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Accession Number
12189316
Author
Cazzoli G. Puzzarini C. Stopkowicz S. Gauss J.
Author/Editor Affiliation
Cazzoli G. Puzzarini C. : Dipartimento di Chimica G. Ciamician, Universita di Bologna, Via Selmi 2, Bologna I-40126, Italy
Stopkowicz S. Gauss J. : Institut fur Physikalische Chemie, Universitat Mainz, Mainz D-55099, Germany
Title
Precise laboratory measurements of trans-DCOOH and trans-HCOOD for astrophysical observations
Source
Astrophysical Journal Supplement Series, vol.196, no.1, Sept. 2011, 10 (7 pp.). Publisher: IOP Publishing Ltd., UK.
Abstract
The rotational spectra of the mono-deuterated isotopologues of trans-formic acid, trans-DCOOH and trans-HCOOD, were investigated. In the millimeter- and submillimeter-wave frequency regions the Lamb-dip technique was exploited to obtain sub-Doppler resolution and to resolve the hyperfine structure due to the deuterium and hydrogen nuclei, thus enabling the accurate determination of the corresponding hyperfine constants. The experimental determination was supported by high-level quantum-chemical calculations at the coupled-cluster level of theory using large atomic-orbital basis sets. The Lamb-dip measurements were also supplemented by THz Doppler-limited measurements in order to extend the predictive capability of the available spectroscopic parameters to higher frequencies. (46 References).