Computer Analysis and Classification of Entanglements in Crystal Structures

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Computer algorithms and programs are developed for the automated analysis and classification of any type entanglements in crystal structures of any complexity and composition. The programs are implemented within a novel version of TOPOS (a program package for multipurpose crystallochemical analysis), where the procedure of recognition of entangled systems is based on the description of a crystal structure as a finite quotient graph. Several levels of the structure representation are provided: strong valence, valence, H bonded, *etc*, to find entanglements in substances of different nature. TOPOS allows one to analyze various entanglement phenomena: interpenetration, polycatenation, polythreading, and polyknotting of any dimensionality. Each entanglement is characterized by a set of topological indices (coordination sequences, Schläfli and vertex symbols). A special classification scheme is proposed and programmed for 3D interpenetration, and a database on topological types of 3D nets is embedded into TOPOS.

These methods and software were applied to the analysis of 3D interpenetrated motifs in the crystal structures of inorganic, organic, and organometallic compounds through the whole ICSD and CSD. More than 500 examples of interpenetration were found and classified, many of them were discovered for the first time. Some unusual crystallographic features of 3D interpenetration are discussed.

Keywords: topology, entanglement, computer analysis