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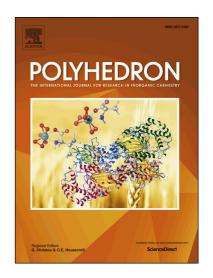
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## ACCEPTED MANUSCRIPT

# The formation of Ca(II) enolato complexes with $\alpha$ - and $\beta$ -ketoglutarate in strongly alkaline solutions

Csilla Dudás,1& Bence Kutus,1& Gábor Peintler,2& István Pálinkó,3& Pál Sipos1&§

#### **ABSTRACT**

In the present study the proton dissociation and calcium complex formation of  $\alpha$ - and  $\beta$ -ketoglutarate (2- and 3-oxopentane-dioate,  $\alpha$ -Ket<sup>2-</sup> and  $\beta$ -Ket<sup>2-</sup>, respectively) in neutral and alkaline aqueous solutions was explored. From potentiometric measurements, the equilibrium constants of the  $[Ca(\alpha-Ket)]^0$  and  $[Ca(\beta-Ket)]^0$  complexes formed in neutral medium were determined to be  $\log K_{1,1}^{\alpha} = 1.15 \pm 0.02$  and  $\log K_{1,1}^{\beta} = 0.78 \pm 0.02$ , respectively. In alkaline medium, it was found for both ligands that the methylene group underwent deprotonation yielding the carbanion-enolate anion. The deprotonation constants,  $pK_a^{\alpha}$  and  $pK_a^{\beta}$ , were found to be  $15.16 \pm 0.01$  and  $14.41 \pm 0.01$ , respectively. The calcium complexing behaviour of the two ligands was also studied in strongly alkaline medium. Under these conditions, the Ca<sup>2+</sup> ion was capable of promoting the deprotonation of the ligands and forming various enolato-type complexes. The formation of both mono- and binuclear species were deduced, their formulae are suggested to be  $[Ca(\alpha-Ket)H_{-1}]^-$ ,  $[Ca_2(\alpha-Ket)H_{-3}]^-$ ,  $[Ca(\beta-Ket)H_{-1}]^-$ ,  $[Ca_2(\beta-Ket)H_{-1}]^+$  with the formation constants of  $\log \beta_{1,1,-1}^{\alpha} = -11.91 \pm 0.02$ ,  $\log \beta_{2,1,-3}^{\alpha} = -36.10 \pm 0.06$ ,  $\log \beta_{1,1,-1}^{\beta} = -36.10 \pm 0.06$  $11.58 \pm 0.01$ ,  $\log \beta_{2.1.-1}^{\beta} = -10.80 \pm 0.03$ , respectively. Beside the formation of the rare Ca<sup>2+</sup>enolato complexes, the deprotonation of the hydrating water molecules around the Ca<sup>2+</sup> ion was also invoked in some cases.

#### 1. Introduction

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