

## Frequency shift or intensity shift? The origin of spectral changes in vibrational spectra.

### Autorzy

Mirosław A. Czarnecki

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It has been shown that the frequency shift for a single band can be reconstructed by a linear combination of contributions from adjacent bands with fixed positions. Assuming discrete distribution of the peaks in a specified spectral range and an appropriate response function one can generate diverse patterns of spectral changes. This diversity was clearly manifested in the corresponding two-dimensional (2D) asynchronous contour plots that are very sensitive to the pattern of spectral variations in the input data. In the condensed phases the shape of spectral envelopes results from the superposition of numerous bands. Hence, in most cases the apparent 'frequency shift' actually means the 'intensity shift' due to variations in population of the species absorbing at different wave numbers.

### Słowa kluczowe

Frequency shift, Origin of spectral changes, Vibrational spectra, 2D correlation spectroscopy, Simulated spectra, Hydrogen bonding, Cyclohexanol

### Adres publiczny

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### Strona internetowa wydawcy

<http://www.elsevier.com>