COMPARISON OF INDEPENDENTLY CALCULATED AB-INITIO NORMAL-MODE DISPLACEMENTS FOR THE THREE C-H STRETCHING VIBRATIONS OF METHANOL ALONG THE INTERNAL ROTATION PATH

LI-HONG XU, RONALD LEES, *Department of Physics, University of New Brunswick, Saint John, NB, Canada*; JON T. HOUGEN, *Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD, USA*; JOEL BOWMAN, *Department of Chemistry, Emory University, Atlanta, GA, USA*; XINCHUAN HUANG, *SETI, NASA Ames Research Center, Moffett Field, CA, USA*; STUART CARTER, *Department of Chemistry, Emory University, Atlanta, GA, USA*.

Graphical displays of C-H stretching normal-mode coefficients from recent quantum chemical projected-frequency calculations are compared with analogous displays constructed after reexamination of results from more extensive higher-level calculations described earlier in the literature. Such comparisons confirm the facts that: (i) no geometrical phase is accumulated in these coefficients when the methyl top undergoes one complete internal-rotation revolution with respect to the frame, and (ii) some of the coefficients, when plotted against the internal rotation angle, exhibit near-cusp-like behavior at one or two angles. The connection between these graphical displays and the magnitude of "Jahn-Teller-like" and "Renner-Teller-like" torsion-vibration interaction terms in a previously reported model Hamiltonian, as well as the connection between the lack of geometric-phase accumulation in these graphs and the number of conical intersections enclosed by one full internal-rotation motion, will also be briefly discussed.