

Supporting Information
for
Synthesis, structure and (spectro)electrochemistry of hybrid
metal(IV)phthalocyaninato-capped 3d-metal pyrazoloximates as prospective
precursors of ET and/or optically operated stimuli-induced and stimuli-
responsive single-molecule magnets, logic gates and qubits

Svetlana A. Belova,^a Semyon V. Dudkin,^a Alexander S. Belov,^a Anastasia A. Danshina,^{a,c} Pavel V. Dorovatovskii,^d Yulia H. Budnikova,^e Vera V. Khrizanforova,^e Svetlana Yu. Bratskaya,^f Denis V. Balatskiy,^f Yan Z. Voloshin^{a,b}

^a*Nesmeyanov Institute of Organoelement Compounds of the Russian Academy of Sciences, Vavilova str., bld. 1, 119334 Moscow, Russia*

^b*Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, 31 Leninsky pr., 119991 Moscow, Russia*

^c*Moscow Center for Advanced Studies, 20 Kulakova Str., 123592, Moscow, Russia*

^d*NRC Kurchatov Institute, 1 Kurchatova pl., 123098 Moscow, Russia*

^e*Arbuzov Institute of Organic and Physical Chemistry of the Russian Academy of Sciences, 8 Arbuzov st., 420088 Kazan, Russia*

^f*Institute of Chemistry, Far Eastern Branch of the Russian Academy of Sciences, 159 100-letiya Vladivostoka pr., 690022 Vladivostok, Russia*

*Corresponding author E-mail: voloshin@ineos.ac.ru, voloshin@igic.ras.ru

Spectral data

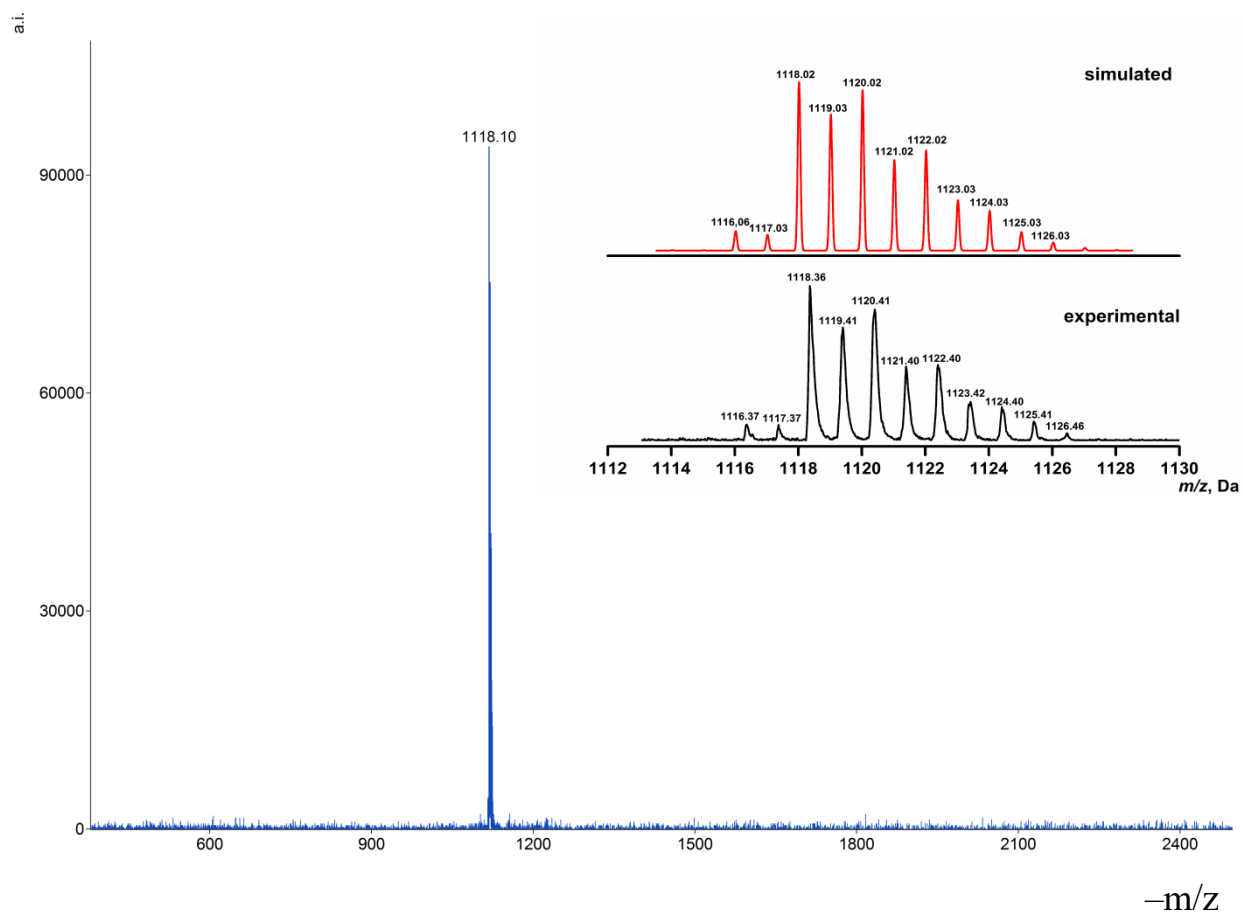
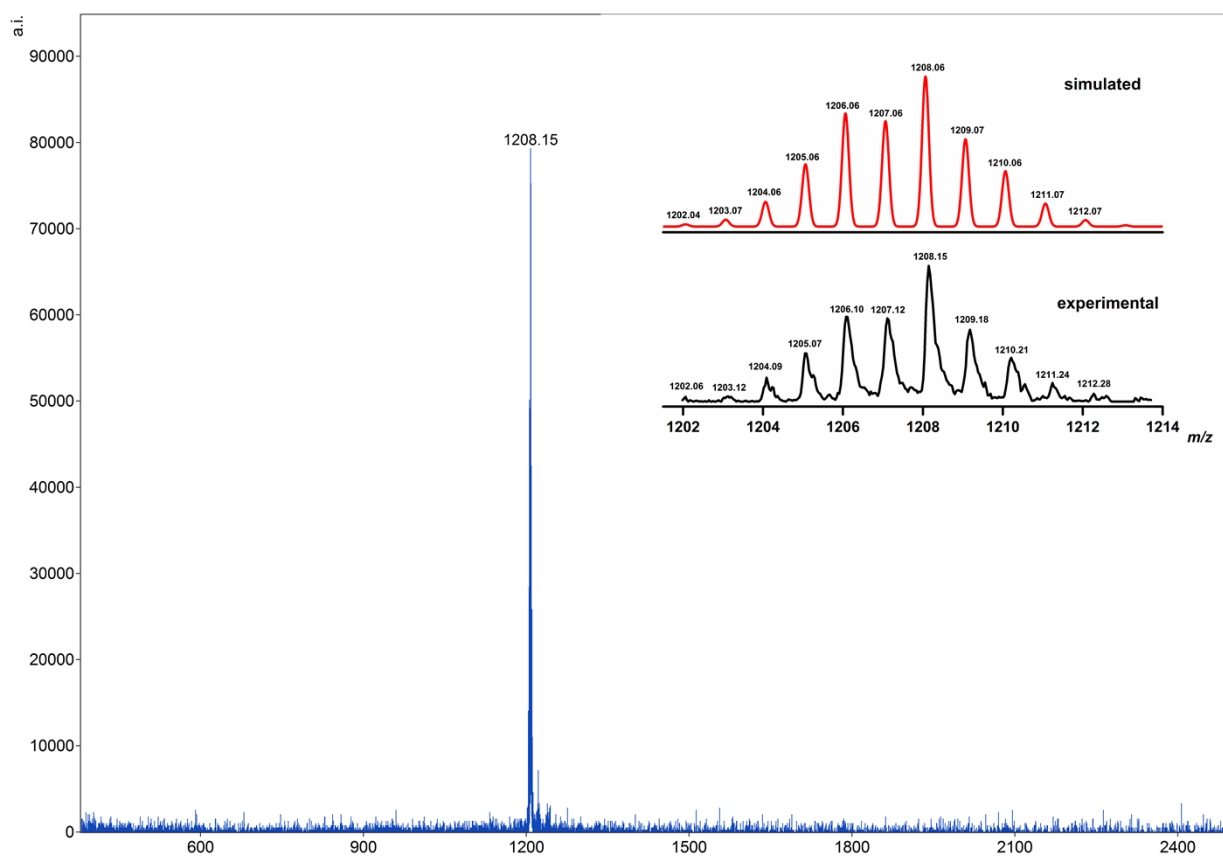


Fig. S1. MALDI-TOF mass spectrum of the hybrid complex $[\text{Fe}(\text{PzOx})_3(\text{ZrPc})\text{Cl}]$ in the negative range. Inset: the experimental and the theoretically calculated isotopic distribution of the peak of its formed anionic cluster.



–m/z

Fig. S2. MALDI-TOF mass spectrum of the hybrid complex $[\text{Fe}(\text{PzOx})_3(\text{HfPc})\text{Cl}]$ in the negative range. Inset: the experimental and the theoretically calculated isotopic distribution of the peak of its formed anionic cluster.

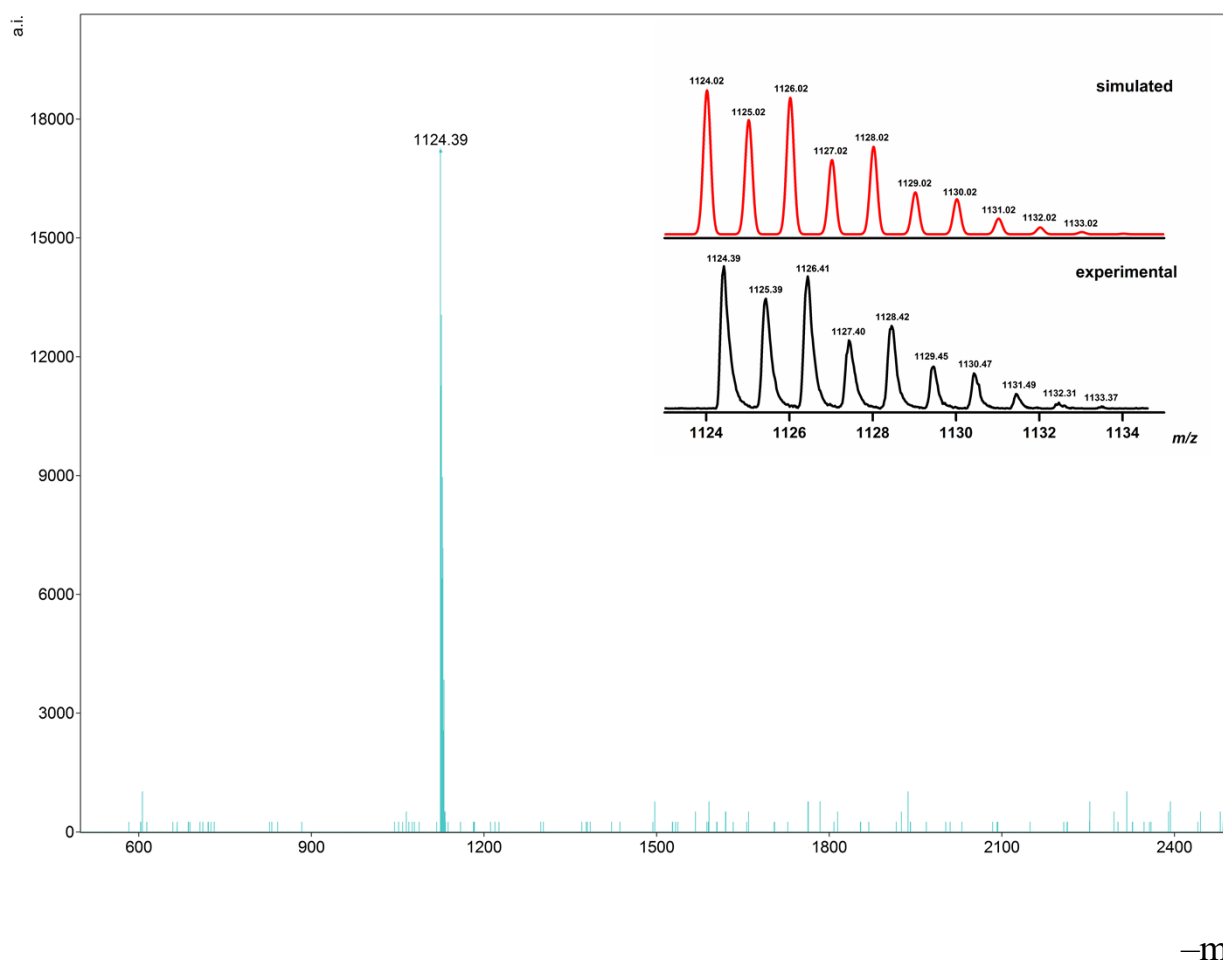


Fig. S3. MALDI-TOF mass spectrum of the hybrid complex $[\text{Co}(\text{PzOx})_3(\text{ZrPc})\text{Cl}]\text{Cl}$ in the negative range. Inset: the experimental and the theoretically calculated isotopic distribution of the peak of its formed anionic cluster.

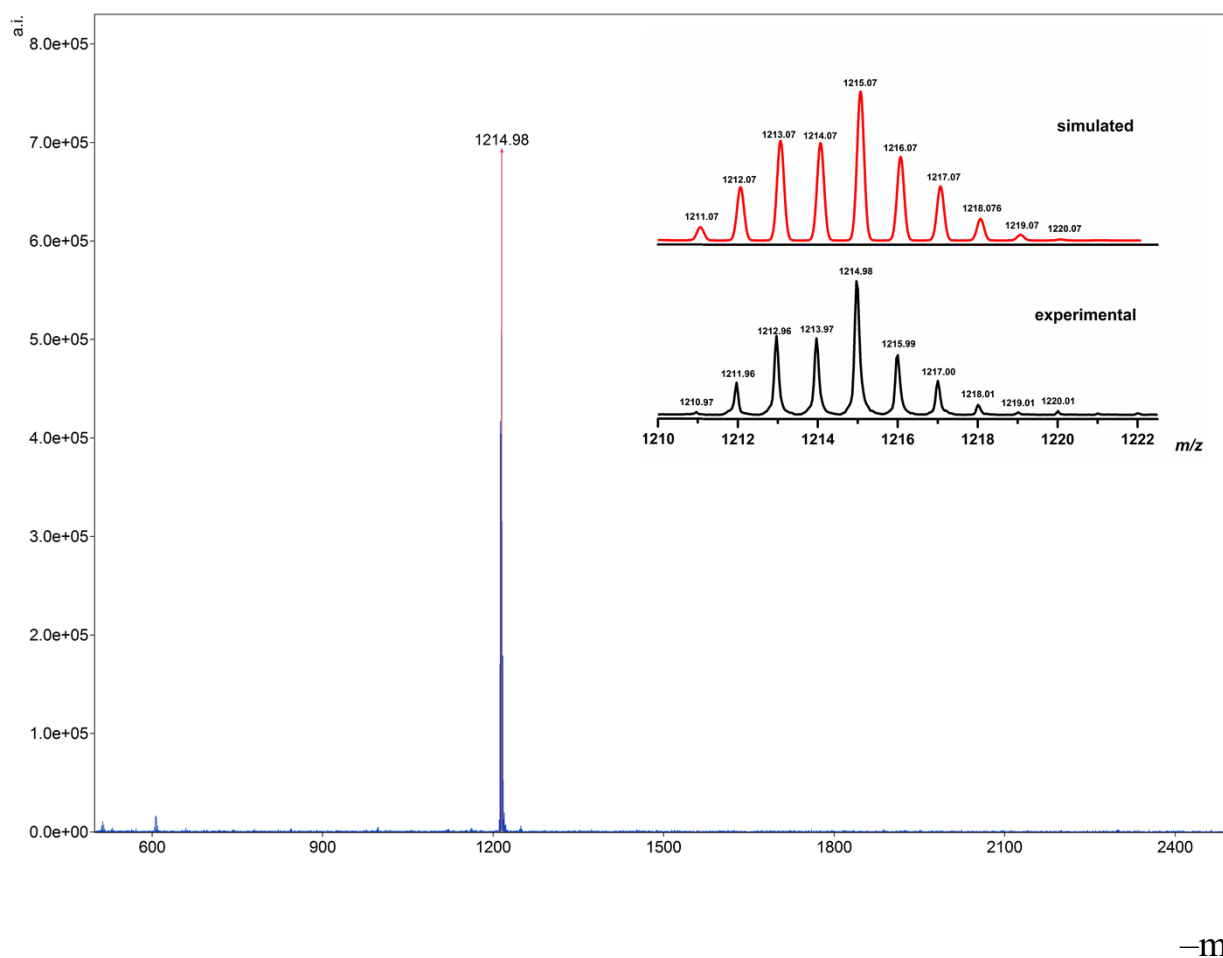


Fig. S4. MALDI-TOF mass spectrum of the hybrid complex $[\text{Co}(\text{PzOx})_3(\text{HfPc})\text{Cl}]\text{Cl}$ in the negative range. Inset: the experimental and the theoretically calculated isotopic distribution of the peak of its formed anionic cluster.

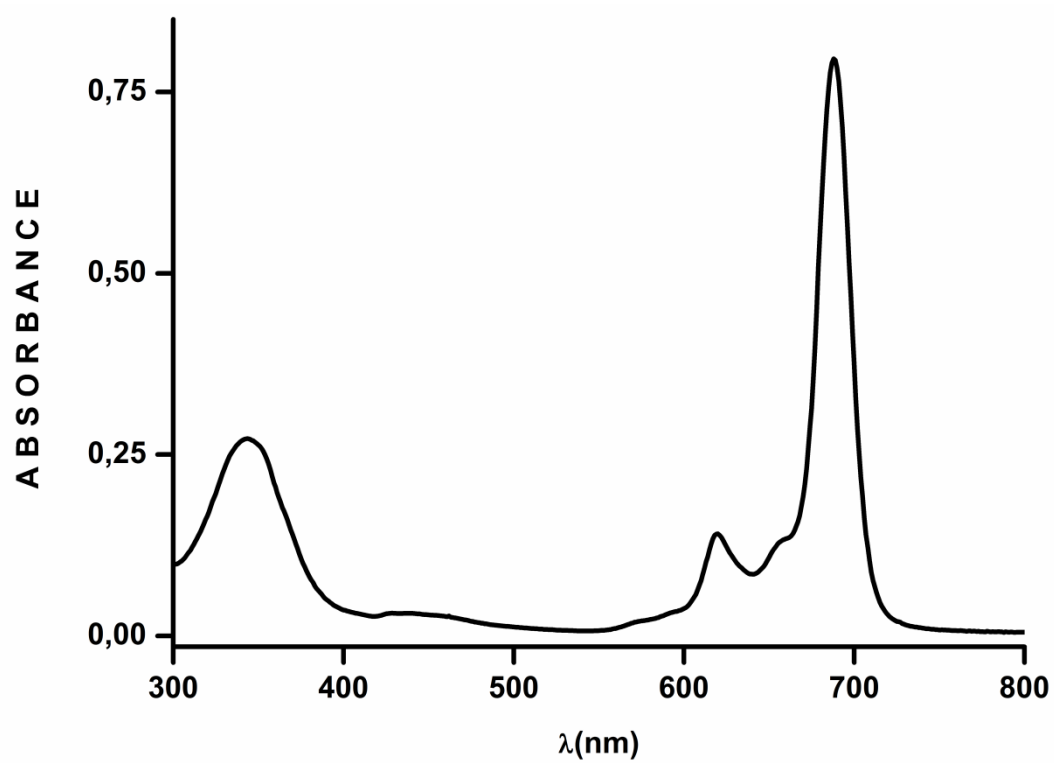


Fig. S5. Solution UV-vis spectrum of the complex [Fe(PzOx)₃(HfPc)Cl] in DMSO.

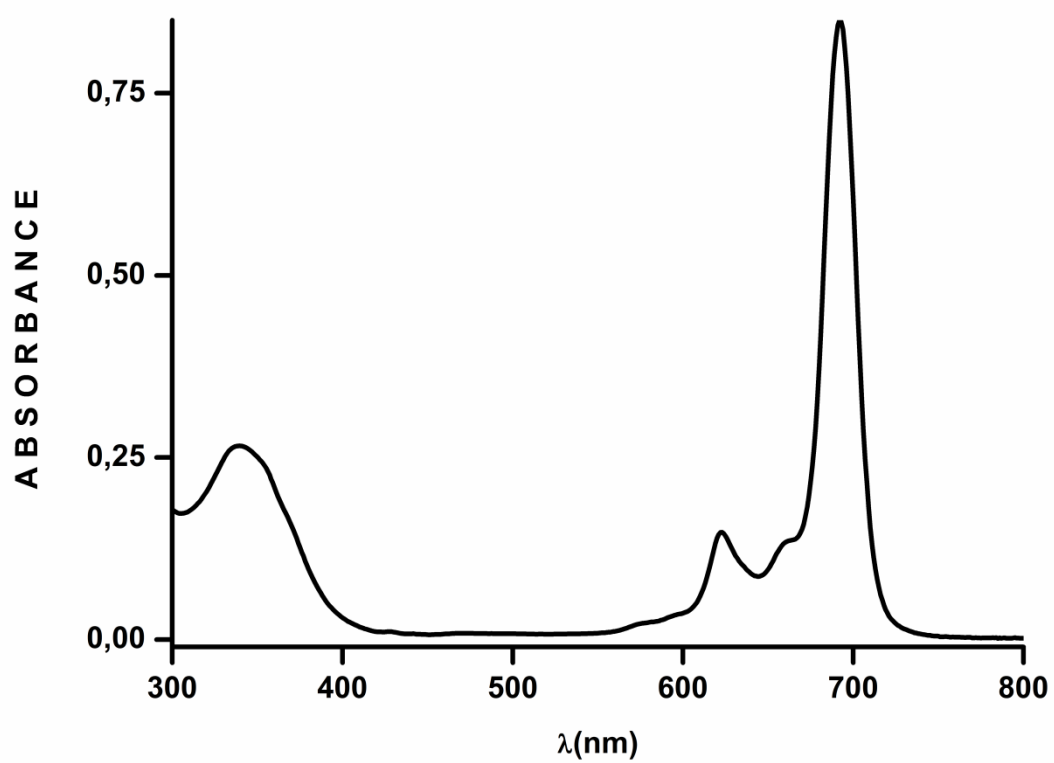


Fig. S6. Solution UV-vis spectrum of the complex [Co(PzOx)₃(HfPc)Cl]Cl in DMSO.

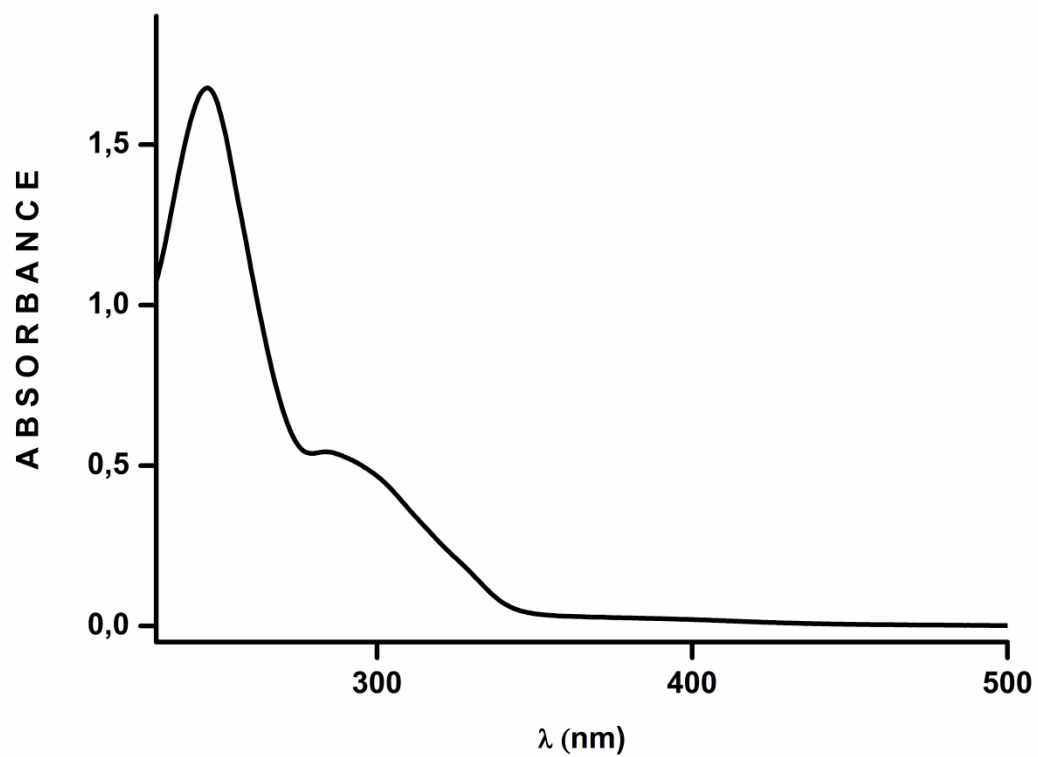


Fig. S7. Solution UV-vis spectrum of the complex [Fe(PzOx)₃B(C₆H₅)Cl] in DMSO.

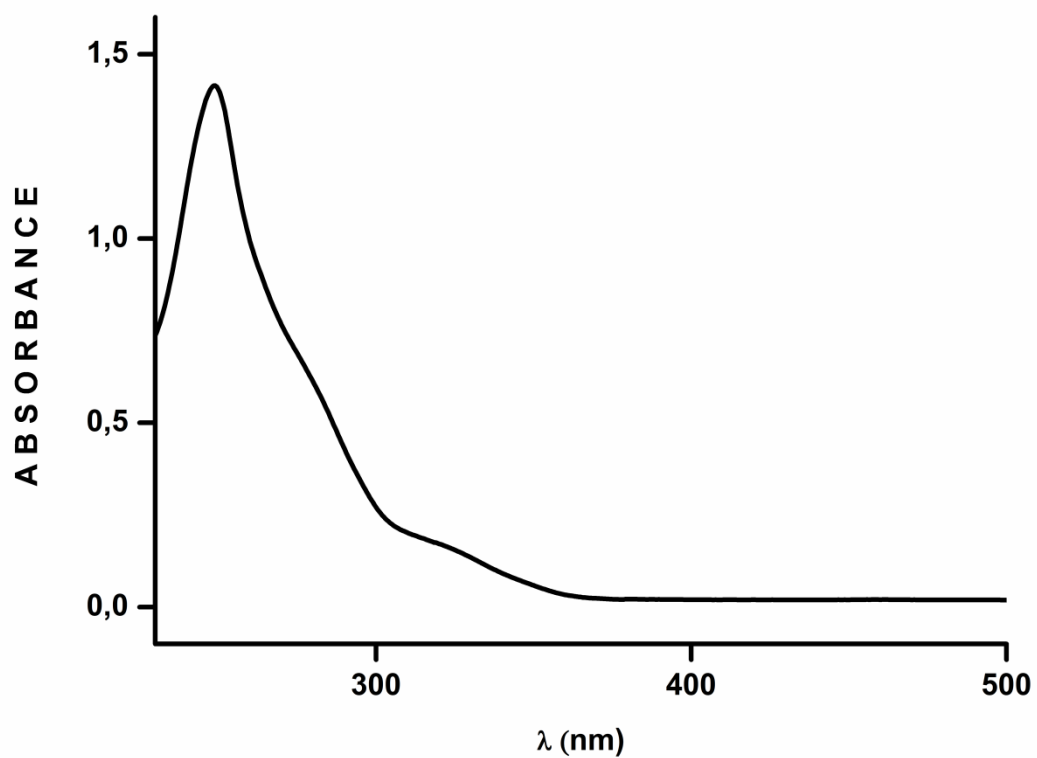


Fig. S8. Solution UV-vis spectrum of the complex [Co(PzOx)₃B(C₆H₅)Cl] in DMSO.

Table S4. Main ^{57}Fe Mössbauer parameters for the obtained binuclear hybrid iron(II) complexes and those for their mononuclear phenylboron-capped analog

Compound	δ	ΔE_q	Γ	Relative area %	Assignment
	<i>mm/s</i>				
[Fe(PzOx) ₃ (BC ₆ H ₅)Cl] [37d]	0.99	3.55	0.28	76.7	HS Fe(II)
Fe ³⁺ -containing admixture [37d]	0.41	0.72	0.57	23.3	HS Fe(III)
[Fe(PzOx) ₃ (HfPc)Cl]	0,99	3.11	0.29	100	HS Fe(II)
[Fe(PzOx) ₃ (ZrPc)Cl]	1.00	3.11	0.24	100	HS Fe(II)