

## Green's function application to normal vibration of dichlorosilane ( $\text{SiH}_2\text{Cl}_2$ ) molecule

R NAMASIVAYAM and S VISWANATHAN

Department of Physics, Annamalai University, Annamalainagar 608 101, India

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**Abstract.** The Green's function analysis of substituted and perturbed molecules is applied to the study of dichlorosilane vibrations. The isotopic rules have been formulated. The potential energy constants, mean amplitudes of vibration, Coriolis coupling constants and rotation distortion constants have been computed and reported.

**Keywords.** Green's function analysis; dichlorosilane  $\text{SiH}_2\text{Cl}_2$ ; mixing parameter; isotopic rules; molecular constants.

### 1. Introduction

In the Green's function analysis of substituted and perturbed molecules (De Wames and Wolfram 1964, 1966; De Wames *et al* 1964, 1966) isotopic rules are derived without recourse to a force field model. However, the isotopic Green's function equations could be important for the more complicated case of an unsymmetrical molecule, when the higher order secular determinants are solved. Thus in the case of vibrational species containing four vibrational modes difficulties arise in generation of mixing parameter matrix ( $A$ ). To study the suitability of this method for solving ( $4 \times 4$ ) secular determinants in the vibrational problem, the potential energy constants of dichlorosilane ( $\text{SiH}_2\text{Cl}_2$ ) have been evaluated. The isotopic rules are derived and the product rules are verified.

### 2. Isotopic rules for $\text{XY}_2\text{Z}_2 \rightarrow \text{XY}_2^i\text{Z}_2$ molecule

$\text{XY}_2\text{Z}_2$  type molecules have  $C_{2v}$  symmetry. The nine normal modes are divided into four of the  $A_1$  species, two of the  $B_1$  species, two of the  $B_2$  species and one of the  $A_2$  species. The isotopic rules for different vibrational species can be determined by solving the secular determinant (DeWames and Wolfram 1964)

$$|\epsilon\omega^2 G(\omega^2) + I| = 0. \quad (1)$$

In this equation  $G(\omega^2)$  is the Green's function for the unperturbed molecule,  $\omega$  the frequency of vibration,  $I$  the identity matrix and  $\epsilon = (m^t - m)/m$ , where  $m^t$

is the mass of the substituted isotopic atom and  $m$  is the mass of the parent atom in the unperturbed molecule. The Green's function for the unperturbed molecule is related to the matrix of transformation  $l$  between the normal and mass weighted Cartesian coordinates. To obtain  $l$ , a set of orthonormalised Cartesian symmetry coordinates  $S$ , which includes rotations and translations, is constructed. A linear combination of these symmetry coordinates with proper mixing parameters yields a set of normal coordinates. The main difficulty lies in the determination of the proper combination of symmetry coordinates with the suitable mixing parameters to represent the actual normal modes of vibration in a single species. For example in the  $A_1$  species there are four symmetry coordinates and using them we can write a number of sets of normal coordinates. But only one of them will be the proper and true set and will give the real solution for this species. This set is as follows :

$$\begin{aligned} Q_1 &= (aS_1 - bS_3)/\sqrt{a^2 + b^2}, \\ Q_2 &= (bS_2 - aS_4)/\sqrt{a^2 + b^2}, \\ Q_3 &= (bS_1 + aS_3)/\sqrt{a^2 + b^2}, \\ Q_4 &= -(aS_2 + bS_4)/\sqrt{a^2 + b^2}. \end{aligned} \quad (2)$$

For this representation of the normal coordinates, consistent values of the ratio ( $a/b$ ) of the mixing parameters is obtained from the sum rule and the sum of the ( $3 \times 3$ ) and ( $2 \times 2$ ) product rules which yield a very good fit for the various equations involving the isotopic sum and product rules.

The normal coordinates for the other species are chosen as follows :

$$A_2 \text{ species : } Q_5 = S_5, \quad (3)$$

$$\begin{aligned} B_1 \text{ species : } Q_6 &= (S_6 + cS_7)/\sqrt{1 + c^2}, \\ Q_7 &= (S_7 - cS_6)/\sqrt{1 + c^2}, \end{aligned} \quad (4)$$

$$\begin{aligned} B_2 \text{ species : } Q_8 &= (S_8 + dS_9)/\sqrt{1 + d^2}, \\ Q_9 &= (S_9 - dS_8)/\sqrt{1 + d^2}, \end{aligned} \quad (5)$$

where  $Q$  and  $S$  represent the normal coordinates and the Cartesian symmetry coordinates.  $a$ ,  $b$ ,  $c$  and  $d$  are the mixing parameters of the respective species. The six translational and rotational symmetry coordinates are themselves normal coordinates.

The frequencies of the isotopically substituted  $XY_2Z_2$  molecule can be obtained from equation (1) and the perturbation associated with the six rows of the  $l$  matrix, representing the two  $y$  atoms. The resulting determinant is a polynomial in  $\omega^2$ . In the present case, equation (1) reduces to

$$\begin{aligned} &[\{\epsilon\omega^2 G_{41}(\omega^2) + 1\} - \{\epsilon\omega^2 G_{47}(\omega^2)\}] [\{\epsilon\omega^2 G_{66}(\omega^2) + 1\} + \{\epsilon\omega^2 G_{69}(\omega^2)\}] \\ &\quad - [\{\epsilon\omega^2 G_{79}(\omega^2) + \epsilon\omega^2 G_{67}(\omega^2)\}^2] = 0, \end{aligned} \quad (6)$$

$$[\{\epsilon\omega^2 G_{55}(\omega^2) + 1\} - \{\epsilon\omega^2 G_{58}(\omega^2)\}] = 0, \quad (7)$$

$$\begin{aligned} &[\{\epsilon\omega^2 G_{44}(\omega^2) + 1\} + \{\epsilon\omega^2 G_{47}(\omega^2)\}] [\{\epsilon\omega^2 G_{66}(\omega^2) + 1\} + \{\epsilon\omega^2 G_{69}(\omega^2)\}] \\ &\quad - [\{\epsilon\omega^2 G_{79}(\omega^2) - \epsilon\omega^2 G_{67}(\omega^2)\}^2] = 0, \end{aligned} \quad (8)$$

$$\text{and } [\{\epsilon\omega^2 G_{55}(\omega^2) + 1\} + \{\epsilon\omega^2 G_{58}(\omega^2)\}] = 0. \quad (9)$$

The solutions of these equations provide the frequencies corresponding to the species of isotopically substituted molecule. The isotopic rules thus obtained are given in the appendix in an abbreviated form with suitable contractions. The product rules are verified in all the cases.

Vibrational frequencies of Ohno *et al* (1973) and Christensen and Nielson (1968, 1970) and the molecular parameters of Davis and Gerry (1976), presented in table 1, are used in the present calculation. The symmetry coordinates are essentially the same as reported by Shimanouchi and Suzuki (1962). The inverse kinetic energy matrix has been constructed using Wilson's  $S_{kt}$  vectors (Wilson *et al* 1955).

### 3. Molecular constants

#### 3.1. Potential energy constants

From the various isotopic rules given in the appendix, the mixing parameters are calculated and the symmetry force constant matrix is obtained from the relation,

$$F = \tilde{B}^{-1} A \Lambda \tilde{A} B^{-1}, \quad (10)$$

where  $\Lambda$  is a diagonal matrix of vibrational eigenvalues.  $B$  is the transformation matrix between the internal and Cartesian symmetry coordinates and  $A$  is the unitary matrix of the mixing parameters. The symmetry force constant elements obtained are presented in table 2 along with the important valence constants.

Table 1. Vibration frequencies and structural parameters.

Vibrational species	Vibration frequencies (in $\text{cm}^{-1}$ ) by Ohno <i>et al</i> (1973)		Structural parameters by Davis and Gerry (1976)
	$\text{SiH}_2\text{Cl}_2$	$\text{SiD}_2\text{Cl}_2$	
$A_1$	2224	1608	$r(\text{Si-Cl}) = 2.033 \pm 0.003 \text{ \AA}$ $r(\text{Si-H}) = 1.480 \pm 0.015 \text{ \AA}$
	527	519	
	954	695	$\angle(\text{Cl-Si-Cl}) = 109^\circ 43' \pm 20'$ $\angle(\text{H-Si-H}) = 111^\circ 18' \pm 40'$
	188	187	
$B_1$	2237	1637	
	602	466	
$B_2$	876	663	
	590	566	
$A_2$	710	506*	

\* Value from force constant calculations.

Table 2. The symmetry force constants and the important valence constants of dichlorosilane.\*

Symmetry species	Force constant values	Valence constants (present work)	Drake <i>et al</i> (1969)
$A_1$	$F_{11} = 2.4131$	$f_r \text{SiH} = 2.6035$	2.865111
	$F_{22} = 4.3003$		
	$F_{33} = 0.8512$		
	$F_{44} = 1.3651$	$f_R \text{SiCl} = 3.8414$	3.329051
	$F_{12} = 0.0499$		
	$F_{13} = -0.8152$	$f_\alpha \text{HSiH} = 0.4953$	0.456407
	$F_{14} = 0.0994$		
	$F_{23} = -0.1676$	$f_\beta \text{ClSiCl} = 0.6782$	0.770425
	$F_{24} = 1.8997$		
$F_{34} = -0.1764$			
$A_2$	$F_{55} = 0.4320$		
$B_1$	$F_{66} = 2.7939$	$f_{rr} = -0.1904$	0.032767
	$F_{77} = 1.3069$		
	$F_{67} = 1.2560$	$f_{dd} = 0.4588$	0.262003
$B_2$	$F_{88} = 0.5160$		
	$F_{99} = 3.3826$		
	$F_{89} = -0.1127$		

\* Bond stretching constants are expressed in mdynes/Å bending constants in mdynes Å and stretch-bend interaction constants are in mdynes.

### 3.2. Mean amplitudes of vibration

The mean square amplitude ( $\Sigma$ ) matrix for the various atom pairs are obtained from Cyvin's (1959) relation. The mean square amplitude for non-bonded atom pairs are calculated by the method of Ramaswamy *et al* (1962). The  $\Sigma$  matrix elements and the important mean amplitudes are reported in table 3.

### 3.3. Coriolis coupling constants

The Coriolis coupling constants for interaction of the vibrations belonging to various species are calculated using the relation

$$\zeta = L^{-1} C^\alpha \tilde{L}^{-1} \quad (11)$$

given by Meal and Polo (1956) which are given in table 4.

Table 3. Elements of  $\Sigma$  matrix of mean square amplitude ( $\text{\AA}^2$ ) of vibration and mean amplitude of vibration ( $\text{\AA}$ ).

$\Sigma$	Present work ( $\text{\AA}^2$ ) $\times 10^{-3}$	$\Sigma$	Present work ( $\text{\AA}^2$ ) $\times 10^{-3}$	Mean amplitude of vibration ( $\text{\AA}$ )
$\Sigma_{11}$	9.5163	$\Sigma_{66}$	9.3556	$\sigma_{\text{Si-H}}$ 0.0974
$\Sigma_{22}$	3.1381	$\Sigma_{77}$	9.0264	$\sigma_{\text{Si-Cl}}$ 0.0512
$\Sigma_{33}$	18.0942	$\Sigma_{67}$	-3.6003	$\sigma_{\text{H...H}}$ 0.1309
$\Sigma_{44}$	8.5832			$\sigma_{\text{Cl...Cl}}$ 0.0939
$\Sigma_{12}$	-0.0883	$\Sigma_{88}$	16.3562	
$\Sigma_{13}$	3.9124	$\Sigma_{99}$	2.1073	
$\Sigma_{14}$	0.2948	$\Sigma_{89}$	-0.2712	
$\Sigma_{23}$	0.0477			
$\Sigma_{24}$	-3.8085			
$\Sigma_{34}$	1.3688			
$\Sigma_{55}$	17.4224			

Table 4. Coriolis coupling coefficients of dichlorosilane.

Coupling species	$\zeta_{ij}^x$	Coupling species	$\zeta_{ij}^y$	Coupling species	$\zeta_{ij}^z$	
$A_1 \times B_2$	$\zeta_{18}^x = -0.7785$	$A_1 \times B_1$	$\zeta_{18}^y = 0.2222$	$A_1 \times A_2$	$\zeta_{18}^z = 0.4992$	
	$\zeta_{26}^x = 0.1292$		$\zeta_{26}^y = 0.0433$		$\zeta_{26}^z = -0.1070$	
	$\zeta_{38}^x = 0.4532$		$\zeta_{38}^y = -0.9712$		$\zeta_{38}^z = 0.8576$	
	$\zeta_{48}^x = -0.4145$		$\zeta_{48}^y = -0.0743$		$\zeta_{48}^z = -0.0623$	
	$\zeta_{19}^x = 0.3695$		$\zeta_{17}^y = 0.9241$		$B_1 \times B_2$	$\zeta_{48}^z = 0.5767$
	$\zeta_{39}^x = 0.0965$		$\zeta_{27}^y = -0.1691$			$\zeta_{78}^z = 0.7794$
	$\zeta_{59}^x = -0.2151$		$\zeta_{37}^y = 0.1817$			$\zeta_{69}^z = -0.3619$
	$\zeta_{49}^x = -0.8988$		$\zeta_{47}^y = 0.2905$			$\zeta_{79}^z = -0.0249$
$A_2 \times B_1$	$\zeta_{58}^x = 0.7219$	$A_2 \times B_2$	$\zeta_{58}^y = 0.9119$			
	$\zeta_{57}^x = -0.6171$		$\zeta_{59}^y = 0.0457$			

### 3.4. Rotation distortion constants

The rotation distortion parameters  $\tau_{\alpha\beta\gamma\delta}$  can be obtained from the theoretical formulation for the vibration-rotation interaction by Kivelson and Wilson (1952). The parameters are defined as

$$\hbar^4 \tau_{\alpha\beta\gamma\delta} = - \frac{K}{I_{\alpha\alpha}^0 I_{\beta\beta}^0 I_{\gamma\gamma}^0 I_{\delta\delta}^0} \sum \frac{a_i^{\alpha\beta} a_i^{\gamma\delta}}{\omega_i^2}, \quad (12)$$

where  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\delta$  are in turn  $x$ ,  $y$  or  $z$ . If these parameters are expressed in MHz, the constant  $K$  assumes a value of  $5.7498 \times 10^8$  and the vibrational frequen-

cies are in  $\text{cm}^{-1}$ . The principal components of moment of inertia tensor  $I_{\alpha\alpha}^0$  are evaluated from the ground state and in the centre of mass of the molecule and the coefficients  $a_i^{\alpha\beta}$  are related to  $l$  matrix (Oka and Morino 1961; Alti *et al* 1965) and they are evaluated by the relation by Savariraj and Jayapandian (1971). The distortion constants thus calculated are presented in table 5.

#### 4. Results and discussion

The isotopic rules derived here are similar to that of Teller-Redlich product rule (Herzberg 1945) and are derived without assuming any force field model.

From the symmetry force constants (table 2) the valence force constants are calculated. As seen from table 2, the Si-H stretching force constant ( $f_s$ ) value of 2.4131 mdyne/Å compares reasonably well with the value 2.865111 mdyne/Å of Drake *et al* (1969) and 2.84 mdyne/Å of Christensen and Nielson (1970). The Si-Cl stretching force constant ( $f_R$ ) value of 3.8414 mdyne/Å is in favourable comparison with the value 3.329051 mdyne/Å of Drake *et al* (1969). However, the  $f_R$  value of the present work is slightly higher than the one reported by Christensen and Nielson (1970). This may be due to the constraints involved in different methods. In the Green's function approach no constraints are involved and the results obtained are much dependable because they form an absolute set of force constants which are derived directly from the nature of mixing of the vibrations in the different species. The stronger silicon halogen bonds caused by the ( $p \rightarrow d$ ) $\pi$  bonding and perhaps  $p - \sigma^*$  (SiH) bonding may be one of the reasons for having higher Si-Cl ( $f_R$ ) and lower Si-H ( $f_s$ ) values. Further it is noticed that the bending force constant values are also in harmony with the reported values of Drake *et al* (1969).

The mean amplitudes of vibration for both bonded and non-bonded atom pairs are calculated and reported in table 3. Since electron diffraction data are not available direct comparison is not made. However the  $\sigma_{\text{Si-H}}$  value of present work (0.0974 Å) reasonably agrees with the values of the molecules having a similar bond (Balakrishnan and Ramaswamy 1979 for  $\text{SiHCl}_3$ ) and also with the studies of Venkateswarlu and Malathidevi (1965). A similar trend is also observed for the bonded  $\sigma_{\text{Cl-Cl}}$  and the non-bonded  $\sigma_{\text{H...H}}$  and  $\sigma_{\text{Cl...Cl}}$  values. These values along with the mean square amplitude quantities are as shown in table 3.

Table 5. Values of rotation distortion constants in MHz.

$D_J$	0.0904
$D_K$	0.0987
$D_{JK}$	-0.1884
$\delta_J$	-0.0604
$R_5$	-0.0322
$R_6$	-0.0153

The Coriolis coupling constants obtained for interaction of vibrations belonging to various species (table 4) are found to obey the following sum rules:

$$(\zeta_{16}^e)^2 + (\zeta_{28}^e)^2 + (\zeta_{38}^e)^2 + (\zeta_{48}^e)^2 = 1,$$

$$(\zeta_{19}^e)^2 + (\zeta_{29}^e)^2 + (\zeta_{39}^e)^2 + (\zeta_{49}^e)^2 = 1,$$

$$(\zeta_{16}^y)^2 + (\zeta_{26}^y)^2 + (\zeta_{36}^y)^2 + (\zeta_{46}^y)^2 = 1,$$

$$(\zeta_{17}^y)^2 + (\zeta_{27}^y)^2 + (\zeta_{37}^y)^2 + (\zeta_{47}^y)^2 = 1,$$

$$(\zeta_{15}^e)^2 + (\zeta_{25}^e)^2 + (\zeta_{35}^e)^2 + (\zeta_{45}^e)^2 = 1.$$

The rotation distortion constants computed by the linear combination of  $\tau$  elements are reported in table 5. No experimental values are available for direct comparison of these constants.

The calculated frequencies of the isotopically substituted  $\text{SiD}_2\text{Cl}_2$  molecule lie very close to the observed values. Hence, it may be concluded that the Green's function and partitioning technique appears to be a very elegant procedure in the determination of molecular constants for this type of molecules which are representative of the dynamics of the molecule.

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### Appendix

#### Isotopic rules for $\text{XY}_3\text{Z}_2 \rightarrow \text{XY}_2\text{Z}_3$ molecules

##### $A_1$ species

$$\begin{aligned} \omega_1^{i^2} \omega_2^{i^2} \omega_3^{i^2} \omega_4^{i^2} &= \frac{\omega_1^2 \omega_2^2 \omega_3^2 \omega_4^2 P_1}{(1 + \epsilon)^2} \\ \omega_1^{i^2} \omega_3^{i^2} (\omega_3^{i^2} + \omega_4^{i^2}) + \omega_3^{i^2} \omega_4^{i^2} (\omega_1^{i^2} + \omega_2^{i^2}) \\ &= \frac{\omega_1^2 \omega_2^2 \omega_3^2 (P_1 + P_2) + \omega_1^2 \omega_2^2 \omega_4^2 (P_1 + P_4) + \omega_1^2 \omega_3^2 \omega_4^2 (P_1 + P_3) + \omega_2^2 \omega_3^2 \omega_4^2 (P_1 + P_5)}{(1 + \epsilon)^2} \\ \omega_1^{i^2} (\omega_2^{i^2} + \omega_3^{i^2} + \omega_4^{i^2}) + \omega_2^{i^2} (\omega_3^{i^2} + \omega_4^{i^2}) + \omega_3^{i^2} \omega_4^{i^2} \\ &= \frac{\omega_1^2 \omega_2^2 (P_1 + P_2 + P_4) + \omega_1^2 \omega_3^2 (P_1 + P_2 + P_3 + P_6) + \omega_1^2 \omega_4^2 (P_1 + P_3 + P_4 + P_7) + \omega_2^2 \omega_3^2 (P_1 + P_2 + P_5 + P_8) + \omega_2^2 \omega_4^2 (P_1 + P_4 + P_5 + P_{10}) + \omega_3^2 \omega_4^2 (P_1 + P_3 + P_5 + P_9)}{(1 + \epsilon)^2} \end{aligned}$$

$$\omega_1^{i^2} + \omega_2^{i^2} + \omega_3^{i^2} + \omega_4^{i^2} \\ = \frac{(\omega_1^2 + \omega_2^2 + \omega_3^2 + \omega_4^2) P_1 + (\omega_1^2 + \omega_2^2 + \omega_3^2) P_2 + (\omega_1^2 + \omega_3^2 + \omega_4^2) P_3 \\ + (\omega_1^2 + \omega_2^2 + \omega_4^2) P_4 + (\omega_2^2 + \omega_3^2 + \omega_4^2) P_5 + (\omega_1^2 + \omega_3^2) P_6 \\ + (\omega_1^2 + \omega_2^2) P_7 + (\omega_2^2 + \omega_3^2) P_8 + (\omega_2^2 + \omega_4^2) P_{10} + (\omega_3^2 + \omega_4^2) P_9}{(1 + e)^2}$$

**B<sub>1</sub> species**

$$\omega_6^{i^2} \omega_7^{i^2} = \frac{\omega_6^2 \omega_7^2 (R_8 + R_7 + R_{10} + R_{11})}{R_1 + R_2 + R_3 + R_4 + R_5 + R_6 + R_7 + R_8 + R_9 + R_{10} + R_{11}} \\ \omega_6^{i^2} + \omega_7^{i^2} = \frac{(\omega_6^2 + \omega_7^2) (R_8 + R_9 + R_{10} + R_{11}) + \omega_6^2 (R_3 + R_5 + R_6) \\ + \omega_7^2 (R_2 + R_4 + R_7)}{R_1 + R_2 + R_3 + R_4 + R_5 + R_6 + R_7 + R_8 + R_9 + R_{10} + R_{11}}$$

**B<sub>2</sub> species**

$$\omega_8^{i^2} \omega_9^{i^2} = \frac{\omega_8^2 \omega_9^2 (U_3 + U_4 + U_5)}{U_1 + U_2 + U_3 + U_4 + U_5} \\ \omega_8^{i^2} + \omega_9^{i^2} = \frac{(\omega_8^2 + \omega_9^2) (U_3 + U_4 + U_5) + \omega_8^2 U_2 + \omega_9^2 U_1}{(U_1 + U_2 + U_3 + U_4 + U_5)}$$

**A<sub>2</sub> species**

$$\omega_5^{i^2} = \frac{\omega_5^2 (V_2 + V_3)}{V_1 + V_2 + V_3}$$

Here  $P_1, P_2, \dots, P_{10}$ ;  $R_1, R_2, \dots, R_{11}$ ;  $U_1, U_2, \dots, U_5$  and  $V_1, V_2, V_3$  are the constants involving molecular parameters.

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