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Letter

The crystal structure of a samarium complex with β-alanine

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1. Introduction

The increasing effort for a better understanding of the biological effects of rare earth elements has led to considerable interest in amino acid complexes of rare earth elements [1–5]. Moreover, the crystal structures of rare earth complexes with amino acids have some interesting characteristics. In the present work the crystal structure of a samarium complex with β-alanine, $[Sm_2(C_3H_7NO_2)_6(H_2O)_4](ClO_4)_6 \cdot H_2O$, has been determined by the single-crystal X-ray diffraction technique.

2. Experimental details

Diffraction data were collected on a Nicolet R3m/E four-circle diffractometer with Mo Kα radiation ($\lambda = 0.710\ 69$ Å). A total of 11 542 reflections were measured using the ω scan mode (scan speed 7.32 deg min^{-1}, scan width 1.4°) within the range $3.0° < 2\theta < 55.0°$, of which 6614 reflections with $I > 3\sigma(I)$ were used for structure refinement. Intensities were corrected for Lp factors and the absorption effect. The structure was solved by the heavy atom method and refined by the block diagonal least-squares technique. The refinement finally converged to $R = 0.045$, $Rw = 0.048$ and $\omega^{-1} = \sigma^2(F_0) + 0.000\ 15\ (F_0)^2$.

3. Results and discussion

The complex $[Sm_2(C_3H_7NO_2)_6H_2O)_4](ClO_4)_6 \cdot H_2O$ (molecular weight 1522.05) crystallizes in the triclinic space group $P\bar{1}$ with the following lattice and other parameters: $a = 12.926(3)$ Å, $b = 21.707(9)$ Å, $c = 9.316(2)$ Å,

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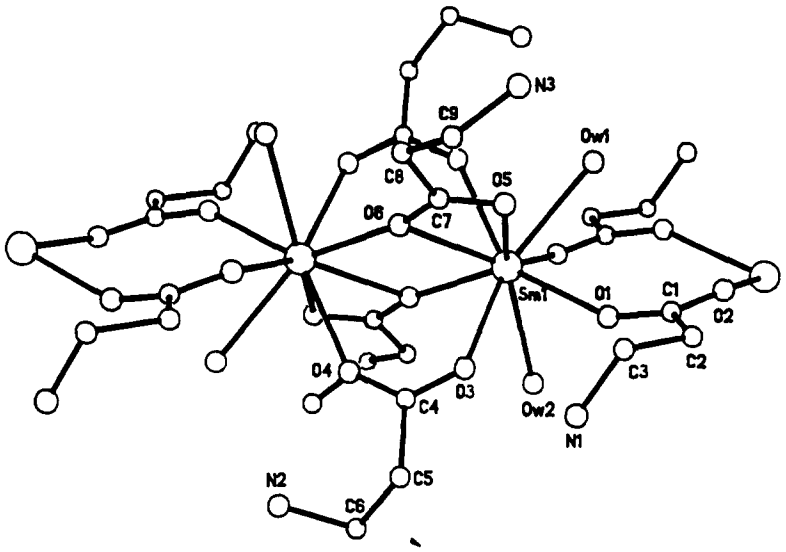

Fig. 1. The configuration of samarium complex with β-alanine.

$\alpha = 98.89(3)°$, $\beta = 96.93(2)°$, $\gamma = 76.89(3)°$, $V = 2505(1)$ Å^3, $Z = 2$, $D_{calc} = 2.017$ g cm^{-3}, $F(000) = 1512$ and μ(Mo Kα) $= 28.0$ cm^{-1}.

The configuration of the complex is shown in Fig. 1. The amino groups of β-alanine molecules remain protonated and so do not participate in bonding with samarium ions. β-Alanine molecules are coordinated to central samarium ions with their carboxyl groups. The average bond length of Sm–O(carboxyl) is 2.433 Å. Four water molecules are coordinated to samarium ions with oxygen donors. The average bond length of Sm–O(aqueous) is 2.579 Å. The Sm–Sm distances are more than 4.060 Å, so it is believed that there is no Sm–Sm bond in the complex. It is quite interesting that two bridging–chelating ligands of carboxyl groups from two β-alanine molecules are coordinated to two samarium ions in a structural unit $[Sm_2(C_3H_7NO_2)_6(H_2O)_4]^{6+}$ and so these carboxyl groups are tridentate ligands. For a structural unit two samarium ions are bridged by two bidentate ligands of carboxyl groups from two other β-alanine molecules and each samarium ion is bonded to two water molecules. Each samarium ion in a structural unit is connected with a samarium ion in its neighboring structural unit by two bidentate ligands of carboxyl groups from two more β-alanine molecules to form an infinite chain structure. The coordination number of the central samarium ion is nine. The coordination polyhedron of the samarium complex with β-alanine is a monocapped square antiprism.

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References

1 F. Gao, C.-J. Niu and J.-Z. Ni, *Wuli Huaxue Xuebao*, *7* (1991) 276.
2 F. Gao, C.-J. Niu and J.-Z. Ni, *Wuli Huaxue Xuebao*, *7* (1991) 362.
3 J.-M. Ren, C.-J. Niu, F.-K. Pei, W.-Y. Wang and J.-Z. Ni, *Chinese J. Magn. Reson.*, *8* (1991) 89.
4 F. Gao, C.-J. Niu and J.-Z. Ni, *Yingyong Huaxue*, *7* (1990) 10.
5 J. Legendziewicz, E. Huskowska, Gy. Argay and A. Waskowska, *Inorg. Chim. Acta*, *95* (1984) 57.