

THE INFRARED SPECTRUM OF CO₂-Kr, INCLUDING THE INTERMOLECULAR BENDING MODE AND SYMMETRY BREAKING OF THE CO₂ BEND

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The infrared spectrum of CO₂-Kr in the region of the carbon dioxide ν_3 fundamental vibration (near 2350 cm⁻¹) was first studied by Randall *et al.*^a Here we reexamine this spectrum, using a tunable OPO laser source to probe a pulsed supersonic slit jet expansion of a dilute mixture of CO₂ and Kr in helium. The bending combination band, which is observed near 2378 cm⁻¹, yields an intermolecular bending frequency of 29.43 cm⁻¹, in fairly good agreement with a theoretical prediction of 30.02 cm⁻¹ by Chen *et al.*^b

The spectrum of CO₂-Kr in the region of the CO₂ (01¹1) - (01¹0) hot band is also observed, following on our recent study of this transition in CO₂-Ar.^c This gives a measurement of the symmetry breaking of the CO₂ ν_2 bending mode caused by the Kr atom. The out-of-plane mode turns out to be about 1.42 cm⁻¹ higher than the in-plane mode for CO₂-Kr, as compared to splittings of 0.06 cm⁻¹ for CO₂-Ne, 0.88 cm⁻¹ for CO₂-Ar, and 2.14 cm⁻¹ for CO₂-Xe.

^aR.W. Randall, M.A. Walsh, and B.J. Howard, *Faraday Discuss. Chem. Soc.* **85**, 13 (1988).

^bR. Chen, H. Zhu, and D. Xie, *Chem. Phys. Lett.* **511**, 229 (2011).

^cT.A. Gartner, A.J. Barclay, A.R.W. McKellar, and N. Moazzen-Ahmadi, *Phys. Chem. Chem. Phys.* **22**, 21488 (2020).