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RAMAN SCATTERING FROM POWDERED BENZIL

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The Raman spectrum of solid benzil is of interest because of the high symmetry of the crystal (D_3^4 or D_3^6). The present author observed a few lines in the spectrum of powderous benzil.[1] Solin and Ramdas[2] report 18 lines in the single crystal spectrum. The present investigation was performed in order to detect weak lines and possible splitting of lines. The region 100-1750 cm^{-1} was examined.

Spectra were excited with a Spectra Physics Model 125 He-Ne laser operated at 6328Å. Pellets pressed from powderous benzil (reagent grade) were used as specimens. The scattered light was analyzed with a Spex 1400 double monochromator with photon counting equipment. The pulses were stored in a multichannel analyzer. The slit widths were about 3, 3 and 12 cm^{-1}.

Thirty-nine lines were observed. They are listed in Table I together with those observed by Solin and Ramdas[2] and the infrared spectrum of crystalline benzil as observed by Mann and Thompson.[3] The intensities are given as peak heights. The frequencies are given in cm^{-1} and are accurate to ±2 cm^{-1}. An original spectrogram of the region 1550-1700 cm^{-1} is reproduced in Fig. 1.

The spectrum shows several new lines as well as splitting of lines. Split lines are e.g. the pairs at 160-70, 1166-1177, and 1666-1676 cm^{-1}. The splitting is small, indicating weak coupling between the molecules in the unit cell. Also, most of the frequencies observed by Thompson

and Mann have their counterpart in the Raman spectrum. This supports the hypothesis of weak coupling, as it can be assumed that some of these corresponding lines are components of the same fundamental in the isolated molecule.

Among the new lines observed, the ones at 399, 844, 1048 and 1492 cm^{-1} have counterparts in the vibrational spectrum of benzene. This is a possible indication of localization of the corresponding vibrational modes in the phenyl groups, which observation also was made by Solin and Ramdas[2] for some of the lines they observed.

Because of the large number of Raman-active vibrations to be expected, 109[2], it is difficult to decide about the assignment of the lines on the basis of these measurements alone. Several weak lines, however, seem to be assignable to combination vibrations: 1059 or 1073 cm^{-1} (797 + 273), 1224 (2×615), 1328 (725 + 615; 1170 + 160), 1453 (1292 + 160), 1565 (1292 + 273), 1594 (2×797) and 1614 (999 + 615).

In conclusion, the spectrum reveals several interesting features specifically related to the benzil crystal. Therefore, additional investigations of the infrared and Raman spectra of single crystals under high resolution would be welcome in order to clarify these questions further.

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1. F. Stenman, Comm. Phys. Math. 33, 8 (1967).
2. S. A. Solin and A. K. Ramdas, Phys. Rev. 174, 1069 (1968).
3. J. Mann and H. W. Thompson, Proc. Roy. Soc. (London), 211A, 168 (1951).

Table I. Raman lines in the region 100-1700 cm^{-1} from crystalline benzil.

$\Delta\nu$ (cm^{-1})	Int.	Ref. 2	Ref. 3	$\Delta\nu$	Int.	Ref. 2	Ref. 3
160	180	159		1020	95	1021	1016
170	50			1048	25		1046
253	8	267		1059	5		
273	55			1073	8	1076	1070
337	15			1099	3		1094
399	15			1166	75	1168	~1164
423	20			1177	15		
459	12			1212	35	1215	~1208
470	35	469		1224	4		
615	140	613		1292	22	1293 }	1290-1350
640	35	642		1328	19	1331 }	
700	25	704					1395
715	6			1453	12		1450
725	55	727	719	1492	9		1490
797	35	794	797	1565	8		
844	6			1579	24		
859	6		874	1594	190	1594	1586-1599
939	5		930	1620	6		
986	20			1666	95	} 1671	1670
999	500	999	995	1676	80		
						3067	

FIGURE CAPTION

Fig. 1 The region 1550-1700 cm^{-1} in the Raman spectrum of powdered benzil. The lines marked C are calibration lines.

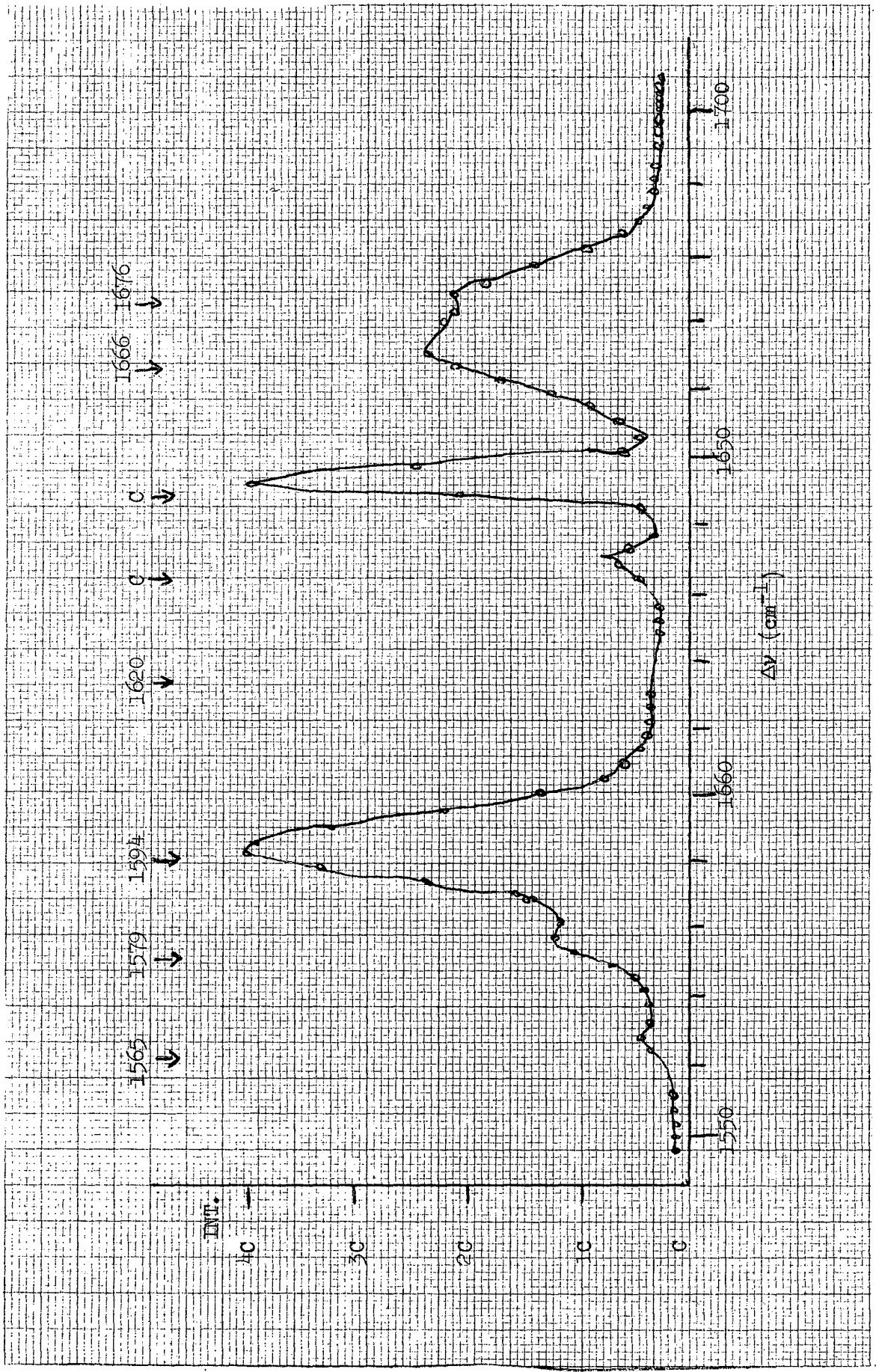
1565
1579
1594
1620
C
C
1666
1676
INT.
4C
3C
2C
1C
C
1550
1660
1650
1700
Δν (cm⁻¹)

Fig. 1

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