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High-pressure crystal structure of kosmochlor, $NaCrSi_2O_6$, and systematics of anisotropic compression in pyroxenes

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ABSTRACT

The crystal structure of synthetic kosmochlor, $NaCrSi_2O_6$, was studied using single crystal X-ray diffraction at high pressure. A four-pin diamond anvil cell, with 4:1 methanol:ethanol pressure medium, was used to achieve pressures to 9.28 GPa. Unit-cell data were collected at 20 pressures, and intensity data were collected at 13 of these pressures. Fitting the *P-V* data to a third-order Birch-Murnaghan equation yields V_0 = 418.84(3) Å^3, K_0 = 134(1) GPa^{-1}, and K_0' = 2.0(3). Anisotropic compression was observed with unit strain axial ratios of 1:1.82:2.08. The CrO_6 octahedron has a bulk modulus K_0 = 90(16) GPa^{-1}, while the SiO_4 tetrahedron has K_0 = 313(55) GPa^{-1}, both with $K_0' \equiv$ 4. An o-type rotation of the O3-O3-O3 linkage was observed with pressure, with ∠O3-O3-O3 decreasing from 172.8(2)° to 166.1(7)°. Compression in kosmochlor is related to the stacking directions of distorted cubic closest packed O atom monolayers. Unit strain ellipsoids for diopside, hedenbergite, spodumene (*C*2/*c* and $P2_1/c$), $LiScSi_2O_6$ (*C*2/*c* and $P2_1/c$), clinoenstatite, orthoenstatite, and $Mg_{1.54}Li_{.23}Sc_{.23}Si_2O_6$ (*Pbcn* and $P2_1cn$) were generated and discussed in terms of closest packing systematics. A relationship between the anisotropy of compression of olivines and pyroxenes is established. A strategy to determine not only the direction of a stress field in deformed rocks, but also an estimate of the magnitude of stress is discussed in terms of comparing the anisotropy of olivine and pyroxene.