Inorganic Structure Prediction with GRINSP

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The computer program GRINSP (Geometrically Restrained INorganic Structure Prediction) [1], allows to explore the possibilities of occurence of 3, 4, 5 and 6-connected 3D networks. Hypothetical binary models (as well as known frameworks) are produced with exclusive connections of polyhedra by corners, such as $[MX_3]$ triangles in M_2X_3 formulation, $[MX_4]$ tetrahedra in MX_2 (zeolites or dense SiO_2 polymorphs), $[MX_5]$ polyhedra in M_2X_5 and finally $[MX_6]$ octahedra in MX_3 polymorphs. Moreover, hypothetical ternary $M_aM'_bX_c$ compounds are built up by combinations of either two different polyhedra or two different cations adopting the same coordination but with two different radii. The cost function is based on the agreement of the model interatomic distances with ideal distances provided by the user. The Monte Carlo algorithm explores randomly a range of cell parameters. First are found rough structure candidates, selected after the verification of the expected geometry, and then are optimized the cell parameters and the atomic coordinates. A satellite software (GRINS) can use the predicted models and produces the characteristics of isostructural compounds which would be obtained by cationic substitutions. CIF files (>1000) of hypothetical boron oxyde polymorphs (including nanotubes), zeolites, fluoroaluminates, borosilicates, titanosilicates, gallophosphates, are available at the PCOD (Predicted Crystallography Open Database) [2].

[1] a) Le Bail A., *J. Appl. Cryst., submitted*; b) http://www.cristal.org/grinsp/
[2] http://www.crystallography.net/pcod/

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