

Supplementary Data

Cation Complexation with *p*-*tert*-butylcalix[5]arene Pentacarboxylic Acid Derivative: An Allosteric Regulation of The First Metal Ion For Stepwise Extraction of The Second Ion

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Fig SF1 ¹H NMR spectrum of Na complexed **2** in CDCl₃ (solvent peak at 7.26 ppm)

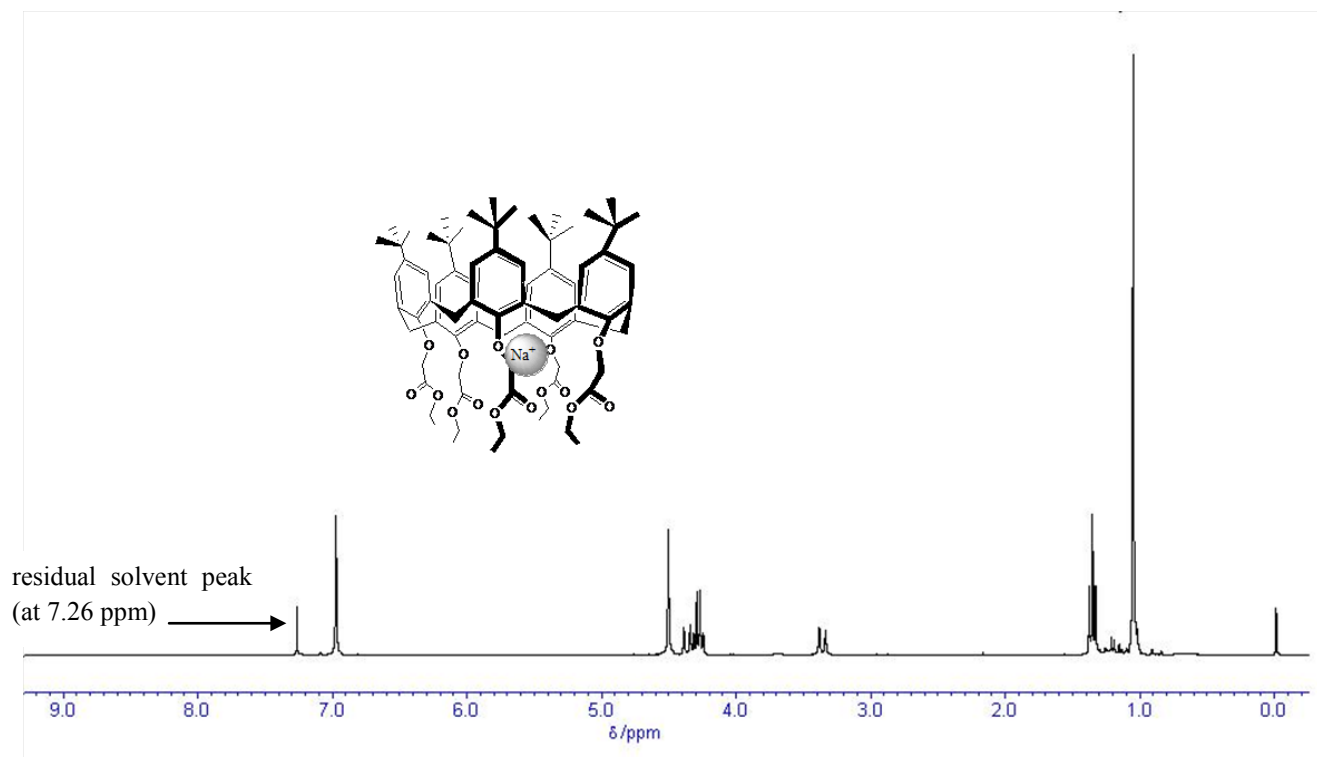


Fig SF2 $^1\text{H-NMR}$ spectrum of Na free **2** in CDCl_3

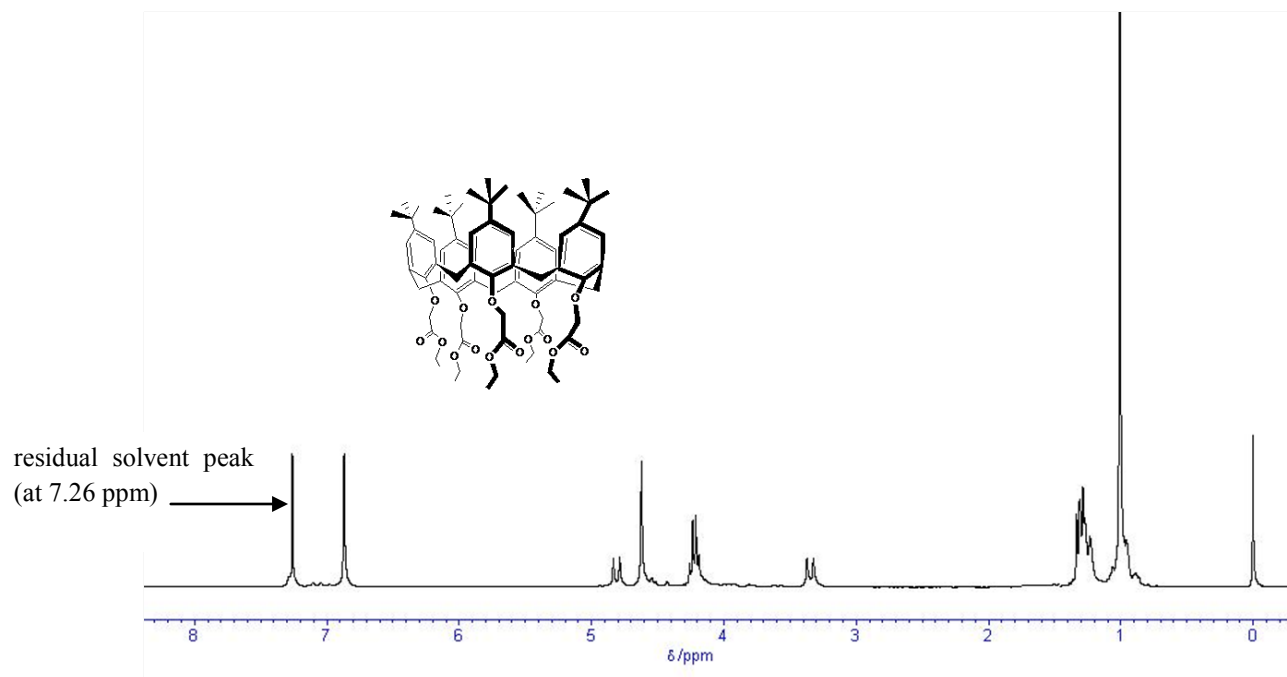


Fig SF3 ^1H -NMR spectrum of **3** in CDCl_3

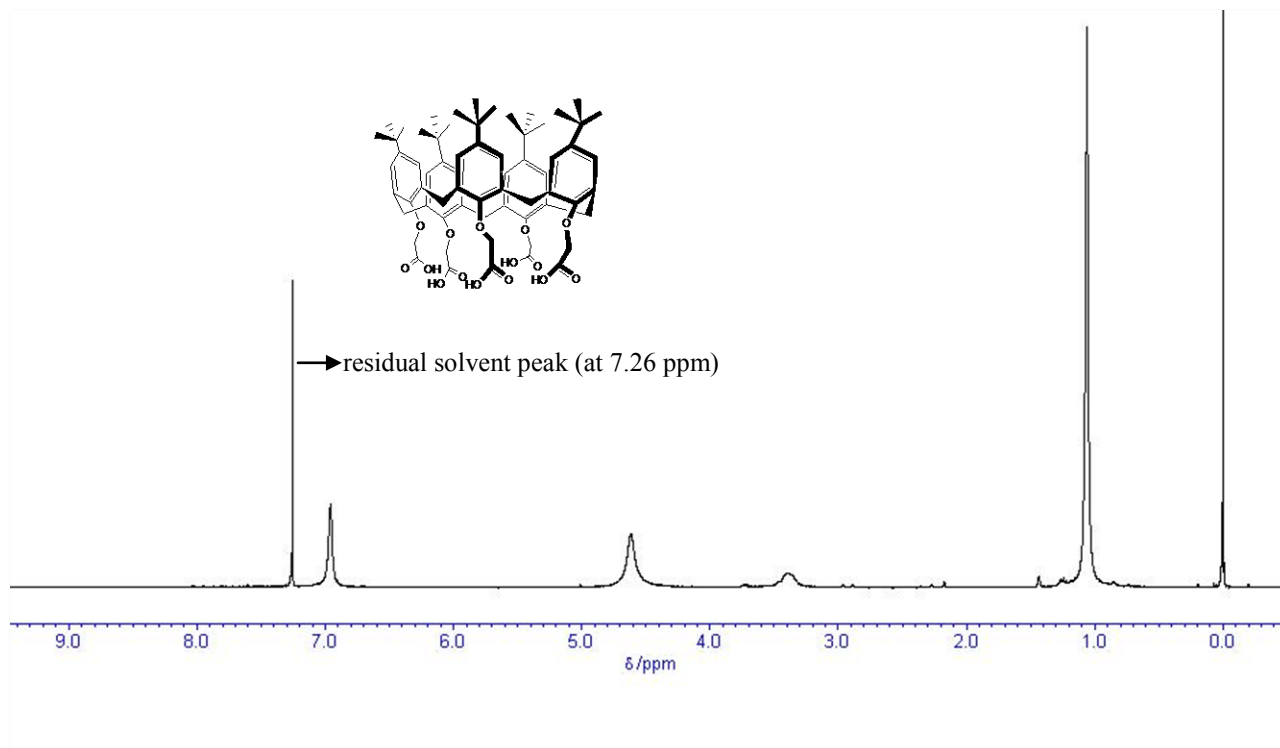


Fig. SF4 Typical Job's plot for extraction of (a) Zn(II), (b) Co(II) and (c) Ni(II) with **3**.

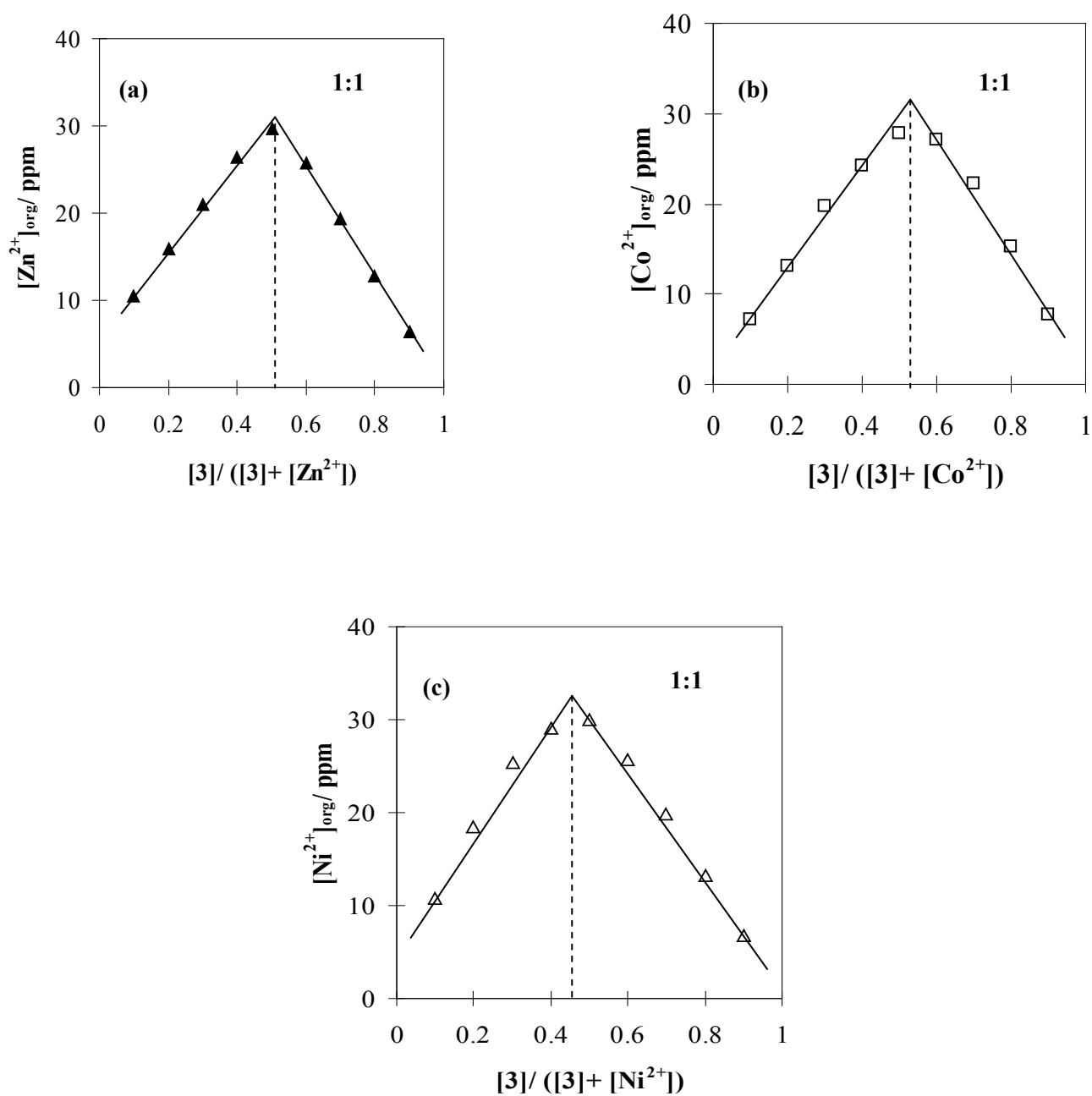


Fig. SF5 Nitrate dependency test for the extraction of lead ion with **3**. $[3] = 2.0 \text{ mM}$, $[\text{Pb}^{2+}] = 0.1 \text{ mM}$, adjustment of $[\text{NO}_3^-] = 1.0 \text{ M LiNO}_3$ in 0.05 M HNO_3 , phase ratio = 1, shaking time = 8.0 h at 303 K.

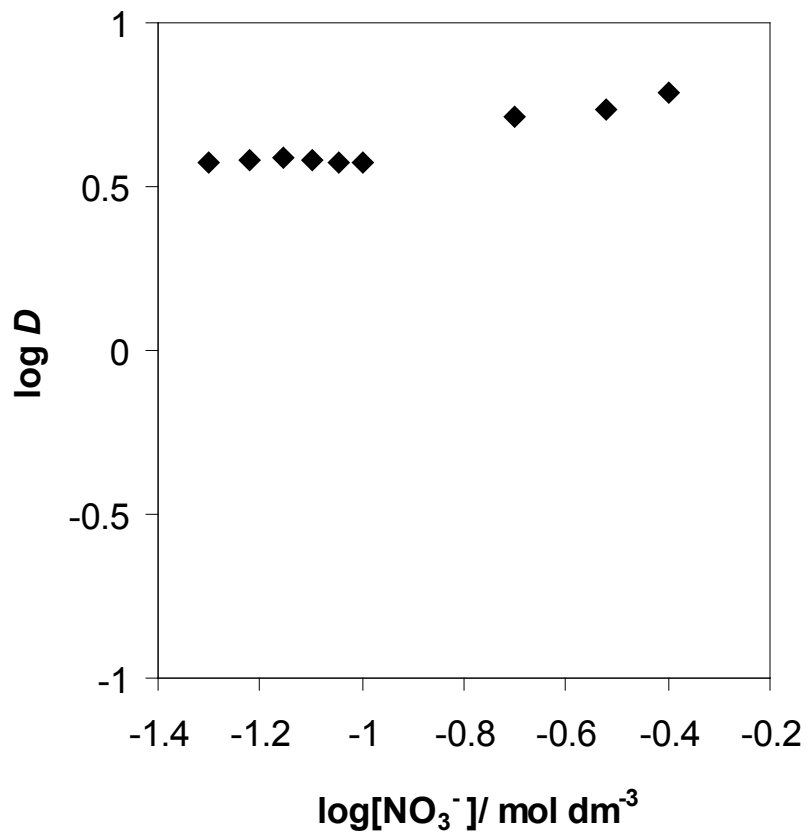


Fig. SF6 Effect of added lead on percentage shift (Δ) of aryl peak with corresponding percentage loading (\blacklozenge) of metal ion on **3**.

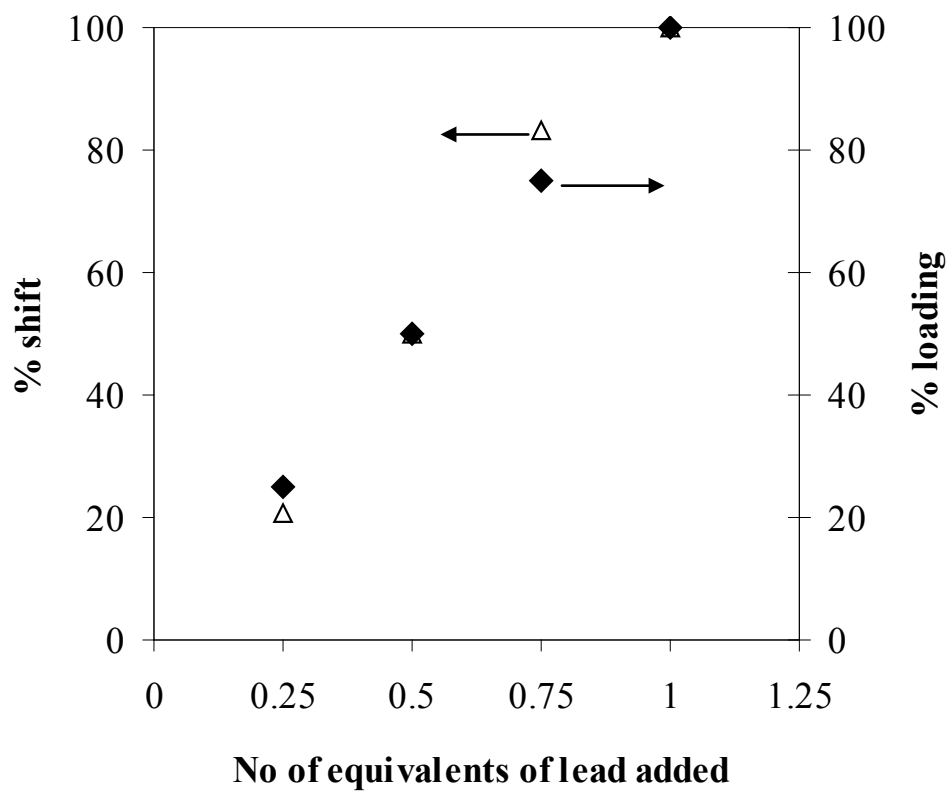


Fig SF7 IR spectra (KBr) of **3**, **3**•Cu²⁺ and **3**•(Pb²⁺)₂ complexes

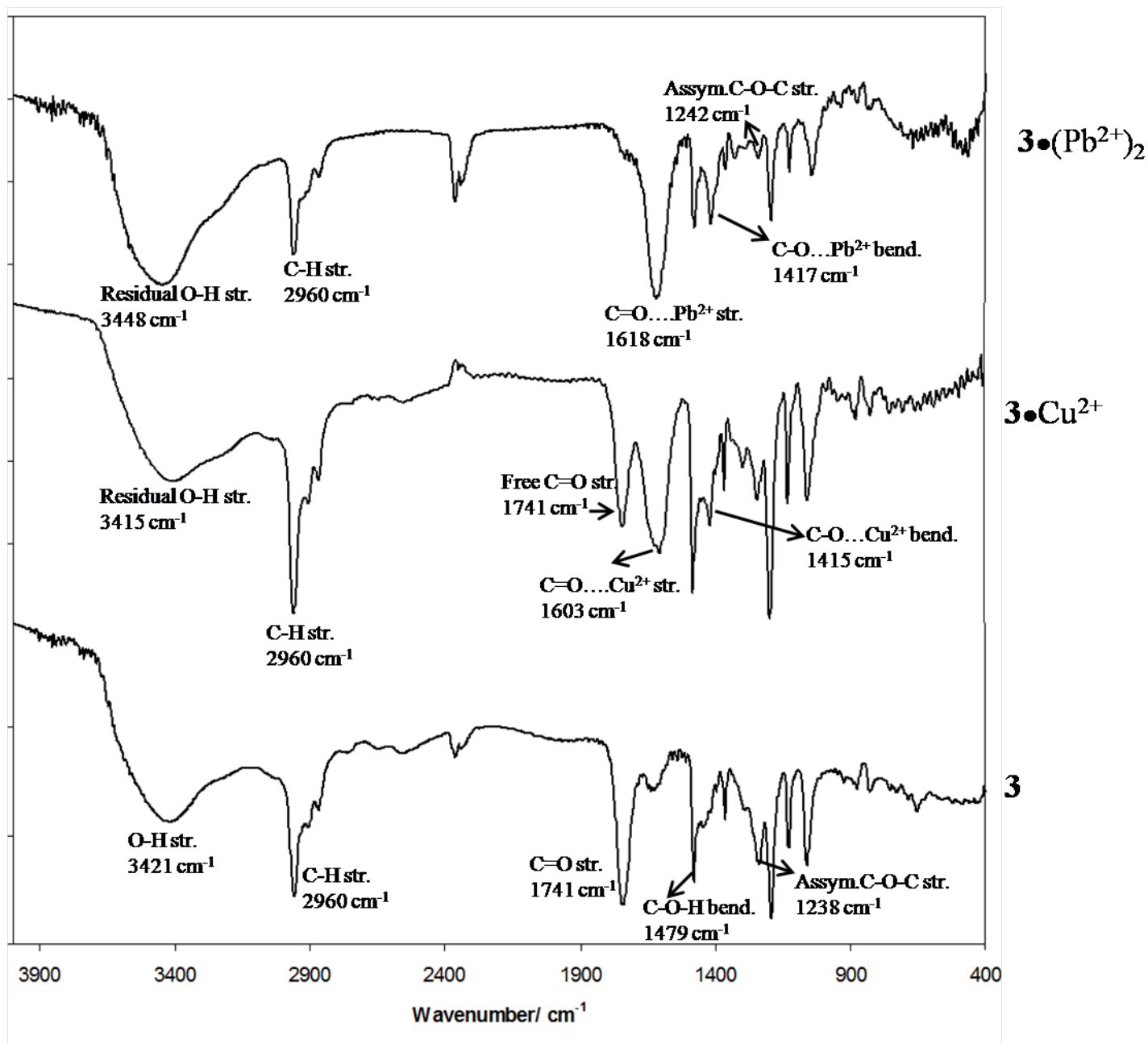


Fig SF8 FT-IR spectrum (KBr) of $3 \cdot \text{Pb}^{2+}$ complex

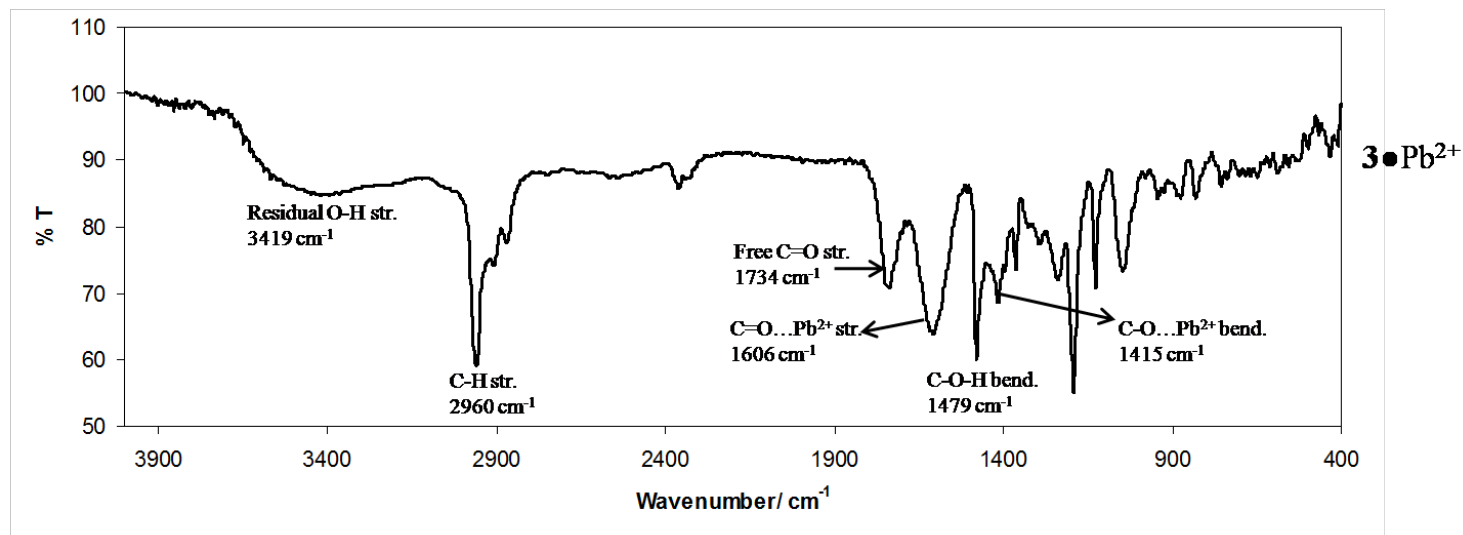


Fig. SF9 Effect of acid concentration on percentage stripping of loaded Pb(II).
[Pb(II)]_{loaded} = 0.1 mM, [3] = 2.0 mM, phase ratio = 1, shaking time = 8 h at 303 K,
[Pb]_{loaded} = 0.1 mM.

