UNDERSTANDING THE METHANOL $5\nu_{OH} - 4\nu_{OH}/1\nu_{CH}$ IVR FRAGMENTATION ASYMMETRY

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The 1:1 resonance between the $5\nu_{OH}$ overtone and the $4\nu_{OH}/1\nu_{CH}$ combination band studied by Rizzo and coworkers exhibits wildly different IVR fragmentation patterns for the two resonant states. Efforts to explain this through hidden symmetries of the wavefunction have met with limited success. We apply an improved version of our vibrational matrix element factorization scheme to a fully anharmonic methanol potential energy surface based on Monte-Carlo sampled *ab-initio* calculations to predict the IVR lineshapes for rotationless transitions. We find that the different linewidths of the resonant pair can be explained based on fluctuations of the local density of coupled states.