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论文

$CaCl_2$在甘氨酸+水和丙氨酸+水混合溶剂中的活度系数

张心宽[1,2], 卓克垒[1], 马晶晶[1], 刘宏勋[1], 王键吉[1]

1. 河南师范大学化学与环境科学学院, 新乡 453007;
2. 新乡学院化学与化工学院, 新乡 453003

摘要:

利用离子选择性电极(ISE)测定了298.15 K时$CaCl_2$在甘氨酸+水和丙氨酸+水混合溶剂中的活度系数. $CaCl_2$的质量摩尔浓度变化范围为0.01～0.20 mol/kg, 氨基酸的质量摩尔浓度变化范围为0.10～0.40 mol/kg. 用Debye-Hückel扩展方程和Pitzer方程进行理论计算得到的活度系数基本一致. 依据McMillan-Mayer理论, 计算了$CaCl_2$从纯水到氨基酸水溶液的标准转移Gibbs自由能, 利用最小二乘法拟合求得了对相互作用参数(g_{EA})和盐效应常数(k_s). 讨论了这两种氨基酸的加入对$CaCl_2$的活度系数、热力学稳定性及盐效应常数的影响.

关键词: 活度系数; Gibbs自由能; 氯化钙; 甘氨酸; 丙氨酸

Activity Coefficients of $CaCl_2$ in Glycine+Water and Alanine+Water Mixtures at 298.15 K

ZHANG Xin-Kuan[1,2], ZHUO Ke-Lei[1*], MA Jing-Jing[1], LIU Hong-Xun[1], WANG Jian-Ji[1]

1. School of Chemistry and Environmental Science, Henan Normal University, Xinxiang 453007, China;
2. School of Chemistry and Chemical Engineering, Xinxiang University, Xinxiang 453003, China

Abstract:

Activity coefficients of $CaCl_2$ in glycine+water and alanine+water mixtures at 298.15 K were determined by cell potential measurements using ion selective electodes(ISE). The molalities of $CaCl_2$ ranged from 0.01 to 0.20 mol/kg, and those of amino acids ranged from 0.1 to 0.4 mol/kg. The cell potentials were analyzed by the Debye-Hückel extended equation and the Pitzer equation to calculate activity coefficients. The results obtained from the two theoretical models are in good agreement with each other. Standard transfer Gibbs free energy, pair interaction parameters(g_{EA}) and salting constants (k_s) were also evaluated. The results are disscussed in terms of the stereo-chemistry of amino acid molecules and structures and electrostatical interaction models. Activity coefficient of $CaCl_2$ increases with increasing of molalities of amino acids. Standard transfer Gibbs free energy decreases with increasing molalities of amino acids, indicating that the interactions of the amino acides with $CaCl_2$ are thermodynamically attractive in aqueous solution. Values of g_{EA} are negative, indicating that the interactions of these two amino acides with $CaCl_2$ result mainly from the electrostatical attraction.

Keywords: Activity coefficient; Gibbs free energy; $CaCl_2$; Glycine; Alanine

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通讯作者: 卓克垒, 男, 博士, 教授, 博士生导师, 主要从事溶液理论研究. E-mail: klzhuo@263.net

作者简介:

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