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Crystal Chemical Controls on Equation of State

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Minerals are known to compress through a number of mechanisms, ranging from polyhedral distortion to electronic transitions. Two mechanisms which can produce significant volume decreases are angle-bending and bond compression. The crystal chemical effects of these two mechanisms have been studied and documented for years. With more recent advances in theory and software enabling the accurate determination of bonding topologies, M-O bonding to bridging oxygens has been shown to modify compressibility by changing angle-bending force constants. Minerals that compress mainly through angle-bending tend to be soft. Good examples are quartz and cristobalite, minerals composed solely of corner-sharing silicate tetrahedra with bulk moduli of 37 and 12 GPa, respectively. Rock salt structured oxides must compress strictly by bond compression, and are much stiffer – lime and periclase have bulk moduli of 111 and 156 GPa, respectively. Feldspars have bulk moduli intermediate to the above examples. Based solely on the presence of Al-O-Si angles, theoretically softer than Si-O-Si angles, feldspars should be softer than quartz or cristobalite, but the T-O-T angles are stiffened by bonds to interstitial cations. The number and nature of these bonds affects compressibility sufficiently to create exceptions to Bridgman's law, which correlates bulk modulus with ambient unit cell volume in isostructural materials. In this paper, we present new high-pressure refinements of the crystal structures of jadeite, aegirine, and NaGa-clinopyroxene. Bulk moduli of these pyroxenes and all other end-member clinopyroxenes we could find in the literature (19 total) are plotted vs. unit cell volumes to test Bridgman's law. The data fall along two trends, each of which is separately consistent with Bridgman's law. Pyroxenes in one trend are dramatically stiffer than those in the other trend, with bulk moduli that differ by approximately 40 GPa. The only difference between the topologies of the structures in the two trends is in the bonding around M2. Structures in the less compressible trend have M2-O3 bonds that oppose Si-O-Si angle-bending in the tetrahedral chains. This angle-bending is an important compression mechanism in pyroxenes.

McCarthy et al. (in press) term these bonds "antipathetic". Pyroxenes in the more compressible trend lack these bonds. There are other M2-O3 bonds that visual inspection suggests might tend to encourage angle-bending, but do not appear to have an effect. McCarthy et al. term these bonds "apathetic," and suggest the term "sympathetic" for M-O bonds that actually soften angles. Other examples from the literature will be presented including one from the feldspars that may be a truly sympathetic bond. McCarthy, A. C., Downs, R.T., and Thompson, R.M. (in press) Compressibility trends of the clinopyroxenes, and in- situ high-pressure single-crystal X-ray diffraction study of jadeite. *American Mineralogist*.

3620 Mineral and crystal chemistry (1042)

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