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Fe-dolomite (teruelite) from the Keuper of the southern sector of the Iberian Mountain Range, Spain

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RESUMEN

En la parte meridional del Keuper de la Cordillera Ibérica una variedad de dolomita ferrosa es de interés como curiosidad mineralogica (teruelita). Los análisis químicos y el estudio cristalografico por medio de las técnicas de difracción de rayos X de monocristales confirman que se trata de una variedad de la dolomita y no de la ankerita. Solo ligeras diferencias morfológicas han sido apreciadas entre dolomita y teruelita. Así, la teruelita cristaliza en la forma (40$\bar{4}$1) mientras que la dolomita cristaliza preferentemente en la forma (10$\bar{1}$1).

INTRODUCTION

A ferroan variety of dolomite occurs in the Keuper of the southern sector of the Iberian Mountain Range. This variety of dolomite (teruelite) is a typical mineralogical curiosity of the Iberian Peninsula, the most important localities of which are Monte Calvario and Barranca del Salobrel (Teruel, Spain) (Maestre, 1845; Quiroga, 1873; Chaves, 1891; Calderon, 1910; Martin-Cardoso and Garrido, 1931; Muñoz and Piñeiro, 1951; Fernández- Galiano, 1954; Sinkankas, 1964; Marfil, 1970).

Chemical and crystallographic studies of teruelite and its comparison with the known crystal structures of dolomite and Fe-ankerite (Althoff, 1977; Beran and Zemann, 1977) confirm the hypothesis of Martin-Cardoso and Garrido (1931) that there is no crystallographic reason which would suggest that teruelite is a different species or variety of dolomite. From the morphologic point of view, however, slight differences in the habit of teruelite and dolomite can be appreciated. This justify this study.

EXPERIMENTAL AND RESULTS

1. Crystal habit. — Teruelite appears as small black rhomboedral crystals, can vary in their longest dimension between 1 mm and 2 cm; their average size is 5 mm. The habit of teruelite (Martin-Cardoso and Garrido, 1931; Fernández-Galiano, 1954; Sinkankas, 1964) is mainly (4041) whereas the dolomite habit is (10$\bar{1}$1). Other combinations are (40$\bar{4}$1) and (0001), and (40$\bar{4}$1), (10$\bar{1}$1) and (0001) (Fig. 1).

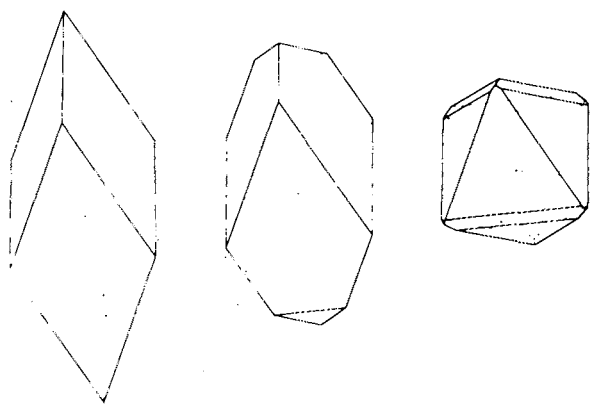

Fig. 1. Teruelite crystals: e (40$\bar{4}$1) rhombohedron, r (10$\bar{1}$1) thomboedron and c (0001) pinacoid.

2. Chemical analysis. — In Table 1 the chemical analysis of some teruelites are given.

3. Optical properties. — The refraction indices have been determined using a monocromatic sodium light (λ = 5893Å). The obtained results are n_ω = 1.688 and n_e = 1.509. They coincide with the ones available in the bibliography («Dana's System of Mineralogy», 1966) about ferroan dolomite.

4. X-ray investigation. — Single crystals of the type specimen were examined and suitable fragment was ground to an sphere 0.3 mm in diameter. According to Althoff (1977) the hexagonal unit-cell parameters are a = 4.8033(9) and c = 15.984(4)Å, and the space group is R$\bar{3}$. These parameters were confirmed by our measurements on an single crystal diffractometer with graphite-monochromatized Mo$K\alpha_1$ (λ = 0.71069Å) radiation: a = 4.81(1) and c = 16.00(9)Å.

321 reflections were measured and considered as observed ($I \geq 2.5\sigma(I)$). These were used in the subsequent analysis. The intensities were corrected for Lorentz and polarization factors. No corrections were made for absorption

The refinement was carried out by the programme SHELX76 (Sheldrick, 1976) with anisotropic thermal parameters to a

Table 1.- Chemical analysis of some Fe-dolomites ("teruelite")

	1		2	
FeO	3.00		3.31	
MnO	0.58		0.81	
MgO	16.83		18.40	
CaO	33.06		30.08	
CO_2	46.51		47.00	
Total	99.98		99.60	
	NUMBER OF IONS ON THE BASIS OF 6(O)			
Mg	0.075		0.008	
Fe	0.014	1.88	0.019	1.78
Mn	0.740		0.805	
Ca	1.046		0.946	
C	2.063		2.074	
Analytical method	Atomic absorption spectrometry		Wet chemical analysis	

1. Barranca del Salobrel (Teruel, Spain). Anal.: Insto.Carboquímica, C.S.I.C., Zaragoza

2. Barranca del Salobrel (Teruel, Spain). Anal.: J.Mandado

Table 2.- Fractional atomic coordinates and thermal parameters ($\times 10^4$)

	x	y	z	U11	U22	U33	U12	U13	U23
C1	0	0	2425(3)	78(11)	78(11)	50(17)	39(5)	0	0
O1	321(6)	-2500(6)	2442(1)	131(10)	85(9)	135(9)	79(8)	11(8)	8(7)
[illegible]	0	0	0	72(4)	72(4)	73(5)	36(2)	0	0
[illegible]	0	0	5000	27(22)	27(22)	24(16)	13(11)	0	0
	0	0	5000	84(103)	84(103)	315(104)	42(51)	0	0

final R value of 0.0543. The final positional and thermal parameters are given in Table 2. Observed and calculated structure factors with standard deviations are available upon request from the «Departamento de Cristalografía y Mineralogía de la Universidad del País Vasco».

DISCUSSION

The teruelite structure is essentially the same as that of other dolomite-ankerite solid solutions (Steinfink and Sands, 1959; Althoff, 1977; Beran and Zemann, 1977). Interatomic distances and bond angles are reported in Table 3 and compared with the data of Althoff (1977) and Beran and Zemann (1977).

We can give some results of our refinements. The CO_3 group does not deviate appreciably from planarity compared with the data in this sense reported by other authors (Beran and Zemann, 1977; Knobloch, Pertlik and Zemann, 1980).

The Ca-O distance in teruelite is 2.371(2)Å, which is comparable to the values found in dolomite (2.378(1)Å, Althoff, 1977; 2.381(1)Å, Beran and Zemann, 1977) and ankerite (2.371(1)Å, Beran and Zemann, 1977).

The (Mg,Fe^{2+})-O distances are 2.093(3)Å, which are more similar to those found in dolomite (2.081(1)Å, Althoff, 1977; 2.087(1)Å, Beran and Zemann, 1977) than to those found in ankerite (2.126(1)Å, Beran and Zemann, 1977).

From the value of the site occupation factor of the cation at (0,0,1/2) we conclude that teruelite has the formula $Ca(Mg_{0.91}Fe_{0.09})(CO_3)_2$. This formula coincide with the data obtained by chemical analysis.

Summing up, from the chemical, optical and crystallographic point of view teruelite is a ferroan variety of dolomite. The only difference is the presence of (4041) rhomboedron in teruelite.

Table 3.- Means interatomic distances and bond angles in teruelite, dolomite and ankerite.

Carbonate group	teruelite[a]	dolomite[b]	dolomite[c]	ankerite[c]
C-O	1.287(3)Å	1.2835(15)Å	1.286(1)Å	1.284(1)Å
O-O	2.229(3)	2.222(2)	2.228(2)	2.224(2)
O-C-O	119.96(0)°	119.95(1)°	119.983(6)°	119.992(4)°
CaO_6 octahedron				
Ca-O	2.371(2)Å	2.378(1)Å	2.381(1)Å	2.371(1)Å
O-O[d]	3.279(3)	3.294(2)	3.295(2)	3.277(2)
O-O[e]	3.425(3)	3.432(3)	3.438(2)	3.428(2)
O-Ca-O[f]	87.51(7)°	87.66(5)°	87.56(4)°	87.42(5)°
O-Ca-O[g]	92.49(7)	92.33(5)	92.44(4)	92.58(5)
$(Mg,Fe^{2+})O_6$ octahedron				
(Mg,Fe^{2+})-O	2.093(3)Å	2.081(1)Å	2.087(1)Å	2.126(1)Å
O-O[d]	2.919(3)	2.903(3)	2.911(2)	2.959(2)
O-O[e]	3.001(2)	2.985(3)	2.992(2)	3.053(2)
O-(Mg,Fe^{2+})-O[f]	88.43(7)°	88.38(6)°	88.42(4)°	88.21(5)°
O-(Mg,Fe^{2+})-O[g]	91.57(7)	91.61(6)	91.58(4)	91.79(5)

[a] this work

[b] ALTHOFF

[c] BERAN and ZEMANN

[d] parallel {00.1}

[e] others

[f] to two oxygens with the same z-coordinate

[g] to another pair of oxygens

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