Zeitschrift für Kristallographie 185, 604 (1988) — P07 4.FR

Crystal structure refinement of a synthetic Fe-Mg-Ca-carbonate phase

G. Heiss
Institut für Mineralogie und Kristallographie,
Universität Wien, Dr. Karl Lueger-Ring 1, A-1010 Wien.

Synthesis experiments in the system $CaCO_3$ - $MgCO_3$ - $FeCO_3$ carried out with a hydrothermal apparatus at T = 250°C and p = 1200 bars produced besides dolomite and siderite phases also a disordered solid solution phase with the average composition $CaCO_3$: $MgCO_3$: $FeCO_3$ = 10 : 33 : 57. The size of the clear rhombohedral single crystals was about 0.1 - 0.2 mm. The crystal structure was refined with 103 independent X-ray diffraction data to R = 0.020 (R_w = 0.021) by using a 4-circle diffractometer. The structure proved to be calcite-type. Compared to pure phases the line width is significantly spreaded.

a_o = 4.704(3) Å	C - O = 1.286(1) Å
c_o = 15.460(10) Å	Me - O = 2.154(1) Å
V = 269.26 Å^3	MeO_6-octahedra distortion
space group $R\bar{3}2/c$	(longer edge / shorter edge): Δ = 1.037

Structural parameters:

6 Me on (0,0,0), etc.	U_{11} = 0.0112(2),	U_{33} = 0.0183(3);
6 C on (0,0,1/4), etc.	U_{11} = 0.0150(10),	U_{33} = 0.0180(14);
18 O on (x,x,1/4), etc.	x = 0.7268(3),	
	U_{11} = 0.0144(6),	U_{33} = 0.0275(8),
	U_{12} = 0.0050(8),	U_{13} = 0.0001(3).

The crystallographic data and the interatomic distances are similar to those of siderite, the elongation of the MeO_6-octahedra parallel (00.1) likewise. The anisotropic temperature factors are about twice as large than those of the end-member carbonates of the system /1/.

/1/ Effenberger, H., Mereiter, K. and Zemann, J. - Z. Kristallogr. 156, 233 (1981).