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VIBRATIONAL ANALYSIS OF G -X SYSTEM OF K_2 MOLECULE

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Abstract

The ultraviolet band spectra of K_2 molecule has been investigated in the absorption in the region 3070-3890Å using a 3.4 m Ebert spectrograph in the first order giving reciprocal desperation of 5.1Å mm^{-1}. The spectrum was recorded with an exposure time of 20 to 30 minutes on Kodak X-Omat X-ray plates. A high pressure xenon arc (450 W) served as the background source. The E-X, F-X and G-X systems have been reproduced. This work reports the vibrational analysis of G-X system. A number of bands have been discovered in the G-X system, which are not reported previously. Vibrational analysis was performed using computer programming.

Keywords: Band spectra, Vibrational analysis, K_2 molecule

Introduction

Seven electronic states of the K_2 molecule have been studied so far. McLennan and Ainslie (1923) in the visible region made the first observation of K_2 spectrum. Yamamoto (1929) studied the C-X system. Later Crane and Christy (1930) analysed A-X system. Loomis (1931) Loomis and Nusbaum (1932) and later on Tango *et. al.* (1970) extended this study to the rotational and vibrational structure of B -X system in the red region. The D-X system was observed by Sinha (1948). Yoshinaga (1937) was the first to report several systems named E-X, F-X and G-X in the ultraviolet region. Later Sinha (1950) also recorded these systems, however, found the analysis of Yoshinaga (1937) unsatisfactory and reanalysed E-X system. The band heads of F-X and G-X systems were measured but left out without analysis. Khalid *et. al.* (1998) recorded the ultraviolet band spectra of K_2 molecule in the region 3070 - 3890Å. This work reports the observation of the E-X, F-X, G-X systems and a new system named H-X in absorption. It is worthwhile to note that all the known systems are degraded toward red. In the present work a study of G-X system was undertaken in the region 3416-3553Å and observed the new bands which are not reported previously, and vibrational analysis has been done using computer methods.

Experiment

The spectra of K_2 molecule were recorded in absorption. Spectroscopically pure potassium was heated in a 1.5m long furnace to about 600°C in an atmosphere of hydrogen. The hydrogen pressure was 400 toor. The spectrogram was taken in the first order on a 3.4m Jarrel-Ash plane grating spectrograph with reciprocal dispersion of about 5.1Å mm^{-1}. Exposure time ranged from 20 to 30 minutes on Kodak X-Omat X-ray plates. A high current xenon arc (450W) was used as background source. The measurement of the plates was made by comparison with the iron arc lines, the wavelengths being taken from the MIT wavelength tables (Harrison 1939). A polynomial fitting computer programming was used to obtain the wavelengths and was estimated to be accurate to ± 0.5Å. The vacuum wave numbers of the wavelengths were obtained from the data of Coleman *et. al.* (1960).

A comparison of band heads position of G-X system is given in Table-1 The vibrational assignments, calculated and measured position of band heads are reported in Table -2.

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Result and discussion

The spectra of G-X system of K_2 molecule have been recorded which lie in the region of 3416-3553Å and contains bands degraded towards red. This system consists of eleven bands. In the present work, assignments of vibrational quantum numbers have been calculated. Some of the band heads were not measurable due to masking by the atomic lines and diffuse structure. This system contains five new bands. Correlation diagram and Morse potential curves have already been drawn by Khalid *et al.* (1998). In this diagram the F-state dissociates into 4 ^2D + 4 ^2S and G-state dissociates 6 ^2S + 4 ^2S. Morse potential curves suggest that F and G states are predissociated by E-state resulting in the diffuse appearance of both the systems. However, further work in higher order would bring further information.

Table 1: Comparison of band heads/position of G-X system.

S. No	λ Authors Å	λ Sinha(1950) Å
1	3552.2	3552.5
2	3545.2	3545.4
3	3539.5*	-
4	3535.3	3537.5
5	3532.3*	-
6	-	3529.9? **
7	3526.1*	-
8	3519.1	3520.0
9	-	3511.7? **
10	3508.0*	-
11	-	3505.0? **
12	3502.9	3503.3
13	-	3501.1**
14	3491.1	3491.1
15	-	3483.6**
16	-	3474.6**
17	-	3461.8**
18	-	3451.6**
19	-	3441.5**
20	-	3434.3**
21	-	3429.9**
22	3416.8*	-

* New bands observed

** Too weak to be measure

Table 2: The vibrational assignments

Band (v', v")	$\bar{v}$ meas. (cm^{-1})	$\bar{v}$ calc. (cm^{-1})
(7, 4)	28143.53	28138.45
(8, 4)	28199.42	28194.55
(11, 5)	28260.72	28267.06
(16, 8)	28244.67	28250.37
(13, 6)	28279.84	28280.73
(10, 4)	28302.23	28303.45
(11, 4)	28352.04	28356.25
(12, 4)	28408.50	28407.95
(14, 4)	28498.14	28508.05
(13, 3)	28539.68	28548.30
(15, 3)	28636.43	28646.20

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