

Supporting Information

Interactions of inosine 5'-monophosphate with Ca^{2+} and Mg^{2+} : a thermodynamic and spectroscopic study in aqueous solution

Paola Cardiano, Donatella Chillè, Massimiliano Cordaro, Claudia Foti* and Ottavia Giuffrè

Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, Università di Messina, Viale F. Stagno d'Alcontres 31, 98166 Messina, Italy

Table S1. Calculated formation constants of H⁺, Ca²⁺ and Mg²⁺ -IMP species at different ionic strengths and at T = 298.15 K

		Species					
	<i>I</i> ^{b)}	HL⁻	H₂L⁰	CaL⁰	CaLH⁺	MgL⁰	MgLH⁺
logβ	0.1	8.99±0.01	15.16±0.01	2.62±0.04	11.20±0.04	2.47±0.05	10.88±0.03
	0.25	8.90±0.01	14.97±0.01	2.46±0.03	10.98±0.03	2.36±0.04	10.74±0.03
	0.5	8.85±0.01	14.86±0.01	2.45±0.05	10.88±0.03	2.43±0.03	10.76±0.02
	1	8.92±0.02	14.79±0.03	2.68±0.09	10.91±0.08	2.80±0.05	11.03±0.05

a) Refer to the equilibrium: M + L + H = MLH; b) in mol·kg⁻¹; c) ±3 std. dev.

Table S2. Calculated formation constants of H^+ , Ca^{2+} and Mg^{2+} -IMP species, at different temperatures and at $I = 0.1 \text{ mol}\cdot\text{kg}^{-1}$

	Species						
	T /K	HL⁻	H₂L⁰	CaL⁰	CaLH⁺	MgL⁰	MgLH⁺
logβ^{a)}	288.15	9.03±0.01 ^{b)}	15.03±0.01 ^{b)}	2.41±0.03 ^{b)}	11.02±0.03 ^{b)}	1.94±0.04 ^{b)}	10.46±0.04 ^{b)}
	298.15	8.98±0.01	15.16±0.01	2.61±0.02	11.19±0.02	2.24±0.02	10.72±0.02
	308.15	8.93±0.01	15.29±0.01	2.79±0.02	11.35±0.02	2.52±0.02	10.96±0.02
	310.15	8.92±0.01	15.31±0.01	2.82±0.02	11.38±0.02	2.58±0.03	11.00±0.03
	318.15	8.88±0.01	15.40±0.01	2.96±0.03	11.50±0.02	2.79±0.04	11.18±0.03

^{a)} Refer to the equilibrium: $M + L + H = MLH$; ^{b)} ±3 std. dev.