Oral Contributions

[MS18] From nature to laboratory: crystallography of minerals and mineral-related materials

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[MS18-01] Prediction of New Structural Arrangements and Chemical Compositions in Ti Silicates.

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Sokolova [1] developed general structural principles and established the relation between structure topology and chemical composition for Ti disilicate minerals containing the block, which is composed of a central trioctahedral (O) sheet and two adjacent (H) sheets of [5-7]-coordinated polyhedra and Si_2O_7 groups. All structures consist of a TS block and may or not have an I (intermediate) block that comprises atoms between two TS blocks. Usually, the I block consists of alkali and alkaline – earth cations, (H_2O) groups and the oxyanions $(PO_4)^{3-}$, $(SO_4)^{2-}$and $(CO_3)^{2-}$. Structures of Ti-disilicate minerals with the TS-block fall into four groups, each characterized by the topology and stereochemistry of the TS block: Groups I, II, III and IV, with Ti = 1, 2, 3 and 4 apfu, respectively. The general formula of the TS block is $A^P_2B^P_2M^H_2M^O_4(Si_2O_7)_2X_{4+n}$, where M^H2 and M^O4 = cations of the H and O sheets; M^H= Ti, Nb, Zr, Mn^{2+}, Mg, Ca; M^O= Ti, Zr, Mg, Mn^{2+}, Ca, Na; $A^P$and B^P= cations at the peripheral (*P*) sites = Na, Ca, K, Ba, Sr; X = anions = O, OH, F, H_2O; $X_{4+n} = X^O_4 + X^P_n$, n = 0, 1, 2, 1.5, 4. The stoichiometry HO Oof core part of the TS block, $M^H_2M^O_4(Si_2O_7)_2X^O_4$, is invariant. There are two types of structures with the TS block. Basic TS-block structure contains one type of TS and I blocks (or TS blocks link directly, additional cations do not occur and the I block is absent) and is characterized by one type of self-linkage of TS blocks; the two H sheets of one TS block are invariably identical. Derivative TS-block structure contains one or more types of TS and I blocks, is characterized by one or more types of self-linkage of TS blocks and is related to several basic structures of the same group. Basic and derivative structures occur in 28 and 4 TS-block minerals (Groups II and III), respectively. Based on established relationships between derivative and basic structures, atomic arrangements and chemical formulae have been predicted for 2 basic structures (Groups III and IV) and 13 derivative structures (Groups II and III).

[1]Sokolova, E. (2006) *Can. Min.* 44, 1273-1330.

Keywords: structure topology; Ti-silicates; derivative structures