GC2024-STP061

Electronically excited molecular nitrogen in the upper and middle atmospheres of Titan and Earth

Andrey S. Kirillov[1]

[1] Polar Geophysical Institute of the Kola Scientific Center of the Russian Academy of Sciences

kirillov@pgia.ru

Molecular nitrogen N_2 is the main molecular gas in the atmospheres of the Earth, Titan (a moon of Saturn), Triton (a moon of Neptune) and Pluto. In the Earth's atmosphere, the second gas in total concentration is molecular oxygen O_2; in the atmospheres of the other mentioned planets it is methane CH_4. We study the kinetics of the triplet $A^3\Sigma_u^+$, $B^3\Pi_g$, $W^3\Delta_u$, $B'^3\Sigma_u^-$, $C^3\Pi_u$ states of molecular nitrogen at altitudes of the upper (700-1200 km) and middle (50-250 km) atmosphere of Titan during the precipitation of solar UV photons and galactic cosmic rays into the atmosphere. The calculations take into account intramolecular and intermolecular electron energy transfer during inelastic collisions of electronically excited molecular nitrogen with N_2, CH_4 and CO molecules. The interaction constants of electronically excited molecular $N_2(A^3\Sigma_u^+)$ with N_2 and CO molecules are calculated according to quantum chemical approximations and show good agreement with the available experimental data [1]. It is shown that there is a significant contribution of electronically excited N_2 in the excitation of $CO(a^3\Pi)$ at the altitudes of 700-1200 km of the Titan’s upper atmosphere. The interaction of electronically excited N_2 molecules with molecules of methane CH_4, acetylene C_2H_2, ethylene C_2H_4, ethane C_2H_6 in the Titan’s middle atmosphere at altitudes of 50-250 km was studied. The dominance of reactions with metastable molecular nitrogen $N_2(A^3\Sigma_u^+)$ in the formation of C_2H and C_2H_3 radicals at these altitudes was shown for the first time [2]. Similar kinetic calculations involving triplet electron-excited molecular nitrogen were carried out for the Earth’s middle atmosphere of 30-80 km during the precipitation of high-energy relativistic electrons into the atmosphere [3]. The interaction constants of metastable molecular nitrogen $N_2(A^3\Sigma_u^+)$ with oxygen molecules O_2 were calculated and compared with the available experimental data [4]. The emission intensities of the bands of the first positive and second positive N_2 systems during the precipitation of high-energy electrons were calculated. It is shown that there is a significant decrease in the emission intensities of the bands of the first positive system with decreasing altitude due to the influence of collision processes on the populations of vibrational levels of the $N_2(B^3\Pi_g)$ molecule. The influence of intermolecular processes of energy transfer from $N_2(A^3\Sigma_u^+)$ on the formation of singlet oxygen and the emission of the Atmospheric and Infrared atmospheric bands of O_2 at altitudes of the Earth’s middle atmosphere was studied.

[1] A.S. Kirillov, Chem. Phys. Lett. 643 (2016) 131.

[2] A.S. Kirillov, R. Werner, and V. Guineva, Bull. Russ. Acad. Sci.: Physics, 87 (2023) 985.

[3] A.S. Kirillov and V.B. Belakhovsky, Geophys. Res. Lett., 46 (2019) 7734.

[4] A.S. Kirillov and V.B. Belakhovsky, J. Geophys. Res.: Atmos., 126 (2021) e2020JD033177.