QUANTITATIVE IR SPECTRA AND VIBRATIONAL ASSIGNMENTS OF CH_2I_2, AN ATMOSPHERIC AEROSOL PRECURSOR

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As part of the Northwest Infrared (NWIR) database of quantitative infrared spectra, we have recently completed quantitative spectra of diiodomethane, CH_2I_2. Photolysis of this molecule in the presence of ozone, O_3, has been suggested as an immediate precursor to new particle formation over the oceans, particularly in coastal areas. Combined with the quantitative medium (0.1 cm^{-1}) resolution vapor-phase IR spectra, liquid-phase IR and FT-Raman spectra, as well as *ab initio* calculations have been used to update and extend the vibrational assignments of earlier workers. Two strong b_2 symmetry A-type bands at 584 and 1114 cm^{-1} are observed, but are not resolved at 760 Torr and appear as B-type. In contrast, the b_1 symmetry C-type bands near 5953, 4426 and 3073 cm^{-1} are resolved with rotational structure, including Q-branches with widths < 1 cm^{-1}. Potential use of these bands for atmospheric monitoring will be discussed.