LASER-INDUCED FLUORESCENCE STUDY OF TUNGSTEN MONOXIDE (WO) AND TUNGSTEN MONOSULFIDE (WS)

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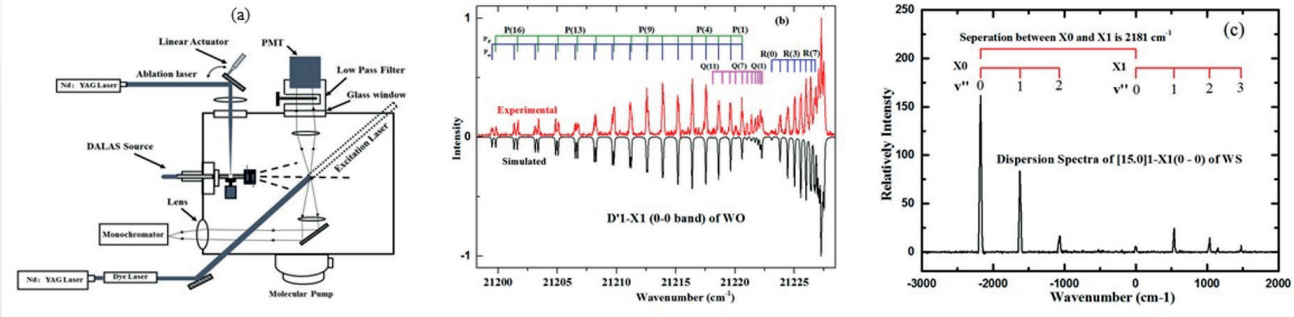
The characters of transition metal compounds WO and WS have partially filled d-electron shell, which give rise to a complex electronic structure with plentiful low-lying electronic states and high multiplicities. The strong spin-orbit interactions lead to complex spectra in which independent assignment of the dominant projection of electronic orbital Λ and electronic spin Σ contributions is difficult. Moreover, the ground state of WO and WS have the $X^3\Sigma^-$ symmtry that contains two components X0 and X1 in Hund's case (c) scheme, but the seperation between these two states are remained unknown up to date.[1-2]



In the present work, we investigated the laser-induced fluorescence (LIF) spectra of jet-cooled WO and WS molecules. Fig.1(a) shows the experimental set-up, the gas phase WO and WS molecules were produced by the reaction to O_2 and SF_6 molecules with the tungsten atoms ablated from a pure tungsten target, respectively. For WO molecule, the electronic transitions to the X0 and X1 states were not experimentally observed in the dispersion spectra. However, based on the e/f spliting of the D'1–X1 (0 – 0) band as shown in Fig.1(b), we can estimate the spin-spin constant λ value is about 212(20) cm^{-1} in the ground state, therefore the separation between X0 and X1 is about $2\lambda = 424$ cm^{-1}. For WS molecule, as shown in Fig.1(c), we experimentally observed the electronic transitions to lower X0 and X1 states in dispersion spectra, and the separation between X0 and X1 states is 2181(1) cm^{-1}, which means that WS molecule has a very strong spin-spin interaction comparing to WO molecule.

References
1. R. S. Ram, Bernath, J. Mol. Spectrosc. 2009, 256, 216 – 227.
2. L.F. Tsang, A.S.-C. Cheung, J. Mol. Spectrosc. 2019, 359, 31 – 36.