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The quantitative infrared and NIR spectrum of CH₂I₂ vapor: vibrational assignments and potential for atmospheric monitoring

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Abstract. Diiodomethane (CH₂I₂) has recently become a molecule of significant atmospheric interest as it can contribute to coastal IO formation. As part of the PNNL database of gas-phase infrared spectra, the quantitative absorption spectrum of CH₂I₂ has been acquired at 0.1 cm⁻¹ resolution. Two strong b₂ symmetry A-type bands at 584 and 1114 cm⁻¹ are observed, but are not resolved when broadened to 760 Torr with nitrogen and appear as B-type. In contrast, the b₁ symmetry C-type bands near 5953, 4426 and 3073 cm⁻¹ are resolved with rotational structure, including Q-branches with widths ≤ 1 cm⁻¹. The quantitative infrared and near-infrared vapor-phase spectra (600–10 000 cm⁻¹) are reported for the first time. Some bands are discussed in terms of their potential for atmospheric monitoring and theoretical detection limits on a selected basis. FT-Raman spectra and ab initio calculations are used to complete vibrational assignments in the C_{2v} point group.

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