CRYSTAL FIELD THEORY ANALYSIS OF ROVIBRATIONAL SPECTRA OF CARBON MONOXIDE MONOMERS IN SOLID PARAHYDROGEN

MARIO E. FAJARDO, *AFRL/MNME, Energetic Materials Branch, Ordnance Division, U.S. Air Force Research Lab, 2306 Perimeter Rd., Eglin AFB, FL 32542-5910. mario.fajardo@eglin.af.mil*; TAKAMASA MOMOSE, *Division of Chemistry, Graduate School of Science, Kyoto University, Kyoto, 605-8502, Japan*.

We report our analysis of high-resolution rovibrational infrared absorption spectra of carbon monoxide (CO) molecules isolated in solid parahydrogen (pH_2). Experimental data, comprising roughly a dozen transitions for each isotopomer, are presented for $^{12}C^{16}O$, $^{13}C^{16}O$, $^{12}C^{18}O$, and $^{13}C^{18}O$. Assignments are made using a Hamiltonian derived using crystal field theory for a diatomic rotor in a D_{3h} symmetry single-substitutional trapping site in hexagonal-close-packed solid pH_2. Successful fitting of these spectra requires treating the CO rotational constants (B_e, D_e, α_e) as adjustable parameters; the resulting $B_e(pH_2)$ values are reduced to roughly 80% of their gas phase values.