ANHARMONIC VIBRATIONAL ANALYSIS OF BUCKMINSTERFULLERENE

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The vibrational self-consistent field method[a] is used to calculate selected overtone and combination bands in the infrared and Raman spectra of buckminsterfullerene. A potential energy surface by Feldman et al.[b] has been slightly modified to generate anharmonicity. The potential consists of four terms: nearest neighbor bond stretching and angle bending, the so-called Keating term, which describes torsion motions, and a "puckering" term, which describes radial distortions. It is hypothesized that the latter two will contribute most strongly to anharmonicity in buckminsterfullerene, whereas the former will be only weak contributors. This hypothesis is investigated via a series of computational experiments, and the results will be reported.

[a] D. A. Jelski, R. H. Haley and J. M. Bowman, J. Comput. Chem., **17**, 1645 (1996); J. M. Bowman, Acc. Chem. Res., **19**, 202 (1986).
[b] J. L. Feldman, J. Q. Broughton, L. L. Broyer, D. E. Reich and M. D. Kluge, Phys. Rev **B46**, 12731 (1992).