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SUPPLEMENTARY MATERIAL TO

Iron(III) complexes with ditopic macrocycles bearing crown-ether and bis(salicylidene) isothiosemicarbazide moieties

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ANALYTICAL AND SPECTRAL DATA

*$[Fe^{III}LClBa(CH_3OH)(H_2O)_{0.5}(ZnCl_4)]\cdot CH_3OH$ (**1·CH_3OH**)*

Anal. Found, %: C, 29.91; H, 3.29; N, 4.05. Calcd for $C_{24.5}H_{33}BaCl_5FeN_3O_{8.5}SZn$ (M_r 973.43), %: C, 30.23; H, 3.42; N, 4.32. ESI positive: *m/z* 513 $[FeL]^+$; ESI negative: *m/z* 169 $[ZnCl_3]^-$; FAB: *m/z* 685 (100%), *m/z* 720 (50%), *m/z* 571 (47%).

*$[Fe^{III}LCl]\cdot CH_2Cl_2$ 0.5H_2O (**2·CH_2Cl_2 0.5H_2O**)*

Anal. Found, %: C, 43.11; H, 3.99; N, 7.01. Calcd for $C_{23}H_{26}FeN_3O_{6.5}SCl_3$ (M_r 642.73), %: C, 42.98; H, 4.08; N, 6.54. IR spectra, selected bands, ν, cm^{-1}: 2984(w), 2921(w), 1599(s) (C=N), 1577(m), 1244(m), 738(m).

*$[Fe^{III}L(N_3)]$ (**3**)*

Anal. Found, %: C, 47.31; H, 3.99; N, 15.05. Calcd for $C_{22}H_{23}FeN_6O_6S$ (M_r 555.37), %: C, 47.58; H, 4.17; N, 15.13. IR spectra, selected bands, ν, cm^{-1}: 2924(w), 2034(m) (N_3^-), 1578(s) (C=N), 1246(m) (C–N), 736(m).

*$[(Fe^{III}L)_2O]\cdot H_2O$ (**4·H_2O**)*

Anal. Found, %: C, 49.91; H, 4.54; N, 7.79; S, 5.81. Calcd for $C_{44}H_{48}Fe_2N_6O_{14}S_2$ (M_r 1060.71), %: C, 49.82; H, 4.56; N, 7.92; S, 6.05. IR spectra, selected bands, ν, cm^{-1}: 2919(w), 2982(w), 1600(s), 1578(s), 1248(m) (C–N), 840(m) (FeOFe), 731(s).

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Table S-I. Crystal Data and Details of Data Collection for $[Fe^{III}LClBa(CH_3OH)(H_2O)_{0.5}(ZnCl_4)]\cdot H_2O$ (**1·H$_2$O**), $[Fe^{III}LCl]\cdot CH_2Cl_2\cdot 0.5H_2O$ (**2·CH$_2$Cl$_2$·0.5H$_2$O**) and $[(Fe^{III}L)_2O]\cdot CHCl_3$ (**4·CHCl$_3$**)

Compound	**1·H$_2$O**	**2·CH$_2$Cl$_2$·0.5H$_2$O**	**4·CHCl$_3$**
empirical formula	$C_{23}H_{30}BaCl_5FeN3O_{8.5}SZn$	$C_{23}H_{26}Cl_3FeN_3O_{6.5}S$	$C_{45}H_{47}Cl_3Fe_2N_6O_{13}S_2$
fw	952.37	642.73	1162.05
space group	*P*-1	$P2_1/c$	*P*-1
a / Å	10.1054(2)	19.8072(9)	12.926(2)
b / Å	10.2497(2)	18.0736(8)	13.460(2)
c / Å	18.7003(4)	16.8200(8)	14.438(2)
α / °	90.031(1)		93.451(9)
β / °	93.822(1)	113.778(2)	96.088(9)
γ / °	119.201(1)		94.944(10)
V / Å^3	1685.79(6)	5510.2(4)	2482.4(7)
Z	2	4	2
λ / Å	0.71073	0.71073	0.71073
ρ_{calcd} / g cm^{-3}	1.876	1.550	1.555
cryst size / mm^3	0.70 × 0.35 × 0.14	0.33 × 0.18 × 0.07	0.50 × 0.25 × 0.25
T / K	100(2)	100(2)	100(2)
μ / mm^{-1}	2.793	0.959	0.900
R_1[a]	0.0502	0.0644	0.0430
wR_2[b]	0.1372	0.1753	0.1129
GOF[c]	1.069	1.071	1.048

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

[c] GOF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{1/2}$, where n is the number of reflections and p is the total number of parameters refined.