Millimeter Wave Spectroscopy of Titanium Monoxide and Titanium Dioxide

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***Abstract*—The pure rotational transitions of titanium monoxide and titanium dioxide have been detected by means of laser-ablation molecular beam millimeter-wave spectroscopy. These submillimeter-wave data were analyzed together with previous low frequency data using Pickett's programs and the precise rotational, leading centrifugal distortion, and fine structure constants were determined.**

I. Introduction And Background

TITANIUM monoxide, TiO, is well known astronomical molecule that exhibits prominent electronic absorption lines in the spectra of M and S stars. But there is no final radio-astronomical detection of TiO towards stellar atmospheres yet. Improved rotational transition frequencies of TiO for an astronomical search in the radio band [1] are presented here.

The recent laboratory detection of TiO_2 in the cm-wave region and its tentative detection in the oxygen-rich supergiant star VY CMa [2] prompted us to record its rotational spectrum in the mm-wave region because it is also possible that titanium forms in space a molecular form different from TiO, e.g. as TiO_2 which can play a role of active material for making high-molecular-weight organic molecules in space [3].

II. Results

The measurements on TiO and TiO_2 were carried out in the frequency range 248-345 GHz using a BWO Cologne spectrometer combined with a laser ablation supersonic jet apparatus. Both species were produced by focusing a Q-switched Nd:YAG laser (1064 nm - Minilite, Continuum) onto a rotating and translating rod of either pure titanium or titanium dioxide and adding small amounts of oxygen to the He buffer gas. The formed species were rotationally cooled to a temperature about 20 K as the plasma expanded adiabatically into the vacuum chamber. The strongest lines were detected with the laser output power 40-45 mJ per pulse and concentration of added oxygen about 1 % for TiO and 2-3 % for TiO_2. For TiO_2, forty-two *b*-type rotational transitions of the main isotopologue $^{48}TiO_2$ (see Figure 1) and six transitions of $^{46}TiO_2$ in natural abundance have been measured up to J = 22 and K_a = 8.

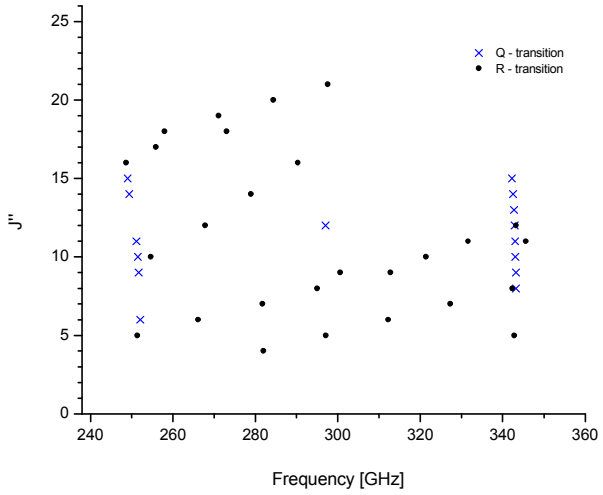

Figure 1: Fortrat diagram of measured transitions of TiO_2 in the ground vibrational state.

The $^3\Delta$ ground electronic state of TiO radical is due to spin-orbit coupling split in to three sublevels $^3\Delta_1$, $^3\Delta_2$, and $^3\Delta_3$. In this study, the rotational transitions with values of J'' from 7 to 10 were measured in sublevels $^3\Delta_1$ and $^3\Delta_2$ and in ground vibrational state. All these transitions were also recorded for three isotopologues ^{46}TiO, ^{48}TiO, and ^{50}TiO (see Figure 2).

The rotational lines were measured using a pair of gated boxcar integrators since it makes possible carry out the time resolved detection of the weak signals and a more subtle numerical evaluation of the spectral background. The numerical fitting of lines was done to the Voigt profile.

The new transitions of TiO_2 have been analyzed together with previously reported low frequency data [2] using Pickett's program suite. A standard *A*-reduced Hamiltonian was used for analysis of this closed shell asymmetric rotor (κ = -0.84) and the set of rotational and leading centrifugal distortion constants was improved and extended.

The spectra of TiO radical were analyzed using Dunham formalism and precise rotational, centrifugal distortion and fine structure constants were determined.

The obtained molecular parameters of TiO and TiO_2 will provide accurate transition frequencies for their future astronomical searches.

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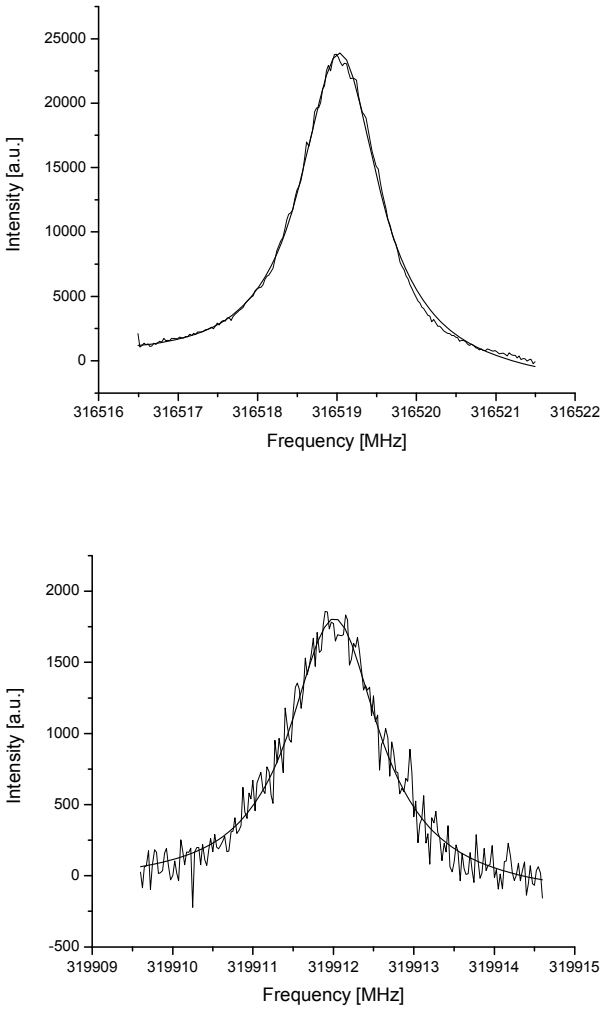

Figure 2: The J = 10 ← 9 e/f pure rotational transition of TiO in $^3\Delta_1$ state. The upper record is a spectrum of main isotopologue ^{48}TiO and lower one of the ^{46}TiO.

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