

12.108
Structure of Earth Materials
Problem Set #1

Point Groups and Symmetry

1. (5 points) The 3-D point groups are generated by the interaction of symmetry operations. 13 of the point groups are monoaxial, and the remainder of the 32 groups are generated by 2 or 3 symmetry elements.

Use a stereographic representation of the axes and/or matrix multiplication methods to examine the consequences of a 4-fold combined with inversion and a 2-fold rotation axis that is perpendicular to the 4-bar.

Bonding and Crystal chemistry

2. (5 points) Pauling's first rule sets out constraints for the way in which a cation will be surrounded by anions in an ideal ionic structure. The radius ratio rule determines the ideal coordination number (CN) of a cation by an anion and is based on the ratio r_c/r_a . Assuming that the radius of the anion is 0.5, derive the optimal cation radius (r_c) for CN = 3, 4, 6, 8 and 12.

3. (15 points) In an idealized ionic crystal the coordination number (CN) of a cation by anions is determined using the radius ratio rule.

a) For the cations given below use the atomic radii (in nm) to calculate the radius ratio for coordination with O^{2-} . From this value and Pauling's 1st law determine the preferred coordination number of each atom. Assume an ionic radius of 0.140 nm for O^{2-} .

Si ⁴⁺	0.026
Al ³⁺	0.039
Mg ²⁺	0.072
Ca ²⁺	0.100
Na ¹⁺	0.102

b) Now using your class notes and part II of Zoltai and Stout (your xeroxed handout) determine the coordination numbers of the cations in the following structures and evaluate the extent to which they satisfy Pauling's 2nd law:

spinel	MgAl ₂ O ₄
olivine	Mg ₂ SiO ₄
silicate perovskite	MgSiO ₃

c) Evaluate the extent to which the three structures satisfy Pauling's 1st law? Comment on the validity of Pauling's laws for ionic crystals.