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Accession number:20123015268740
Title:High resolution spectral analysis of oxygen. I. Isotopically invariant Dunham fit for the X³Σ<inf>g</inf>⁻, a ¹Δ<inf>g</inf>, b¹Σ<inf>g</inf>⁺ states
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Source title:Journal of Chemical Physics
Abbreviated source title:J Chem Phys
Volume:137
Issue:2
Issue date:July 14, 2012
Publication year:2012
Article number:024304
Language:English
ISSN:00219606
CODEN:JCPSA6
Document type:Journal article (JA)
Publisher:American Institute of Physics, 2 Huntington Quadrangle, Suite N101, Melville, NY 11747-4502, United States
Abstract:We have developed a simultaneous global fit to the MW, THz, infrared, visible, and UV transitions of all six oxygen isotopologues, ¹⁶O ¹⁶O, ¹⁶O¹⁷O, ¹⁶O¹⁸O, ¹⁷O¹⁷O, ¹⁷O¹⁸O, ¹⁸O ¹⁸O, with the objective of predicting all transitions below the O(³P) O(³P) dissociation threshold as well as the B ³Σ<inf>u</inf>⁻ state from O(³P)O(¹D) within state-of-the-art experimental uncertainty. Here, we report an isotopically invariant Dunham fit for the lowest three electronic states, X³Σ<inf>g</inf>⁻, a¹Δ<inf>g</inf>, and b¹Σ<inf>g</inf>⁺. Experimental transition frequencies involving these three states of all six O<inf>2</inf> isotopologues were critically reviewed and incorporated into the analysis. For the ¹⁶O¹⁶O isotopologue, experimental data sample vibrational states v 0-31 for X³Σ<inf>g</inf>⁻, v 0-10 for a¹Δ<inf>g</inf>, and v 0-12 for b¹Σ <inf>g</inf>⁺. To the best of our knowledge, this is the first analysis that simultaneously fits spectra from all six O<inf>2</inf> isotopologues. © 2012 American Institute of Physics.
Number of references:133

Main heading:Oxygen
Controlled terms:Spectrum analysis
Uncontrolled terms:Dissociation threshold - Experimental data - Experimental uncertainty - High-resolution spectral analysis - Isotopologues - Transition frequencies - Vibrational state
Classification code:804 Chemical Products Generally - 921 Mathematics - 941 Acoustical and Optical Measuring Instruments - 942 Electric and Electronic Measuring Instruments - 943 Mechanical and Miscellaneous Measuring Instruments - 944 Moisture, Pressure and Temperature, and Radiation Measuring Instruments
DOI:10.1063/1.4719170
Database:Compendex