ACCURATE SPECTROSCOPIC CHARACTERIZATION OF OXIRANE: A VALUABLE ROUTE TO ITS IDENTIFICATION IN TITAN'S ATMOSPHERE AND THE ASSIGNMENT OF UNIDENTIFIED INFRARED BANDS

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Streszczenie

In an effort to provide an accurate spectroscopic characterization of oxirane, state-of-the-art computational methods
and approaches have been employed to determine highly accurate fundamental vibrational frequencies and rotational parameters. Available experimental data were used to assess the reliability of our computations, and an accuracy
on average of 10 cm−1 for fundamental transitions as well as overtones and combination bands has been pointed
out. Moving to rotational spectroscopy, relative discrepancies of 0.1%, 2%–3%, and 3%–4% were observed for rotational, quartic, and sextic centrifugal-distortion constants, respectively. We are therefore confident that the highly accurate spectroscopic data provided herein can be useful for identification of oxirane in Titan’s atmosphere and the assignment of unidentified infrared bands. Since oxirane was already observed in the interstellar medium and some astronomical objects are characterized by very high D/H ratios, we also considered the accurate determination of the spectroscopic parameters for the mono-deuterated species, oxirane-d1. For the latter, an empirical scaling procedure allowed us to improve our computed data and to provide predictions for rotational transitions with a relative accuracy of about 0.02% (i.e., an uncertainty of about 40 MHz for a transition lying at 200 GHz).

Słowa kluczowe

ISM: molecules, line: identification, methods: data analysis, molecular data

Adres publiczny

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