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On the $e^1\Sigma^+$–$d^1\Sigma^+$ Transition of TiO Related to Cool Star Spectra

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Based on the calculated intensity factors for the bands of the $e^1\Sigma^+$–$d^1\Sigma^+$ transition of the TiO molecule, expected positions of unobserved bands are indicated, for use in studies of cool star spectra. The need for further laboratory investigation of the transition is suggested.

INTRODUCTION

The astrophysical significance of the spectrum of the diatomic TiO molecule is well known, as it is the main feature of the absorption spectra of M-type stars, as well as of sunspot spectra. It is, therefore, important to learn all that is possible, through experimental and theoretical work, regarding the electronic transitions of the molecule.

At the present time, three triplet band systems, involving four triplet states, and five singlet systems, involving six states, have been assigned with certainty, in the region between 3000–12,000 Å. Compared to our knowledge of the triplet systems (Phillips, 1973), far less is known about the singlet transitions. Linton and Nicholls (1969) reported the Morse potential Franck–Condon factors for the $\beta(c^1\Phi$–$a^1\Delta)$, $\delta(b^1\pi$–$a^1\Delta)$ and $\phi(b^1\pi$–$d^1\Sigma)$ systems, in addition to the calculation of the expected positions of unobserved sequences of each system and the assignment of previously unidentified infrared bands to the above systems. It is interesting to note that the assignments of the bands are entirely in agreement with those reported by Lockwood (1969), who, in addition, observed seven bands in the 1-μm region of the spectra of late-type Mira variable stars (stars later than M6).

Following the above studies, it seemed desirable to undertake a similar theoretical study, in order to extend our knowledge of the other two singlet systems ($f^1\Delta$–$a^1\Delta$ and $e^1\Sigma$–$d^1\Sigma$). A single band (0–0) is known (Linton 1972) for the f–a system and therefore, as no equilibrium molecular constants are available, the present paper concerns the e–d system, for which approximate vibrational and accurate rotational constants are available (Phillips and Davis, 1971; Lindgren, 1972; Linton and Singhal, 1974).

RESULTS

For the calculation of intensities of a band system, Franck–Condon factors ($q_{v'v''}$) are required. These, in turn, require a knowledge of the vibrational constants for the states involved. For the present study, accurate vibrational and rotational constants are available for the $d^1\Sigma^+$ state (Pettersson, 1959; Pettersson and Lindgren, 1962). For the $e^1\Sigma^+$ state, the constants used are those reported by Lindgren (1972). It is noted that the vibrational constants for the $e^1\Sigma^+$ state are determined from the observed three bands only and, therefore, they are approximate. Franck–Condon intensity factors are calculated by the method described by Fraser and Jarmain (1953), in which a Morse potential is assumed to represent the electronic states involved. The r-centroids ($\bar{r}_{v'v''}$) of the bands, which will be useful for a study of the variation of the electronic transition moment with internuclear separation, are also evaluated by the method of Nicholls and Jarmain (1956). The calculated values of $q_{v'v''}$ and $\bar{r}_{v'v''}$ for the bands up to $v' = v'' = 0$ to 5 are included in Table 1. The band head (R heads) positions of the unobserved bands of the e–d system are calculated using the well known energy equation for an electronic–vibration transition (Herzberg, 1950). The calculated wavenumbers and wavelengths of the band heads are also included in Table 1, along with the band head assignments.

DISCUSSION

The calculated $q_{v'v''}$ values (Table 1) help to indicate which bands should be present in the e–d system. The magnitude of the Franck–Condon factors of the bands suggests that the intensities of the un-

TABLE 1

Calculated band head data of the $e^1\Sigma^+$–$d^1\Sigma^+$ system of TiO

v'	v''	λ	ν	$q_{v'v''}$	$\bar{r}_{v'v''}$
0	5	5174.0	19321.7	0.006	1.846
1	5	4957.4	20166.2	0.097	1.807
0	4	4924.8	20299.8	0.033	1.801
2	5	4760.3	21001.3	0.223	1.771
1	4	4728.1	21144.0	0.214	1.765
0	3	4696.5	21286.5	0.115	1.759
3	5	4580.2	21827.0	0.007	1.738
2	4	4548.5	21979.1	0.094	1.732
1	3	4517.3	22131.0	0.237	1.726
0	2	4486.5	22282.7	0.263	1.720
4	5	4415.1	22643.3	0.128	1.707
3	4	4383.8	22804.8	0.091	1.701
2	3	4353.0	22966.1	0.010	1.695
1	2	4322.7	23127.2	0.057	1.689
0	1	4292.8	23288.1	0.359	1.683
5	5	4263.2	23450.2	0.007	1.677
4	4	4232.3	23621.1	0.012	1.671
3	3	4201.9	23791.8	0.096	1.665
2	2	4172.0	23962.3	0.169	1.659
1	1	4142.6	24132.6	0.057	1.654
0	0	4113.6	24302.7	0.221	1.648
5	4	4092.5	24428.0	0.105	1.644
4	3	4062.6	24608.1	0.105	1.638
3	2	4033.1	24788.0	0.029	1.631
2	1	4004.0	24967.7	0.024	1.626
1	0	3975.5	25147.2	0.305	1.620
5	3	3933.6	25415.0	0.009	1.611
4	2	3904.5	25604.3	0.016	1.605
3	1	3875.9	25793.4	0.134	1.599
2	0	3847.7	25982.3	0.234	1.593
5	2	3785.2	26411.2	0.093	1.580
4	1	3757.0	26609.7	0.165	1.574
3	0	3729.2	26808.0	0.133	1.568
5	1	3646.4	27416.6	0.125	1.550
4	0	3619.0	27624.3	0.063	1.544
5	0	3516.3	28431.2	0.026	1.522

observed bands of the $\Delta v = +3$, $\Delta v = -1$, $\Delta v = -2$ and $\Delta v = -3$ sequences are comparable with the intensities of the observed 0–0, 1–0, and 2–0 bands. Thus, at least the bands 2–5, 1–4, 0–2, 1–3, 0–1 and 4–1, should be observable in the regions 4760 Å, 4728 Å, 4486 Å, 4517 Å, 4293 Å, and 3757 Å respectively, suggesting that a further search for these bands of the spectrum of TiO is desirable. Therefore, in order to obtain a more complete knowledge of the *e–d* system, a thorough experimental investigation of the wavelengths of the bands in the region 3640–4800 Å is required. This would help to determine the validity of the assignments made in Table 1 and improved wavelength measurements would lead to accurate vibrational constants which in turn would improve the Franck–Condon factors.

Linton and Nicholls (1970) reported measurements of relative band strengths of the α ($c^3\Delta$–$x^3\Delta$) and β ($c^1\Phi$–$a^1\Delta$) transitions and they have shown that in both systems, the variation of the electronic transition moment is negligible and that the band strengths can therefore be represented by the Franck–Condon factors. A successful identification of the bands of the v''-progression of the *e–d* system would enable a study of the band intensity measurements and, hence, the determination of the absolute *f*-values for the bands, as in the case of the α and γ-band systems (Price *et al.*, 1971 and 1974), which are of great use, in spectral studies of cool stars, as well as, in the identification of many unassigned lines in sunspot spectra.

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