

The A-center Defect in Diamond. A Quantum Mechanical Characterization Through the Infrared Spectrum Supplemental Material

S. Salustro,¹ G. Sansone,¹ C. M. Zicovich-Wilson,² Yves Noël,³ L. Maschio,¹ and R. Dovesi¹

¹Dipartimento di Chimica, Università di Torino and NIS - Nanostructured Interfaces and Surfaces - Centre of Excellence, Via Giuria 5, 10125 Torino, Italy

²Centro de Investigación en Ciencias-(IICBA), Universidad Autónoma del Estado de Morelos, Av. Universidad, 1001, Col. Chamilpa, 62209 Cuernavaca, Morelos (Mexico)

³Institut des Sciences de la Terre de Paris (UMR 7193 UPMC-CNRS), UPMC, Sorbonne Universités, Paris, France

I. IR SPECTRA

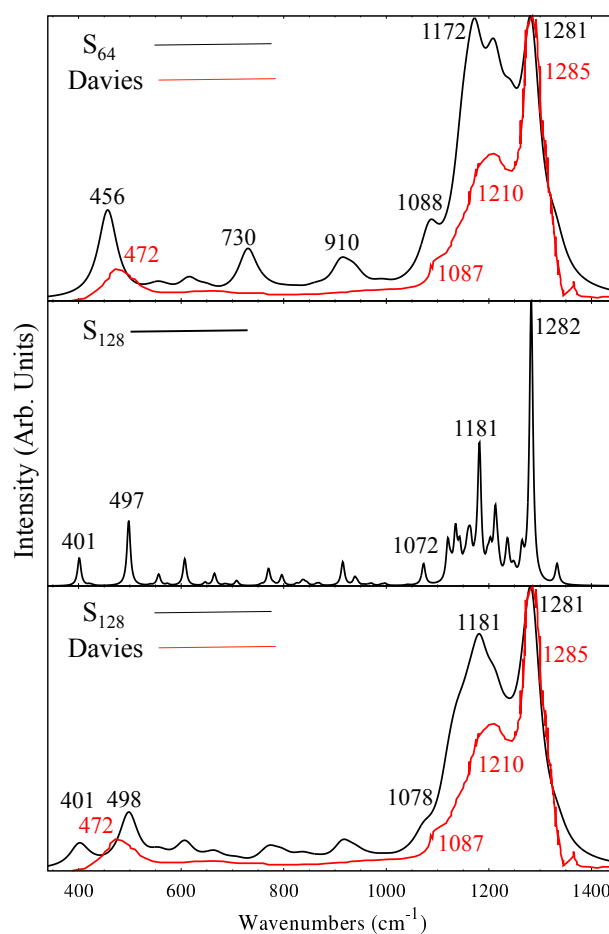


Figure S1: Simulated and experimental IR spectra of the A-center defect in diamond. In the top panel the S_{64} spectrum, computed with a $\text{FWHM}=45 \text{ cm}^{-1}$ is compared with the experimental spectrum reported in Ref. 2 of the manuscript. In the middle panel the simulated IR spectrum of the S_{128} with a $\text{FWHM}=8 \text{ cm}^{-1}$ is shown. Finally, in the bottom panel, the comparison with the experimental spectrum and the S_{128} with a $\text{FWHM}=45 \text{ cm}^{-1}$ is reported.