**Solvation Structure of Manganese(II) Ion in Water-*N*,*N*-Dimethylformamide**

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著者名：

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 **and Water-1,1,3,3-Tetramethylurea Mixed Solvents**

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 The solvation structure of manganese(II) ion in water-*N*,*N*-dimethylformamide (DMF) and water-1,1,3,3-tetramethylurea (TMU) solvent mixtures has been studied by the extended X-ray absorption fine structure (EXAFS) method. It has been revealed that manganese(II) ion has a six-coordinate structure with the Mn-O length of 217(2) pm in water-DMF mixed solvents. In neat TMU, the coordination number of Mn(II) ion is five and the Mn-O length is 210(1) pm due to the bulkiness of a TMU molecule. Therefore, it is expected that the coordination number decreases from 6 to 5 with increasing TMU contents in water-TMU mixed solvents. Result of the EXAFS analysis indicates that the decrease of the coordination number with increasing mole fractions of TMU corresponds to the shortening of the Mn-O distance.

Abstract：

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1. **Introduction**

 In two component solvent mixtures, an ion is solvated with two different kinds of solvent molecules. The solvent composition in the first coordination sphere of the ion may usually not be the same as that in the bulk. Such preferential solvation phenomena affect t

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1. **Experimental**

*Preparation of Sample Solutions*

 Manganese(II) perchlorate hydrate was prepared by dissolving the manganese carbonate in dilute perchloric acid and then recrystallized from water. Manganese(II) perchlorate ……………..

1. **Results and Discussion**

 The extracted EXAFS oscillations of Mn(II) in the water-DMF solvents are shown in Fig. 1. The phase and amplitude of each curve are similar, although the shape at *k* = 3 to 6 ….

**Table 1**  Structural parameters for Mn(II) in water-DMF mixturesa

|  |  |  |  |
| --- | --- | --- | --- |
|  | *n* | *r* / pm | **2 / 10 pm2 |
| Water | 6b | 217(1) | 6(1) |
| *X*DMF = 0.1 | 5.9(0.4) | 216(1) | 6(1) |
| 0.9 | 5.9(0.5) | 216(1) | 6(1) |
| DMF | 5.7(0.4) | 216(1) | 6(1) |

a The standard deviations are given in parentheses.

bThe value was kept constant during the least-squares calculations.

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**Fig. 1** The extracted EXAFS oscillations in the form of *k*3**(*k*) for Mn(II) ion in water-DMF solvents.

1. **Conclusions**

The values show that th****e solvated structure of Mn(II) ion in water-DMF mixtures is six-coordinate and the Mn-O distance is 217(2) pm on average at all mole fractions.

**Acknowledgement**

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**Fig. 2** The radial structure functions |*F*(*r*)| for Mn(II) ion in water-DMF solvents, phase shift uncorrected. The dashed lines are obtained experimentally, and the solid lines are calculated.

**References**

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