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Computer Simulation of Insoluble Pr(III) Speciation in Human Interstitial Fluid

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Abstract: A multi-phase model of Pr(III) speciation in human interstitial fluid was constructed and insoluble Pr(III) speciation was studied. When the total concentration of Pr(III) is below 8.401E-10 mol/L, soluble Pr(III) species are main species. With rising the total concentration of Pr(III), Pr(III) is firstly bound to phosphate to form precipitate of $PrPO_4$, then bound to carbonate and another precipitate of $Pr_2(CO_3)_3$ was obtained. When the total concentration is between 1.583E-9 mol/L and 4.000E-3 mol/L, the insoluble species are predominant Pr(III) species.

Keyword: Computer simulation, praseodymium(III), speciation, human interstitial fluid.

Due to the wide application of rare earths, more and more rare earths enter into environment, and human body *via* food chain *etc*[1,2]. It becomes very urgent to study the biological effect of rare earths. It is well known that biological effects of metal ions depend on their speciation in biological systems. Therefore, the research on rare earth speciation is a key to understand their distribution, metabolism and biological effects. Previous researches were devoted to rare earth speciation in human blood plasma, but rare earth speciation in human interstitial fluid has not been studied. However, human interstitial fluid, which constitutes the environment of the cells and is regulated by body homeostasis, is a very important biofluid. In this work, the insoluble Pr(III) speciation in human interstitial fluid was studied.

A muti-phase model was established, including 3 metals and 30 ligands, such as Ca(II), Zn(II), Pr(III), PO_4^{3-}, CO_3^{2-}, HSA, IgG and a lot of important low-molecular-weight ligands. In this work, the MINTENQA2 program developed by U.S. Environment Protection Agency in 1991 was used to simulate the distribution of insoluble Pr(III) speciation in human interstitial fluid. Almost all the stability constants of the complexes of Pr(III), Ca(II) and Zn(II) with the low-molecular-weight biological ligands contained in this model were determined accurately under physiological conditions(T=37°C, I=0.15mol/L)[3]. The binding constants of Pr(III) with inorganic ligands and proteins were mostly cited from references[2].

Table 1 shows the distribution of insoluble Pr(III) species. The background value of Pr(III) in human interstitial fluid for a normal man is about 5.7E-10 mol/L[4]. At this concentration all the Pr(III) species are soluble. With rising the total concentration of

Pr(III) to 8.401E-10 mol/L, the precipitate of $PrPO_4$ forms. When the total concentration reaches to 1.000E-8 mol/L, the precipitate becomes predominant species. At the same time, the percentage of soluble Pr(III) decreases greatly from 100% to 7.4%, but the concentration of soluble Pr(III) still remains at a low level(about 7.3E-10 mol/L). When the total concentration gets to 6.213E-4 mol/L, the amount of available phosphate are exceeded and another precipitate of $Pr_2(CO_3)_3$ begins to appear. At this moment, the concentration of soluble Pr(III) dramatically increases to 1.606E-5 mol/L, but the percentage of soluble Pr(III) varies a little. At the LD_{50} concentration of $PrCl_3$ (4 mmol/L), the percentage of the soluble Pr(III) is only 0.5% and the percentage of insoluble Pr(III) gets to 99.5%. Obviously, the precipitate species remain as main species in a wide concentration range. It is in good accordance with Luckey's conclusion that lanthanides tend to form insoluble complexes with phosphate[5]. Since the precipitates are main species, which affect the transportation of rare earths and the accumulation of rare earths in organs and tissues.

Table 1 Distribution of insoluble Pr(III) species (%) (T=37°C, I=0.15mol/L, pH=7.4)

Species	Total concentration of Pr(III)(mol/L)					
	5.764E-10	8.401E-10	1.583E-9	1.000E-8	6.213E-4	4.000E-3
$PrPO_4$	0.0	0.3	50.1	92.6	97.38	14.4
$Pr_2(CO_3)_3$	0.0	0.0	0.0	0.0	0.04	85.1
Soluble Species*	100.0	99.7	49.9	7.4	2.6	0.5
	(5.764E-10)	(7.353E-10)	(7.353E-10)	(7.322E-10)	(1.606E-5)	(2.018E-5)

*The values in parentheses are concentrations of soluble Pr(III)

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