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ACCURATE FIRST-PRINCIPLES SPECTRA PREDICTIONS FOR ETHYLENE FROM FULL 12D AB INITIO SURFACES

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Knowledge of rovibrational transitions of hydrocarbons (C_2H_4, CH_4) is of primary importance in many fields but remains a formidable challenge for the theory and spectral analysis. Essentially two theoretical approaches for the computation and prediction of spectra exist. The first one is based on empirically-fitted effective spectroscopic models. Several databases aim at collecting the corresponding data but the information about C_2H_4 spectrum present in these databases remains limited, only some spectral ranges around 1000, 3000 and 6000 cm^{-1} being available. Another way for computing energies, line positions and intensities is based on global variational calculations using *ab initio* surfaces. Although they do not yet reach the spectroscopic accuracy, they could provide reliable predictions which could be quantitatively accurate with respect to the precision of available observations and as complete as possible. All this thus requires extensive first-principles quantum mechanical calculations essentially based on two necessary ingredients: (i) accurate intramolecular potential energy surface and dipole moment surface components and (ii) efficient computational methods to achieve a good numerical convergence. We report predictions of vibrational and rovibrational energy levels of C_2H_4 using our new ground state potential energy surface obtained from extended *ab initio* calculations¹. Additionally we introduce line positions and line intensities predictions based on a new dipole moment surface for ethylene. These results are compared with previous works on ethylene and its isotopologues.

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¹T. Delahaye, A. V. Nikitin, M. Rey, P. G. Szalay, and V. G. Tyuterev, *J. Chem. Phys.* 2014, 141, 104301