GREEN'S FUNCTION ANALYSIS OF THE VIBRATIONS OF BORINE CARBONYL

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Using the Green's function technique the molecular constants of borine carbonyl have been calculated by making use of the boron atom substitution. The molecular constants thus obtained agree well with the available experimental values.

1. Introduction

The electron diffraction study of Bauer [1] and microwave investigations of Gordy et al. [2] on borine carbonyl have established a symmetric C_{3v} structure for this molecule. The earliest investigation of the infrared spectrum of borine carbonyl, made Cowan [3], left uncertain the assignment of the B–C–O bending and B–H symmetrical and unsymmetrical vibrations. Bethke and Wilson [4] reported the complete infrared spectrum of gaseous and solid phase of $^{10}BH_3CO$, $^{11}BH_3CO$, $^{10}BD_3CO$ and $^{11}BD_3CO$ and the Raman spectra of these compounds in the gaseous phase as well as a normal coordinate analysis. Taylor [5] reported the Raman spectra of $^{11}BH_3CO$ and $^{11}BD_3CO$ in the liquid state along with the results of a normal coordinate analysis using GVFF. Using a propoer ortho-normalized set of symmetry coordinates, Sundaram and Cleveland [6], obtained the potential energy constants and rotational distortion constants for these molecules using GVFF. The presence of a large number of isotopic frequencies makes it ideal for the application of Green's function analysis [7–9] to obtain an accurate description of the molecular force fields [10] for these molecules. The present paper deals with the applicability of Green's function analysis, in evaluating the molecular constants of borine carbonyl.

2. Isotopic rules for $XY_3ZW \rightarrow X^iY_3ZW$ molecules

According to De Wames and Wolfram [7] in the case of vibrational analysis by the Green's function approach the secular determinant to be solved is of the form

$$|\varepsilon\omega^2 G(\omega^2)+I| = 0 \tag{1}$$

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where $\varepsilon = (m^i - m)/m$ (m stands for mass) ω is the vibrational frequency, $G(\omega^2)$ is the Green's function for the unperturbed molecule. Green's function for the motion of the molecule is given by

$$G_{ij}(\omega^2) = \Sigma_k \frac{X_{il}X_{jl}}{(\omega^2 - \omega_l^2)} \qquad (2)$$

where ω_k's are the vibrational, translational and rotational frequencies (the values of translational and rotational frequencies are zero) and X_{il} is the lth component of the normal coordinate for the mode whose frequency is ω_l. The normal coordinates are the linear combinations of the external symmetry coordinates S, through suitable mixing parameters. In the A_1 species, the normal coordinates chosen are

$$Q_1 = (S_1 + aS_3)/\sqrt{1+a^2}$$

$$Q_2 = (S_2 + bS_4)/\sqrt{1+b^2}$$

$$Q_3 = (S_3 - aS_1)/\sqrt{1+a^2}$$

and

$$Q_4 = (S_4 - bS_2)/\sqrt{1+b^2} . \qquad (3)$$

The combination of two or more mixing parameters in one normal coordinate leads to complications and an unreliable set of force constants. The normal coordinates given above are the nearest true representation of the normal vibrations, since of the various combinations possible they alone give a reliable set of isotopic rules and force constants. The normal coordinates representing the E species are,

$$Q_5 = (S_5 + cS_6)/\sqrt{1+c^2}$$

$$Q_6 = (S_6 - cS_5)/\sqrt{1+c^2}$$

$$Q_7 = (S_7 + dS_8)/\sqrt{1+d^2}$$

$$Q_8 = (S_8 - dS_7)/\sqrt{1+d^2}. \qquad (4)$$

In the above two equations a, b, c and d are the mixing parameters.

The frequencies of the X^iY_3ZW molecules can be obtained from equation (1) and the perturbation is associated with the three rows of equation (2) representing the X atom. The isotopic rules governing the X atom substitution are given in the Appendix. The molecular parameters used in our calculations are presented in Table I.

The values of the mixing parameters obtained in the present calculation for $^{10}BH_3CO$ are $a = -1.324401$, $b = 2.864723$, $c = 1.251445$ and $d = -0.663400$.

TABLE I

Fundamental frequencies of borine carbonyls in cm^{-1}

Species and activity	Assignment	$^{10}BH_3CO$	$^{11}BH_3CO$	
A_1 IR, || Raman, pol.	ω_1	2166.0	2164.7	
	ω_3	707.0	691.4	
	ω_3	2385.0	2379.0	$D = 1.131$ Å
	ω_4	1083.1	1073.4	$R = 1.540$ Å
				$r = 1.194$ Å
E IR $\perp$ Raman, depol.	ω^5	2456.0	2441.0	$\alpha = 113° 52'$
	ω_6	1100.0	1100.0	$\beta = 104° 36'$
	ω_7	818.8	809.3	
	ω_8	313.7	313.2	

3. Potential energy constants

The relation between the force constant matrix F and the mixing parameter matrix A has been shown to be [9]

$$F = \tilde{B}^{-1} A \Lambda \tilde{A} B^{-1}. \tag{5}$$

Using this relation the F matrix elements are determined and from that the valence force constants are evaluated, as shown in Table II.

TABLE II

Valence force constants of borine carbonyl in millidynes per Angstrom

	Present work	Ref. [4]	Ref. [5]	Ref. [6]
f_D	21.6130	18.966	17.9900	18.0450
f_R	2.4332	2.629	2.7750	2.7283
f_r	3.6401	3.236	3.1607	3.2059
f_α	0.3584	0.212	0.2125	0.2048
f_β	0.3692	0.167	0.2250	0.1758
f_δ	0.3841	0.297	0.2744	0.2331
f_{rr}	0.0831	0.078	0.0687	0.0495
$f_{R\alpha}$	−0.1703	−0.088	−0.0670	−0.0710
$f_{R\beta}$	0.2128	0.097	0.0836	0.0887
$f_{\alpha\alpha}$	−0.0513	−0.030	−0.0309	0.0374
$f_{\beta\beta}$	−0.0112	0.009	0.0048	−0.0121
$f_{\beta\delta}$	−0.0972	−0.088	0.0647	−0.0797
$f_{\alpha\beta}$	−0.0723	−0.056	−0.0627	−0.0419

4. Mean amplitudes of vibration

The mean square amplitude matrix can be obtained from Cyvin's relation [11]

$$\Sigma = L\Delta\tilde{L} \tag{6}$$

where $\Delta_i = \dfrac{h}{8\pi^2 c\omega_i} \cot h \dfrac{hc\omega_i}{2kT}$ and $L = BA$. In the above equation h is the Planck

constant, k the Boltzmann constant, and T is the absolute temperature. The mean amplitude quantities computed from the Σ matrix, are given in Table III.

TABLE III

Important mean amplitudes of vibration of borine carbonyl in Å

	Present work	Ref. [17]
σ_D	0.03367	0.03464
σ_R	0.05875	0.04951
σ_r	0.09604	0.10680

5. Rotational distortion constants

The rotational distortion parameters $\tau_{\alpha\beta\gamma\delta}$ can be obtained from the theoretical formulation for vibration-rotation interactions by Wilson and Howard [12] and by Nielson [13]. These parameters are defined as

$$\hbar^4 \tau_{\alpha\beta\gamma\delta} = -\frac{K}{I^0_{\alpha\alpha}I^0_{\beta\beta}I^0_{\gamma\gamma}I^0_{\delta\delta}} \sum_i \frac{a_i^{\alpha\beta}a_i^{\gamma\delta}}{\omega_i^2} \tag{7}$$

where α, β, γ and δ can be taken in turn as x, y or z. If these are expressed in MHZ, the constant K assumes the value 5.7498×10^8, the vibrational frequencies ω_i are in cm^{-1}, the principal components of the moment of inertia tensor $I^0_{\alpha\alpha}$ are evaluated for the ground state and in the centre of mass of the molecule, and the coefficient $a_i^{\alpha\beta}$ are expressed in a. m. u Å^2.

The coefficients $a_i^{\alpha\beta}$ are related to the $l\ (=S\tilde{A})$ matrix by

$$a_i^{\alpha\alpha} = 2\sum_K m_K^{1/2}(\beta_K^0 l_{Ki}^\beta + \gamma_K^0 l_{Ki}^\gamma)$$

$$a_i^{\alpha\beta} = -2\sum_K m_K^{1/2}\alpha_K^0 l_{Ki}^\beta (\alpha \neq \beta) \tag{8}$$

where α_K^0, β_K^0 and γ_K^0 represent the equlibrium Cartesian coordinates and m_K the mass of the Kth atom. The D_J, D_K and D_{JK} values calculated are given in Table IV.

TABLE IV

Rotational distortion constants of borine carbonyl in MHZ

	Present work	Ref. [18]	Ref. [6]
D_J	0.2153	0.1770	—
D_K	2.1062	—	1.7054
D_{JK}	0.4486	0.3900	—

6. Coriolis coupling constants

The Coriolis coupling constants, according to Meal and Polo [14] are given in terms of the l matrix as

$$\zeta^\alpha = lM^\alpha\tilde{l}; \quad \alpha = x, y, z \tag{9}$$

M^x, M^y and M^z are as defined in reference [14]. The ζ elements calculated are given in Table V.

Coriolis coupling constants of borine carbonyl

	Present work	Ref. [4]
ζ_5	0.1238	0.13
ζ_6	0.1152	0.17
ζ_7	0.5849	0.56
ζ_8	0.2119	0.17
$\Sigma\zeta_i$	1.0358	$\dfrac{I_A}{2I_B}+1 = 1.03$

7. Results and discussion

In the present study, the internal coordinates, symmetry coordinates and the molecular parameters used are the same as the ones used by Sundaram and Cleveland [6]. The elements of the kinetic energy matrix obtained are in general the same as the ones obtained by them.

As seen from equations (3) and (4), the mixing is predominant between S_1 and S_3, and S_2 and S_4. This indicates the presence of strong interaction between the $C = 0$ stretch and the BH_3 symmetric stretch. Also there is considerable mixing between the $B = C$ stretch and BH_3 bending modes. This result is in good agreement with the results of normal coordinate analysis by Bethke and Wilson.

The electronic structure of borine carbonyl has been discussed by Gordy *et al.* The resonant structures postulated by them are as follows:

(I) $H_3B^- - C \equiv 0^+$; (II) $H_3B^- - C \equiv 0$; (III) $H_3^+B^- = C = 0$; (IV) $H_3^+B^- = C^+ - 0^-$ and (V) H_3BCO.

According to Gordy *et al.*, the (V) structure contributes the most (50 percent) towards stability and this explains the low stability of BH_3CO. In this case the borine group is loosely bound to the $C = 0$ group. This will result in the boron atom tending to have a planar sp^2 hybridization while the other structures lead to tetrahedral sp^3 hybridization. The value of 113°52' for the HBH angle is indicative of the intermediate state.

These facts are well represented in the force constant calculations. As seen from Table II, the value of the $C = 0$ stretching force constant is 21.613 mdynes/Å, which is of the order expected for a double bond, indicating the predominance of the structure III. The B–H stretching obtained here is 3.64 mdynes/Å, where the B–H distance is 1.194 Å, which is consistent with the values of 3.60 mdynes/Å and 2.848 mdynes/Å obtained from diborane [15] and borohydride ions [16], whose bond lengths are respectively 1.2 Å and 1.255 Å. It can be observed from the above force constant values that as the nuclear seperation of the B–H bond increases the B–H stretching constant decreases which is to be expected. No such conclusion can be drawn the HBH bending constants.

The positive sign of the bond-bond interaction term, f_{rr}, implies that as one B–H bond is stretched, the other contracts. As a B–H bond is stretched, a change in hybridization towards the sp^3 configuration would decrease the B–H bond strength and produce a negative interaction constant. On the other hand, as one B–H bond is lengthened, ionic repulsion between the hydrogens would allow the other two bonds to shorten, resulting in a positive interaction constant. As f_{rr} is found to be positive, the B–H stretch is most strongly influenced by ionic or other repulsion terms while the hybridization effect is comparatively small.

The negative stretch-bend interaction term, $f_{R\alpha}$, is probably due to an increasing contribution from structure (V) during the BC stretch, which would result in both greater sp^2 boron hybridization and less mutual hydrogen repulsion. Both of these should decrease the H–B–H bending constant, producing a negative interaction constant. Similar explanations can be given for the positive stretch bend interaction constant, $f_{R\beta}$. In general, the set of force constant values obtained by us compares favourably with those obtained by previous workers.

The mean amplitudes of vibration, calculated using the L matrix obtained from this Green's function procedure, compares well with the corresponding values calculated by Venkateswarlu and Purushothaman [17], as shown in Table III. No experimental values are available for this molecule.

Rotational distortion constants of borine carbonyl have been reported by Strandberg et al. [18] and by Gordy et al. [2]. The D_J value obtained here, 0.2153 MHZ, is in agreement with the value of Strandberg et al. The value of D_{JK}, 0.4486 MHZ compares well with the value reported by Gordy et al. No experimental values are available for comparing the D_K value. However, this is also in good agreement with the calculated value of Sundaram and Cleveland. These facts are shown in Table IV.

The Coriolis sum rule derived by Cowman [3] for axially symmetric YX_3ZW molecules is, for the fundamental vibrations of the E species

$$\zeta_5 + \zeta_6 + \zeta_7 + \zeta_8 = \frac{I_A}{2I_B} + 1 = \frac{B}{2A} + 1$$

where I_A and I_B are the moments of inertia about axes which lie along and perpendicular to the symmetric axis respectively, and $A \, (= h/8\pi^2 cI_A)$ and B are the corresponding rotational constants. The structure of borine carbonyl has been determined from the microwave spectra of the normal and deutrated compounds by Gordy et al. From their results, the calculated values of A and B are 4.17 and 0.29 cm^{-1}, respectively. This gives $\Sigma\zeta_i = 1.03$. From the theoretical expressions $\Delta\gamma = 2(A-B) - 2A$ for the separation of successive Q maxima, one obtains $\zeta_5 = 0.13$; $\zeta_6 = 0.17$; $\zeta_7 = 0.56$ and $\zeta_8 = 0.17$. Our values are in fairly good agreement with those values and the ζ sum rule is also obeyed as shown in Table V.

APPENDIX

Product rule: A_1 species

$$\omega_1^{i2}\omega_2^{i2}\omega_3^{i2}\omega_4^{i2} = \omega_1^2\omega_2^2\omega_3^2\omega_4^2 \frac{[(\varepsilon m_X + d_4^2)/\varepsilon d_4^2]}{[Q_1^2 + Q_2^2 + Q_3^2 + Q_4^2 + (\varepsilon m_X + d_4^2)/\varepsilon d_4^2]}$$

$$\{\omega_1^{i2}\omega_2^{i2}\omega_3^{i2} + \omega_1^{i2}\omega_2^{i2}\omega_4^{i2} + \omega_1^{i2}\omega_3^{i2}\omega_4^{i2} + \omega_2^{i2}\omega_3^{i2}\omega_4^{i2}\} =$$

$$= \left\{\frac{\begin{array}{c}\omega_1^2\omega_2^2\omega_3^2 Q_4^2 + \omega_1^2\omega_2^2\omega_4^2 Q_3^2 + \omega_1^2\omega_3^2\omega_4^2 Q_2^2 + \omega_2^2\omega_3^2\omega_4^2 Q_1^2 + \\ + (\omega_1^2\omega_2^2\omega_3^2 + \omega_1^2\omega_2^2\omega_4^2 + \omega_1^2\omega_3^2\omega_4^2 + \omega_2^2\omega_3^2\omega_4^2)(\varepsilon m_X + d_4^2)/\varepsilon d_4^2\end{array}}{[Q_1^2 + Q_2^2 + Q_3^2 + Q_4^2 + (\varepsilon m_X + d_4^2)/\varepsilon d_4^2]}\right\}$$

$$\{\omega_1^{i2}\omega_2^{i2} + \omega_1^{i2}\omega_3^{i2} + \omega_1^{i2}\omega_4^{i2} + \omega_2^{i2}\omega_3^{i2} + \omega_2^{i2}\omega_4^{i2} + \omega_3^{i2}\omega_4^{i2}\} =$$

$$= \frac{\begin{array}{c}\{\omega_1^2\omega_2^2 + \omega_1^2\omega_3^2 + \omega_2^2\omega_3^2\}Q_4^2 + \{\omega_1^2\omega_2^2 + \omega_1^2\omega_4^2 + \omega_2^2\omega_4^2\}Q_3^2 + \{\omega_1^2\omega_3^2 + \omega_1^2\omega_4^2 + \omega_3^2\omega_4^2\}Q_2^2 + \\ + \omega_2^2\omega_3^2 + \omega_2^2\omega_4^2 + \omega_3^2\omega_4^2 Q_1^2 + \{\omega_1^2\omega_2^2 + \omega_1^2\omega_3^2 + \omega_1^2\omega_4^2 + \omega_2^2\omega_3^2 + \omega_2^2\omega_4^2 + \omega_3^2\omega_4^2\}\dfrac{\varepsilon m_X + d_4^2}{\varepsilon d_4^2}\end{array}}{[Q_1^2 + Q_2^2 + Q_3^2 + Q_4^2 + (\varepsilon m_X + d_4^2)/\varepsilon d_4^2]}$$

$$\{\omega_1^{i2} + \omega_2^{i2} + \omega_3^{i2} + \omega_4^{i2}\} =$$

$$= \frac{\begin{array}{c}\{(\omega_1^2 + \omega_2^2 + \omega_3^2)Q_4^2 + (\omega_1^2 + \omega_2^2 + \omega_4^2)Q_3^2 + (\omega_1^2 + \omega_3^2 + \omega_4^2)Q_2^2 + \\ + (\omega_2^2 + \omega_3^2 + \omega_4^2)Q_1^2 + (\omega_1^2 + \omega_2^2 + \omega_3^2 + \omega_4^2)(\varepsilon m_X + d_4^2)/\varepsilon d_4^2\}\end{array}}{[Q_1^2 + Q_2^2 + Q_3^2 + Q_4^2 + (\varepsilon m_x + d_4^2)/\varepsilon d_4^2]}$$

where

$$Q_1 = \left\{\frac{\sqrt{3m_Y}\,C_\beta}{d_1} + \frac{a\sqrt{m_X m_Z}}{d_2 d_3}\right\}\frac{1}{\sqrt{1+a^2}};$$

$$Q_2 = \left\{\frac{\sqrt{3m_X m_Y}\,S_\beta}{d_1 d_2} + \frac{\sqrt{m_X m_W}\,b}{d_3 d_4}\right\}\frac{1}{\sqrt{1+b^2}};$$

$$Q_3 = \left\{\frac{\sqrt{m_X m_Z}}{d_3 d_4} - \frac{\sqrt{3m_Y}\,C_\beta a}{d_1}\right\}\frac{1}{\sqrt{1+a^2}};$$

$$Q_4 = \left\{\frac{\sqrt{m_W m_Z}}{d_3 d_4} - \frac{b\sqrt{3m_X m_Y}\,S_\beta}{d_1 d_2}\right\}\frac{1}{\sqrt{1+b^2}}$$

$$d_1 = (m_X + 3m_Y C_\beta^2)^{1/2}; \quad d_2 = (m_X + 3m_Y)^{1/2};$$

$$d_3 = (m_X + m_Z + 3m_Y)^{1/2}; \quad \text{and} \quad d_4 = (m_W + m_X + m_Z + 3m_Y)^{1/2}.$$

Product rules: E species

$$\omega_5^{i2}\omega_6^{i2}\omega_7^{i2}\omega_8^{i2} = \omega_5^2\omega_6^2\omega_7^2\omega_8^2 \frac{[\varepsilon m_X\{I_Y+l^2d_4^2+I_Yd_4^2\}]/I_Yd_4^2}{\varepsilon(\Phi_1^2+\Phi_2^2+\Phi_3^2+\Phi_4^2)+[\varepsilon m_X\{I_Y+l^2d_4^2\}+I_Yd_4^2]/I_Yd_4^2}$$

$$\omega_5^{i2}\omega_6^{i2}\omega_7^{i2}+\omega_5^{i2}\omega_6^{i2}\omega_8^{i2}+\omega_5^{i2}\omega_7^{i2}\omega_8^{i2}+\omega_6^{i2}\omega_7^{i2}\omega_8^{i2} =$$

$$= \frac{\varepsilon(\Phi_1^2\omega_6^2\omega_7^2\omega_8^2+\Phi_2^2\omega_5^2\omega_7^2\omega_8^2+\Phi_3^2\omega_5^2\omega_6^2\omega_8^2+\Phi_4^2\omega_5^2\omega_6^2\omega_7^2)+\dfrac{[\varepsilon m_X\{I_Y+l^2d_4^2\}+I_Yd_4^2]}{I_Yd_4^2}[\omega_5^2\omega_6^2(\omega_7^2+\omega_8^2)+\omega_7^2\omega_8^2(\omega_5^2+\omega_6^2)]}{\varepsilon(\Phi_1^2+\Phi_2^2+\Phi_3^2+\Phi_4^2)+[\varepsilon m_X\{I_Y+l^2d_4^2+I_Yd_4^2\}]/I_Yd_4^2}$$

$$\omega_5^{i2}\omega_6^{i2}+\omega_5^{i2}\omega_7^{i2}+\omega_5^{i2}\omega_8^{i2}+\omega_6^{i2}\omega_7^{i2}+\omega_6^{i2}\omega_8^{i2}+\omega_7^{i2}\omega_8^{i2} =$$

$$= \frac{\varepsilon\Phi_1^2[\omega_6^2(\omega_7^2+\omega_8^2)+\omega_7^2\omega_8^2]+\Phi_2^2[\omega_5^2(\omega_7^2+\omega_8^2)+\omega_7^2\omega_8^2]+\Phi_3^2[\omega_5^2(\omega_6^2+\omega_8^2)+\omega_6^2\omega_8^2]+\Phi_4^2[\omega_5^2(\omega_6^2+\omega_7^2)\omega_6^2\omega_7^2]+[\varepsilon m_X\{I_Y+l^2d_4^2\}+I_Yd_4^2]/I_Yd_4^2[\omega_5^2(\omega_6^2+\omega_7^2+\omega_8^2)+\omega_6^2(\omega_7^2+\omega_8^2)+\omega_7^2\omega_8^2]}{\varepsilon(\Phi_1^2+\Phi_2^2+\Phi_3^2+\Phi_4^2)+[\varepsilon m_X\{I_Y+l^2d_4^2\}+I_Yd_4^2]/I_Yd_4^2}$$

$$\omega_5^{i2}+\omega_6^{i2}+\omega_7^{i2}+\omega_8^{i2} =$$

$$= \frac{\varepsilon\Phi_1^2(\omega_6^2+\omega_7^2+\omega_8^2)+\Phi_2^2(\omega_5^2+\omega_7^2+\omega_8^2)+\Phi_3^2(\omega_5^2+\omega_6^2+\omega_8^2)+\Phi_4(\omega_5^2+\omega_6^2+\omega_7^2)+\dfrac{[\varepsilon m_X\{I_Y+l^2d_4^2\}+I_Yd_4^2]}{I_Yd_4^2}(\omega_5^2+\omega_6^2+\omega_7^2+\omega_8^2)}{\varepsilon(\Phi_1^2+\Phi_2^2+\Phi_3^2+\Phi_4^2)+[\varepsilon m_X(I_Y+l^2d_4^2)+I_Yd_4^2]/I_Yd_4^2}$$

where

$$\Phi_1 = \left(\frac{\sqrt{3m_Y}\,S_\beta}{d_5}+\frac{c\sqrt{3m\;\;m_Y}\,S_\beta^2}{d_5d_6}\right)\frac{1}{\sqrt{1+c^2}};$$

$$\Phi_2 = \left(\frac{\sqrt{3m_Xm_Y}\,S_\beta^2}{d_5d_6}-\frac{c\sqrt{3m_Y}\,S_\beta}{d_5}\right)\frac{1}{\sqrt{1+c^2}}$$

$$\Phi_3 = \left(\frac{\sqrt{3m_Y}\,v}{\sqrt{m_X}\,I_YPd_6}+\frac{2d\sqrt{m_Wm_Xm_Z}}{Pd_6}DS\frac{1}{\sqrt{1+d^2}}\right);$$

$$\Phi_4 = \left(\frac{2\sqrt{m_Wm_Xm_Z}\,DS}{Pd_7}-\frac{d\sqrt{3m_Y}\,v}{\sqrt{m_X}\,I_Y\cdot P\overline{d}_6}\right)\frac{1}{\sqrt{1+d^2}}$$

$$d_5 = (2m_X+3m_YS_\beta^2)^{1/2}; \quad d_6 = (d_5^2-m_XS_\beta^2)^{1/2};$$

$$d_7 = [P^2(m_W+m_Z)-2m_Wm_Z(m_X+3m_Y)D^2], \quad S = [(m_X+3m_Y)1-3m_YrC_\beta],$$

$$l = [3m_YrC_\beta+m_ZR+m_W(R+D)]/d_4; \quad v = [m_Xlr(d_4^2-m_XS_\beta^2)-2m_XI_YC_\beta]$$

$$\text{and} \quad I_Y = \left\{m_W(R+D-1)^2+m_Xl^2+3m_Y\left[(l-rC_\beta)^2+\frac{r^2S_\beta^2}{2}\right]+m_Z(R-l)^2\right\}.$$

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