ISOTOPIC LINES OF SiO IN SUNSPOTS

(*Research Note*)

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Abstract: As the isotopic shift for the vibration rotation band is generally much larger than the isotopic shift for the corresponding electronic transitions and thus facilitating separation of isotopic lines, the vibration rotation bands of SiO may find use in the determination of isotopic abundance ratio $Si^{28} : Si^{29} : Si^{30}$. To help identify the isotopic lines of SiO the wavenumbers for $Si^{29}O^{16}$ and $Si^{30}O^{16}$ have been calculated with an uncertainty of ± 0.05 cm^{-1}.

   Taking note of the fact that SiO shows strong vibration rotation bands in the spectra of some cool stars the equivalent width calculations for P(40) and R(40) lines of the 1–0 and 2–1 vibration rotation bands of $Si^{29}O^{16}$ and $Si^{30}O^{16}$ have been made at the centre of the disc for the model ZSM-74 using two values of isotopic abundance ratio and three values of dissociation energy.

   The search for the isotopic lines of SiO near 7 to 8 μm is recommended in low noise centre to limb sunspot spectrum scans with a view to help improve the isotopic ratio $Si^{28} : Si^{29} : Si^{30}$ and oscillator strengths for the vibration-rotation transitions.

1. Introduction

The molecule SiO shows strong vibration rotation bands in the spectra of some cool stars (Cudaback *et al.*, 1971; Wollman *et al.*, 1973; Beer *et al.*, 1974) and recently Gaur *et al.* (1978) have predicted a possible occurrence of the 1–0 and 2–1 vibration rotation bands of SiO near 7–8 μm in the sunspot spectrum.

   These vibration rotation bands in appropriate regions in the infrared may prove useful in estimating the isotopic ratio $Si^{28} : Si^{29} : Si^{30}$ from the observations of stellar and sunspot spectra. Our aim in the present communication is to give the wavelengths for the lines of the 1—0 and 2—1 vibration rotation bands of $Si^{29}O^{16}$ and $Si^{30}O^{16}$ arising from the ground electronic state $X^1\Sigma^+$, and to discuss the feasibility of detecting these lines in the infrared region of the sunspot spectrum.

   The only effort towards a determination of isotopic abundance ratio $Si^{28} : Si^{29} : Si^{30}$ in the sunspot spectrum has been made by Lambert and Mallia (1970). For this purpose, they utilised the 0—0 band of the electronic transition $A^2\Delta - X^2\Pi$ of SiH in the sunspot spectrum near 414 nm. An inspection of Table II in that paper shows that the strongest lines of $Si^{28}H$ found by them have equivalent widths ≤ 9 mÅ. For a Doppler broadened profile the central depth is $R_0 = [W/\sqrt{\pi}]/\Delta\lambda_D$ where W is equivalent width and $\Delta\lambda_D$ is Doppler width. R_0 is $<30\%$ in case of the lines of SiH corresponding to equivalent widths of <9 mÅ near 410 nm. In contrast, the central depths of the strongest lines of vibration rotation bands of SiO are $R_0 < 12$ to 18% corresponding to equivalent widths in the range 65 to 95 mÅ as predicted by Gaur *et al.* (1978). However, the advantage in selecting the vibration rotation bands is that

the isotopic shifts for the vibration rotation bands are generally much larger than the isotopic shifts for the electronic transitions, thus facilitating a separation of isotopic lines.

2. Calculation of the Isotopic Shifts

For $Si^{28}O^{16}$ the wavenumber calculations for the 1—0 and 2—1 vibration rotation bands of SiO have been reported by Singh (1975). Utilizing Equation (2) as given by Singh (1975), and the following useful relations (Herzberg, 1950) for modified molecular constants: $\omega_e^i = \rho\omega_e$; $(\omega_e x_e)^i = \rho^2\omega_e x_e$; $(\omega_e y_e)^i = \rho^3\omega_e y_e$; $B_e^i = \rho B_e$; $\alpha_e^i = \rho^3\alpha_e$; $D_e^i = \rho^4 D_e$; $\beta_e^i = \rho^5\beta_e$ the wavenumbers for the isotopic lines were calculated. Here the superscript i refers to the isotope and the quantity ρ is given by $\rho^2 = \mu|\mu_i$, where the reduced mass μ of a molecule ab is given by, $\mu = (m_a m_b)/(m_a + m_b)$.

The molecular constants have been adopted from Singh (1975) and the accuracy of the calculated wavenumbers would, therefore, be the same as found by Singh (1975) i.e. there is an uncertainty of ± 0.05 cm^{-1} in the calculated wavenumbers. To facilitate easy calculation of the isotopic shift $\Delta\sigma = \sigma(Si^{28}O^{16}) - \sigma(^iSiO^{16})$ for the P and R branches of the 1—0 and 2—1 vibration rotation bands of $Si^{29}O^{16}$ and $Si^{30}O^{16}$, $\Delta\sigma$ has been expressed by the polynomial expression of the type $\Delta\sigma = a + bJ + cJ^2$. The values of a, b, and c are tabulated in Table II for various cases.

3. Equivalent Width Calculations

The method adopted for equivalent width calculations of the isotopic lines is the same as used by Gaur *et al.* (1978). The three values of dissociation energy viz. $D_0 = 8.33$ eV (Glushko *et al.*, 1962), 8.1 eV (Tsuji, 1964) and 7.93 eV (Hilderbrand and Murad, 1969) and the model ZSM-74 (Zwaan, 1974) have also been used by us. The *JANAF Thermochemical Tables* (Stull *et al.*, 1970) use a $D_0 = 8.24 \pm 0.13$ eV which falls in the range 8.10–8.33 eV adopted by us. The reason for selecting the model ZSM-74 is that this model appears to be a more refined continuum based model than its predecessors (Zwaan, 1974).

The $P(40)$ and $R(40)$ lines of the 1—0 and 2—1 vibration rotation bands of $Si^{29}O^{16}$ and $Si^{30}O^{16}$ were selected for equivalent width calculations at the centre of the disk in the model ZSM-74 using oscillator strengths from Hedelund and Lambert (1972).

Two values for the isotopic abundance ratio $Si^{28} : Si^{29} : Si^{30}$ were adopted, viz., the terrestrial value as quoted by Greenstein (1966) and the upper limit for this ratio as given by Lambert and Mallia (1970). The former author gives this ratio as 92 : 5 : 3 and the latter authors as 1 : 0.2 : 0.15. The results are summarised in Table I.

4. Discussions

An inspection of Table I shows that even in the least favourable case ($D_0 = 7.93$ eV

TABLE I

Computed equivalent widths of selected lines of the vibration rotation bands of $Si^{29}O^{16}$ and $Si^{30}O^{16}$ for ZSM-74

Band	Line	$D_0 = 8.33$ eV		$D_0 = 8.10$ eV		$D_0 = 7.93$ eV	
		L.M.	G	L.M.	G	L.M.	G
Equivalent width in mÅ of $Si^{29}O^{16}$							
1—0	P(40)	26.4	7.1	12.0	3.2	6.7	1.8
1—0	R(40)	24.9	6.9	11.3	3.1	6.3	1.7
2—1	P(40)	31.5	8.4	14.3	3.8	7.9	2.1
2—1	R(40)	31.2	7.6	14.2	3.5	7.9	1.9
Equivalent width in mÅ of $Si^{30}O^{16}$							
1—0	P(40)	19.8	4.3	9.0	1.9	5.0	1.1
1—0	R(40)	18.7	4.1	8.5	1.9	4.7	1.0
2—1	P(40)	23.6	5.0	10.7	2.3	5.9	1.3
2—1	R(40)	23.4	4.6	10.7	2.1	5.9	1.1

and isotopic abundances from Greenstein (1966)), weak lines with equivalent widths of ≤ 2 mÅ are expected for the isotopic molecule $Si^{29}O^{16}$ and the lines of the $Si^{30}O^{16}$ are still fainter. However, the referee has kindly pointed out that presently the value of dissociation energy of SiO appears to be well determined and closely corresponds to the case $D_0^0 = 8.33$ eV considered by us. Further, since observations show that the solar isotopic abundance ratios, for the elements C, O, Mg, and Ti are consistent with the terrestrial case (cf., Hall, 1970; Sotirovski, 1971; Lambert and Mallia, 1972), it seems that the Lambert and Mallia's (1970) upper limit for the isotopic ratios of Si may not be valid. Under these circumstances, column G in Table I for $D_0^0 = 8.33$ eV seems to be the most probable case for the detection of isotopic SiO lines, if the model ZSM-74 and the oscillator strengths adopted by us are acceptable. Thus, a search for the isotopic lines of 2—1 and 1—0 vibration rotation bands of SiO in the regions near 7.0 to 8.0 μm is recommended since it will help in improving the isotopic ratio $Si^{28}:Si^{29}:Si^{30}$ and oscillator strengths for the vibration rotation transitions. Since the central depth of the strongest isotopic lines of the vibration rotation bands of SiO would probably be <1.8%, centre to limb scans with good signal to noise ratio would be required in such a search.

Regarding the limitations of the model chosen by us at this stage we can only say that the model ZSM-74 appears to be a refined version over its predecessors as discussed by Zwaan (1974) himself. We may add here that this model seems to explain the observed rotational temperature of TiO (Sinha, 1977). So, only somewhat hotter and/or somewhat cooler models than ZSM-74 seem plausible to us. Therefore, the molecular abundances calculated by us for the ZSM-74 and a relatively hotter model (Zwaan, 1965) were compared to assess the model effect. The overall SiO abundance decreases by a factor of 1.5 in the hotter (Zwaan, 1965)

model. Consequently, in hotter models the selective opacity due to SiO will decrease and the observations of the normal SiO vibration rotation lines and isotopic vibration rotation lines may also help in refining the ZSM-74 model.

A search of these isotopic lines in the spectra of cool stars is also recommended.

TABLE II

The values of the coefficients a, b, and c used in the polynom for wavenumber calculations

Band		$Si^{30}O^{16}$		$Si^{29}O^{16}$	
		P	R	P	R
	a	14.7847	14.8831	7.6251	7.7074
1—0	b	$-3.6816(-2)$	$3.1596(-2)$	$-1.9717(-2)$	$1.4875(-2)$
	c	$-1.1572(-4)$	$-1.5805(-4)$	$-3.8772(-5)$	$-6.0988(-5)$
	a	14.3835	14.5120	7.3634	7.4742
2—1	b	$-3.1615(-2)$	$3.6719(-2)$	$-1.4891(-2)$	$2.0307(-2)$
	c	$-1.4987(-4)$	$-2.3547(-4)$	$-6.9030(-5)$	$-1.4205(-4)$

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