

## INFRARED SPECTROSCOPY OF BUTYL RADICALS IN He NANODROPLETS

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Butyl radicals (*n*-, *s*-, *i*-, and *tert*-butyl) are formed from the pyrolysis of nitrite precursors (1-pentyl nitrite, 2-methyl-butyl nitrite, 3-methyl-butyl nitrite, and 2,2-dimethyl-propyl nitrite, respectively). The radicals are doped into a beam of liquid helium droplets and probed with infrared action spectroscopy from 2700-3125  $\text{cm}^{-1}$ , allowing for a low temperature measurement of the CH stretching region. The presence of anharmonic resonance polyads in the 2800-3000  $\text{cm}^{-1}$  region complicates assignments. To facilitate spectral assignment, the anharmonic resonances are modeled with two effective Hamiltonian approaches that explicitly couple CH stretch fundamentals to HCH bend overtones and combinations: a VPT2+K normal mode model based on CCSD(T) quartic force fields and a semi-empirical local mode model. Both methods have been previously applied to the *n*- and *i*-propyl radicals.<sup>a</sup> Extension to the butyl radicals allows for examination of the transferability of the empirical local mode coupling parameters to all types of local alkyl radical environment.

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<sup>a</sup>P.R. Franke, D.P. Tabor, C.P. Moradi, G.E. Douberty, J. Agarwal, H.F. Schaefer, E.L. Sibert, Infrared laser spectroscopy of the *n*-propyl and *i*-propyl radicals: stretch-bend Fermi coupling in the alkyl CH stretch region, *J. Chem. Phys.* 145 (2016) 224304.