

SHORT COMMUNICATIONS

POTENTIAL ENERGY CURVES OF D STATES OF SiF AND SiCl

J. B. BHARTIYA and S. H. BEHERE*

Department of Physics, S. B. Science College,
Aurangabad 431001, India.* Department of Physics, Marathwada University,
Aurangabad 431004, India.

THE emission spectrum of SiF has shown a number of electronic states, a few of them being Rydberg states. The potential energy curves of $X^2\pi$, $A^2\Sigma$, $B^2\Sigma$ and $C^2\Sigma$ states have been reported by Singh and Rai¹. Later Ramkrishnarao *et al*² also reported the potential energy curves of $X^2\pi$, $A^2\Sigma$, $A^4\Sigma$, $B^2\Sigma$, $C^2\Delta$, $C'^2\pi$, $D'^2\pi$ and $D^2\Sigma$ states of SiF and estimated the dissociation energy by curve-fitting method in which Hulbert-Hirschfelder³ potential (H-H potential) function was used for the ground state. Recent analysis⁴ of D-X transition of SiF yielded accurate constants compared with those of earlier workers. We have used these constants for the construction of RKR⁵ curves.

The spectrum of SiCl was studied by many workers earlier. Venkataramanaiah and Lakshman⁶ reported the potential energy curves of $X^2\pi$, $B^2\Sigma$, $B'^2\Delta$ and $C^2\pi$ states of SiCl and estimated the dissociation energy of SiCl by curve-fitting method using the H-H potential function for the ground state. The high resolution studies of D-X transition⁷ of SiCl have reported constants of $D^2\Sigma$ state. These constants of the D state of SiCl are used in the present case for the construction of RKR curves.

The molecular constants of the D states of SiF and SiCl are presented in table 1 and the RKR turning points are presented in table 2 respectively.

We have also applied the H-H potential function to the ground states of SiF and SiCl, with revised constants and the dissociation energies are estimated. In the case of SiF the Value of D_0^0 we obtained is 4.75 ± 0.011 eV and for SiCl it is 4.09 ± 0.017 eV. These

Table 1 Molecular Constants* $D^2\Sigma$ states

| Molecule | ω_e | $\omega_e x_e$ | α_e | r_e | B_e |
|----------|------------|----------------|------------|--------|----------|
| SiF | 1001.77 | 5.499 | 0.004794 | 1.5456 | 0.62358 |
| SiCl | 655.98 | 2.85 | 0.001568 | 1.9582 | 0.282792 |

* All constants are in cm^{-1} except r_e which is in A° unit.Table 2 RKR turning points and energy values. SiF $D^2\Sigma$ state
 $T_2 = 47419.64 \text{ cm}^{-1}$

| v | $G(v)$ (cm^{-1}) | $G(v) + T_e$ (cm^{-1}) | r_{min} (A°) | r_{min} (A°) |
|-----|--------------------------------|--------------------------------------|-----------------------------------|-----------------------------------|
| 0 | 499.01 | 47918.65 | 1.4937 | 1.6029 |
| 1 | 1488.78 | 48908.42 | 1.4592 | 1.6493 |
| 2 | 2467.56 | 49887.20 | 1.4369 | 1.6835 |
| 3 | 3435.33 | 50854.97 | 1.4197 | 1.7128 |
| 4 | 4392.11 | 51811.75 | 1.4054 | 1.7394 |
| 5 | 5337.89 | 52757.53 | 1.3931 | 1.7641 |
| 6 | 6272.67 | 53692.31 | 1.3822 | 1.7874 |
| 7 | 7196.46 | 54616.10 | 1.3726 | 1.8098 |
| 8 | 8109.24 | 55528.88 | 1.3635 | 1.8315 |
| 9 | 9011.03 | 56430.67 | 1.3553 | 1.8525 |
| 10 | 9901.82 | 57321.46 | 1.3477 | 1.8731 |

SiCl $D^2\Sigma$ state $T_e = 44843.63 \text{ cm}^{-1}$

| v | $G(v)$ (cm^{-1}) | $G(v) + T_e$ (cm^{-1}) | r_{min} (A°) | r_{min} (A°) |
|-----|--------------------------------|--------------------------------------|-----------------------------------|-----------------------------------|
| 0 | 327.28 | 45170.91 | 1.9031 | 2.0183 |
| 1 | 977.56 | 45821.19 | 1.8660 | 2.0662 |
| 2 | 1622.14 | 46465.77 | 1.8418 | 2.1012 |
| 3 | 2261.02 | 47104.65 | 1.8228 | 2.1310 |
| 4 | 2894.20 | 47737.83 | 1.8070 | 2.1576 |
| 5 | 3521.68 | 48365.31 | 1.7933 | 2.1825 |
| 6 | 4143.46 | 48987.09 | 1.7810 | 2.2058 |
| 7 | 4759.54 | 49603.17 | 1.7700 | 2.2280 |
| 8 | 5369.92 | 50213.55 | 1.7600 | 2.2494 |
| 9 | 5974.60 | 50818.23 | 1.7506 | 2.2700 |
| 10 | 6573.58 | 51417.21 | 1.7420 | 2.2902 |

values are in good agreement with the values 4.846 eV and 4.15 eV reported by Ramkrishnarao *et al*² and Venkataramanaiah *et al*⁶ respectively.

14 May 1985; Revised 30 August 1985

1. Singh, R. B. and Rai, D. K., *Indian J. Pure. Appl. Phys.*, 1966, **4**, 102.
2. Ramakrishna Rao, T. V. and Reddy, R. R., *Curr. Sci.*, 1979, **48**, 96.
3. Hulbert, H. M. and Hirschfelder, J. O., *J. Chem. Phys.*, 1941, **9**, 61.
4. Houbrechts, Y., Dubois, I. and Bredohl, H., *J. Phys.*, 1979, **B12**, 2137.
5. Vanderslice, J. T., Mason, E. A., Maisch, W. G. and Lippincott, E. R., *J. Mol. Spectrosc.*, 1960, **33**, 614.
6. Venkataramanaiah, M. and Lakshman, S. V. J., *J. Quant. Spectro. Radiat. Transfer*, 1981, **26**, 11.
7. Bredohl, H., Cornet, R., Dubois, I. and Melen F., *J. Phys.*, 1982, **B15**, 727.