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Relative Intensities and Predicted New bands of the A (E − X) and B (D − A) Systems of ZrO

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Values of revised molecular constants for the ground state of the ZrO molecule are used to evaluate the Morse potential Franck-Condon intensity factors and r-centroids for bands of the $E\,^1\Sigma^+ - X\,^1\Sigma^+$ and $D\,^1\Delta - A\,^1\Delta$ transitions. The results suggest the need for further laboratory study of the band systems in the 3500 - 6000 Å wavelength region. Expected positions of unobserved bands are presented for use in spectral studies of cool S-stars.

INTRODUCTION

Since the first identification by Merrill (1922), in spectra of a group of long period variables, the zirconium monoxide molecule has been known as an important constituent of the spectra of S-type stars. During the past fifty-five years, a considerable amount of experimental and theoretical work has been devoted to the study of the ZrO molecule, in view of its astrophysical significance. Up to the present time, seven band systems, three triplet and four singlet, have been identified with certainty in the spectrum of ZrO. Compared to our knowledge of the intense triplet systems, very little is known regarding the weaker singlet systems. However, recent identifications of the singlet band systems in the spectrum of R Cyg (Wyckoff and Clegg, 1978) has provided considerable impetus to the theoretical and experimental studies of these systems.

Nicholls and Tyte (1967) reported the Morse Franck-Condon factors and r-centroids for the triplet (α, β and γ) and singlet (A and B) band systems. Using a consistent set of molecular constants, Schoonveld and Sundaram (1974) evaluated new values of Morse FC-factors and r-centroids for the triplet band systems. These new values differ considerably from those of the earlier results.

During the course of a reinvestigation of the spectrum of ZrO, Phillips and Davis (1976) identified eighteen new bands in the 5849 - 8341 A region of the 6495 A (e - X) system. This study resulted in providing accurate molecular constants for the ground state of the molecule. The new vibrational constants differ considerably from those reported by Afaf (1950b). Since the results on the A and B systems by Nicholls and Tyte were based on the molecular constants of Afaf, it is considered desirable to present new values of FC-factors using the improved molecular constants. The results are used to explain the intensity distribution of bands in the systems.

CALCULATIONS AND RESULTS

Molecular constants for the A and B systems used in the present study are given in Table 1. FC-factors are calculated by the method (Fraser and Jarmain, 1953) which involves the use of a Morse model molecular potential function. As a check on the validity of the Morse potential function, the values of α_e are calculated using the Pekeris's (1934) relation. The calculated values of α_e (0.001914 and 0.002 cm^{-1} for the $X\,^1\Sigma^+$ and $E\,^1\Sigma^+$ states, respectively) are found to be in good agreement with the experimental values (0.001954 and 0.0019 cm^{-1}), thus indicating that the Morse potential function is a very good approximation for these states. The values of r-centroids (representing the characteristic internuclear separation for the (v′, v″) transition), which are useful for a study of the variation of electronic transition moment with internuclear distance, are also evaluated by the method described by Nicholls and Jarmain (1956). If it is assumed that the electronic transition moment is constant, the relative band strengths can be represented by the Franck-Condon factors. Presented in Tables 2 and 3, are the values of $q_{v'v''}$, $\bar{r}_{v'v''}$ and $\lambda_{v'v''}$ (experimentally ob-

TABLE 1
Molecular constants for the X $^1\Sigma^+$, A $^1\Delta$, D $^1\Delta$ and E $^1\Sigma^+$ states of ZrO*

State	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	B_e (cm^{-1})	α_e (cm^{-1})	r_e (Å)
X $^1\Sigma^+$	976.51	3.462	0.423608	0.001954	1.711911
A $^1\Delta$	938.1	1.80	0.4173	0.0012	1.725
D $^1\Delta$	839.2	2.56	0.3986	0.0021	1.764
E $^1\Sigma^+$	843.27	3.04	0.3951	0.0019	1.772

* Molecular constants for the X $^1\Sigma^+$ state are from Phillips and Davis (1976); for states A $^1\Delta$ and D $^1\Delta$ are from Afaf (1950a) and Akerlind (1956); for the E $^1\Sigma^+$ state are from Uhler and Akerlind (1956).

served band head positions) for the A and B systems respectively.

DISCUSSION

A, (E $^1\Sigma^+$ - X $^1\Sigma^+$) 3682 Å system

It may be seen from Table 2 that the (0,0) band is the most intense band followed by the bands of the $\Delta v = \pm 1$, ± 2 and ± 3 sequences. From the magnitude of the FC-factors, it may be concluded that the band (0,4) and beyond in the v″ -progression with v′ = 0 and the band (4,0) and beyond in the v′ - progression with v″ = 0 are unlikely to be observed experimentally. This conclusion is consistent with the experimental study of the system. However, it is interesting to note that the intensities of unobserved (2,5), (0,2), (3,5), and (5,3) bands are comparable with those of the observed bands. Thus, additional bands of the $\Delta v = \pm 2$ and ± 3 sequences are expected, suggesting a search for these bands in the ultraviolet spectrum of ZrO. In order to assist in the search for new bands, the expected band head positions are calculated using the molecular constants given in Table 1. The results are presented in Table 4. The regions 3500 - 3560 Å and 4000 - 4200 Å, as seen from Table 4 (column 2), are of particular interest during a reinvestigation of the spectrum of ZrO.

TABLE 2
Franck-Condon factors, r-centroids and observed band heads for bands of the A (E $^1\Sigma^+$ - X $^1\Sigma^+$) system of ZrO*

	v″					
v′	0	1	2	3	4	5
0	0.513	0.349	0.112	0.022	0.003	—
	1.744	1.792	1.841	1.890	1.940	—
	3682.1	3818.3				
1	0.333	0.055	0.319	0.213	0.066	0.012
	1.703	1.751	1.799	1.847	1.896	1.946
	3572.0	3700.1	3836.4	3981.5		
2	0.117	0.281	0.008	0.181	0.257	0.119
	1.661	1.710	1.757	1.805	1.853	1.902
	3468.9	3589.9		3854.2	4000.7	
3	0.030	0.204	0.141	0.082	0.063	0.244
	1.619	1.668	1.716	1.764	1.811	1.859
		3486.7	3607.6			
4	0.006	0.081	0.222	0.037	0.146	0.006
	1.576	1.627	1.676	1.723	1.771	1.818
		3390.0	3504.2		3754.7	
5	—	0.023	0.131	0.182	0.036	0.160
	—	1.584	1.635	1.683	1.730	1.777
			3407.9			3772.9

* First entry: Franck-Condon factor, $q_{v'v''}$. Second entry: r-centroid, $r_{v'v''}$ (Å). Third entry: Band head, $\lambda_{v'v''}$ (Å).

TABLE 3
Franck-Condon factors, r-centroids and observed band heads for bands of the B ($D\ ^1\Delta$ - $A\ ^1\Delta$) system of ZrO*

	v″					
v′	0	1	2	3	4	5
0	0.759	0.208	0.030	0.003	—	—
	1.748	1.818	1.883	1.946	—	—
	5185.3	5448.9				
1	0.210	0.395	0.309	0.075	0.010	—
	1.678	1.756	1.824	1.889	1.952	—
	4969.8	5212.2	5478.4			
2	0.029	0.314	0.171	0.336	0.124	0.023
	1.591	1.687	1.763	1.831	1.895	1.958
		4996.3	5240.2			
3	—	0.073	0.344	0.052	0.313	0.170
	—	1.604	1.696	1.771	1.838	1.902
		4798.9	5023.0			
4	—	0.009	0.123	0.323	0.005	0.262
	—	—	1.617	1.705	1.778	1.845
5	—	—	0.021	0.169	0.273	0.003
	—	—	—	1.629	1.714	1.786

* Entries: as in Table 2.

As regards observational studies of the 3682 Å system, it may be noted that the (0,0), (1,0) and (2,1) bands have been identified in the spectra of R And and *o* Ceti. Merrill (1947) discovered the 3682 Å band in the spectrum of R And and Joy (1947) observed the band in *o* Ceti (1947). Herbig (1949) established the identity of the band, as the (0,0) band of a $^1\Sigma$ - $^1\Sigma$ transition. Herbig further proposed the absorption feature at 3571 Å observed in the spectrum of R And, as due to the (0,0) band of OH^+. Subsequently, Afaf (1950b) identified this absorption feature with the (1,0) 3571.9 Å band of the A system. In addition, Afaf observed a band at 3590 Å in the spectrum of R And, and identified it with the (2,1) band of the A system. It is of considerable interest to note that the (0,1) and (1,2) bands of the A system are more intense than those of the observed (1,0) and (2,1) bands (see Table 2). Thus, the possible presence of the (0,1) and (1,2) bands at 3818 Å and 3836 Å respectively, in the spectra of cool stars (especially, spectra of S stars near minimum light) may not be ignored. It is expected that the band positions given in Table 4, may be helpful in identifying any new absorption features in the spectra of S-stars.

B, (D $^1\Delta$ - A $^1\Delta$) 5185 Å system

The change of Δr_e of the internuclear separation for this transition is very small (0.039 Å). The

TABLE 4
Predicted intense bands (R-heads) of the A ($E\ ^1\Sigma^+$ - $X\ ^1\Sigma^+$) and B ($D\ ^1\Delta$ - $A\ ^1\Delta$) systems of ZrO

Band		A system Wavelength (λ,Å)	B system Wavelength (λ,Å)
v′	v″		
4	2	—	4824.7
5	3	3521.6	4851.3
6	4	3539.3	4878.6
7	5	3557.1	4906.5
4	3	—	5050.7
5	4	—	5078.9
6	5	—	5107.9
7	6	—	5137.6
3	3	3736.4	—
2	3	—	5507.8
3	4	3873.7	5538.2
4	5	—	5569.5
5	6	—	5601.6
6	7	—	5634.6
0	2	3964.2	—
2	4	—	5803.1
3	5	4020.5	5835.7
4	6	4039.3	5869.2
5	7	4058.2	5903.6
2	5	4158.5	—
3	6	4177.6	—
4	7	4196.7	—

primary Condon locus is therefore very narrow and q_{00} is the largest factor for this band system. Thus, it is seen from Table 3 that the (0,0) band is the most intense band followed by the bands of the $\Delta v = \pm 1$ and ± 2 sequences. Afaf (1950a) observed only nine bands in the 4790 - 5480 Å region, with the 5185 Å band as the (0,0) band of the B system. However, for this band system also, many new bands of the $\Delta v = \pm 1$ and ± 2 sequences are yet to be observed, as indicated by the magnitude of the FC-factors. Expected positions of the intense bands are calculated and the results are given in Table 4 (column 3). It is seen that the wavelength regions 4820 - 4910 Å, 5050 - 5140 Å, 5500 - 5640 Å and 5800 - 5910 Å are of considerable interest during a reinvestigation of the spectrum of ZrO. A successful identification of new bands of this system would improve the molecular constants, which in turn would provide accurate data of transition probabilities. It may, however, be noted that a search for new bands of the B system would require high resolution spectrograms, as the blue and yellow regions of the spectrum are dominated by the intense triplet (α and β) band systems of ZrO.

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