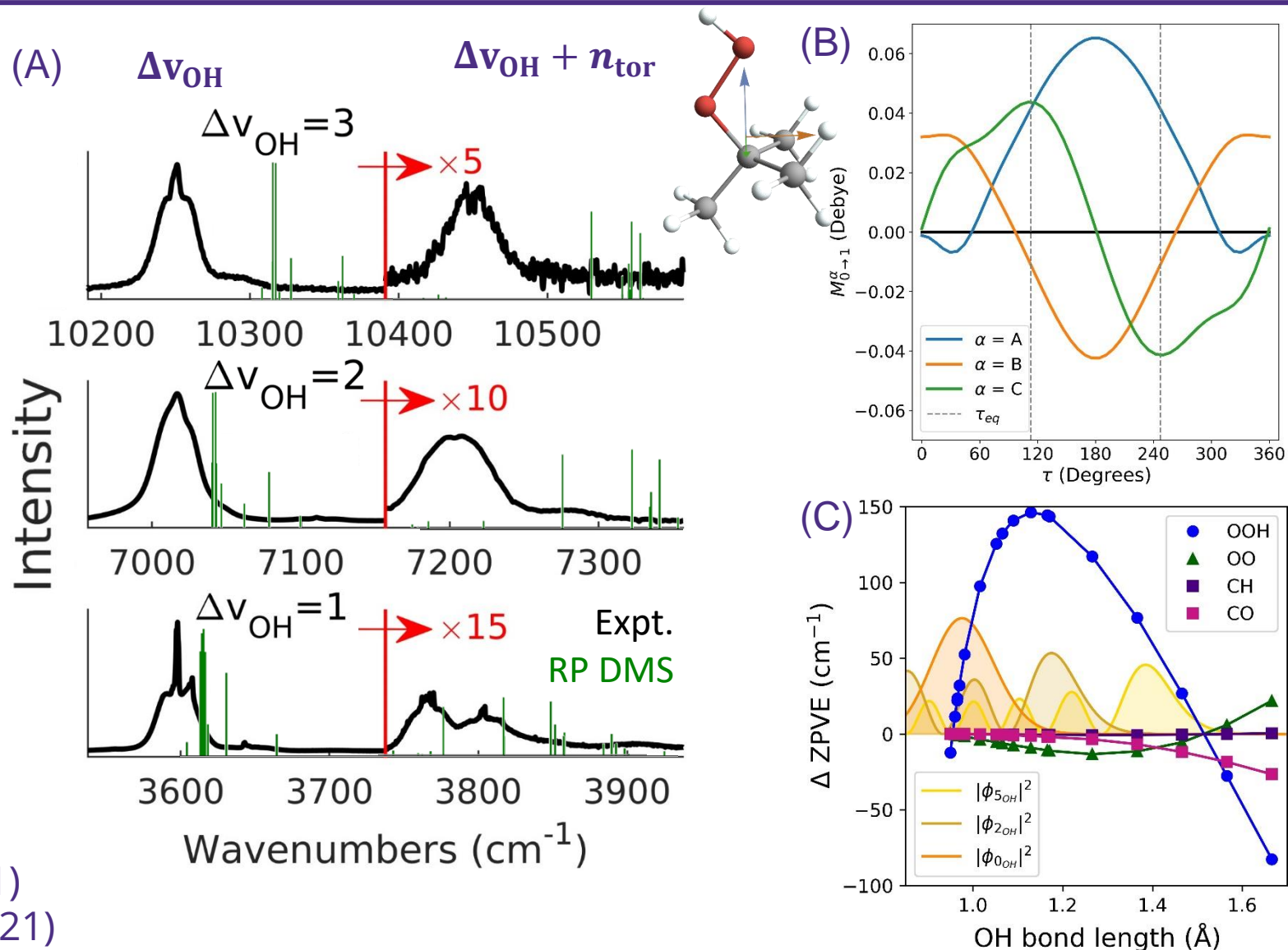


P5353: COUPLING OF TORSION AND OH-STRETCHING IN *TERT*-BUTYL HYDROPEROXIDE AND ITS RADICAL ANALOG, QOOH

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- Using a Reaction Path Model, we were able to qualitatively reproduce experimental spectra of TBHP (A).
- The intensity in the $\Delta v_{\text{OH}} + n_{\text{tor}}$ band is due to the shape of the transition dipole moment (B).
- Transition frequency shifts are due to the level of theory (DFT) and OOH bend OH stretch coupling (C).
- We are working out a similar model for the alkyl radical of TBHP.



$\Delta v_{\text{OH}} = 2$: *J. Chem. Phys.* **154**, 164306 (2021)

$\Delta v_{\text{OH}} = 1-5$: *J. Chem. Phys.* **154**, 164307 (2021)