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SUPPORTING INFORMATION FOR

Comparison of the Ca^{2+} complexing properties of isosaccharinate and gluconate – is gluconate a reliable structural and functional model of isosaccharinate?

Csilla Dudás,[a] Bence Kutus,[a] Éva Böszörményi,[a] Gábor Peintler,[b] Zoltán Kele [c] István Pálinkó,[d] Pál Sipos[a]*

[a] Department of Inorganic and Analytical Chemistry, University of Szeged, Dóm tér 7, Szeged, H−6720 (Hungary)

[b] Department of Physical Chemistry and Material Science, University of Szeged, Aradi vértanúk tere 1, Szeged, H−6720 (Hungary)

[c] Department of Medical Chemistry, University of Szeged, Dóm tér 8, Szeged, H−6720 (Hungary)

[d] Department of Organic Chemistry, University of Szeged, Dóm tér 8, Szeged, H−6720 (Hungary)

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* Corresponding author, e-mail: sipos@chem.u-szeged.hu; phone: +36 62 544 045

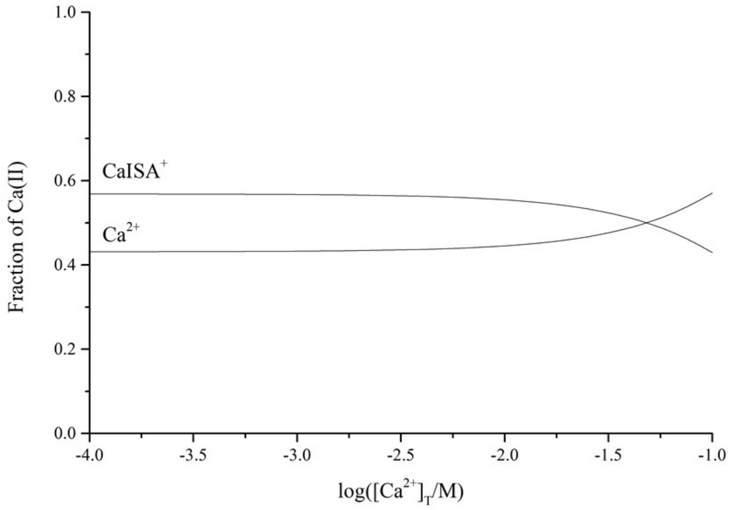


Figure S1. Distribution of Ca(II) among the aqueous species in a solution containing $[Isa^{-}]_T$ = 0.10 M as a function of $\log([Ca^{2+}]_T/M)$ using the formation constant $\log K_{1,1}$ = 1.12.

Table S1. The average coupling constants for the Isa^{-} protons in Hz, determined from the ^{1}H NMR spectrum of aqueous solutions containing $[NaIsa]_T$ = 0.20 M

J(Hz)/J(Hz)	H3	H3'	H4	H5	H5'	H6	H6'
H3		14.5	7.8				
H3'	14.5		4.8				
H4	7.8	4.8		4.2	6.9		
H5			4.2		11.5		
H5'			6.9	11.5			
H6							11.4
H6'						11.4	

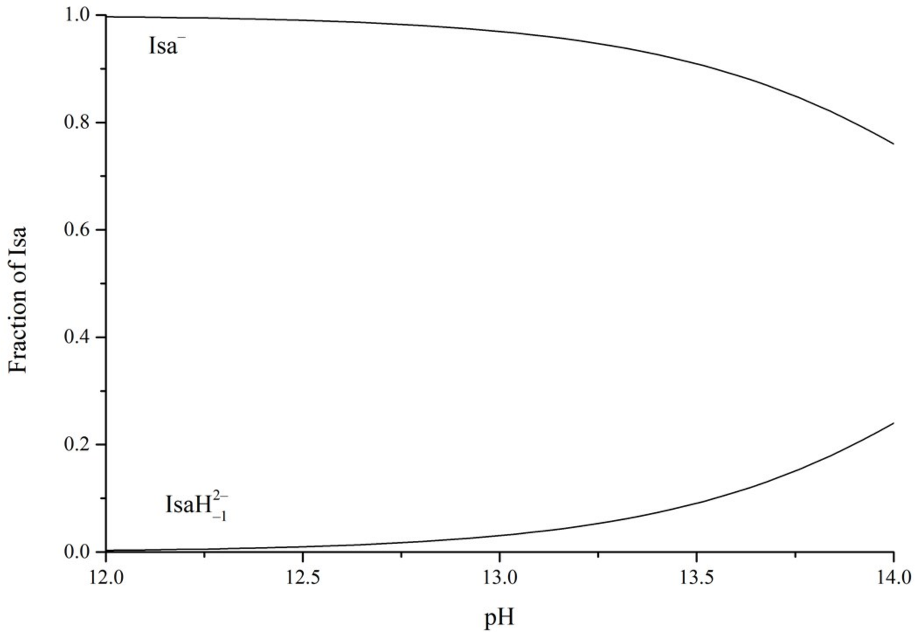


Figure S2. Distribution of Isa among the aqueous species in a solution containing $[Isa^-]_T$ = 0.10 M as a function of pH using the deprotonation constant p*K*a = 14.5.

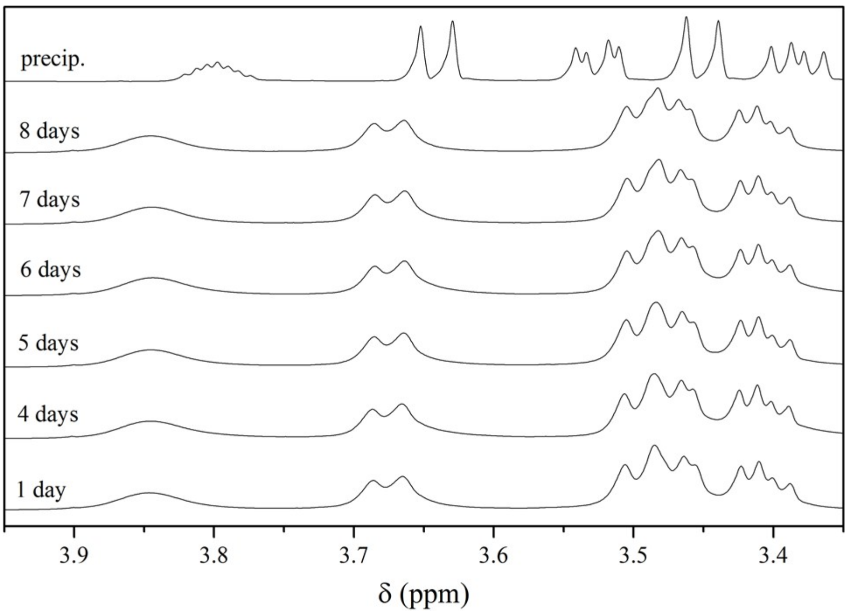


Figure S3. Time dependence of the ^1H NMR spectra of a solution containing $[Isa^-]_T$ = 0.20 M, $[OH^-]_T$ = 0.50 M and $[Ca^{2+}]_T$ = 0.10 M, T = (25 ± 1) °C. The spectrum on the top corresponds to the filtrate after removing the precipitate formed after 8 days.

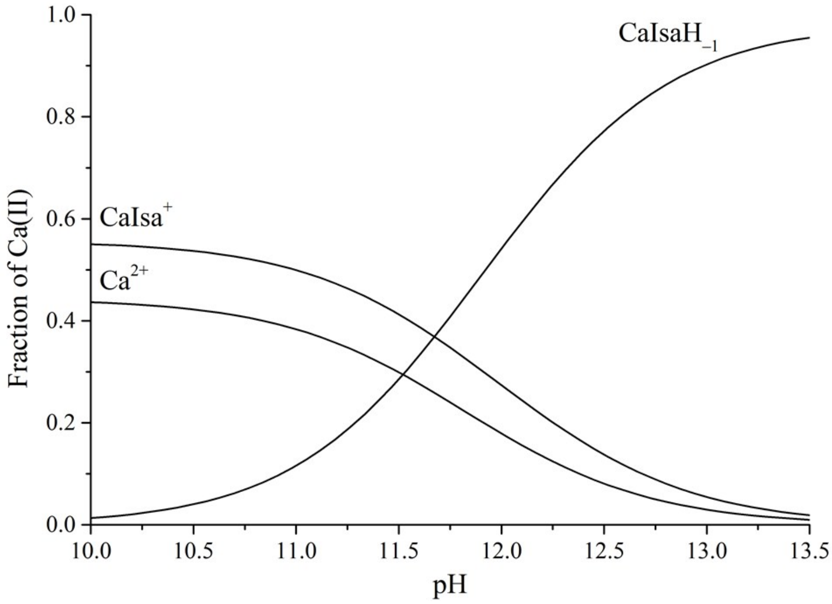


Figure S4. Distribution of Ca(II) among the various aqueous species in a solution containing $[Isa^-]_T$ = 0.10 M and $[Ca^{2+}]_T$ = 0.05 M as a function of pH.

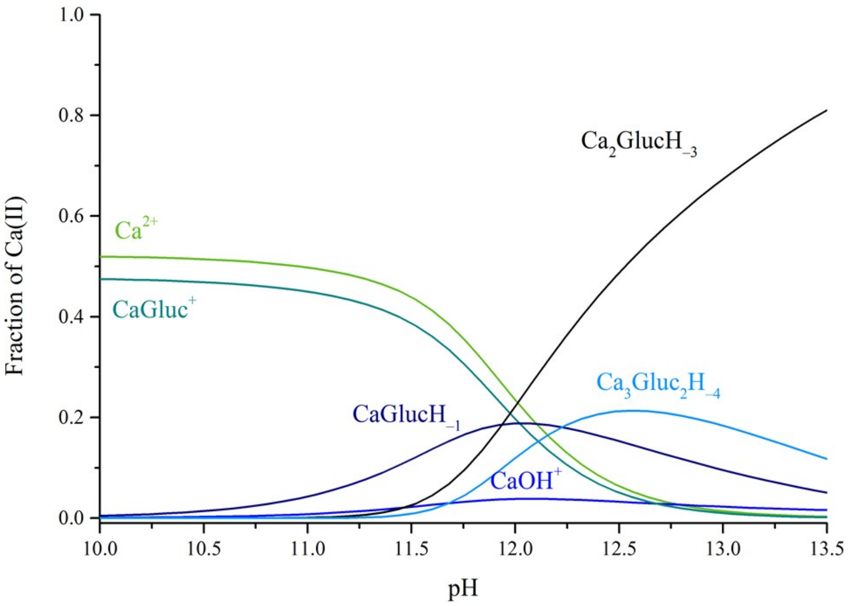


Figure S5. Distribution of Ca(II) among the various aqueous species in a solution containing $[Gluc^-]_T$ = 0.10 M and $[Ca^{2+}]_T$ = 0.05 M as a function of pH.

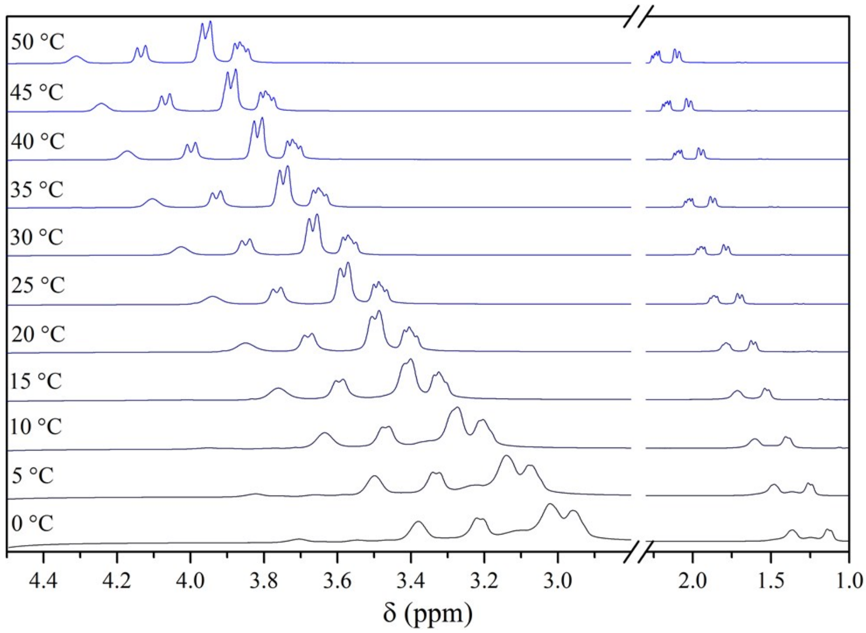


Figure S6. Temperature dependent ^{1}H NMR spectra in the temperature range of 0-50 ^{o}C of a solution containing $[Isa^{-}]_T$ = 0.20 M, $[OH^{-}]_T$ = 0.20 M and $[Ca^{2+}]_T$ = 0.10 M.

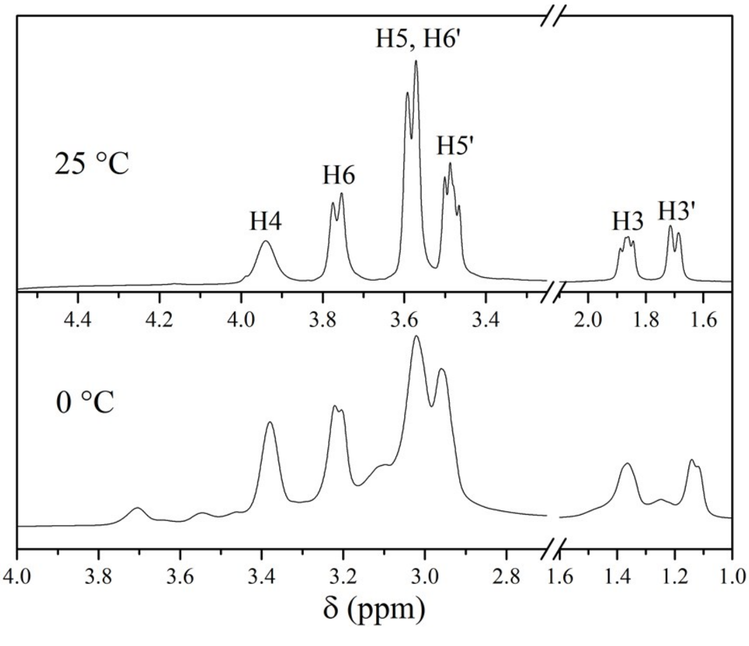
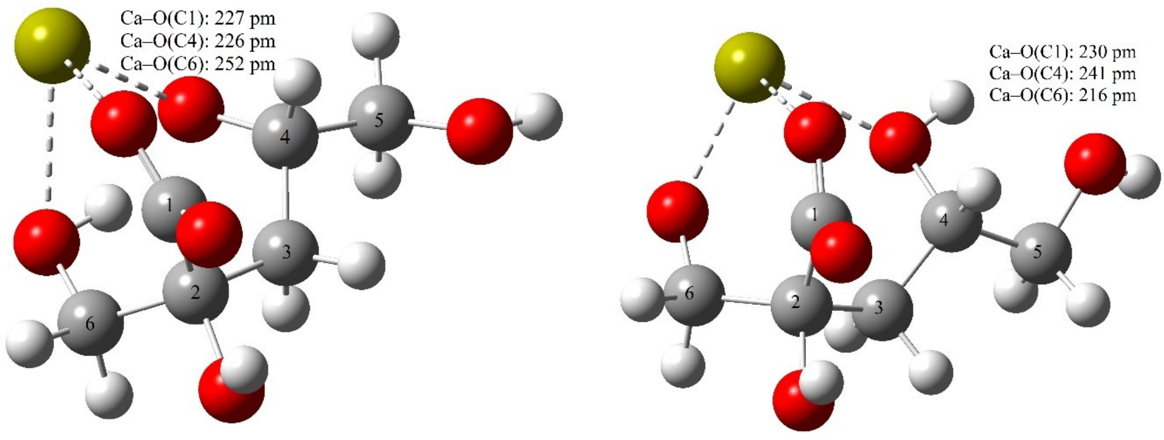


Figure S7. ^{1}H NMR spectra collected at 0 °C and 25 °C of a solution containing $[Isa^{-}]_T$ = 0.20 M, $[OH^{-}]_T$ = 0.20 M and $[Ca^{2+}]_T$ = 0.10 M, T = (25 ± 1) °C, I = 1 M (NaCl).



(a) (b)

Figure S8. The optimum geometries of the CaIsaH_{-1} complex with O(C6) as a binding site calculated at the B3LYP/6-311++G(d,p) level using the PCM model and explicit water molecules.