

force field

Within the molecular mechanics approach, a set of potential functions defining bond stretch, bond angle (both valence and dihedral) distortion energy of a molecule as compared with its non-strained conformation (that characterized by standard values of bond lengths and angles). A set of transferable empirical force constants is pre-assigned and the harmonic approximation is usually employed. Some force fields may contain terms for interactions between non-bonded atoms, electrostatic, hydrogen bond and other structural effects as well as account for unharmonicity effects.

In vibrational spectroscopy, the inverse problem is solved by determining a set of force constants and other parameters of a chosen potential energy function which would match with experimentally observed vibrational frequencies of a given series of congeneric molecules.

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