INTENSITY PARAMETERS FOR THE RAMAN TRACE SCATTERING OF METHYL HALIDES

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We have measured the absolute Raman trace scattering cross sections for the symmetric modes of the methyl halides: CH_3F, CH_3Cl and CH_3Br. The trace cross sections may be expressed in terms of derivatives of the mean molecular polarizability with respect to symmetry coordinates, the latter being invariant to isotopic substitution. In previous studies, it has been found that when a CH bond may be associated with more than one conformationally distinct position, for example the axial and equatorial CH bonds in cyclohexane [a] or with various CH bond positions, as in pentane [b], there may be considerable variation in the intensity parameter for the CH stretch. We have related these variations to field- and vibrationally-induced changes in the charge distribution, through analysis of the wavefunctions from molecular orbital calculations. We present here the results of our current study on the methyl halides, examining in particular both the CH and the CX stretching modes.

[a] K. M. Gough and W. F. Murphy *J. Chem. Phys.* **87**, 1509 (1987).
[b] K. M. Gough and H. K. Srivastava *J. Phys. Chem.* **100**, 5210 (1996).