## Anion disorder in calcite and nitratine

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There is considerable interest in the phase transitions in calcite (CaCO<sub>3</sub>) and the related mineral, nitratine (NaNO<sub>3</sub>). The transition in both isotypic calcite and NaNO3 involves orientational disorder of the CO<sub>3</sub> or NO<sub>3</sub> groups. The temperature dependences of the crystal structure and intensities of the (113) and (211) reflections in calcite, CaCO<sub>3</sub>, and nitratine, NaNO3, were studied using Rietveld structure refinements based on synchrotron powder X-ray diffraction data. Calcite transforms from  $R\overline{3}c$  to  $R\overline{3}m$  at about  $T_c = 1240$ K, whereas nitratine transforms at 552(1) K. A CO<sub>3</sub> or NO<sub>3</sub> group occupies, statistically, two positions with equal frequency in the disordered R3m phase, but with unequal frequency in the partially ordered R3c phase. One position for the CO<sub>3</sub> or NO<sub>3</sub> group is rotated by 180° with respect to the other. The unequal occupancy of the two orientations in the partially ordered R3c phase is obtained directly from the occupancy factor, x, for the O1 site and gives rise to the order parameter, S = 2x - 1. In calcite, the a cell parameter shows a negative thermal expansion at low T, followed by a plateau region at higher T, then a steeper contraction towards  $T_c$ , where the CO<sub>3</sub> groups disorder in a rapid process. In nitratine as well, the **a** axis contracts towards  $T_c$ , where the NO<sub>3</sub> groups disorder rapidly. Using a modified Bragg-Williams model, fits were obtained for the order parameter S, and for the intensities of the (113) and (211) reflections.

## Two contrasting Ordovician and Variscan plutons at Central Iberian Zone (central Portugal)

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In the Central Iberian Zone (CIZ) of the Iberian Massif, most granitic plutons are related to the last ductil deformation phase D3 of the Variscan orogeny. Ordovician granites are rare

The Oledo pluton consists of Early Ordovician granitic rocks (479 - 480 Ma), ranging from tonalite to granite, whereas the Castelo Branco pluton consists of late-D3 Variscan granodiorites and granites (310  $\pm$  1 Ma). The U-Pb ages were determined on zircon and monazite by ID-TIMS. The former pluton was intruded by the latter pluton.

At the Oledo pluton, biotite granodiorite contains biotite tonalitic and granodioritic microgranular enclaves. They are of I-type. Granodioritic enclaves and host granodiorite were derived from tonalitic magma by fractional crystallization. Biotite > muscovite granodiorite shows a sharp contact with biotite granodiorite and is of hybrid origin. Biotite = muscovite granodiorite has tonalitic and granodioritic enclaves. The granodioritic enclaves result from mixing of relatively primitive granodiorite magma with magma derived from crustal melting. Tonalitic enclaves are globules of a more mafic relatively primitive magma. Muscovite > biotite granite is of S-type.

The reversely zoned pluton from Castelo Branco consists of S-type granitic rocks. It has a muscovite > biotite granite at the pluton's core surrounded successively by biotite > muscovite granodiorite, porphyritic biotite > muscovite granodiorite grading to porphyritic biotite = muscovite granite and by muscovite > biotite granite. Porphyritic granodiorite and biotite = muscovite granite were derived from the granodiorite magma by a fractional crystallization process. Both muscovite > biotite granites resulted from two distinct pulses of granite magma.