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ESI

Conformational analysis and synthetic approaches to polydentate perhydro-diazepine ligands for the complexation of gallium(III)

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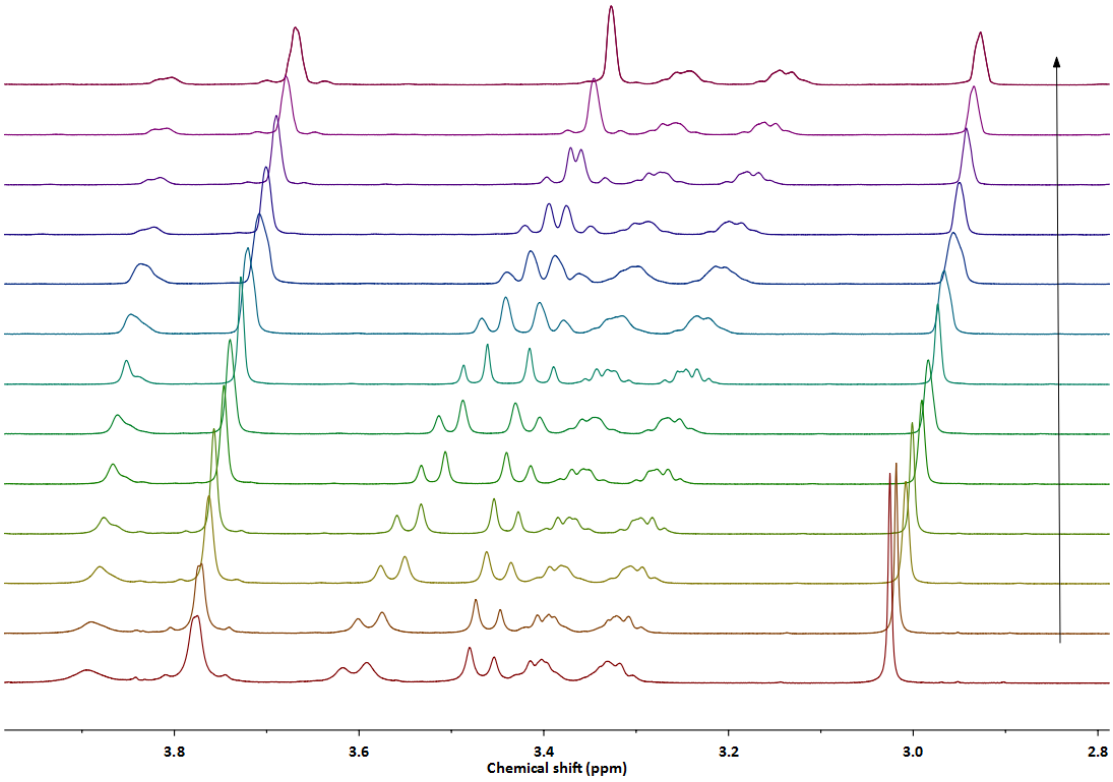
ESI Figure 1 VT 1H NMR spectra of $[H_2L^{4a}]^{2+}$ (D_2O, pD 2.4, 600MHz) showing the coalescence of the NCH_2CCH_2N methylene protons at 3.61 and 3.47 ppm (298K) as the temperature increases from 298K to 358K.



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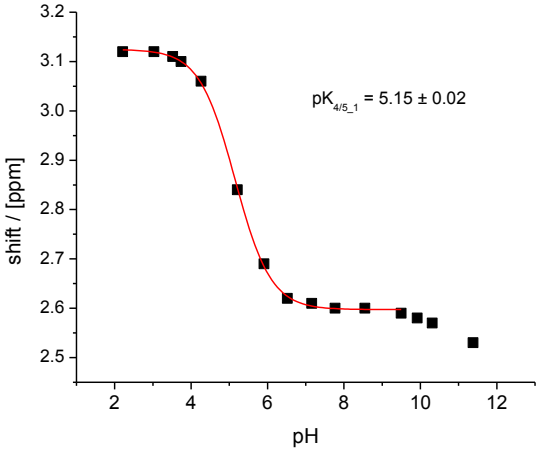
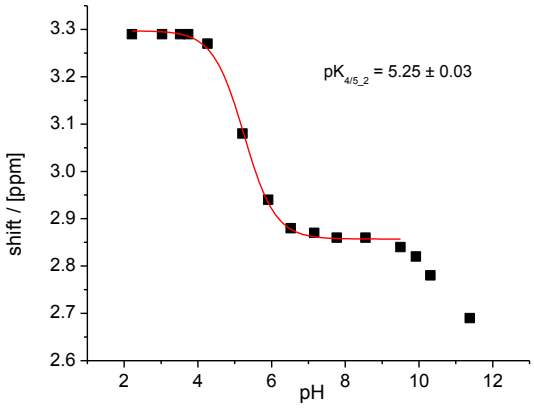
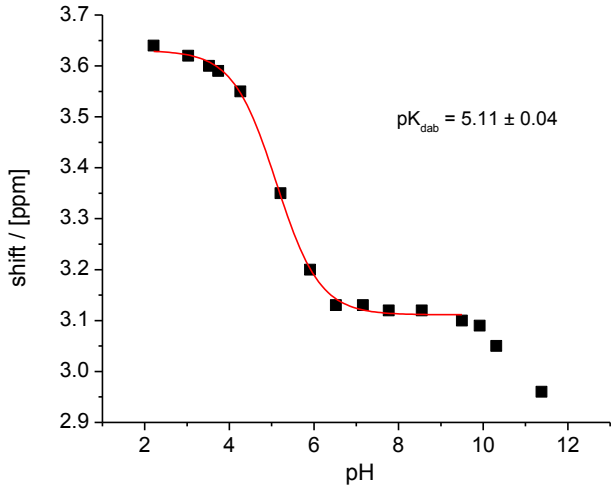
ESI Figure 2 *upper:* Variation of the chemical shift of the endocyclic NCH_2CH_2N protons in $[H_2L^1]$as a function of the meter-reading pH (pD = pH (meter reading) + 0.41: P. K. Glasoe and F. A. Long, *J. Phys. Chem*. 1960, **64**, 188.); *lower:* depicting the change of chemical shift with pH for the NCH_2CCH_2N protons. A value for the apparent pK_a was determined by fitting the data to the line shown, using iterative non-linear least squares methods: pK_a = 5.58 (±0.10) (D_2O, 295K).







Details of the related variation of the ^1H NMR chemical shift with pH for the ligand resonances in L^{4a} in D_2O (295K) have been reported in the ESI of reference 3.