Coordination properties of $N,N'$-bis(5-methylsalicylidene)-2-hydroxy-1,3-propanediamine with $d$- and $f$-electron ions: crystal structure, stability in the solution, spectroscopic and spectroelectrochemical studies

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Supplementary information

Crystallographic data for the structural analysis has been deposited with the Cambridge Crystallographic Data Centre, Nos. CCDC – 1569983 (H$_3$L A), CCDC-1569984 (H$_3$L B), CCDC - 1569985 (1), and CCDC – 1569986 (2). Copies of this information may be obtained free of charge from: The Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK. Fax: +44(1223)336-033, e-mail:deposit@ccdc.cam.ac.uk, or www: www.ccdc.cam.ac.uk.

Fig. S1 The difference Fourier map of H$_3$L.

Fig. S2 The difference Fourier map of H$_3$L.
Fig. S3 The difference Fourier map of H$_3$L.

Fig. S4 The difference Fourier map of H$_3$L.

Fig. S5 A comparison of conformations of H$_3$L molecules from complexes (1) and (2).

Fig. S6 A comparison of experimental and theoretical curves of selected Cu$^{2+}$/H$_3$L system (1:1).
Fig. S7 The cyclic voltammogram of complexes (2) (from synthesis with Dy) (black) and [CuHL] (from synthesis with Tb) (red) measured in anhydrous and deaerated acetonitrile with 0.1 M TBAPF₆ as a supporting electrolyte at a scan rate 100 mV/s scanned in the negative direction.

Fig. S8 Spectroelectrochemistry of complex (2) (from synthesis with Dy) in dehydrated and deaerated acetonitrile with 0.1 M TBAPF₆ as a supporting electrolyte by applying 0 (■), -100 (●), -200 (▲), -300 (▼), -400 (●), -500 (◄), and -600 mV (►) potential versus Ag/AgCl gel reference electrode held for 30 s per potential.

Fig. S9 Spectroelectrochemistry of complex (2) (from synthesis with Tb) in dehydrated and deaerated acetonitrile with 0.1 M TBAPF₆ as a supporting electrolyte by applying 0 (■), -300 (●), -400 (▲), -500 (▼), and -600 mV (○) potential versus Ag/AgCl gel reference electrode held for 30 s per potential.