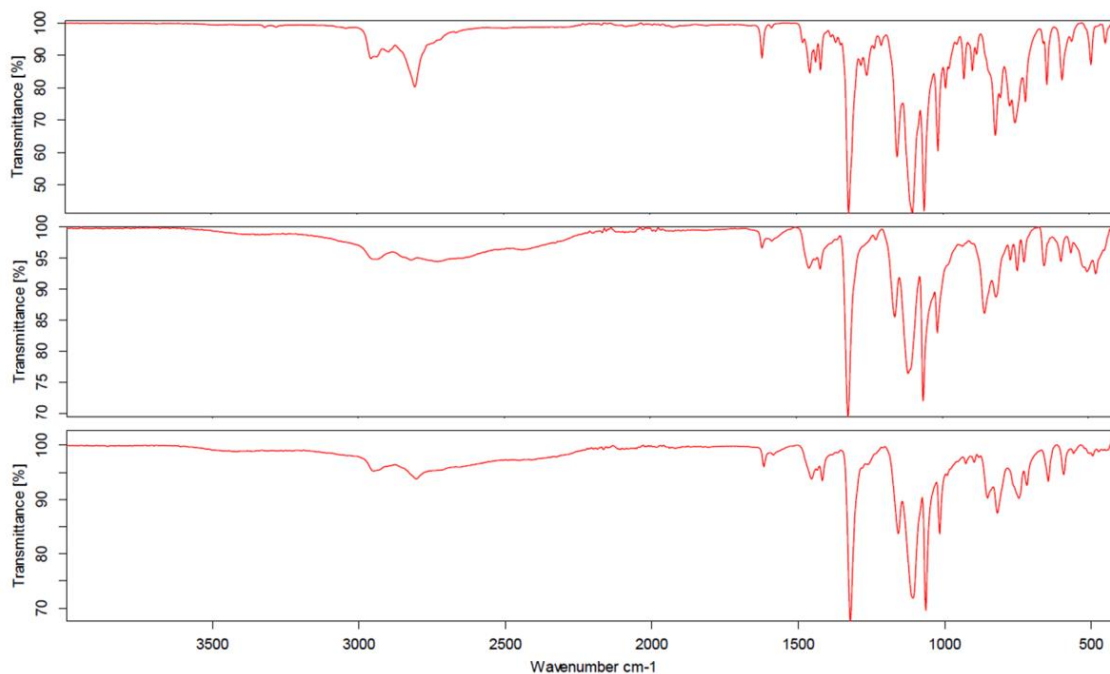


Figure S11 – IR spectra of H₂(⁴-CF₃PhCH₂)₂Cyclam, **1**, (top) and [{H₂(⁴-CF₃PhCH₂)₂Cyclam}FeCl₂]Cl, **2**, obtained in solution (middle) and in the solid state (bottom).

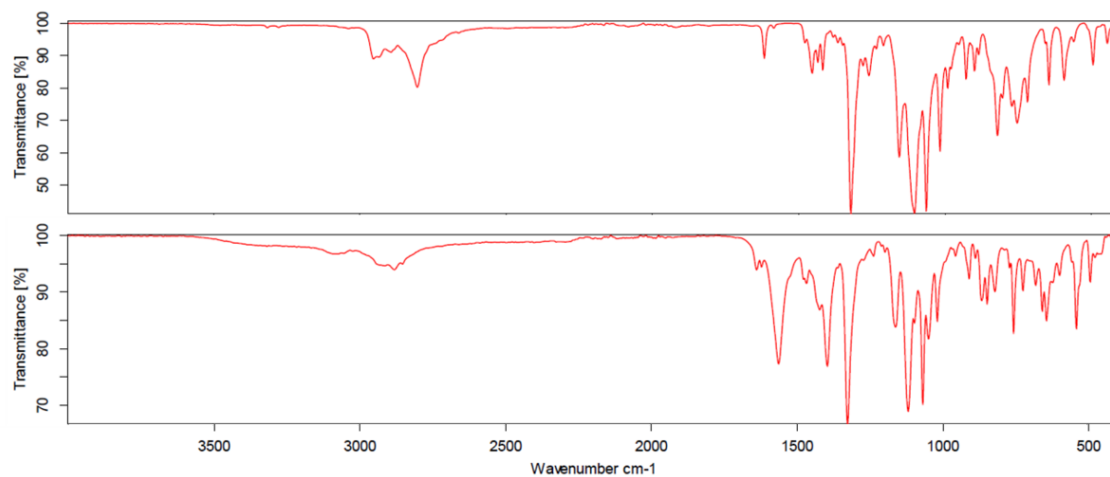


Figure S12 – IR spectra of H₂(⁴-CF₃PhCH₂)₂Cyclam, **1**, (top) and [{H₂(⁴-CF₃PhCH₂)₂Cyclam}Cu](CH₃COO)₂·2H₂O, **3**, (bottom).

Table S11 – Estimated parameters from the ^{57}Fe Mössbauer spectra of [$\{\text{H}_2(^{4-\text{CF}_3}\text{PhCH}_2)_2\text{Cyclam}\}\text{FeCl}_2\text{]Cl$, **2**.

	T (K)	spin state	IS (mm/s)	QS (mm/s)	B_{hf} (T)	I (%)
2 (solution)	80	HS	0.48	0.67	-	71
		LS	0.39	1.54	-	29
2 (solution)	4	HS	0.50	-0.23	47.0	75
		LS	0.40	1.59	-	25
2 (solid state)	80	HS	0.48	0.73	-	75
		LS	0.37	1.32	-	25
2 (solid state)	4	HS	0.48	-0.15	46.7	79
		LS	0.35	1.33	-	21

IS isomer shift relative to metallic $\alpha\text{-Fe}$ at 295 K; QS quadrupole splitting. $2\varepsilon = (e^2V_{zz}Q/4)(3\cos^2\theta-1)$ quadrupole shift estimated for the sextets. B_{hf} magnetic hyperfine field; I relative area. Estimated errors are <0.02 mm/s for IS, QS, ε and $<2\%$ for I

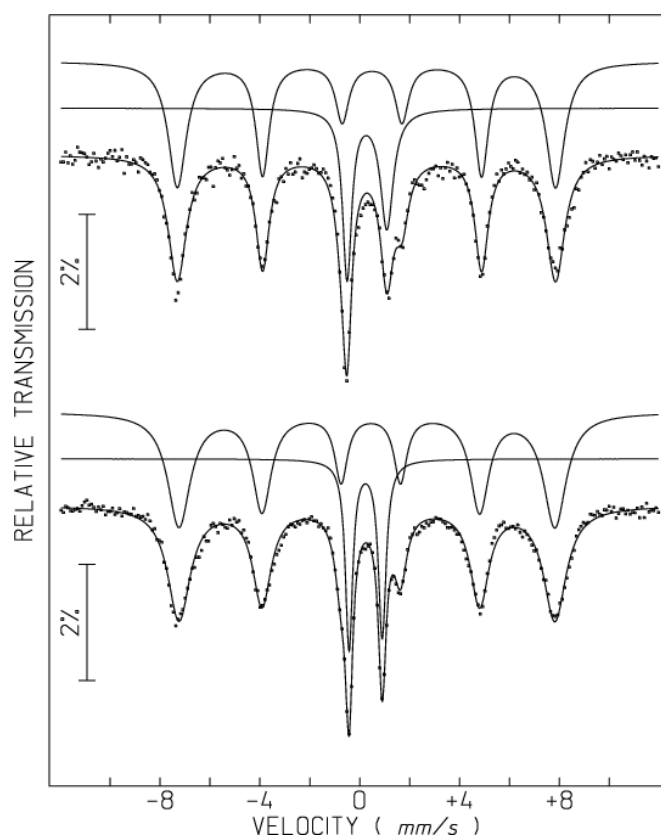


Figure S13 – ^{57}Fe Mössbauer spectra, at 4K, of [$\{\text{H}_2(^{4-\text{CF}_3}\text{PhCH}_2)_2\text{Cyclam}\}\text{FeCl}_2\text{]Cl$, **2**, obtained in solution (top) and in the solid state (bottom).

Table S12 – Hydrogen bond distances (Å) and angles (°) of complexes **3a** and **3b**.

	D-H \cdots A	d(D-H)	d(H \cdots A)	d(D \cdots A)	(D \hat{H} A)	Symmetry operation
3a	O(1)-H(1O) \cdots O(2)	0.82(12)	1.94(11)	2.708(13)	155(12)	1-x, -y, 1-z
	O(1)-H(2O) \cdots O(2)	0.89(11)	2.13(11)	2.970(15)	157(9)	
	O(1)-H(2O) \cdots O(3)	0.89(11)	2.47(11)	3.230(12)	143(8)	
	N(2)-H(2N) \cdots O(3)	1.00(7)	1.84(7)	2.774(10)	154(6)	1-x, -y, -z
3b	O(1)-H(1O) \cdots O(2)	0.86	1.82	2.660(5)	166	1+x, y, z
	O(4)-H(4O) \cdots O(2)	0.96	1.83	2.778(5)	169	
	N(2)-H(2N) \cdots O(3)	1.05(7)	1.78(7)	2.816(6)	167(6)	1+x, y, z

Table S13 – Minimal Inhibitory Concentration (MIC, $\mu\text{g/mL}$) and Minimal Lethal Concentration (MLC, $\mu\text{g/mL}$) for compounds **4** and **5**.

		4	5
<i>Candida albicans</i> ATCC10231	MIC	128	128
	MLC	128	128
<i>Candida albicans</i> H37	MIC	32	64
	MLC	128	64
<i>Candida krusei</i> ATCC6258	MIC	8	8
	MLC	8	8
<i>Candida krusei</i> H9	MIC	8	8
	MLC	8	8
<i>Cryptococcus neoformans</i> CECT1078	MIC	4	4
	MLC	8	8