

## CRYSTAL STRUCTURE OF A NEW COMPLEX

### **bis(4,4,10,10-TETRAMETHYL-1,3,7,9-TETRAAZOSPIRO- [5.5]UNDECANE-2,8-DIONE-O)-DIAQUA- tris(NITRATO-O,O')-LANTHANUM**

**E. E. Netreba**

UDC 54.057:548.736.5:546.654

For the first time, a mononuclear biligand complex of lanthanum nitrate with bicyclic bisurea (4,4,10,10-tetramethyl-1,3,7,9-tetraazospiro[5.5]undecane-2,8-dione, or spirocarbon, Sk)  $[\text{La}(\text{C}_{11}\text{H}_{20}\text{N}_4\text{O}_2)_2(\text{H}_2\text{O})_2 \cdot (\text{NO}_3)_3]$  (**I**) is synthesized and its structure is determined by direct single crystal XRD. The crystals of **I** are monoclinic: space group  $P2_1/c$ ,  $a = 11.1989(15) \text{ \AA}$ ,  $b = 13.015(2) \text{ \AA}$ ,  $c = 24.153(2) \text{ \AA}$ ,  $\beta = 101.129(12)^\circ$ ,  $V = 3454.3(8) \text{ \AA}^3$ ,  $d_{\text{calc}} = 1.618 \text{ g/cm}^3$ ,  $Z = 4$ , CCDC 985760. The structure is molecular. The lanthanum cation is coordinated by two oxygen atoms of two organic ligand molecules, two water molecules, and three bidentate nitrate anions. The coordination number of lanthanum is ten; the coordination polyhedron is an irregular 10-vertex polyhedron. The crystal of **I** represents a non-merohedral twin with the components turned by  $180^\circ$  along the  $a$  axis; the relative weights of the components are 0.76:0.24. To confirm the purity of the sample of **I**, the powder XRD pattern was refined using the Rietveld method; the unit cell parameters at room temperature are as follows:  $a = 11.2777(4) \text{ \AA}$ ,  $b = 13.0774(5) \text{ \AA}$ ,  $c = 24.3453(9) \text{ \AA}$ ,  $\beta = 101.129(3)^\circ$ ,  $V = 3523.0(2) \text{ \AA}^3$ .

**DOI:** 10.1134/S0022476616030173

**Keywords:** lanthanum, spirocarbon, mononuclear, biligand, complex, structure, IR, single crystal XRD, powder XRD.