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ASSIGNMENT AND MODELING OF THE SPECTRUM OF $^{13}\text{CH}_4$ RECORDED AT 80 K BETWEEN 5853 AND 6200 CM^{-1}

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The absorption spectrum of the $^{13}\text{CH}_4$ methane isotopologue has been recently recorded by Differential Absorption Spectroscopy (DAS) at 80 K in the 5853 – 6200 cm^{-1} spectral range¹. This range corresponds to upper part of the tetradecad dominated by the $2\nu_3$ band near 5988 cm^{-1} . An empirical list of 3700 lines was constructed from the DAS spectrum.

In this work, we present the first rovibrational assignments obtained using two theoretical approaches: (i) variational calculations² using *ab initio* dipole moment surface³ and (ii) calculations based on effective Hamiltonian and effective dipole moment operators. Initial non-empirical effective Hamiltonian for the methane polyads was formed using high-order Contact Transformations (CT)⁴ from an *ab initio* PES⁵.

In total, 2300 lines were assigned to transitions of the tetradecad. Their positions were reproduced with an *rms* deviation of 5×10^{-3} cm^{-1} . About 1300 measured line intensities were modeled using the effective dipole transition moments approach with the *rms* deviation of about 10%. These new data were used for the simultaneous fit of the $^{13}\text{CH}_4$ Hamiltonian parameters of the {ground state / dyad / pentad / octad / tetradecad} system and the dipole moment parameters of the {ground state – tetradecad} system.

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