American Mineralogist, Volume 83, pages 126–132, 1998

A systematic approach to general and structure-type formulas for minerals and other inorganic phases

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Abstract

During the preparation of the Mineral Group List Index of the Mineral Powder Diffraction File, it was necessary to develop a consistent scheme for the representation of the structural formulas. Because the fourteen letters B, C, F, H, I, K, N, O, P, S, U, V, W, and Y of the Latin (Roman) alphabet represent chemical elements (element symbols), this system uses twelve letters to represent cations, anions, and molecules occupying various sites of the structure (site symbols). The letters available as structure-site symbols represent cations with decreasing coordination numbers (CN) as follows: **D**, CN ≥ 9; **E**, CN = 8 or 7; **G**, CN = 6; **J**, CN = 5; **Q**, CN = 4 planar or 2 linear; **T**, CN = 4 tetrahedral; and **R**, CN = 3 planar. These definitions leave sufficient remaining letters for other structure-site symbols such as: **A** for all cations without regard to the coordination number; **L** for lone-electron-pair cations; **M** for neutral molecular units; **X** for monatomic anions; and **Z** for polyatomic anions. Structure sites of the same coordination type, yet distinct enough for ordered occupancy of resident cations, may be differentiated by primes (′,′′,′′′, etc.). Variable coordination numbers on a structure site and variable site occupancies are indicated by two symbols or subscripts with the intervening symbol ↔. For example, the general structure-type formula of amphibole may be written as $\mathbf{A}_{7\leftrightarrow8}[\mathbf{T}_4\mathbf{X}_{11}]_2\mathbf{X}'_2$. A specific structure-type formula also allows for a mixture of symbols to represent chemical elements and structure sites such as $\mathbf{A}_{0\leftrightarrow1}(\mathbf{E}'\leftrightarrow\mathbf{G})_2\mathbf{G}'_3\mathbf{G}''_2[Si_4O_{11}]_2(OH)_2$ whereas an example of a chemical formula is $Ca_2Mg_5[Si_4O_{11}]_2(OH)_2$ for the amphibole tremolite.