RE-PRINTS

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RAMAN SPECTRUM OF DANBURITE

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1. INTRODUCTION

THE Raman spectrum of danburite ($CaB_2Si_2O_8$) has been investigated by Nisi (1929, 1932). Working with a colourless transparent specimen (11 mm. × 7 mm. × 5 mm.) and the visible radiations of the mercury arc, he recorded 16 frequency shifts. It was observed that the scattered intensity in danburite was only a third of that of calcite and that the Raman spectrum was accompanied by a fairly strong continuum. In view of the complicated structure of danburite ($CaB_2Si_2O_8$) and the large number of atoms in the unit cell, it appeared that the results obtained by Nisi are incomplete and as such a study of its Raman spectrum using the Rasetti technique has been carried out by the author.

2. EXPERIMENTAL DETAILS AND RESULTS

In the present study, a clear transparent specimen (1·5 cm. × 5 mm. × 5 mm.) with its natural faces 120 and $\bar{1}20$ well developed was used. The incident light was normal to the 120 face and the scattered light was normal to the $\bar{1}20$ face of the crystal. With the medium quartz spectrograph, using a fairly fine slit (·03 mm.) exposures of the order of 12 hours were found to be necessary to obtain moderately exposed spectrograms. The recorded spectrum exhibits 30 Raman lines, 14 of which have been observed for the first time [see microphotometer record (Fig. 1) and (Fig. 2 *a*)]. The frequency shifts are given in Table I along with those reported by Nisi and the observed infra-red reflection maxima (Matossi and Krueger, 1936).

As in phenacite (Narayanan, 1950), all the Raman lines are extremely sharp, and lines separated by a few wave-numbers can be distinguished. Further, as there is some similarity between the spectra of topaz and danburite, the frequency shifts of the Raman lines of topaz recorded by Krishnan (1947) have also been included in Table I (see Fig. 2 also). In both these crystals, the low frequency lines are sharper than the high frequency ones. The lines 269 and 1205 cm.$^{-1}$ reported by Nisi have not been observed

TABLE I

Observed frequency shift in cm.$^{-1}$		Infra-red maxima	Topaz (Krishnan)
Author	Nisi		
115	92		
126	124		
153			156
157			167
183	186		
193			190
209	207		
227			
246	242		241
	269		269
296	289		287
313			317
348	342		335
			362
376	371		374
421	422	*424*	405
444			441
462			459
480		479	490
			520
564			550
609			558
627		*625*	650
		697	705
771			770
865			850
899	884	883	874
			898
926		910	920
			934
949			940
971	970	970	
		1009	
		1045	
1107	1110	1099	985
1171	1158	*1139*	1162
1558	1205		
1581			1235–1280
			1355–1435
			3636
			3649

in the present investigation. It is likely that both these lines are absent in the orientation used by the author and mentioned above.

3. INFRA-RED SPECTRUM

The infra-red spectrum of danburite has been investigated by Matossi and Krueger (1936) and they have reported reflection maxima corresponding to 8·78, 9·10, 9·57, 9·91, 10·31, 10·74, 11·33, 14·35, 16·0, 20·9 and 23·6 μ.

These infra-red reflection maxima have also been listed in column 3 of Table I, the strong ones being shown in italics.

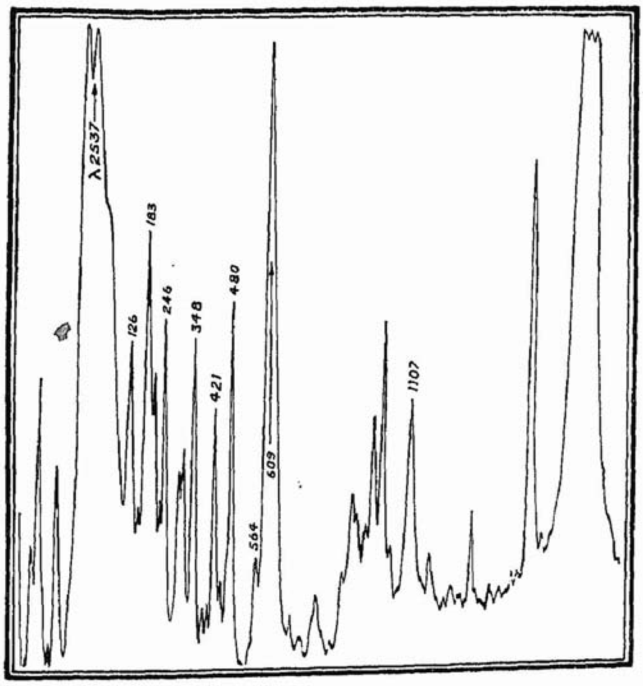

FIG. 1. Microphotometer Curve of the Raman Spectrum of Danburite

4. DISCUSSION

The crystal structure of danburite has been analysed by Dunbar and Machatschki (1930) and it is similar to that of topaz. Danburite belongs to the orthorhombic class and the space group is V_h^{16} and there are four molecules in the unit cell. In the lattice, both silicon and boron nuclei lie within tetrahedral groups of oxygen atoms. These tetrahedral groups are linked by their corners, each oxygen atom being common to two tetrahedra. Thus 8 out of the 32 oxygen atoms in the unit cell occupy special positions and are on reflection planes. The character table for the unit cell may easily be written out and it is seen that 78 frequencies are permitted in Raman effect and 54 in infra-red absorption. The presence of a centre of symmetry makes the infra-red maxima and Raman shifts complementary and no coincidence can be expected. However, it is found that 4 of the observed infra-red maxima have almost the same frequency as the observed Raman lines. It may be accidental, as the infra-red frequencies given here correspond to reflection maxima. Also, the difference between the theoretically expected number of shifts and that actually observed may arise because of two reasons. It is likely that more than one mode has very nearly the same frequency and/or those modes which involve a movement of the boron atoms may not have appreciable intensity. For a more detailed analysis of the spectrum, a detailed investigation of the effect of crystal orientation on intensity and state of polarisation of the Raman lines is necessary.

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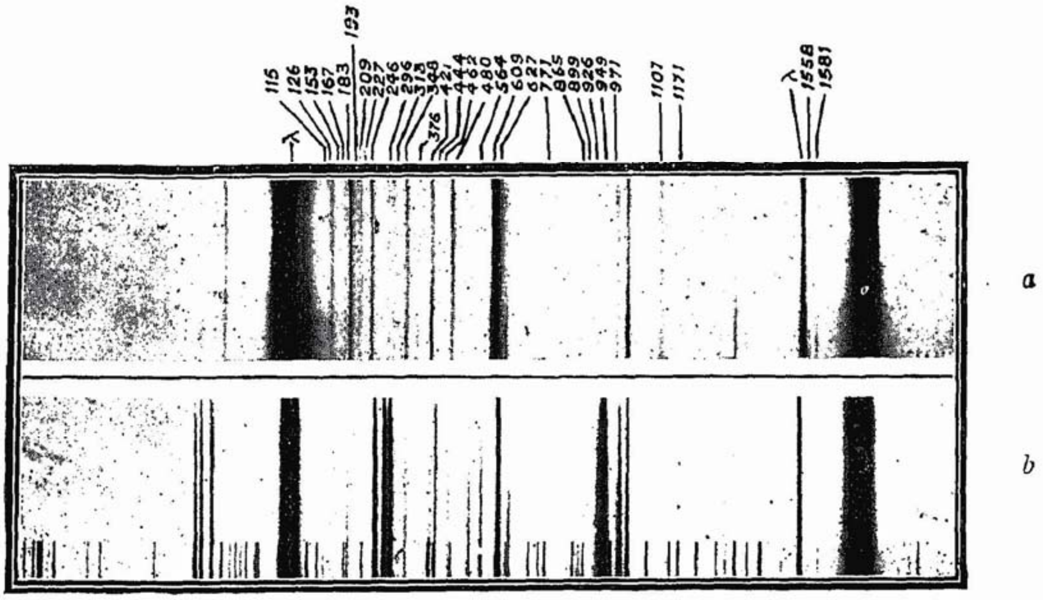

Fig. 2 (*a*). Raman Spectrum of Danburite.
Fig. 2 (*b*). ,, ,, Topaz.