ROTATIONAL SPECTROSCOPY OF PROPYLENE OXIDE RADICALS

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Chirality, the molecular characteristic of having non-superimposable mirror images, is a major component of life as we know it. Investigation of chiral molecules in interstellar space may provide insight into the origins of homochirality in biology. Propylene oxide (CH_3CHCH_2O) was the first chiral molecule to be detected in space. Reactions inolving it and its radical derivatives may provide a means for installing chiral centers in more complex molecules, especially in protostellar regions. We have calculated the equilibrium structures of four radical derivatives of propylene oxide at the CCSD(T)/cc-pwCVTZ level of theory along with spin-rotation interaction terms. In addition, we have explored the barrier to internal rotation of the methyl group in two of the radicals at the CCSD(T)/cc-pwCVDZ level. We will discuss the results of these calculations and searches for the pure rotational spectra of these radicals.