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标题: The rotational spectra of (HDO)-O-17 and (D2O)-O-17: Experiment and quantum-chemical calculations
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来源出版物: JOURNAL OF CHEMICAL PHYSICS 卷: 137 期: 15 文献号: 154311 DOI: 10.1063/1.4758316 出版年: OCT 21 2012
在 Web of Science 中的被引频次: 0
被引频次合计: 0
引用的参考文献数: 57
摘要: Guided by theoretical predictions, the rotational spectrum of (HDO)-O-17 was recorded and assigned for the first time, while the measurements for (D2O)-O-17 were extended up to the THz region. For both isotopic species, a large portion of the rotational spectrum, from 65 GHz (from 200 GHz for the bideuterated isotopologue) up to 1.6 THz, was investigated, thus allowing the accurate determination of the ground-state rotational and centrifugal-distortion constants. Considering that the rotational spectra of water isotopologues are characterized by a very low density of lines and strong centrifugal-distortion effects, the accurate quantum-chemical prediction of the relevant spectroscopic parameters played a crucial role in the line search and assignment as well as in supporting the fitting procedure. In addition to rotational and centrifugal-distortion constants, the knowledge of the oxygen quadrupole-coupling constants was essential, as the corresponding interaction leads to characteristic features (hyperfine structure) that enabled proper line assignments. (C) 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4758316]
入藏号: WOS:000310307100030
语种: English
文献类型: Article
作者关键词: coupled cluster calculations; ground states; hyperfine structure; isotope effects; quadrupole coupling; rotational states; terahertz wave spectra; water
KeyWords Plus: CORRELATED MOLECULAR CALCULATIONS; GAUSSIAN-BASIS SETS; IUPAC CRITICAL-EVALUATION; ANALYTIC 2ND DERIVATIVES; TRANSITION WAVE-NUMBERS; ANHARMONIC-FORCE FIELDS; CONSISTENT BASIS-SETS; VIBRATIONAL SPECTRA; SEXTUPLE ZETA; ENERGY-LEVELS
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出版商: AMER INST PHYSICS
出版商地址: CIRCULATION & FULFILLMENT DIV, 2 HUNTINGTON QUADRANGLE, STE 1 N O 1, MELVILLE, NY 11747-4501 USA
Web of Science 类别: Physics, Atomic, Molecular & Chemical
研究方向: Physics
IDS 号: 026TX
ISSN: 0021-9606
29 字符的来源出版物名称缩写: J CHEM PHYS

ISO 来源出版物缩写: J. Chem. Phys.
来源出版物页码计数: 9