

Vibrational spectroscopy as a confirmation method for structural analysis

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In this work, the results obtained by single X-ray diffraction (XRD); even if for larger R-factor, are confirmed by another independent technique, one can study the vibrational spectroscopy with symmetry and group theory character tables. This method can be applied on the whole molecule or a part of it, mainly we search for function groups such as H₂O, an ionic part such as NH⁴⁺ or metal halide such as (MnBr_x). The fine XRD data results five possible solutions for the same molecule with the same chemical formula, although the R-factor values are so close, this method can distinguish between these possible solutions upon the crystal structure. The study of C₅H₁₀(NH₃)₂(MnCl₄Br₂) results one solution of XRD is confirmed by IR and Raman spectroscopy.

The space group of the molecule Ima2 with R= 3.33, The (MnCl₄Br₂) belongs to D_{4h} of 5 Raman peaks and different 5 IR peaks.

The Mn₂(MnCl₄Br₂) is C₂, C_{2h} or C_s according To the location of Mn atoms to the octahedral, the suitable solution is C_{2h} which expects 12 IR and another 9 Raman peaks with good agreement with IR and Raman results.

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