

Correlating the Force Fields of Methylpyrazines: Vibrational Spectrum of Tetramethylpyrazine

I. López-Tocón, J.F. Arenas, S.P. Centeno, D. Pelaez and J.C. Otero

Department of Physical Chemistry, Faculty of Science, University of Málaga, E-29071 Málaga, Spain.

Raman and Infrared spectra of tetramethylpyrazine (tetra-MPz) have been recorded and the *ab initio* calculated force field has been refined following the scaled quantum mechanical force field (SQMFF) methodology by Pulay [1]. It is well-known that the *ab initio* quantum chemical calculations overestimate the vibrational wavenumbers and then, scale factors are usually employed to fit the calculated frequencies to experimental ones. Moreover, this method allows us to transfer the scale factors among structurally related molecules yielding a priori estimation of the fundamental vibrational frequencies. In this case, the scale factors are directly transferred from 2-methylpyrazine [2]. The scaled frequencies of tetra-MPz agree quite well with the experimental ones in the whole spectral range.

In addition, the assignment of the vibrational spectrum of tetra-MPz has been compared with that of pyrazine and other methylpyrazines in order to determine how affects the substitution of the aromatic ring on the vibrational frequencies and to check the transferability of the scale factors. It is demonstrated that the scaled force fields of the methylpyrazine series obtained by transferring the scale factor reproduce the experimental frequency shifts as happen in substituted benzene derivatives.

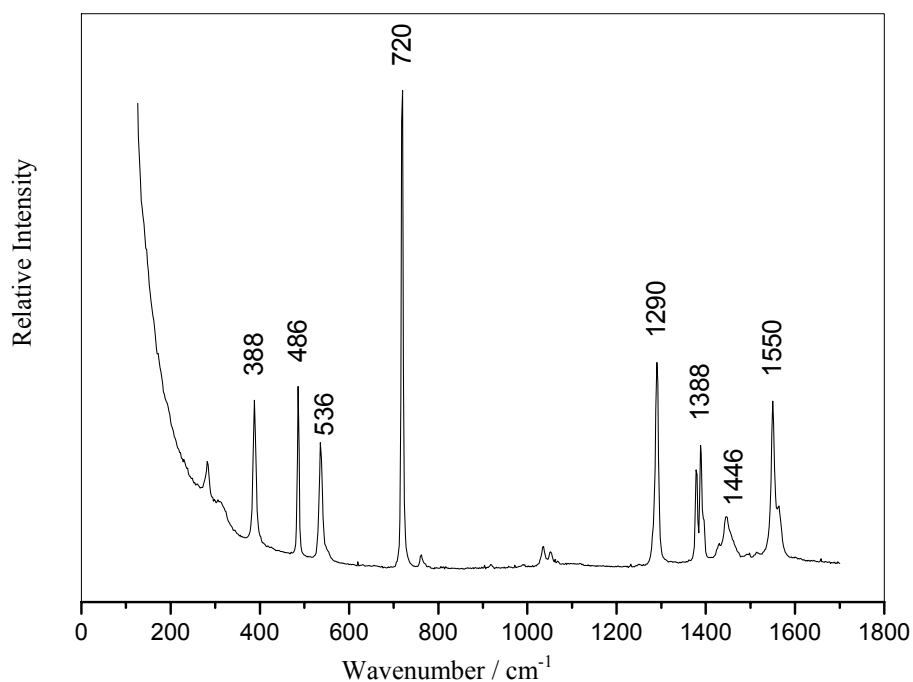


Figure 1: Raman spectrum of a 1M aqueous solution of tetra-MPz.

[1] P. Pulay, G. Fogarasi, J.E. Boggs, J. Chem. Phys. 74 (1981) 3999.

[2] J.F. Arenas, I. López-Tocón, J.C. Otero, J.I. Marcos, Vibr. Spectrosc. 19 (1999) 213.