Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Coincidence Ion-Pair Production (cipp) Spectroscopy of Diiodine

Kristján Matthíasson,[1] Ágúst Kvaran,[1,*] Gustavo A. Garcia,[2] Peter Weidner,[3] and Bálint Sztáray[3,*]

1. *Science Institute, University of Iceland, Dunhagi 3, 107 Reykjavík, Iceland.*
2. *Synchrotron SOLEIL, L'Orme des Merisiers, St. Aubin BP 48, 91192 Gif sur Yvette, France.*
3. *Department of Chemistry, University of the Pacific, Stockton, CA-95211, USA.*

Electronic Supplementary Information

Figures

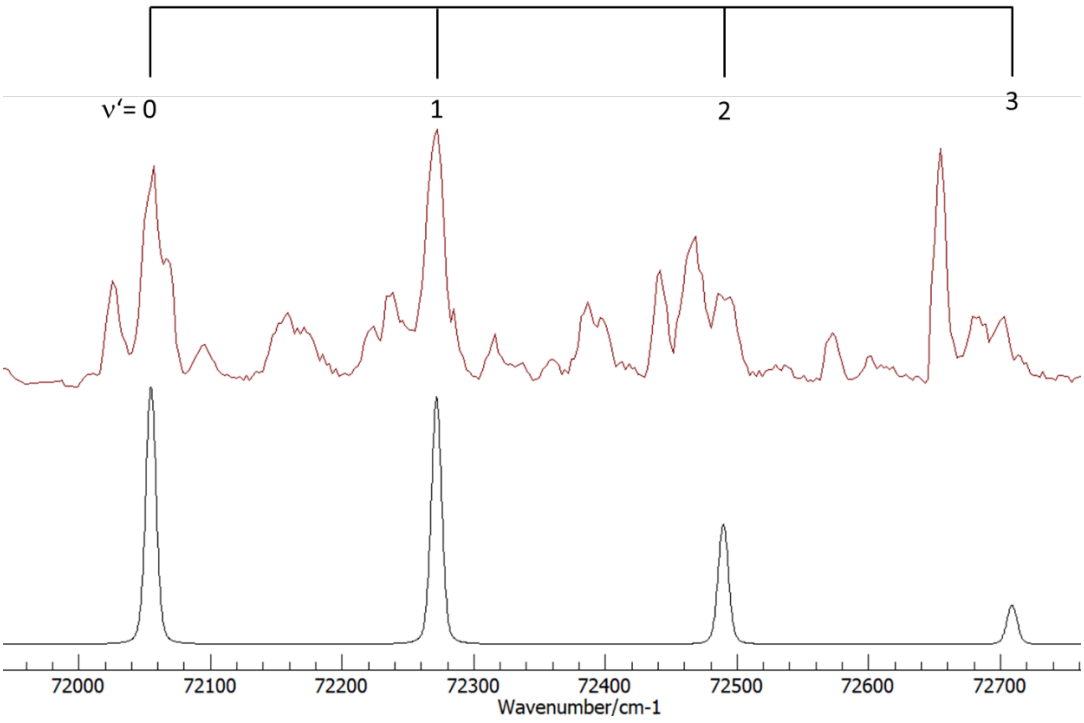

Figure S1: Vibrational simulation of o the $7f\delta_u$ state spectrum using T = 40K, ω_e = 217 cm^{-1} and $\omega_e x_e$= 0.5 cm^{-1}.

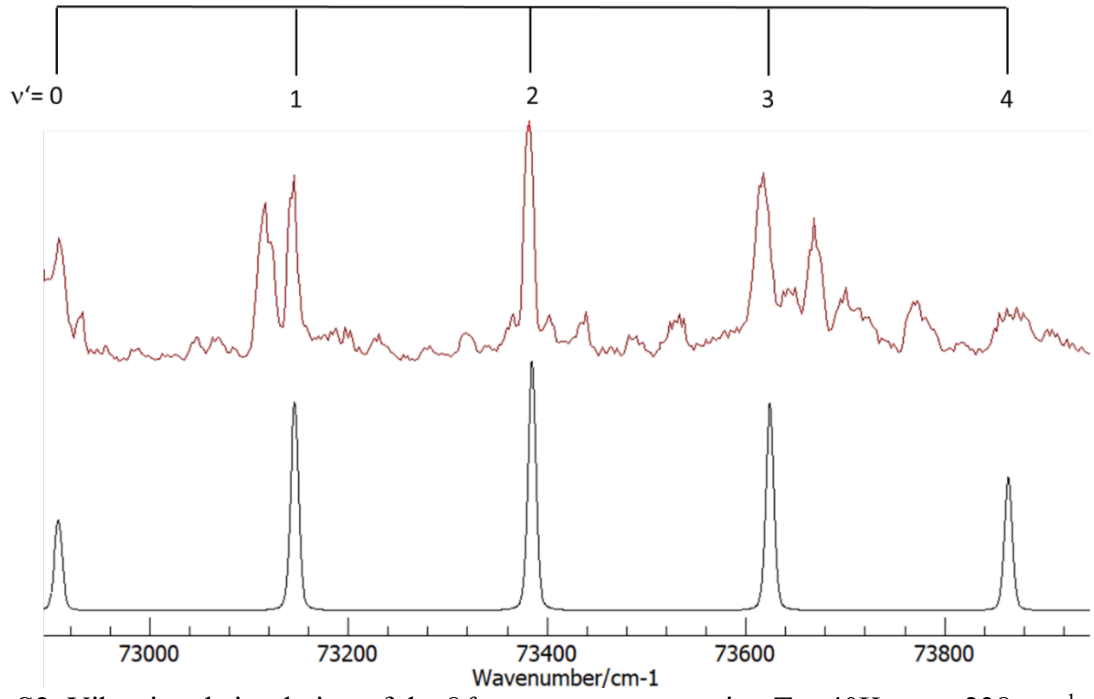

Figure S2: Vibrational simulation of the $8f\pi_u$ state spectrum using T = 40K, ω_e = 238 cm^{-1} and $\omega_e x_e$= 0.2 cm^{-1}.

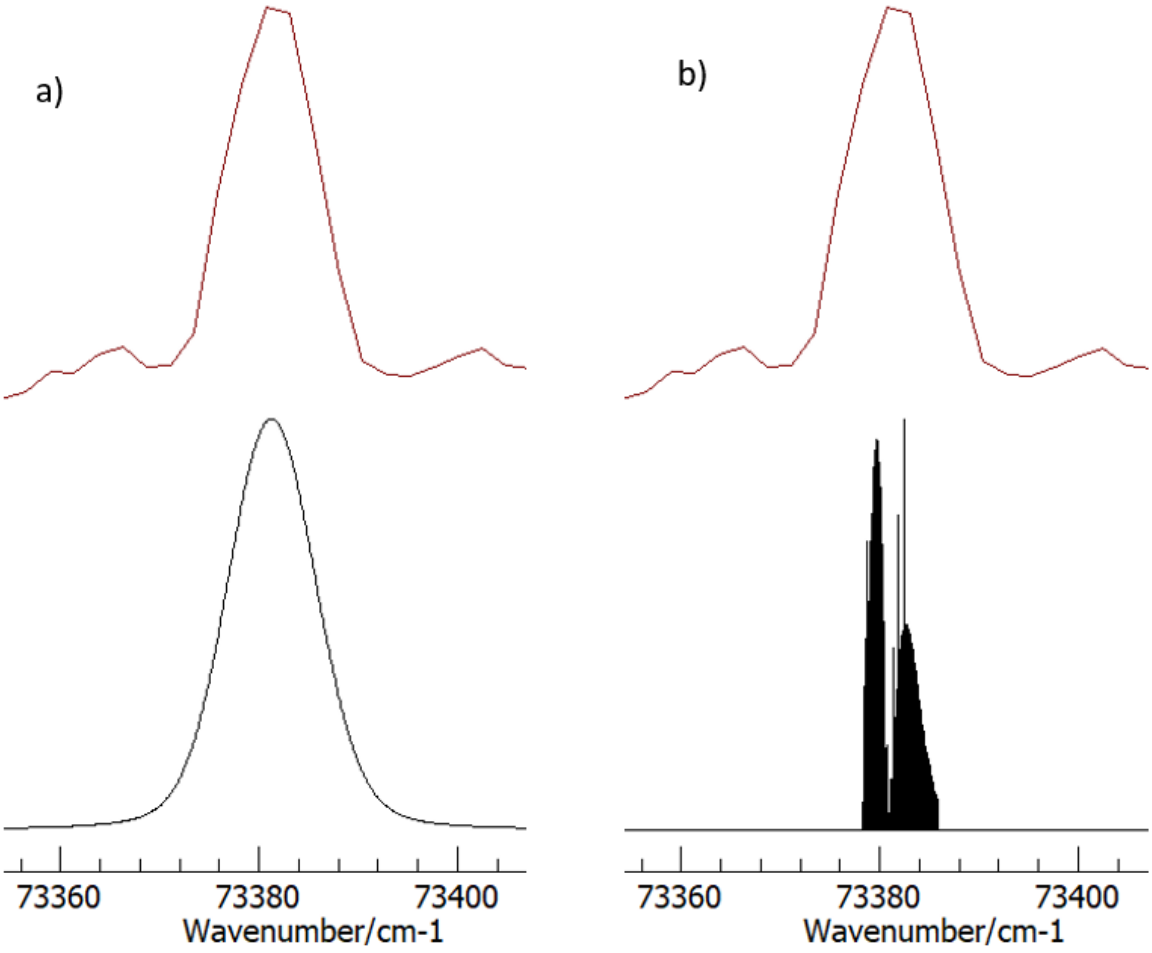

Figure S3: Rotational simulation for the $8f\pi_u$ (v'=2) spectral peak. Rotational constants used for the simulation were B'= 0.0378 cm^{-1}, D' = 4.2x10^{-9} cm^{-1}, B'' = 0.03737 cm^{-1} and D'' = 4.4x10^{-9} with T = 40 K. **a)** Shows the peak shape by using a Voigt band profile with a combination of Gaussian width contribution of 8 cm^{-1} and Lorentzian width contribution of 2 cm^{-1}. **b)** Shows rotational lines as sticks.