

## OPTICAL PROPERTIES OF THE ORTHORHOMBIC MINERAL BARITE

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**ABSTRACT:** Using polarized light infra red and far infrared reflectivity spectra have been obtained for single crystal  $\text{BaSO}_4$  in the range between 40 and  $2000 \text{ cm}^{-1}$  for all three principal directions. Altogether 18 "Restahlen" peaks were observed, five for E//a; six for E//b and seven for E//c. Optical parameters were calculated using a four parameter fitting procedure.

### I. INTRODUCTION

Barium sulphate,  $\text{BaSO}_4$ , is better known as the mineral barite. It crystallizes in an orthorombic  $\text{Pnma}$  ( $D_{2h}^{16}$ ) structure with the lattice constants  $a=0.88701\text{nm}$ ,  $b=0.54534\text{nm}$  and  $c=0.71507\text{nm}$  and  $Z=4$ .

In the last five years the luminescence and thermoluminescence properties of barite /1,2/ were investigated and this mineral can be used as a thermo-luminescent dosimeter of gamma rays /3/, and in the production of paint and paper.

As far as we know the only transmission measurements to be made were obtained using polycrystalline barite /4,5,6,7/. No reflectivity data on single crystals barite has been published yet. In this work complete reflectivity measurements in the infrared and far infrared ranges are reported. The experimental data were numerically analysed using a suitable four parameter fitting procedure and values for the optical parameters were obtained.

## 2. EXPERIMENTAL

Samples of the natural mineral barite were usually about  $30 \times 10 \times 3 \text{ mm}^3$ . They were cleaved and suitable pieces were obtained for both reflectivity and x-ray measurements. Single crystals of barite were usually cleaved parallel to the plane (002). The other two planes were obtained by a standard cutting and polishing procedure. Infrared and far infrared reflectivity measurements were done with polarized light using a Perkin Elmer 457 spectrophotometer and a Fourier spectrometer (Beckmann FS720).

Figures 1 and 2 show the results of infrared and far infrared reflectivity measurements at 300K in the frequency ranges between  $400$  and  $1300 \text{ cm}^{-1}$  and  $40$ -  $400 \text{ cm}^{-1}$  respectively.

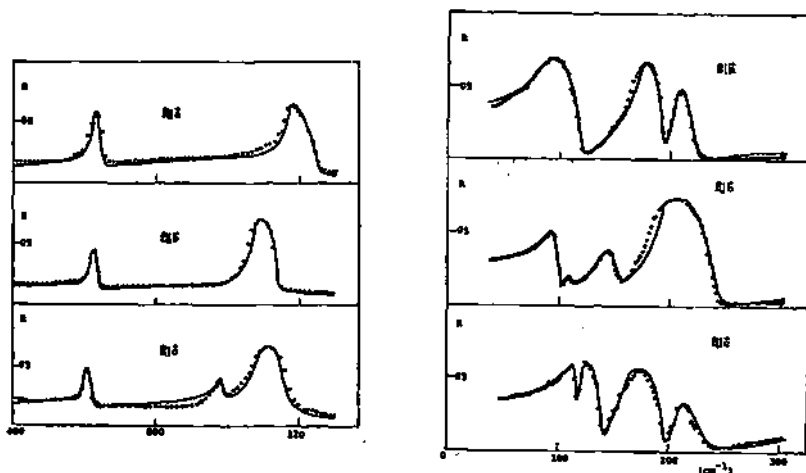


Fig. 1 and 2. Experimental infrared and far infrared data (open circuits) for  $\text{BaSO}_4$ . The solid lines were calculated using the oscillator parameters given in Table 1.

The experimental data are represented by squares. The solid lines were calculated using the oscillator parameters which were obtained by numerical analysis carried out with the help of a fitting procedure according to the Gervais /8/ four parameter model.

Table 1

	$\omega_{TO} (\text{cm}^{-1})$	$\gamma_{TO} (\text{cm}^{-1})$	$\omega_{LO} (\text{cm}^{-1})$	$\gamma_{LO} (\text{cm}^{-1})$	$\epsilon_0$	$\epsilon_\infty$
	82.	19	119	9.3	18.6	5.0
	169.8	8.0	191	8		
E//a	201	7	220	14		
	630	3	643	35		
	1182	15	1240	70		
	91	16.5	100	4.5	12.5	4.62
	106	19	114-	16.5		
E//b	142	13	153	15		
	192	8	239	13		
	621	1	630	24		
	1083	8	1140	70		
	113	28	117	1	12.6	5.45
	118	4	140	6.5		
E//c	168	16	195	8		
	207	11	231	23		
	607	7	617	20		
	984	17	1000	21		
	1100	22	1180	55		

Optical parameters used to fit infrared and far infrared reflectivity spectra of  $\text{BaSO}_4$ .

The values of the frequencies ( $\omega$ ) and damping factors ( $\gamma$ ) of the transverse (TO) and longitudinal (LO) optic modes are given in Table 1, where  $\epsilon_0$  and  $\epsilon_\infty$  represent the low frequency and the high frequency contribution to the dielectric parameter.

### 3. DISCUSSION

In this work reflectivity spectra of  $\text{BaSO}_4$  in the infrared and the far infrared for all three principal polarizations are given for the first time. The experimental results were analysed using a suitable fitting procedure and the values of the optical parameters were obtained. A factor group analysis of the group  $D_{2h}^{16}$  reveals that there are 62 optical phonons; three are inactive 26 ( $10B_{1u} + 6B_{2u} + 10B_{3u}$ ) are infrared active and 36 ( $11A_g + 7B_{1g} + 11B_{2g} +$

$7B_{3g}$ ) are Raman active. Using our experimental data we have identified 18 among 26 infrared active modes. 8 non identified modes surely belong to the oscillators whose energy is at the level of noise. It is not impossible that some of the infrared modes are nearly degenerate but that could only be seen if the experiments are repeated at liquid helium temperature.

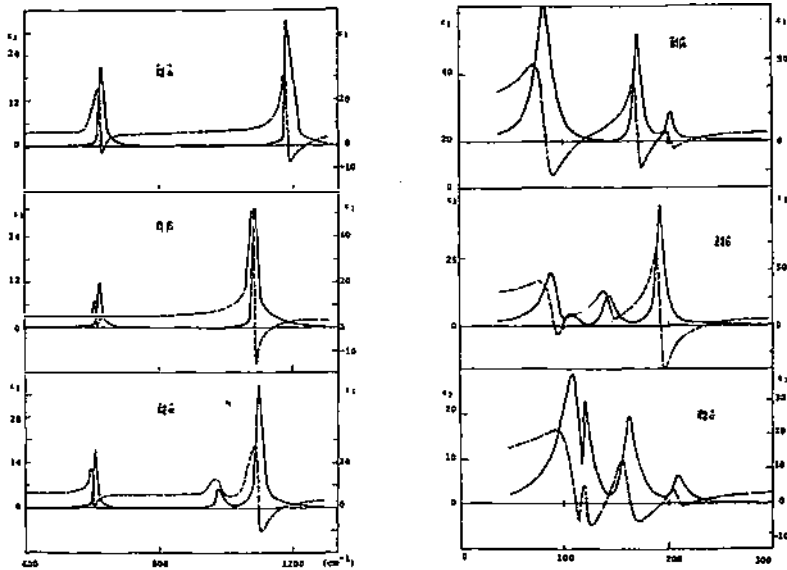


Fig. 3. The change of real (represented by a solid line) and imaginary (represented by a broken line) parts of the complex dielectric function for  $BaSO_4$  in the infrared (a) and far infrared (b) ranges.

Using the obtained values of the optical parameters given in Table 1, we have calculated the change in the real and imaginary parts of the complex dielectric function for  $E//a$ ,  $E//b$ , and  $E//c$ , which are also given in Figs 3a and 3b for the infrared and far infrared ranges respectively.

#### 4. REFERENCES

1. M. Sekulić, PH.D.Thesis, PMF, Beograd, 1977.
2. M.Prokić, PH.D.Thesis, Faculty of Electrical Engineering, Beograd, 1976.
3. K.Omori, P.F. Kerr, Geol. Soc. Amer. Bull. 74, 709, 1963.
4. P.M.Dimitrijević, Ph.D. Thesis Philosophical Faculty, Niš, 1980.

5. H.H. Adler, P.F. Kerr, Amer.Min., 50, 132, 1965.
6. C. Alexanian et al., Bull. Soc. Fr. Ceram., No. 71, 3, 1966.
7. K.Omori, MinerJour., 5, No. 5, 334, 1968.
8. F.Gervais, B. Piriou, Phys. Rev., B,10, No.4, 1642, 1974.