Chinese Chemical Letters Vol. 10, No. 8, pp. 677–678, 1999

Studies on the Coordination of Pr(III) with Adrenaline by Potentiometry and Absorption Spectroscopy

Feng GAO, Jing Fen HAN, Zhi Jian WU, Yue WANG, Kui Yue YANG, Chun Ji NIU,* Jia Zuan NI

Laboratory of Rare Earth Chemistry and Physics, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022

Abstract : The stability constant for complex of Pr(III) with adrenaline has been determined by potentiometric titration under biological conditions (37°C and 0.15mol/L NaCl). The absorption spectra of the Pr(III)-adrenaline system exhibit characteristic bands of Pr(III) at lower pH values. However, the charge transfer band which is due to the coordination of Pr(III) with adrenaline has been observed at higher pH values.

Keywords: Praseodymium, adrenaline, potentiometry, spectroscopy.

As an extension to our previous work [1,2] , the coordination of Pr(III) with adrenaline (3,4-dihydroxy-α-(methylaminomethyl)benzyl alcohol, $(HO)_2C_6H_3CH(OH)CH_2NHCH_3$) has been investigated by potentiometry and absorption spectroscopy in the present work.

Potentiometric titrations were carried out on a pHS-3C pH meter under biological conditions (37°C and an ionic strength of 0.15mol/L NaCl) by using the titration techniques described in previous papers [3,4]. The absorption spectra of Pr(III) - adrenaline system were recorded in visible region at various pH values with a Kontron UV-922 spectrophotometer using 1.000 cm quartz cell. Praseodymium chloride solution for absorption spectra was 5 x 10^{-4} mol/L. The molar ratios of Pr(III) to adrenaline was 1:2.

The potentiometric titration data were treated by means of program SCOGS 2[4] in order to ascertain species in the Pr(III) - adrenaline system and obtain the stability constants (βpqs, where p, q and s denote the stoichiometric coefficients of Pr(III) ion, ligand and proton for a complex molecule, respectively) for the complexes of Pr(III) with adrenaline. The protonation constants for the ligand ($\log\beta_{011}$=9.76, $\log\beta_{012}$=18.21) were used in this calculation[2]. The computational results demonstrate that 121 type of complex is the major species in the Pr(III)-adrenaline system. Meanwhile, $\log\beta_{121}$ value for 121 type of Pr(III)-adrenaline complex has been found to be 16.54±0.07. The complex of Pr(III) with adrenaline is comparatively stable, so the coordination of Pr(III) with adrenaline may be related to the neural and endocrine effect of rare earth.

Spectroscopic data are given in **Table 1**. It can be seen from **Table 1** that the Pr(III) - adrenaline system exhibits the characteristic spectra of Pr(III) ion when pH

Table 1 Data of absorption spectra for the Pr(III) - adrenaline system *

pH	λ_1(nm)	λ_2(nm)	λ_3(nm)	λ_4(nm)	λ_5(nm)
3.29	443 (0.134)	468 (0.077)	481 (0.066)	588 (0.028)	
4.21	443 (0.165)	468 (0.115)	481 (0.106)	588 (0.035)	
5.33	444 (0.550)	467 (0.579)	481 (0.587)	588 (0.135)	
6.30	443 (0.971)	467 (0.784)	481 (0.680)	588 (0.250)	411(0.901)
7.39					411 (2.583)
8.33					412 (3.400)

* Absorbance values are in parentheses.

value of the measured solution is below 6.30. The four bands centered around 433, 468, 481 and 588 nm which are assigned to $^3H_4 \rightarrow {}^3P_2$, $^3H_4 \rightarrow {}^3P_1$, $^3H_4 \rightarrow {}^3P_0$ and $^3H_4 \rightarrow {}^1D_2$ transitions of Pr(III) ion respectively have been observed for the Pr(III)-adrenaline system. The intensity of all bands enhances obviously with the increasing of pH value. This fact reflects the enhanced interaction between Pr(III) ion and the ligand in higher pH region. On the other hand, these bands do not show significant shift in the region of pH 3.29 - 6.30, which indicates that the bonding of Pr(III) to the ligand is predominantly ionic. The absorption spectra of the Pr(III)-adrenaline system show a new band at 411 nm at pH 6.30. In the pH range of 7.39~8.33 the new band is so wide and intensive that the original four bands of the Pr(III)-adrenaline system can not be seen clearly. The intensity of the new band exhibits a big enhancement beyond pH 7.39. In addition, little shift has been observed for the new band when pH value increases toward 8.33. It is known that the spectra of some metal complexes show charge transfer bands[5]. The results obtained in this work are similar to those reported previously [6]. From mentioned above, the band centered around 411 nm may be tentatively ascribed to charge transfer of the Pr(III)-adrenaline system, which indicates that adrenaline is coordinated to Pr(III).

Acknowledgment

The authors thank the National Natural Science Foundation of China for financial support of this work (Project No. 29671029 and Project No. 29890280).

References

1. R. Y. Wang *et al*., *Chinese Science Bulletin*, **1997**, *42*(17),1444.
2. F. Gao *et al*., *Chinese Chemical Letters*, In press.
3. C. J. Niu *et al*., *Inorg. Chim. Acta*, **1987**, *131*, 277.
4. S. F. Zhao *et al*., *Chem. J. Chin. Univ.*, **1995**, *16*(6), 847.
5. A. B. P. Lever, *J. Chem. Educ.*, **1974**, *51*, 612.
6. K. S. Rajan *et al*., *Bioinorg. Chem.*, **1978**, *9*(3), 187.

Received 28 January 1999