Crystallochemical Analysis of Halogenides and Chalcogenides of d-metals

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A comparative crystallochemical analysis and classification are performed for 35 halogenides, 123 chalcogenides M_v[TX₄] (T is dmetal), and 1573 binary compounds A_xB_y using the program IsoTest of the TOPOS package. Two levels of structural relationship are considered: (i) 'grey' isomorphism, when a binary compound $A_x B_y$ relates to a ternary compound M_v[TX₄] if some atoms M, T, or X are topologically equivalent; (ii) partial isotypism when a complex salt $M_v[TX_4]$ is considered as a quasi-binary compound $M_v[T]$ keeping the connectivity of initial net. The examples of 'grey' isomorphism for ternary compounds are found with Tl₂Cl₄, In₂Br₄, magnetite, cristobalite, and C₃N₄. Partial isotypism is much more frequent; the following binary compounds participate in such relations: CsCl, NdS₂, NiAs, FeB, BaF₂-HP, PtS, sphalerite, fluorite, PoCl₂, BiF₃ (gananite), ReO₃. Many of the found correspondences are typical also for other anhydrous inorganic salts: orthosilicates, orthogermanates, arsenates, sulfates, selenates, molybdates, perchlorates, periodates, nitrates, carbonates, and borates.

Topological analysis of ionic arrays shows that in a half of the halogenides and almost in all the chalcogenides there are arrays related to close packings. Using the data on uniformity of these arrays the conclusions are made about their significant structure-forming role.

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