

QUANTITATIVE IR SPECTRA AND VIBRATIONAL ASSIGNMENTS OF CH₂I₂, AN ATMOSPHERIC AEROSOL PRECURSOR

T.J. JOHNSON, T. MASIELLO, S.W. SHARPE, *Pacific Northwest National Laboratory, P.O. Box 999, MSIN K8-88, Richland, WA 99354.*

As part of the Northwest Infrared (NWIR) database of quantitative infrared spectra, we have recently completed quantitative spectra of diiodomethane, CH₂I₂. Photolysis of this molecule in the presence of ozone, O₃, 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 b₂ 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 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. Potential use of these bands for atmospheric monitoring will be discussed.