

# **Supporting Information**

## **Anharmonic Vibrational Properties from Intrinsic *n*-Mode State Densities**

Eugene Kamarchik\* and Ahren W. Jasper\*

*Combustion Research Facility, Sandia National Laboratories, California 94551, USA*

E-mail: ekamarc@sandia.gov; ajasper@sandia.gov

---

\*To whom correspondence should be addressed

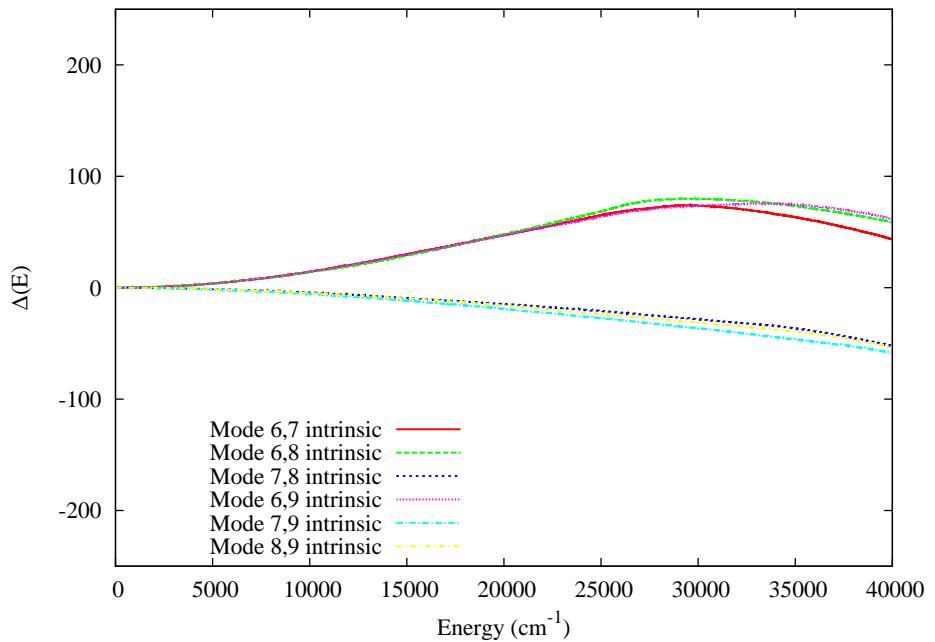


Figure 1: Intrinsic densities of states corresponding to coupling amongst the stretching modes of  $\text{CH}_4$

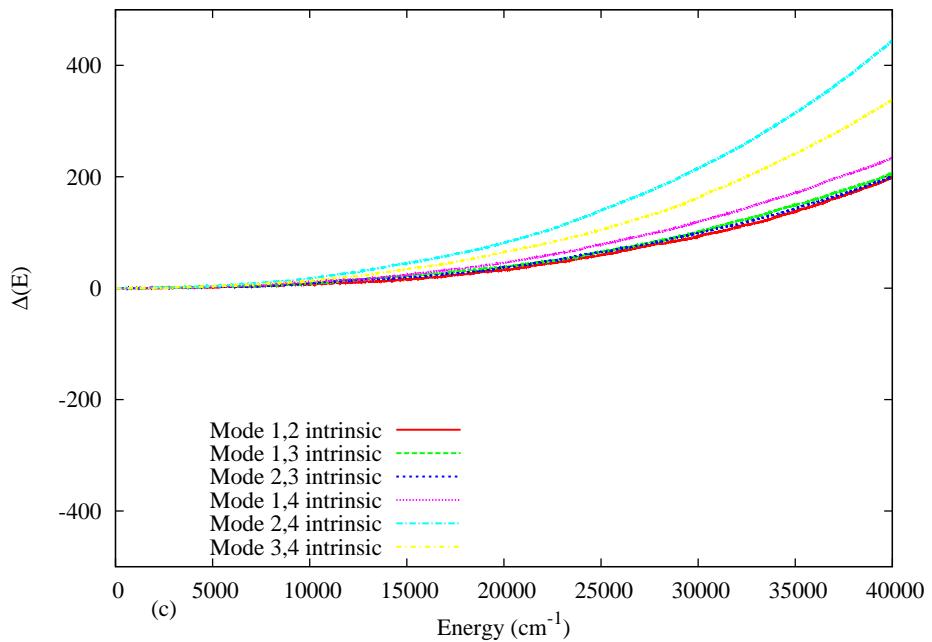


Figure 2: Intrinsic densities of states corresponding to coupling amongst the bending modes of CH<sub>4</sub>.

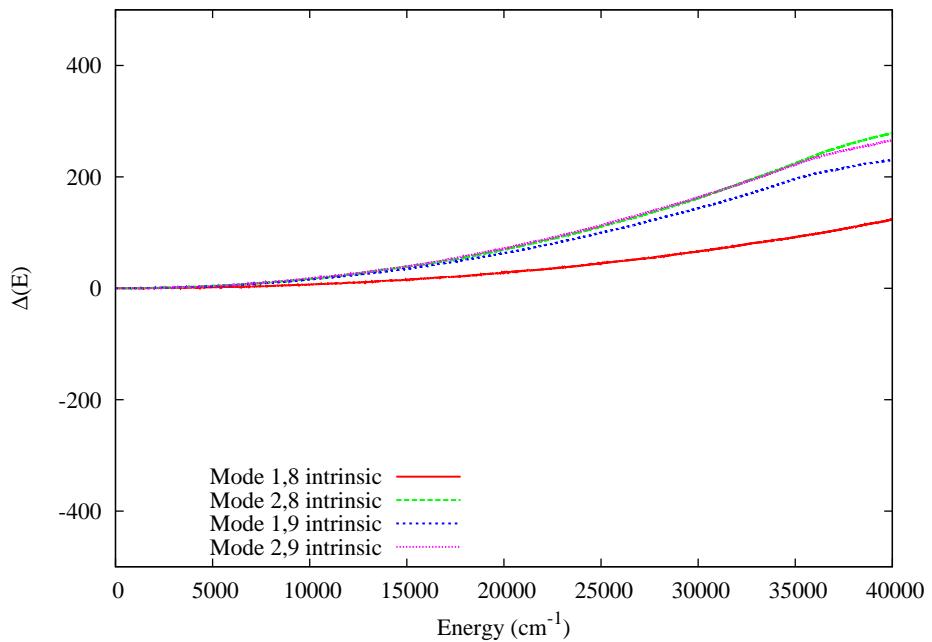


Figure 3: Intrinsic densities of states corresponding to coupling between stretching and bending modes of CH<sub>4</sub>.

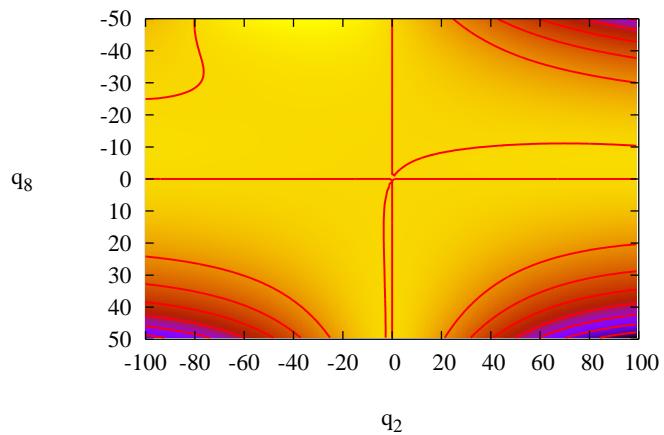


Figure 4: Contour plot of  $V^{(2)}(q_2, q_8)$ . Contour lines are in increments of  $10\,000 \text{ cm}^{-1}$  starting from  $-80\,000 \text{ cm}^{-1}$ . By construction  $V^{(2)}(q_2, q_8)$  is 0 along the x- and y-axes.