

Fig. 3. Raman spectra of  $\text{LiNO}_3$  in the four unique polarization orientations. (Reproduced from R. E. Miller, R. R. Getty, K. L. Treuil and G. E. Leroi, *J. Chem. Phys.*, 51 (1969) 1385.)

of an  $S_4$  site symmetry. The  $\nu_1(a_1)$  band of carbon tetrachloride can be resolved into three components in the Raman spectrum of the polycrystalline solid. It is assigned these bands as being due to isotopic splitting rather than to factor group splitting<sup>172</sup>. This assignment has been confirmed recently since the Raman spectrum of solid  $\text{C}^{13}\text{Cl}_4$  displays only one component for the  $\nu_1(a_1)$  band<sup>173</sup>.

X-Ray diffraction studies have shown that crystalline methyl chloride has a  $C_3$  site symmetry and  $C_{2v}^2$  space group. The vibrational spectra are in accord with such a structure, and the spectra of the crystalline bromide and iodide suggest that these two compounds have a similar structure to that of the chloride (refs. 174, 175) (Fig. 4).

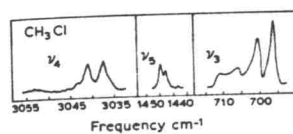


Fig. 4. Raman bands of polycrystalline  $\text{CH}_3\text{Cl}$  at high resolution ( $< 1.0 \text{ cm}^{-1}$  spectral slitwidth). (Reproduced from C. W. Brown and E. R. Lippincott, *J. Chem. Phys.*, 52 (1970) 786.)

The infrared<sup>176-182</sup> and Raman<sup>11,179,181</sup> spectra of the polycrystalline methylene halides have been investigated by several workers. The spectroscopic data indicate that the site symmetries are  $C_2$ ,  $C$ , and  $C_2$ , for the chloride, bromide and iodide, respectively.

Several infrared studies on polycrystalline chloroform have been reported (refs. 183-186). Ito originally reported two components for the doubly degenerate modes in the Raman spectrum<sup>174</sup> of solid  $\text{CHCl}_3$ , but recent work has shown that three components are present<sup>187</sup>. Comparison of the infrared and Raman spectra suggests a  $C_3$  site symmetry in a  $D_{3d}^5$  space group.

The infrared spectra of several matrix-isolated chlorinated tetrahedral molecules have been studied and isotopic splitting of several bands were observed (ref. 188).

Crystalline osmium tetroxide is known to have  $C_2$  site symmetry and space group  $C_{2h}^6$ . The Raman spectrum<sup>189-191</sup> of the solid is consistent with this structure.  $\text{RuO}_4$  gives a similar Raman spectrum which suggests a similar crystal structure.

The infrared and Raman spectra of liquid, crystalline and matrix isolated carbon suboxide<sup>192</sup>, and the gas phase Raman spectrum<sup>193</sup> support a quasilinear structure for the molecule.

The infrared and Raman spectra of a number of sulphate salts have been reported, and attempts have been made to correlate the observed spectra with the known crystal structures. The vibrational spectra of numerous anhydrous sulphate (refs. 194-203) salts have been reported together with low temperature infrared spectra<sup>204</sup> of single crystals of  $\text{K}_2\text{SO}_4$ ,  $\text{BaSO}_4$ ,  $\text{SrSO}_4$  and  $\text{PbSO}_4$ .

Several hydrated sulphate salts have also been investigated<sup>205-210</sup>. An interesting observation is that the  $\nu_1(a_1)$  mode of  $\text{SO}_4^{2-}$  appears as a triplet in the solid state spectra of some rare earth sulphate pentahydrates<sup>207</sup>.

The spectra of several alums<sup>211</sup>, double sulphates<sup>213</sup>, langbeinites<sup>213</sup> and Tutton salts<sup>213,214</sup> have been reported together with a single crystal Raman study<sup>212</sup> of several alums.

Phosphate salts have also been examined, and the spectra are in accord with a  $D_{2d}$  site symmetry<sup>215</sup> for the phosphate ion in  $\text{YPO}_4$  and  $\text{YbPO}_4$ ; a  $C_1$  site symmetry<sup>216</sup> in  $\text{Ca}_8\text{H}_2(\text{PO}_4)_6 \cdot 5\text{H}_2\text{O}$ ;  $C_{3v}$  site symmetry in strontium and barium