

Electronic Supplementary Information (ESI) for: Multinuclear complex formation in aqueous solution of Ca(II) and heptagluconate ions

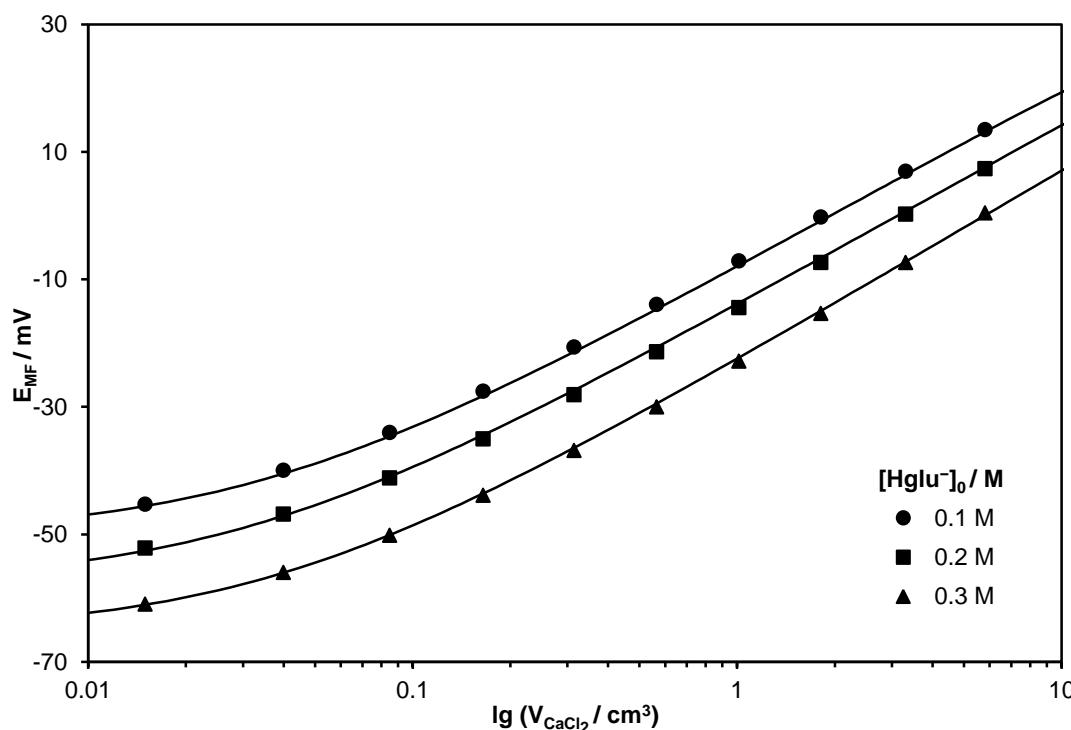
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¹⁵ **Fig. S1** Ca-ISE titration curves of the Ca²⁺/Hglu⁻ binary systems. Symbols represent observed EMF values, solid lines were fitted on the basis of the model discussed in the text. (25.00 ± 0.02 °C; I = 1 M, NaCl, [Ca²⁺]₀ = ~0.1 mM.); titrant: [Ca²⁺] = 0.1 M.

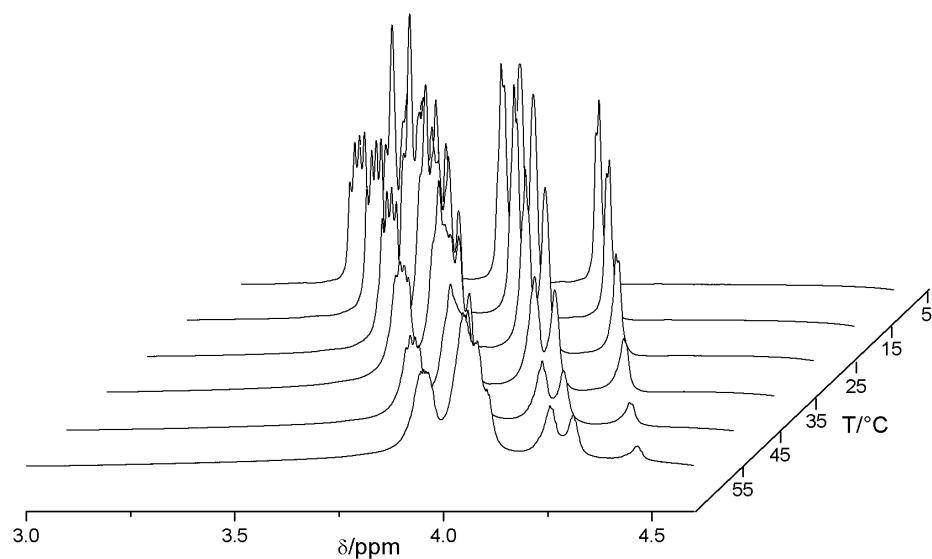


Fig. S2 Temperature dependent ^1H NMR spectra of a system with Hglu^- (0.200 M) and CaCl_2 (0.100 M) in the presence of 0.01 M NaOH.

Multiplicities of the ^1H NMR signals as they appear (Fig. 7, spectrum B): H(C2): doublet; H(C3): triplet; H(C4) triplet; H(C5), H(C7) and H(C7') double doublets, H(C6) multiplet. The values of J-coupling constants are presented in Table S1.

Table S1: The average coupling constants for the Hglu^- protons in Hz, determined from the ^1H NMR spectrum of aqueous solutions containing $[\text{NaHglu}]_T = 0.20 \text{ M}$ and $[\text{NaOH}]_T = 1.0 \text{ M}$. The spectrum is presented in the Fig. 7.

	J/Hz						
	H2	H3	H4	H5	H6	H7	H7'
H2	-	4.5	-	-	-	-	-
H3	4.5	-	~4.0	-	-	-	-
H4	-	~4.0	-	2.4	-	-	-
H5	-	-	2.4	-	7.6	-	-
H6	-	-	-	7.6	-	2.7	6.2
H7	-	-	-	-	2.7	-	11.7
H7'	-	-	-	-	6.2	11.7	-

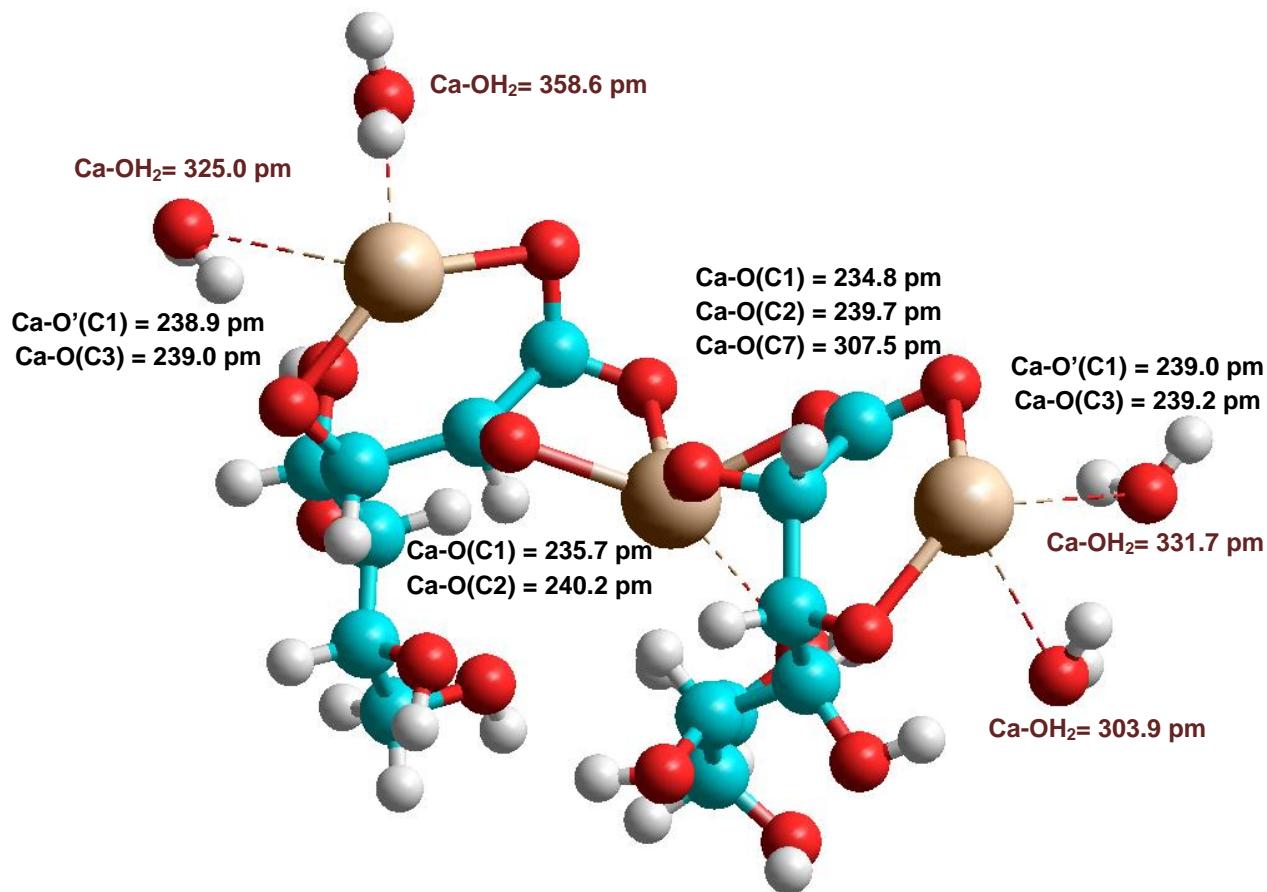


Fig. S3 Structure of the $[\text{Ca}_3\text{Hglu}_2\text{H}_4]^0$ complex in aqueous solution after full geometry optimisation applying explicit water molecules with PM3 semiempirical quantum chemical calculations using the *ab initio* structures as initial geometry.