

## SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE OF 1,3-OXAZOLE FROM MANY ISOTOPOLOGUES

BRIAN J. ESSELMAN, MADELEINE ATWOOD, TAYLOR K. ADKINS, MARIA ZDANOVSKAIA, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI, USA*; MANAMU KOBAYASHI, SHOZO TSUNEKAWA, KAORI KOBAYASHI, *Department of Physics, University of Toyama, Toyama, Japan*; NITAI PRASAD SAHOO, *Department of Chemistry, University of Florida, Gainesville, FL, USA*; JOHN F. STANTON, *Quantum Theory Project, University of Florida, Gainesville, FL, USA*; R. CLAUDE WOODS, ROBERT J. McMAHON, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI, USA*.

The rotational spectrum of 1,3-oxazole (*c*-C<sub>3</sub>H<sub>3</sub>NO, *C*<sub>s</sub>) has been studied from 40 GHz to 750 GHz. Transitions of the main isotopologue and five heavy-atom isotopologues (<sup>15</sup>N, <sup>18</sup>O, and three <sup>13</sup>C) were fit to S- and A-reduced, sextic distorted-rotor Hamiltonians. Rotational spectra have been obtained for several deuterium-enriched samples from 235 to 360 GHz, and rotational constants for more than a dozen deuterium-containing isotopologues have been determined. A highly accurate and precise semi-experimental ( $r_e^{SE}$ ) equilibrium structure of oxazole has been determined using spectroscopic constants for all available isotopologues and CCSD(T) corrections to the rotational constants. Comparison will be made to a CCSD(T)/cc-pCV5Z equilibrium ( $r_e$ ) structure and the  $r_e^{SE}$  structures of other heteroaromatic compounds.