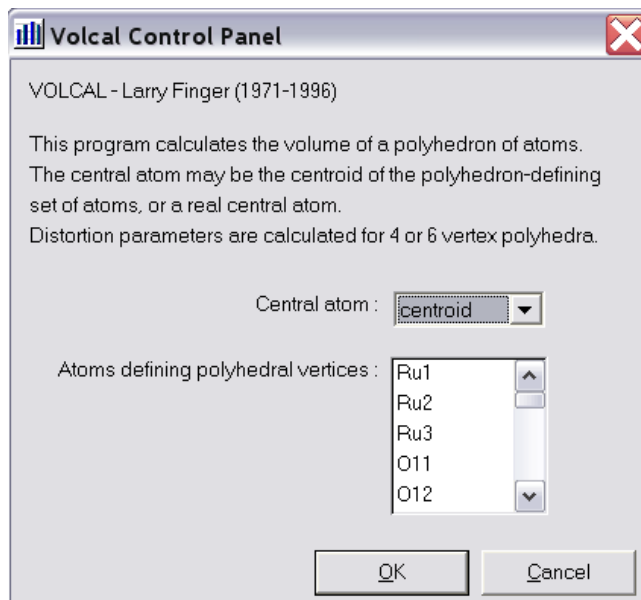


Chapter 9.8

VOLCAL

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The program VOLCAL computes the volume derived from a polyhedron comprising of a set of atoms. For 4-vertex and 6-vertex polyhedra, the distortion parameter away from idealised tetrahedral or octahedral symmetry is also computed



The "central atom" may be a real atom or the centroid of the points defining the polyhedron. A maximum of 20 atoms may be selected to define the polyhedron. The output is given to the TextServer and also to the file *VOLCAL.LST*.