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Journal of Molecular Structure 795 (2006) 9–13

Journal of
MOLECULAR
STRUCTURE

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# The rovibronic energies of the SiNSi radical in its $\tilde{X}^2\Pi_g$ electronic state

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Received 10 July 2005; received in revised form 17 October 2005; accepted 14 February 2006
Available online 19 May 2006

In honor of Dr Gisbert Winnewisser for his many contributions to Science.

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## Abstract

We present the results of a calculation of the rovibronic energies of the SiNSi radical in its $\tilde{X}^2\Pi_g$ electronic ground state. At bent geometries, the electronic degeneracy is split to give a lower state of $A_2$ symmetry and an upper state of $B_2$ symmetry; each state is linear at equilibrium. The rovibronic calculation involves consideration of the Renner effect, and we initially made the calculation using ab initio $A_2$ and $B_2$ potential surfaces. The term values obtained were of help in making vibronic assignments in a newly obtained spectrum of the molecule. Having vibronically assigned the spectrum, we refined the potentials in a fitting to the vibronic term value separations. The optimized potentials allow us, in principle, to predict all rovibronic energies of the $\tilde{X}^2\Pi_g$ state.

*Keywords:* SiNSi; Renner effect; Vibronic energies

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## 1. Introduction

There is considerable contemporary interest in determining the properties of small gaseous silicon nitrides for the purpose of understanding how silicon nitride films are formed in chemical-vapour deposition processes, and for optimizing the production of high performance silicon nitride materials such as $Si_3N_4$. In this paper, we focus on SiNSi. Previous experimental and theoretical studies [1–5] show that the SiNSi molecule has a linear electronic ground state, $\tilde{X}^2\Pi_g$, but no detailed analysis of spectra involving this state has been made (Section 3 of [4]). We provide the basis for that analysis here using the results of a low resolution (experimental precision 3–7 cm$^{-1}$) dispersed laser induced fluorescence spectrum, and of a higher resolution (experimental precision 0.5–1.0 cm$^{-1}$) laser excitation spectrum of SiNSi, both recently obtained by Jakubek et al. [6].

When the SiNSi molecule is bent the $\tilde{X}^2\Pi_g$ state splits into two, giving rise to an upper ($B_2$) electronic state and a lower ($A_2$) electronic state; both states being linear at equilibrium. To calculate the rovibrational energies in such a situation it is necessary to allow for the Renner effect, and in the work reported here we have used our Renner computer program [7–9] with, initially, ab initio $A_2$ and $B_2$ potential energy surfaces. This assisted in the assignment of the vibronic structure in the spectrum, and as a result we assigned 36 vibronic term value separations for the $\tilde{X}$ state. We adjusted the potential surfaces in order to achieve an optimum least squares fitting to the separations. The optimized surfaces that we have obtained can be used to make predictions of any $\tilde{X}$ state rovibronic term value.

## 2. The calculations

Using the program system MOLPRO [10], we made ab initio calculations using the CCSD(T) method [11], with an aug-cc-pVTZ/frozen-core basis set [12,13], at 49 geometries on the lower ($A_2$) state surface and at 40 geometries on the upper ($B_2$) state surface. The calculations covered bending angles from 180 to 80°, and bond lengths from 1.4 to 2.0 Å. The RENNER program uses the analytical expressions given in Eq. (1) below for the two surfaces; we determine the parameters $f^0_{\dots}$ in these expressions by adjusting them to

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doi:10.1016/j.molstruc.2006.02.014

optimize the fitting of the surfaces through the 89 ab initio points.

For SiNSi, the lower and upper potential energy surfaces, $V_{-}(\Delta r_1,\Delta r_3,\bar{\rho})$ and $V_{+}(\Delta r_1,\Delta r_3,\bar{\rho})$, respectively, are written

$$\begin{aligned} V_{\pm}(\Delta r_1,\Delta r_3,\bar{\rho}) = {} & V_0^{(\pm)}(\bar{\rho}) + \sum_j F_j^{(\pm)}(\bar{\rho}) y_j \\ & + \sum_{j\le k} F_{jk}^{(\pm)}(\bar{\rho}) y_j y_k + \sum_{j\le k\le m} F_{jkm}^{(\pm)}(\bar{\rho}) y_j y_k y_m \\ & + \sum_{j\le k\le m\le n} F_{jkmn}^{(\pm)}(\bar{\rho}) y_j y_k y_m y_n, \end{aligned} \tag{1}$$

with

$$y_j = 1 - \exp(-a_1 \Delta r_j), \tag{2}$$

$$F_{jk\ldots}^{(\pm)}(\bar{\rho}) = f_{jk\ldots}^{(0)} + \sum_{i=1}^{N} f_{jk\ldots}^{(i,\pm)} (1-\cos\bar{\rho})^i, \tag{3}$$

and

$$V_0^{(\pm)}(\bar{\rho}) = V_{\mathrm{e}} + \sum_{i=1}^{8} f_0^{(i,\pm)} (1-\cos\bar{\rho})^i. \tag{4}$$

In Eq. (1), $\bar{\rho}$ is the instantaneous value of the bond angle supplement (see Figs. 14 and 15 of Ref. [14]), and $\Delta r_j = r_j - r_{\mathrm{e}}$, where the $r_j$ are the instantaneous N–Si$_j$ bond lengths and $r_{\mathrm{e}}$ is the equilibrium bond length; the indices $j$, $k$, $m$, and $n$ can each be 1 or 3. In Eq. (2), $a_1$ is a molecular parameter. In Eq. (3), the parameters $f_{jk\ldots}^{(0)}$ are common for the two potential energy surfaces and this ensures that the functions are degenerate at linearity when $\bar{\rho}=0$; the function $F_j^{(\pm)}(\bar{\rho})$ has $N=4$, $F_{jk}^{(\pm)}(\bar{\rho})$ has $N=3$, $F_{jkl}^{(\pm)}(\bar{\rho})$ has $N=2$, and $F_{jklm}^{(\pm)}(\bar{\rho})$ has $N=1$. In Eq. (4), $V_{\mathrm{e}}$ is the value of the two potential energy functions at equilibrium. The adjustable parameters $f_{\ldots}^{()}$ in $V_{-}$ and $V_{+}$ are constrained to ensure that $V_{-}$ and $V_{+}$ are totally symmetric under the interchange of $\Delta r_1$ and $\Delta r_3$ which they must be for a symmetrical molecule like SiNSi.

We experienced some difficulty in adjusting the parameters $f_{\ldots}^{()}$ and $a_1$ to fit the surfaces through the ab initio points. The problem was not with the precision of the fitting but rather with the shape of the obtained surfaces; they had unreasonable multiple inflexion points (i.e. 'wiggles') and they extrapolated to wildly high or low values. As a result, we decided to sacrifice the precision of the fitting in order to maintain acceptable smooth surfaces having appropriate qualitative behaviour. With this limitation we found that we could determine 27 parameters and obtain a root mean square deviation of 25 cm$^{-1}$. The values of these parameters are given in Table 1.

Table 1
The ab initio potential energy parameters[a] obtained for the $A_2$ and $B_2$ surfaces of the $\tilde{X}^2\Pi_g$ state of SiNSi (Eqs. (1)–(4))

| | |
|---|---|
| $V_{\mathrm{e}}/E_{\mathrm{h}}$ | −632.7397742 (14)[b] |
| $r_{\mathrm{e}}$ (Å) | 1.648294 (5) |
| $a_1$ (Å$^{-1}$) | 1.8[c] |
| $f_1^{(0)}$ | 0.0 |
| $f_{11}^{(0)}$ | 35071.6 (7.2) |
| $f_{13}^{(0)}$ | 22724 (12) |
| $f_{111}^{(0)}$ | −9101 (97) |
| $f_{113}^{(0)}$ | 8766 (97) |
| $f_{1111}^{(0)}$ | 14359 (23) |
| $f_{1113}^{(0)}$ | −13265 (21) |

| | $A_2$ ($\sigma = -$) | B$_2$ ($\sigma = +$) |
|---|---|---|
| $f_0^{(1,\sigma)}$ | 3273.1 (6.7) | 12181 (10) |
| $f_0^{(2,\sigma)}$ | 9100 (30) | 8715 (72) |
| $f_0^{(3,\sigma)}$ | −9441 (43) | 317 (167) |
| $f_0^{(4,\sigma)}$ | 12953 (19) | 7281 (116) |
| $f_1^{(1,\sigma)}$ | −3852.0 (6.8) | −8253 (17) |
| $f_1^{(2,\sigma)}$ | −7436 (11) | −8553 (74) |
| $f_{11}^{(1,\sigma)}$ | 1539 (40) | −8609 (37) |
| $f_{11}^{(2,\sigma)}$ | −12098 (103) | |
| $f_{13}^{(1,\sigma)}$ | −3815 (57) | 17222 (63) |
| $f_{13}^{(2,\sigma)}$ | 23070 (151) | |

[a] Units are cm$^{-1}$ unless otherwise indicated.

[b] One standard error given in parentheses in units of the last figure quoted for the parameter.

[c] Held fixed after a preliminary determination in the least squares fitting.

We next used these parameters in our Renner program to calculate rovibronic energies and wavefunctions. In the calculation, we took the spin-orbit coupling constant $A_{\mathrm{SO}} = 150$ cm$^{-1}$, based on a preliminary experimental determination of the vibronic splittings in the (0 0 0) and (0 1 0) states. The Morse oscillator rigid bender basis set was chosen after making convergence tests to ensure that all states of interest were converged to within 1 or 2 cm$^{-1}$. For the lower surface we used the $N_{\mathrm{Bend}} = 11$ lowest bending basis functions, and for the upper surface we used the $N_{\mathrm{Bend}} = 7$ lowest bending basis functions. The stretching function basis was selected using Morse oscillator functions $|n_1 n_3>$ having $n_1 + n_3 \le N_{\mathrm{stretch}} = 15$. Of these functions we used the $N_A = 6$ lowest stretching basis functions of $A_1$ symmetry, and the $N_B = 3$ lowest stretching basis functions of $B_2$ symmetry for both electronic states. In column 7 of Table 2 we compare the ab initio term value separations with experiment.

After successive partial vibronic assignments and optimizations of the potential we arrived at what we considered to be our 'final' optimized potential by fitting the 36 observed vibronic term value separations given in Table 2. In the fitting, six term value separations (from the laser excitation spectrum) were given a weight five times larger than the rest (from the dispersed fluorescence spectrum) because they were determined more precisely; the weights are given in column 8 of Table 2. Test fittings showed that only four parameters can be determined by the data set to be significantly different (in a statistical sense) from their ab initio values, and the optimized values of these four parameters are given in Table 3. The rest of the parameters were kept at their ab initio values in the final term value calculation. The comparison of the term value

Table 2
The comparison of the ab initio and fitted term value separations (cm$^{-1}$) with the observations

| $J$ | $N$ | Sym | $(v_1\ v_2\ v_3)$ | $(\mu/\kappa)K_P$ | Obs. | Ab initio | Fitted | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | O–C | Weight | O–C |
| Relative to the [1/2, 0, $A_1$ (0 1 0) $\mu\Sigma_{1/2}$] state | | | | | | | | |
| 1/2 | 0 | $B_1$ | (0 1 0) | $\kappa\Sigma_{1/2}$ | 230 | −3.4 | 0.2 | −1.9 |
| 1/2 | 0 | $B_1$ | (1 1 0) | $\kappa\Sigma_{1/2}$ | 856 | 3.5 | 0.2 | −5.7 |
| 1/2 | 0 | $B_1$ | (2 1 0) | $\kappa\Sigma_{1/2}$ | 1499 | 29.9 | 0.2 | 10.1 |
| 1/2 | 0 | $A_1$ | (0 3 0) | $\mu\Sigma_{1/2}$ | 289 | −5.8 | 0.2 | −11.5 |
| 1/2 | 0 | $A_1$ | (1 3 0) | $\mu\Sigma_{1/2}$ | 946 | 25.3 | 0.2 | 6.5 |
| 1/2 | 0 | $A_1$ | (2 1 0) | $\mu\Sigma_{1/2}$ | 1261 | 32.9 | 0.2 | 8.8 |
| 3/2 | 2 | $A_1$ | (0 1 0) | $\Delta_{3/2}$ | 32.4 | −1.2 | 1.0 | 2.7 |
| 3/2 | 2 | $A_1$ | (0 3 0) | $\mu\Delta_{3/2}$ | 297 | 6.5 | 0.2 | −0.6 |
| 3/2 | 2 | $A_1$ | (1 1 0) | $\Delta_{3/2}$ | 631 | −9.8 | 0.2 | −16.3 |
| 3/2 | 2 | $A_1$ | (2 1 0)[a] | $\Delta_{3/2}$ | 1261 | 10.9 | 0.2 | −7.8 |
| 5/2 | 2 | $A_1$ | (0 1 0) | $\Delta_{5/2}$ | 151.7 | 5.4 | 1.0 | −0.8 |
| 5/2 | 2 | $A_1$ | (0 3 0) | $\mu\Delta_{5/2}$ | 350 | 9.8 | 0.2 | 2.7 |
| 5/2 | 2 | $A_1$ | (1 1 0) | $\Delta_{5/2}$ | 791 | 22.8 | 0.2 | 5.5 |
| 5/2 | 2 | $A_1$ | (2 1 0) | $\Delta_{5/2}$ | 1410 | 20.9 | 0.2 | −7.1 |
| Relative to the [1/2, 1, $B_2$ (0 0 0) $\Pi_{1/2}$] state | | | | | | | | |
| 1/2 | 1 | $B_2$ | (0 2 0) | $\mu\Pi_{1/2}$ | 286.0 | 11.5 | 1.0 | 0.4 |
| 1/2 | 1 | $B_2$ | (0 4 0) | $\mu\Pi_{1/2}$ | 568 | 23.2 | 0.2 | 6.1 |
| 1/2 | 1 | $B_2$ | (0 2 0)[b] | $\kappa\Pi_{1/2}$ | 618 | 19.3 | 0.2 | 11.4 |
| 1/2 | 1 | $B_2$ | (1 0 0)[b] | $\Pi_{1/2}$ | 632 | 14.6 | 0.2 | 8.8 |
| 1/2 | 1 | $B_2$ | (1 2 0) | $\mu\Pi_{1/2}$ | 910 | 14.0 | 0.2 | −9.1 |
| 1/2 | 1 | $B_2$ | (1 4 0) | $\mu\Pi_{1/2}$ | 1204 | 26.6 | 0.2 | −1.8 |
| 1/2 | 1 | $B_2$ | (2 0 0) | $\Pi_{1/2}$ | 1225 | 22.8 | 0.2 | 1.0 |
| 1/2 | 1 | $B_2$ | (3 0 0) | $\Pi_{1/2}$ | 1830 | 33.9 | 0.2 | −3.7 |
| 3/2 | 1 | $B_2$ | (0 0 0) | $\Pi_{3/2}$ | 141.5 | 7.4 | 1.0 | −1.8 |
| 3/2 | 1 | $B_2$ | (0 2 0) | $\mu\Pi_{3/2}$ | 309.0 | 10.0 | 1.0 | −0.4 |
| 3/2 | 1 | $B_2$ | (0 2 0)[c] | $\kappa\Pi_{3/2}$ | 530 | 7.3 | 0.2 | −4.2 |
| 3/2 | 1 | $B_2$ | (0 4 0)[c] | $\mu\Pi_{3/2}$ | 627 | 0.2 | 0.2 | −8.5 |
| 3/2 | 1 | $B_2$ | (1 0 0) | $\Pi_{3/2}$ | 768 | 27.8 | 0.2 | 6.8 |
| 3/2 | 1 | $B_2$ | (1 2 0) | $\mu\Pi_{3/2}$ | 940 | 21.8 | 0.2 | −0.6 |
| 3/2 | 1 | $B_2$ | (1 2 0) | $\kappa\Pi_{3/2}$ | 1183 | 27.6 | 0.2 | 5.5 |
| 3/2 | 1 | $B_2$ | (1 4 0) | $\mu\Pi_{3/2}$ | 1268 | 17.2 | 0.2 | −4.5 |
| 3/2 | 1 | $B_2$ | (2 0 0) | $\Pi_{3/2}$ | 1380 | 35.9 | 0.2 | 3.1 |
| 3/2 | 1 | $B_2$ | (2 2 0) | $\mu\Pi_{3/2}$ | 1572 | 36.4 | 0.2 | 2.0 |
| 3/2 | 1 | $B_2$ | (3 0 0) | $\Pi_{3/2}$ | 1984 | 36.6 | 0.2 | −7.9 |
| 5/2 | 3 | $B_2$ | (0 2 0) | $\Phi_{5/2}$ | 340 | 13.5 | 0.2 | 6.5 |
| 7/2 | 3 | $B_2$ | (0 2 0) | $\Phi_{7/2}$ | 438.0 | 18.1 | 1.0 | 0.9 |
| 7/2 | 3 | $B_2$ | (1 2 0)[d] | $\Phi_{7/2}$ | 1093 | 37.8 | 0.2 | 10.9 |

The quantum number $v_2$ is that appropriate for a linear molecule.

[a] Heavily mixed with (1 3 0) $\kappa\Delta_{3/2}$; gains that label using the ab initio potential.

[b] Heavily mixed pair; both labeled (1 0 0) $\Pi_{1/2}$ using the ab initio potential.

[c] Heavily mixed pair; gain each others label using the ab initio potential.

[d] Heavily mixed with (0 4 0) $\kappa\Phi_{7/2}$; gains that label using the ab initio potential.

separations obtained using the optimized potentials with experiment is given in column 9 of Table 2. In Table 2 the state labels are those obtained using the optimized potentials; each label is that of the basis function having the largest coefficient in the eigenfunction. When there is heavy mixing of basis states, as is the case here in many places, more than one state can gain the same label.

In Table 4, we list some calculated rovibronic energies chosen to show the bending and stretching vibronic energy level structure. In Table 5 we list some calculated rovibronic energies chosen to show how the bending energy level pattern depends on the level of stretching excitation.

## 3. Conclusion

We hope that the results in Tables 4 and 5 will prove helpful in further experimental work on this fascinating molecule.

Table 3
The optimized parameters (in cm$^{-1}$) obtained by fitting to the data

| | | |
|---|---|---|
| $A_{\mathrm{SO}}$ | 158.2(2.5) | |
| $f_{11}^{(0)}$ | 36924 (179) | |
| | A$_2$ ($\sigma=-$) | $B_2$ ($\sigma=+$) |
| $f_0^{(1,\sigma)}$ | 3525 (46) | 11960 (210) |

The remaining parameters are as in Table 1.

Table 4
Bending and stretching term values $F$ (in cm$^{-1}$) calculated using the optimized parameters

| $(v_1\ v_2\ v_3)$ | $(\mu/\kappa)K_P$ | $N$ | $J$ | Sym | $F$ |
|---|---|---|---|---|---|
| (0 5 0) | $\kappa\Sigma_{1/2}$ | 0 | 1/2 | $B_1$ | 1242.2 |
| | $\kappa\Delta_{3/2}$ | 2 | 3/2 | $B_1$ | 1280.0 |
| | $\kappa\Delta_{5/2}$ | 2 | 5/2 | $B_1$ | 1221.5 |
| | $\kappa\Gamma_{7/2}$ | 4 | 7/2 | $B_1$ | 1265.9 |
| | $\kappa\Gamma_{9/2}$ | 4 | 9/2 | $B_1$ | 1241.7 |
| | $I_{2/2}$ | 6 | 13/2 | $B_1$ | 878.8 |
| | $I_{2/2}$ | 6 | 11/2 | $A_1$ | 812.0 |
| | $\mu\Gamma_{9/2}$ | 4 | 9/2 | $A_1$ | 825.1 |
| | $\mu\Gamma_{7/2}$ | 4 | 7/2 | $A_1$ | 753.9 |
| | $\mu\Delta_{5/2}$ | 2 | 5/2 | $A_1$ | 697.4 |
| | $\mu\Delta_{3/2}$ | 2 | 3/2 | $A_1$ | 713.0 |
| | $\mu\Sigma_{1/2}$ | 0 | 1/2 | $A_1$ | 696.7 |
| (0 4 0) | $\kappa\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 1053.0 |
| | $\kappa\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 1039.5 |
| | $\kappa\Phi_{5/2}$ | 3 | 5/2 | $B_2$ | 961.8 |
| | $\kappa\Phi_{7/2}$ | 3 | 7/2 | $B_2$ | 1008.2 |
| | $H_{11/2}$ | 5 | 11/1 | $B_2$ | 729.9 |
| | $H_{9/2}$ | 5 | 9/2 | $B_2$ | 653.8 |
| | $\mu\Phi_{7/2}$ | 3 | 7/2 | $B_2$ | 659.7 |
| | $\mu\Phi_{5/2}$ | 3 | 5/2 | $B_2$ | 594.1 |
| | $\mu\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 635.5 |
| | $\mu\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 561.9 |
| (0 3 0) | $\kappa\Sigma_{1/2}$ | 0 | 1/2 | $B_1$ | 831.8 |
| | $\kappa\Delta_{3/2}$ | 2 | 3/2 | $B_1$ | 835.3 |
| | $\kappa\Delta_{5/2}$ | 2 | 5/2 | $B_1$ | 823.2 |
| | $\Gamma_{9/2}$ | 4 | 9/2 | $B_1$ | 582.8 |
| | $\Gamma_{7/2}$ | 4 | 7/2 | $A_1$ | 494.1 |
| | $\mu\Delta_{5/2}$ | 2 | 5/2 | $A_1$ | 486.4 |
| | $\mu\Delta_{3/2}$ | 2 | 3/2 | $A_1$ | 436.6 |
| | $\mu\Sigma_{1/2}$ | 0 | 1/2 | $A_1$ | 439.5 |
| (0 2 0) | $\kappa\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 606.6 |
| | $\kappa\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 534.2 |
| | $\Phi_{7/2}$ | 3 | 7/2 | $B_2$ | 437.1 |
| | $\Phi_{5/2}$ | 3 | 5/2 | $B_2$ | 333.5 |
| | $\mu\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 309.4 |
| | $\mu\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 285.6 |
| (0 1 0) | $\kappa\Sigma_{1/2}$ | 0 | 1/2 | $B_1$ | 370.9 |
| | $\Delta_{5/2}$ | 2 | 5/2 | $B_1$ | 291.5 |
| | $\Delta_{3/2}$ | 2 | 3/2 | $A_1$ | 168.7 |
| | $\mu\Sigma_{1/2}$ | 0 | 1/2 | $A_1$ | 139.0 |
| (0 0 0) | $\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 143.3 |
| | $\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 0.0 |
| (1 0 0) | $\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 623.2 |
| (0 0 1) | $\Pi_{1/2}$ | 1 | 1/2 | $A_1$ | 997.1 |
| (2 0 0) | $\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 1224.0 |
| (1 0 1) | $\Pi_{1/2}$ | 1 | 1/2 | $A_1$ | 1610.9 |
| (3 0 0) | $\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 1833.7 |
| (0 0 2) | $\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 1997.0 |

Table 5
Bending term values $F$ (in cm$^{-1}$) in the (1 0 0) and (2 0 0) stretching states calculated using the optimized parameters

| $(v_1\ v_2\ v_3)$ | $(\mu/\kappa)K_P$ | $N$ | $J$ | Sym | $F$ |
|---|---|---|---|---|---|
| (1 3 0) | $\kappa\Sigma_{1/2}$ | 0 | 1/2 | $B_1$ | 848.8 |
| | $\kappa\Delta_{3/2}$ | 2 | 3/2 | $B_1$ | 855.8[a] |
| | $\kappa\Delta_{5/2}$ | 2 | 5/2 | $B_1$ | 845.4 |
| | $\Gamma_{9/2}$ | 4 | 9/2 | $B_1$ | 566.7 |
| | $\Gamma_{7/2}$ | 4 | 7/2 | $A_1$ | 509.5 |
| | $\mu\Delta_{5/2}$ | 2 | 5/2 | $A_1$ | 503.1 |
| | $\mu\Delta_{3/2}$ | 2 | 3/2 | $A_1$ | 455.2 |
| | $\mu\Sigma_{1/2}$ | 0 | 1/2 | $A_1$ | 455.3 |
| (1 2 0) | $\kappa\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 632.2 |
| | $\kappa\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 554.3 |
| | $\Phi_{7/2}$ | 3 | 7/2 | $B_2$ | 458.9 |
| | $\Phi_{5/2}$ | 3 | 5/2 | $B_2$ | 427.0[a] |
| | $\mu\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 317.4 |
| | $\mu\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 295.9 |
| (1 1 0) | $\kappa\Sigma_{1/2}$ | 0 | 1/2 | $B_1$ | 377.5 |
| | $\Delta_{5/2}$ | 2 | 5/2 | $B_1$ | 301.3 |
| | $\Delta_{3/2}$ | 2 | 3/2 | $A_1$ | 163.2 |
| | $\mu\Sigma_{1/2}$ | 0 | 1/2 | $A_1$ | 142.6 |
| (1 0 0) | $\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 138.0 |
| | $\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | (623.2) |
| (2 3 0) | $\kappa\Sigma_{1/2}$ | 0 | 1/2 | $B_1$ | 887.0 |
| | $\kappa\Delta_{3/2}$ | 2 | 3/2 | $B_1$ | 808.8[a] |
| | $\kappa\Delta_{5/2}$ | 2 | 5/2 | $B_1$ | 773.7[a] |
| | $\Gamma_{9/2}$ | 4 | 9/2 | $B_1$ | 590.8 |
| | $\Gamma_{7/2}$ | 4 | 7/2 | $A_1$ | 546.0 |
| | $\mu\Delta_{5/2}$ | 2 | 5/2 | $A_1$ | 540.1 |
| | $\mu\Delta_{3/2}$ | 2 | 3/2 | $A_1$ | 495.5 |
| | $\mu\Sigma_{1/2}$ | 0 | 1/2 | $A_1$ | 492.7 |
| (2 2 0) | $\kappa\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 666.9 |
| | $\kappa\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 597.0 |
| | $\Phi_{7/2}$ | 3 | 7/2 | $B_2$ | 434.3 |
| | $\Phi_{5/2}$ | 3 | 5/2 | $B_2$ | 366.5 |
| | $\mu\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 346.0 |
| | $\mu\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | 326.3 |
| (2 1 0) | $\kappa\Sigma_{1/2}$ | 0 | 1/2 | $B_1$ | 404.0 |
| | $\Delta_{5/2}$ | 2 | 5/2 | $B_1$ | 332.1 |
| | $\Delta_{3/2}$ | 2 | 3/2 | $A_1$ | 183.9 |
| | $\mu\Sigma_{1/2}$ | 0 | 1/2 | $A_1$ | 167.2 |
| (2 0 0) | $\Pi_{3/2}$ | 1 | 3/2 | $B_2$ | 152.8 |
| | $\Pi_{1/2}$ | 1 | 1/2 | $B_2$ | (1224.0) |

[a] Heavily perturbed level.

## Acknowledgements

The work of PJ is supported in part by the Deutsche Forschungsgemeinschaft and the Fonds der Chemischen Industrie. PRB and ZJJ acknowledge with thanks the financial support received from an NRC(Canada)–NSC(Taiwan) Cooperation Agreement. PJ and SNY acknowledge support from the European Commission through the contract no.

MRTN-CT-2004-512202 ‘Quantitative Spectroscopy for Atmospheric and Astrophysical Research’ (QUASAAR).

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