TRAJECTORY-BASED SIMULATION OF FAR-INFRARED CIA PROFILES OF CH_4-N_2 FOR MODELING TITAN'S ATMOSPHERE

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Far-infrared opacity of tropospheric and lower stratospheric layers in Titan's atmosphere is dominated by collision-induced absorption (CIA) in various molecular pairs containing N_2, CH_4, and H_2. The presently available spectra of these pairs are often insufficiently accurate for reliably analyzing observed Titan spectra. Analysis of emission spectra from Titan's atmosphere recorded with the Cassini Composite Infrared Spectrometer (CIRS)[a] suggests that the Borysow et al. model[b] for CH_4-N_2 CIA coefficients underestimates absorption by about 50%.

We present the trajectory-based study of the rototranslational CIA band in CH_4-N_2. Assuming rigid monomers, potential energy and induced dipole are characterized quantum-chemically at the CCSD(T)/CCSD(T)-F12b levels of theory. The Monte Carlo strategy is adopted to obtain the dipole autocorrelation function. The original procedure is employed to sample initial conditions throughout the phase space of a molecular pair. The autocorrelation function is derived from an ensemble of 5 to 10 million classical trajectories obtained through the solution of Hamilton equations in the space-fixed reference frame. The Fourier transform of the autocorrelation function yields the CIA band profile. We propose a new semiempirical model for CH_4-N_2 CIA that allows us to reproduce CIRS spectra recorded at low and high emission angles in the equatorial region[a]. This work is partially supported by RFBR-CNRS grant 18-55-16006 and NASA HITRAN grant.

[a] Bézard et al. (2020). Icarus. 344, 113261.

[b] Borysow, et al. (1993). Icarus. 105, 175.