ISOTOPE EFFECTS IN THE RO-VIBRATIONAL SPECTRUM OF FORMALDEHYDE

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Abstract

We present ro-vibrational line lists for three isotopologues of formaldehyde (H_2CO), $D_2{}^{12}C^{16}O$, $H_2{}^{13}C^{16}O$ and $D_2{}^{13}C^{16}O$, computed using the variational nuclear-motion program TROVE (Theoretical ROVibrational Energies)[1] in conjunction with an empirical potential energy surface (PES) by Al-Refaie et al. (2015)[2] H2CO-AYTY. In order to take into account the effects introduced by the isotope substitutions, a mass-dependent correction to the H2CO-AYTY PES was constructed by fitting to the ro-vibrational energies of $D_2{}^{12}C^{16}O$, $H_2{}^{13}C^{16}O$ and $D_2{}^{13}C^{16}O$, experimentally derived through the MARVEL procedure.[3] We show that the mass-depended PES constructed using this procedure retains the quality of the parent molecule for all three isotopologues. We aim to use it for production of accurate ro-vibrational line lists for other isotopologues as part of the ExoMol project.[4]

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