

THE DETERMINATION OF C_0 (OR A_0), D_0^K , H_0^K , AND SOME DARK STATES FOR SYMMETRIC-TOP MOLECULES FROM INFRARED SPECTRA WITHOUT THE NEED FOR LOCALIZED PERTURBATIONS

A. MAKI, 15012 24th Ave. S.E., Mill Creek, WA 98012-5718; T. MASIELLO, National Institute of Standards and Technology, Gaithersburg, MD, 20899-8393; T.A. BLAKE, Pacific Northwest National Laboratory, P.O. Box 999, Mail Stop K8-88, Richland, WA 99352; J.W. NIBLER, Department of Chemistry, Oregon State University, Corvallis, OR 97331-4003; A. WEBER, National Institute of Standards and Technology, Gaithersburg, MD 20899-8393.

Several different combinations of allowed and apparently unperturbed rovibrational transitions are used to obtain the K -dependent rotational constants, C_0 , D_0^K , and H_0^K . A necessary ingredient for the application of this technique is a band with selection rules $\Delta k = \pm 1$, $\Delta l = \mp 2$, and appropriate hot or difference bands. Examples are given for boron trifluoride (BF_3), sulfur trioxide (SO_3), and cyclopropane (C_3H_6) for which there are microwave measurements that provide a check on the derived constants. Examples are also given for the determination of dark states from difference bands, and/or hot bands, and also whole forbidden bands that arise from mixing with distant energy levels.