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简单体系水溶液包裹体pH和Eh的计算

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摘要：

流体包裹体pH和Eh参数的计算一直处于探索阶段。已经发表的计算公式,由于缺少高压(>1bar)环境下化学组分反应平衡常数,常常利用常压(1大气压)下化学组分反应平衡常数代替而推导出的,对于大多数自然界捕获的包裹体,不可避免地产生较大计算误差。根据水溶液包裹体中离子反应热力学特征,结合前人推导的计算公式,我们分别建立简单体系水溶液包裹体pH和Eh计算公式。由于利用较高压(>1bar)化学反应平衡常数,基本上解决不同条件下、特别在较高温度、压力下捕获的水溶液包裹体pH和Eh的计算难题。4种简单体系水溶液包裹体pH计算公式:① H_2O包裹体:$pH=pK_w$ ② CO_2-H_2O包裹体: $^3-(m_{CO_2}K_{a,1}+K_W)\cdot\ -2m_{CO_2}K_{a,1}K_{a,2}=0$ ③ NaCl-H_2O包裹体: $^2=$ ④ CO_2-H_2O-NaCl包裹体: $^3+\ ^2-(m_{CO_2}\cdot K_{a,1}+K_W)\cdot\ -2m_{CO_2}\cdot K_{a,1}\cdot K_{a,2}\ -\ =0$ 计算数值精度分析表明:CO_2-H_2O和NaCl-H_2O包裹体的pH值按照公式计算,相同或接近于实际测定的天然酸雨、海水pH数值范围。CO_2-H_2O-NaCl包裹体与Crerar(1978)公式计算误差不超过10%。4种简单体系水溶液包裹体Eh的计算,引用Ryzhenko and Bryzgalin (1984)年推导的Eh公式。文中列举了3个实例,详细叙述不同类型包裹体捕获温度、压力下pH和Eh计算过程。自然界中水溶液包裹体成分十分复杂,本文涉及的只是自然界几种简单体系水溶液包裹体,给出的pH和Eh公式只对特定组分组合反应平衡条件有效,它不适合另外一种组分组合平衡条件下的关系,因此使用时务必注意平衡的组分组合条件。

英文摘要：

The calculation of pH and Eh parameters for fluid inclusions is still under an investigation stage. Because of lacking of equilibrium constants of chemical components in reactions at high pressure (>1bar) environment, the published calculation formulas are deduced by using the equilibrium constants at normal pressure (1atm.). A bigger calculating error is produced inevitably for most fluid inclusions in the nature. Based on the thermodynamic property of ion reactions in aqueous inclusions, and combined with the formulas deduced by predecessor, we have established the pH and Eh calculation formulas for the aqueous inclusions of simple systems. By using of the equilibrium constants of chemical reactions under higher pressure (>1bar), we have solved basically the tough problem of calculating pH and Eh parameters for the aqueous inclusions trapped under different conditions, especially at higher temperatures and pressures. The pH calculation formulas for the aqueous inclusions of four simple systems are as follows:① for H_2O inclusions: $pH=pK_w$ ② for CO_2-H_2O inclusions: $^3-(m_{CO_2}K_{a,1}+K_W)\cdot\ -2m_{CO_2}K_{a,1}K_{a,2}=0$ ③ for NaCl-H_2O inclusions: $^2=$ ④ for CO_2-H_2O-NaCl inclusions: $^3+\ ^2-(m_{CO_2}\cdot K_{a,1}+K_W)\ ^2\ -2m_{CO_2}\cdot K_{a,1}\cdot K_{a,2}\ -\ =0$Accuracy analysis of calculated values has shown that the calculated results by using the pH formulas for the CO_2-H_2O and NaCl-H_2O inclusions, are the same or close to the range of actually measured pH values of natural acid rain and sea water. For the CO_2-H_2O-NaCl inclusions, a computed error by our formula is not more 10% as compared with Crerar's (1978) formula. The Eh calculation formula for four types of aqueous inclusions of simple system is adapted from the formula deduced by Ryzhenko and Bryzgalin (1984). Three calculated examples are listed. In this paper the computation process of pH and Eh values under the trapping temperature and pressure conditions for different types of inclusions is described in detail. The composition of aqueous inclusions is very complicated in the nature. This paper only involves a few simple systems in the nature and the pH and the Eh formulas given are validated to the reaction equilibrium conditions for the particular components, but is n t suitable for other component assemblages under equilibrium conditions. So the equilibrium assemblage conditions must be noted when use these formulas.

关键词：离子反应热力学特征 4种类型离子反应 简单体系水溶液包裹体 pH和Eh计算公式

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