Crystal structure and Hirshfeld surface analysis of a new Eu(III)/Cr(III) double-complex salt

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Hirshfeld surface analysis and two-dimensional fingerprint plot are used to study the intermolecular interactions in a new double-complex salt: diaqua pentakis (tetramethylurea) europium(III) hexa (isothiocyanato) chromate(III) tetrakis (tetramethylurea) solvate, $[Eu(H_2O)_2(C(O)(N(CH_3)_2)_2)_5][Cr(NCS)_6].4C(O)(N(CH_3)_2)_2$ (I). The contacts received by the four symmetry-different components in the structure, including cationic complex, counter-anion complex and two symmetry-independent tetramethylurea molecules are discussed, with considering the relative contributions percentages of all contacts existing in the crystal packing. The highlighted interactions are S…C contacts (between cation and anion) and relatively strong Eu—O—H···O hydrogen bonds, which are manifested as red spots in the related Hirshfeld surface maps. These highlighted contacts in the title structure are compared with those found from the Cambridge Structural Database (CSD) [1] in the structures including similar contacts.

Keywords: Double-complex Salt, Hirshfeld Surface Analysis, Crystal Structure

Reference

[1] C.R. Groom, I.J. Bruno, M.P. Lightfoot, S.C. Ward, *Acta Cryst.*, **2016**, B72, 171–179.