SOME FEATURES OF VIBRATIONAL SPECTRA OF CYCLOPROPENE AND ITS METHYL AND FLUORO DERIVATIVES AND THEIR DEUTERO ANALOGUES

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Calculations of quantum mechanical force fields which were followed by their corrections using the scale factor technique resulted in unambiguous assigments of all the experimental vibrational frequencies of the compounds mentioned above.
Analysis of the vibrational spectra of the deutero analogues of 3,3-difluorocyclopropene and 1,3,3-trifluorocyclopropene revealed inverse isotopic shifts [1]. These shifts result in increasing certain frequencies by about 50 cm^{-1}.
The largest increases of the ν(C=C) stretching frequencies are observed in the series cyclopropene (1653 cm^{-1}), 1-methylcyclopropene (1788 cm^{-1}), and 1,2-dimethylcyclopropene (1890 cm^{-1}). These changes are not accompanied by an increase in the corresponding force constants. In contrast, the scaled diagonal force constants were found to decrease very slowly, being equal to 10.16, 10.06, and 9.99 mdyn/Å [2]. Only small changes in the formal C=C and C–C bond lengths are observed in this molecular series. All these effects were shown to be brought about primarily by kinematic factors.

References:

1. M. S. Baird, K. Spencer, S. V. Krasnoshchiokov, Yu. N. Panchenko, N. F. Stepanov, G. R. De Maré, *J. Phys. Chem. A*, (1998) *in press*.
2. G. R. De Maré, S. V. Krasnoshchiokov, Yu. N. Panchenko, N. F. Stepanov, *Russ. J. Org. Chem.*, **33** (1997) 860–866 (*Russian pagination*).