

ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Internal hydrogen bonding and amide co-ordination in zinc(II) complexes of a tripodal N4 ligand: Structural, spectroscopic and reactivity studies.

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Figure captions

Fig. S1 An ORTEP plot drawn with 30 % probability thermal ellipsoids showing intermolecular N(7)-H(7N)···N(12) hydrogen bonding in the crystal structure of bppapa.

Fig. S2 An ORTEP plot drawn with 50 % probability thermal ellipsoids showing hydrogen bonding between the [(bppapa)Zn]²⁺ cation and one of the PF₆⁻ anions in the crystal structure of **1**·0.5MeOH.

Fig. S3 Aromatic and NH region of the ¹H NMR spectra (360.1 MHz, CD₃CN) of **1** at 323 K (*top*) and 293 K (*bottom*).

Fig. S4 Aromatic and NH region of the ¹H NMR spectra (360.1 MHz, CD₃CN/CD₃OH 6:1, 323 K) of (i) **1** (0.046 mM), (ii) **1** (0.046 mM) mixed with MeNOH·5H₂O (0.046) after 60 s; (iii) **1** (0.046 mM) mixed with MeNOH·5H₂O (0.046) after 7.5 h; (iv) [(bpapa)Zn(NCCH₃)](PF₆)₂ (0.046 mM) mixed with

MeNOH·5H₂O (0.046) and (CH₃)₃CCOOH (0.046 mM) after 60 s and (v) [(bpapa)Zn(NCCH₃)](PF₆)₂ (0.046 mM).

Fig. S5 Aromatic and NH region of the ¹H NMR (360.1 MHz, CD₃CN/CD₃OH 6:1, 323 K) of (i) bppapa (0.046 mM), (ii) bppapa (0.046 mM) mixed with MeNOH·5H₂O (0.046) after 7.5 h s; (iii) bppapa (0.046 mM) mixed with MeNOH·5H₂O (0.046) after 10 days; (iv) bpapa (0.046 mM).

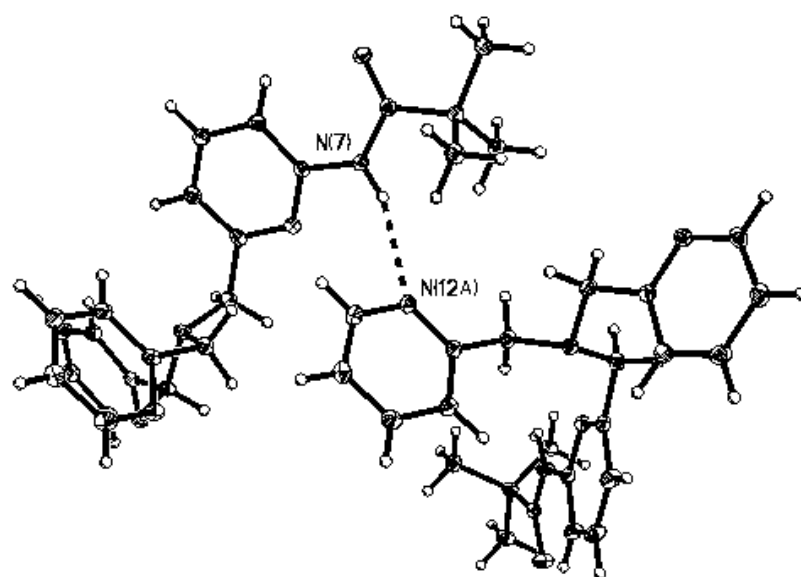


Fig. S1 Mareque Rivas, Torres and Parsons.

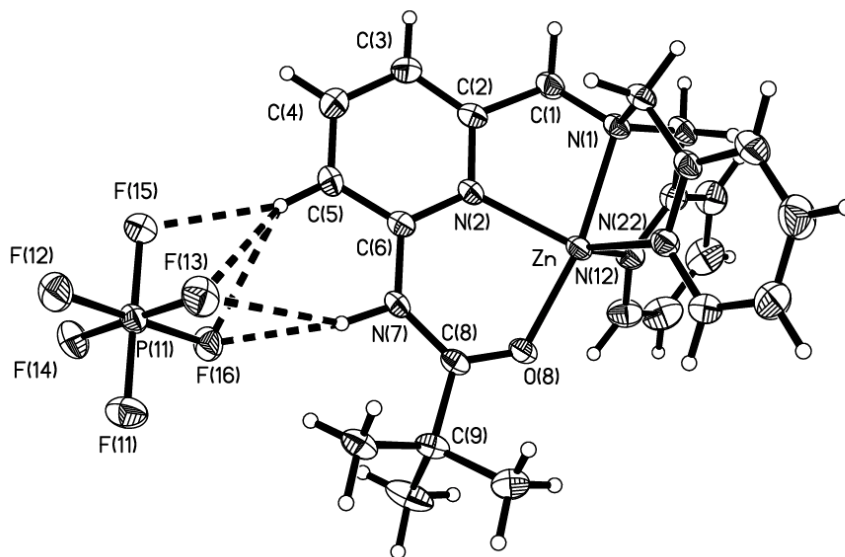


Fig. S2 Mareque Rivas, Torres and Parsons.

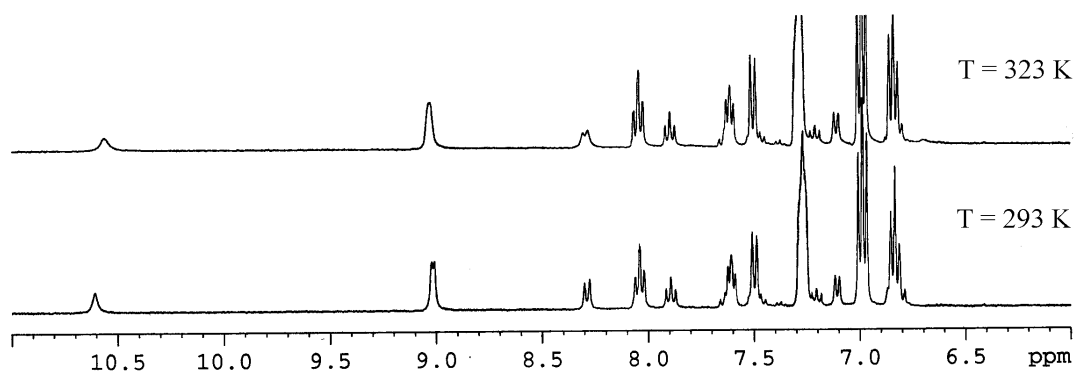


Fig. S3 Mareque Rivas, Torres and Parsons.

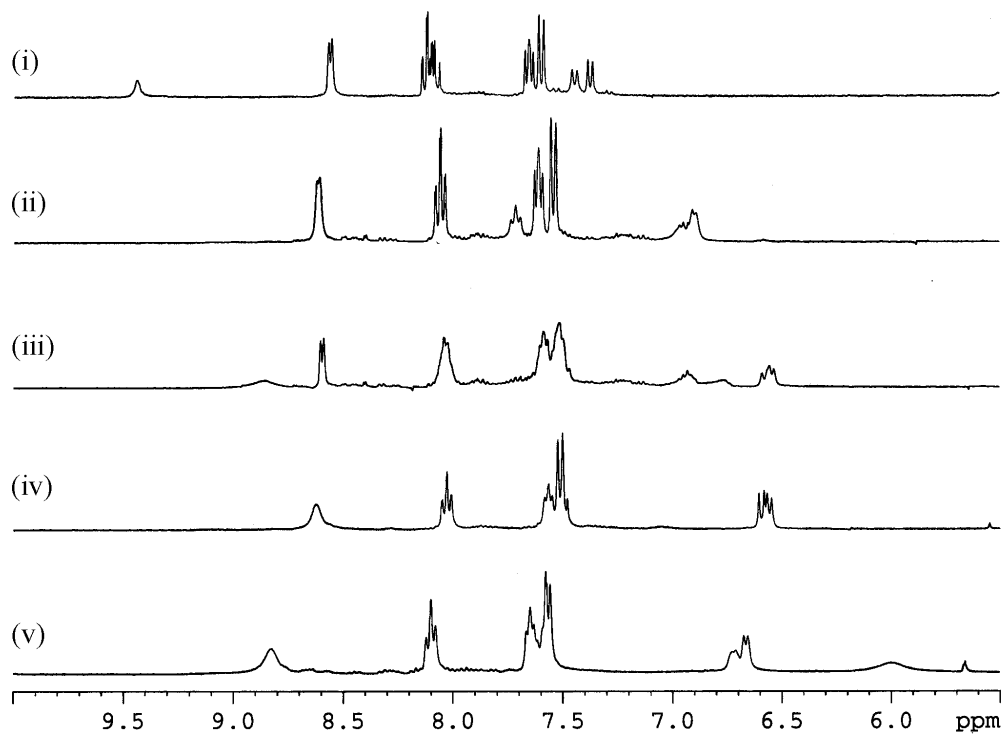


Fig. S4 Mareque Rivas, Torres and Parsons.

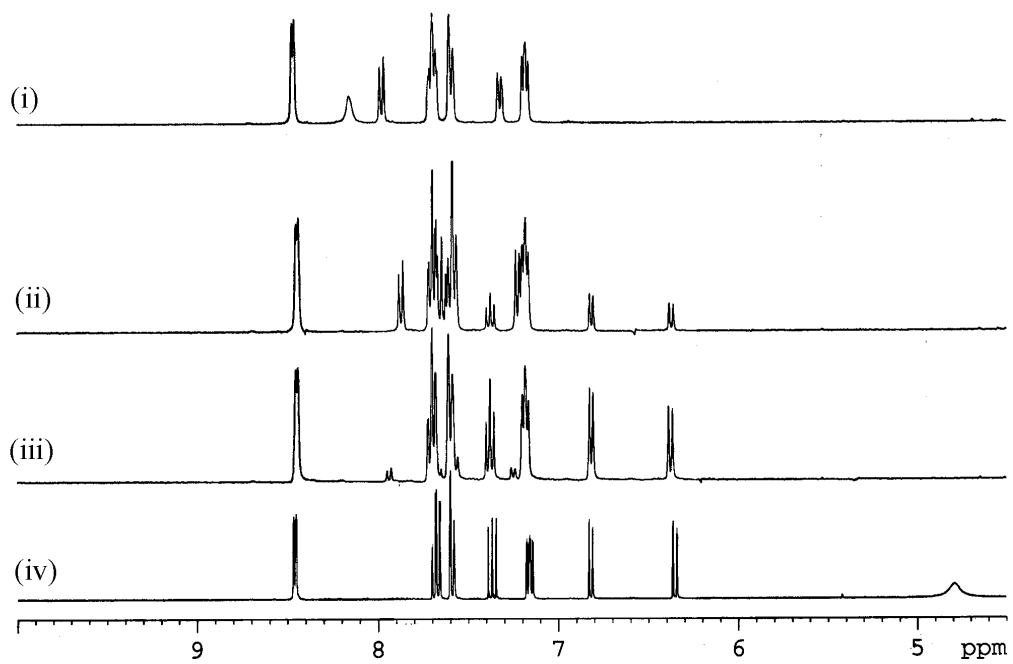


Fig. S5 Mareque Rivas, Torres and Parsons.