NEW ELECTRONIC STATES OF YO IN THE UV REGION

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Laser excitation spectra of the yttrium monoxide (YO) molecule in the ultra violet region between the 280 and 320 nm have been recorded and studied using optical-optical double resonance (OODR) spectroscopy. The YO molecule was prepared by the reaction of laser ablated yttrium atom with oxygen under supersonic jet cooled conditions. Thirteen vibration bands have been observed via the intermediate $B^2\Sigma^+$ state from the $X^2\Sigma^+$ state. The excited states analyzed so far are generally in good case (c) coupling scheme. Besides the observation of excited $\Omega = 0.5$ and 1.5 sub-states, and $^2\Sigma^+$ state, we have also identified and studied a forbidden transition, the $[33.7]^4\Sigma^-$ - $B^2\Sigma^+$ transition. Molecular constants for the newly observed electronic states were determined by least squares fitting the measured rotational lines.

A number of low-lying Λ-S states and Ω sub-states of the YO molecule have been calculated using SA-CASSCF (state-averaged complete active space self-consistent field) followed by MS-CASPT2 (multi-state complete active space second-order perturbation theory). Since the active Y 5p shell is very important to get some low-lying electronic states with the correct principal configurations, the active space consists of 7 electrons in 12 orbitals corresponding to the Y 4d5s5p and O 2p shells. The molecular orbitals from Y 4s4p and O 2s are inactive but are also correlated, whereas the lower core-shells are relaxed only by SA-CASSCF and then kept frozen at the CASPT2 level. Spin-orbit coupling (SOC) is treated via the state-interaction (SI) approach with the one-center atomic mean field integral (AMFI) approximation for one- and two-electron spin-orbit integrals. In the SOC calculations of potential energy curves (PECs), the SA-CASSCF wavefunctions are adopted where the diagonal elements in the SOC matrix are replaced by the corresponding MS-CASPT2 energies calculated above. A comparison of the spectroscopic properties of electronic states determined experimentally and from calculations will be presented.