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X-ray Structures of Carbonate Apatite. M.E. Fleet, Dept. of Earth Sciences, Univ. of Western Ontario, London, Ontario N6A 5B7, Canada.

Composite single crystals of type A and A-B carbonate apatites [CAp; $\text{Ca}_{10}(\text{PO}_4)_{6-y}(\text{CO}_3)_{x+2y}(\text{OH})_{2-2x-y}$] have been synthesized at 2-4 GPa, 1400-1500EC. Single crystals of type A CAp ($x = 0.75$, $y = 0.0$; ν_3 IR bands at 1540 and 1455 cm^{-1} ; space group $P-3$ are domain disordered with multiplicity of six about the c -axis. The carbonate ion is ordered along the apatite channel at $z = 0.5$, and oriented with two oxygen atoms close to the c -axis and its plane tilted -9° . Structure refinements have been made with carbonate oxygen atoms both unconstrained ($R = 0.024$) and constrained to ideal geometry ($R = 0.025$), with similar results. There are three structural locations for the carbonate ion in disordered type A-B CAp ($x = 0.7$, $y = 0.6$; $P6_3/m$; $R = 0.023$): A1 (of type A CAp) and A2 in the apatite channel, and B (ν_3 IR bands at 1475 and 1410 cm^{-1}) representing carbonate substituting for the orthophosphate ion. The A2 carbonate ion (ν_3 IR bands at 1570 and 1505 cm^{-1}) is bisected by the c -axis in a stuffed channel position, and appears to charge compensate carbonate-for-phosphate substitution at high pressure. The type B carbonate ion is located close to the sloping faces of the PO_4 tetrahedron, but is not well resolved in the present X-ray structures. Correspondence with the structure of carbonated HAp of bone and dental enamel will be discussed.