

Lanthanides Stereochemistry in the Structure of Oxygencontaining Compounds

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The crystallographic analysis of 3476 compounds containing 4044 coordination polyhedrons LnO_n ($\text{Ln} = \text{La} - \text{Lu}$) has been carried out (data have been taken from [1] and [2]). Coordination numbers (CN) of all atoms, coordinates of missing hydrogen atoms and characteristics of Voronoi-Dirichlet polyhedrons (VDP) of Ln atoms have been calculated by means of program complex TOPOS [3]. It was found out that CN(Ln) changes from 3 to 12, growth of CN is accompanied by increase of $r(\text{Ln}-\text{O})$ but VDP volume (V_{VDP}) of Ln atom depends only on Ln nature and its oxidation state. In our opinion this fact may be an evidence of a viewpoint in which complexing atom should be described as soft (that is able for deformation) sphere with a volume equal to V_{VDP} (radius of the sphere is R_{SD}). It was established that $R_{\text{SD}}(\text{Ln}^{3+})$ meanings reduce from La to Lu. Decrease of oxidation state of Ln atom is corresponded by growth of their VDP volumes on 1 – 4 Å³. It was shown that the VDP characteristics may be used for determination of oxidation state of Ln atoms in crystal structure, description and analysis of nonvalent (for example agostic $\text{Ln} \cdots \text{H}-\text{C}$) interactions and bonds between two metal atoms.

[1] *Inorganic crystal structure database, Release 2002/1*, FIZ Karlsruhe & NIST Gaithersburg, 2002. [2] *Cambridge structural database system, Version 5/25*, Cambridge Crystallographic Data Centre, 2003. [3] Blatov V.A., Shevchenko A.P., Serezhkin V.N., *J. Appl. Cryst.*, 1999, **32**, 377.

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