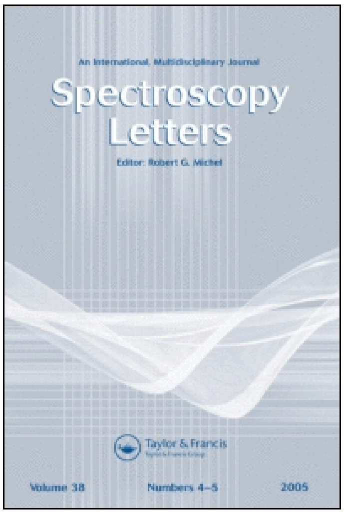

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G-, F-, and ε-Matrices for XY_4Z Molecules of C_{4V} Symmetry

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G-, F-, AND Σ-MATRICES FOR XY_4Z MOLECULES OF C_{4v} SYMMETRY

KEY WORDS: XY_4Z molecules (C_{4v}), logarithmic steps method

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XY_4Z molecules or ions with a square-pyramid structure (C_{4v}) are relatively rare. This explains the infrequency of investigations of their vibrational spectra, with analysis in normal coordinates and computation of the mean-square amplitudes of vibration.

In order to determine the force constants, the authors:

(1) have mainly used simple force fields such as the Urey-Bradley[1,2] force field(U.B.F.F.),the modified U.B.F.F.[3-6], the orbital valence force field[7](O.V.F.F.), and simplified valence force fields[8-17]. For the latter, they calculated 8 to 12 constants of a foreseeable total of 20 within the framework of the generalized valence force field (G.V.F.F.). Only Goulet[18] used the G.V.F.F. and determined all the constants for ClF_5. Unfortunately, for five of these: $f_{R\alpha}$, $f_{r\alpha}$, $f'_{r\alpha}$, $f_{\alpha\beta}$ and $f'_{\alpha\beta}$, the values are meaningless;

(2) did not use the general G-matrix accounting for three possible types of structure for an XY_4Z group with C_{4v} symmetry: as shown in the figure, the X atom, in effect, can be above, in or below the plane of the four Y atoms.The G-

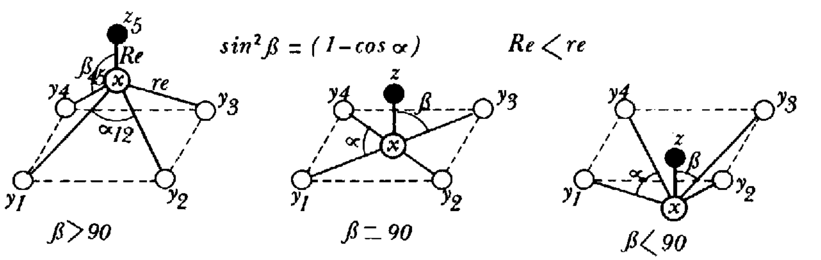
matrices proposed by Stephenson[8] and Khanna[9] are intended to be general, but they are in fact incorrect (see remark concerning the U-matrix). Moreover, these authors set the ratio $\rho=(r_e/R_e)$ at 1 (see figure). As for the **G**-matrix suggested by Begun et al[10], it is specific to the case in which $\beta=90°$, whereas that of Brunvoll and Cyvin[19] has not been published.

Hence it proved interesting to reconsider the determination of **G**-, **F**-, and Σ-matrices, in order to compute all the force constants f and mean-square amplitudes of vibration σ of the XY_4Z (C_{4v}) within the framework of the G.V.F.F., and thanks to the logarithmic steps method (L.S.M.)[20,21].

The notations used here are similar to those in References 20 and 21, and are therefore not redefined here.

Only the results will be given here, but it can be readily seen from the tables that formal analogies exist between the **G'**-, **F'**-, and Σ'-, the **G***-, **F***-, and Σ^*-, and finally the **G**-, **F**-, and Σ-matrices

For a molecule XY_4Z of C_{4v} symmetry, the numbering of the ligands and the notation for the internal co-ordinates can be seen from the figure.



figure

The general quadratic potential function may be expressed $2V = R\,F'\tilde{R}$. R is the column matrix(Δr_1, Δr_2, Δr_3, Δr_4, $\Delta\alpha_{12}$, $\Delta\alpha_{23}$, $\Delta\alpha_{34}$, $\Delta\alpha_{41}$, ΔR, $\Delta\beta_{15}$, $\Delta\beta_{25}$, $\Delta\beta_{35}$, $\Delta\beta_{45}$). $\tilde{R}$ is its transpose. Then, the elements of the 13x13 G'-, F'-, and Σ'-matrices can be written as indicated on table 1. The expressions for the G'-, and F'-matrix elements are given in table 2. μ_X, μ_Y, and μ_Z denote respectively the reciprocal masses of the atoms X,Y, and Z. The expressions for the Σ'-matrix elements are derived from those of the F'-matrix by substituting σ for f, $|(1/r_e)\sigma|$ for $|r_e f|$, $|(1/r_e^2)\sigma|$ for $|r_e^2 f|$, $|(1/\sqrt{r_e R_e})\sigma|$ for $|(\sqrt{r_e R_e})f|$, $|(1/r_e R_e)\sigma|$ for $|(r_e R_e)f|$, and $|(1/r_e\sqrt{r_e R_e})\sigma|$ for $|(r_e\sqrt{r_e R_e})f|$, whereby the indices remain unchanged.

The G.V.F.F. leads to 20 force constants and to 20 mean--square amplitudes of vibration. Their corresponding definitions are readily derived from table 1.

TABLE 1

G'-, F'-, AND Σ'-MATRICES

	Δr_1	Δr_2	Δr_3	Δr_4	$\Delta\alpha_{12}$	$\Delta\alpha_{23}$	$\Delta\alpha_{34}$	$\Delta\alpha_{41}$	ΔR	$\Delta\beta_{15}$	$\Delta\beta_{25}$	$\Delta\beta_{35}$	$\Delta\beta_{45}$
Δr_1	A	B	C	B	D	E	E	D	I	J	K	L	K
Δr_2		A	B	C	D	D	E	E	I	K	J	K	L
Δr_3			A	B	E	D	D	E	I	L	K	J	K
Δr_4				A	E	E	D	D	I	K	L	K	J
$\Delta\alpha_{12}$					F	G	H	G	M	N	N	O	O
$\Delta\alpha_{23}$						F	G	H	M	O	N	N	O
$\Delta\alpha_{34}$							F	G	M	O	O	N	N
$\Delta\alpha_{41}$								F	M	N	O	O	N
ΔR									P	Q	Q	Q	Q
$\Delta\beta_{15}$										R	S	T	S
$\Delta\beta_{25}$											R	S	T
$\Delta\beta_{35}$												R	S
$\Delta\beta_{45}$													R

TABLE 2

	G'-MATRIX ELEMENTS	F'-MATRIX ELEMENTS
A	$G_r = \mu_X + \mu_Y$	f_r
B	$G_{rr} = \cos^2\beta\mu_X$	f_{rr}
C	$G'_{rr} = (2\cos^2\beta - 1)\mu_X$	f'_{rr}
D	$G_{r\alpha} = -(1/r_e)\sin\beta\sqrt{1+\cos^2\beta}\ \mu_X$	$r_e\ f_{r\alpha}$
E	$G'_{r\alpha} = -(1/r_e)[\sin\beta(3\cos^2\beta-1)/\sqrt{1+\cos^2\beta}]\mu_X$	$r_e\ f'_{r\alpha}$
F	$G_\alpha = (1/r_e^2)(2\sin^2\beta\mu_X + 2\mu_Y)$	$r_e^2\ f_\alpha$
G	$G_{\alpha\alpha} = (1/r_e^2)[\sin^2\beta/(1+\cos^2\beta)](4\cos^2\beta\mu_X - \mu_Y)$	$r_e^2\ f_{\alpha\alpha}$
H	$G'_{\alpha\alpha} = (1/r_e^2)[2\sin^2\beta(3\cos^2\beta - 1)/(1+\cos^2\beta)]\mu_X$	$r_e^2\ f'_{\alpha\alpha}$
I	$G_{rR} = \cos\beta\ \mu_X$	f_{rR}
J	$G_{r\beta} = -(1/r_e)\rho\sin\beta\mu_X$	$\sqrt{r_eR_e}\ f_{r\beta}$
K	$G'_{r\beta} = -(1/r_e)\cos\beta\ \sin\beta\mu_X$	$\sqrt{r_eR_e}\ f'_{r\beta}$
L	$G''_{r\beta} = -(1/r_e)\sin\beta(2\cos\beta-\rho)\mu_X$	$\sqrt{r_eR_e}\ f''_{r\beta}$
M	$G_{R\alpha} = -(1/r_e)(2\cos\beta\ \sin\beta/\sqrt{1+\cos^2\beta})\mu_X$	$r_e\ f_{R\alpha}$
N	$G_{\alpha\beta} = (1/r_e^2)(1/\sqrt{1+\cos^2\beta})[\sin^2\beta(\cos\beta+\rho)\mu_X + \cos\beta\mu_Y]$	$r_e\sqrt{r_eR_e}\ f_{\alpha\beta}$
O	$G'_{\alpha\beta} = (1/r_e^2)[(3\cos\beta-\rho)\sin^2\beta/\sqrt{1+\cos^2\beta}]\mu_X$	$r_e\sqrt{r_eR_e}\ f'_{\alpha\beta}$
P	$G_R = \mu_X + \mu_Z$	f_R
Q	$G_{R\beta} = -(1/r_e)\sin\beta\mu_X$	$\sqrt{r_eR_e}\ f_{R\beta}$
R	$G_\beta = (1/r_e^2)[(1+\rho^2-2\rho\cos\beta)\mu_X + \mu_Y + \rho^2\mu_Z]$	$r_eR_e\ f_\beta$
S	$G_{\beta\beta} = (1/r_e^2)\sin^2\beta\mu_X$	$r_eR_e\ f_{\beta\beta}$
T	$G'_{\beta\beta} = -(1/r_e^2)\{[\rho^2 - 1 - 2\cos\beta(\rho-\cos\beta)]\mu_X + \rho^2\mu_Z\}$	$r_eR_e\ f'_{\beta\beta}$

Remarks about units:

In order to express all the force constants of the G.V.F.F. in mdyne Å^{-1}, we have, as suggested by L.H.Jones[22], multiplied:

- the bond-angle interaction constants of type $f_{r\theta}$, by r_0
- the angle-angle interaction constants of type $f_{\theta\theta'}$, by $r_0r'_0$
- the angular deformation constants of type f_θ, by r_0^2

where $r_0 = \sqrt{r_ir_j}$ and $r'_0 = \sqrt{r'_ir'_j}$. r_i (or r'_i) and r_j (or r'_j) are the lengths at equilibrium of the bonds forming the angle θ (or θ').

The orthogonal matrix U is formed by the 13 following symmetry coordinates: $S_1(A_1)$, $S_2(A_1)$, $S_3(A_1)$, $S_4(B_1)$, $S_5(B_1)$, $S_6(B_2)$, $S_{7a}(E)$, $S_{8a}(E)$, $S_{9a}(E)$, $S_{10}(A_1)$, $S_{7b}(E)$, $S_{8b}(E)$, $S_{9b}(E)$.

The basic equation $UG'\tilde{U} = G^*$ leads to a blocked out diagonal G^*-matrix , with the elements noted '$0^\dagger$' all null (see below). Similar equations are applicable to the F' and Σ' matrices, and also lead to blocked out diagonal F^*-, and Σ^*-matrices.

The elements of the G^*-, F^*-, and Σ^*-matrices can be written as indicated on table 3. The various elements are assigned as follows: 1,1; 1,2; 1,3; 2,2; 2,3; and 3,3 refer to the normal vibrations $\nu_1(A_1)$, $\nu_2(A_1)$, and $\nu_3(A_1)$. 4,4; 4,5; and 5,5 refer to $\nu_4(B_1)$ and $\nu_5(B_1)$. 6,6 refers to $\nu_6(B_2)$. 7,7; 7,8; 7,9; 8,8; 8,9; and 9,9 refer to $\nu_7(E)$, $\nu_8(E)$, and $\nu_9(E)$. The elements 1,10; 2,10; 3,10; and 10,10 are noted '$0^\dagger$'. The

TABLE 3

G^*-, F^*-, AND Σ^*-MATRICES

1,1	1,2	1,3	0	0	0	0	0	0	$0^\dagger$	0	0	0
1,2	2,2	2,3	0	0	0	0	0	0	$0^\dagger$	0	0	0
1,3	2,3	3,3	0	0	0	0	0	0	$0^\dagger$	0	0	0
			4,4	4,5	0	0	0	0	0	0	0	0
			4,5	5,5	0	0	0	0	0	0	0	0
					6,6	0	0	0	0	0	0	0
						7,7	7,8	7,9	0	0	0	0
	S Y M.					7,8	8,8	8,9	0	0	0	0
						7,9	8,9	9,9	0	0	0	0
									$0^\dagger$	0	0	0
										7,7	7,8	7,9
										7,8	8,8	8,9
										7,9	8,9	9,9

existence of the redundant coordinate $S_{10}(A_1)$ leads to the voiding of these elements.

In the literature we noted the symmetry coordinates proposed by Stephenson[8], Khanna[9], Begun[10], Pillai[3], Brunvoll[19] and Ramaswamy[4]. By comparing these symmetry coordinates (after uniformization of notations), one observes:

- that only the U-matrix of Brunvoll[19] is not orthogonal;
- that the symmetry coordinates $S_{10}(A_1)$ of Stephenson[8] and Khanna[9] do not nullify all the elements noted '$0^{\dagger}$' irrespective of the value of the angle β. It follows that the U-matrices proposed by Stephenson[8] on the one hand, and Khanna[9] on the other, are not acceptable, and lead to incorrect G^{*}-matrices;
- the U-matrices proposed by Begun[10], Pillai[3] and Ramaswamy[4], all three orthogonal, lead to the same G^{*}-matrix and nullify all the elements noted '$0^{\dagger}$' irrespective of the value of angle β: they are said to be equivalent.

Remarks:

- The symmetry coordinate noted S(E) by Begun[10] is erroneous. This is certainly due to a typographic error. It must be written $S(E)=(1/\sqrt{2})(-\Delta\alpha_2+\Delta\alpha_4)$ instead of: $(1/2)(-\Delta\alpha_2+\Delta\alpha_4)$.
- This applies also to the symmetry coordinate noted S_{11a} by Ramaswamy[4]. The latter must be written: $S_{11a}=(1/\sqrt{2})(\Delta d_1-\Delta d_3)$ instead of: $(1/\sqrt{2})(\Delta d_1-\Delta d_2)$.

By adopting one or the other of these three latter U-matrices, one can determine the expressions of the elements of the G^{*}-, and F^{*}-matrices. Those expressions are given in table 4 and 5. The Σ^{*}-matrix elements can be derived from those of the F^{*}-matrix in the same way as for the Σ'-, F'-matrix pair.

TABLE 4

G^*-MATRIX ELEMENTS

1,1	$\mu_X + \mu_Z$
1,2	$2\cos\beta\ \mu_X$
1,3	$(-1/r_e)[2\sin\beta\ \sqrt{(5\cos^2\beta + 1)/(1 + \cos^2\beta)}\ ]\ \mu_X$
2,2	$4\cos^2\beta\ \mu_X + \mu_Y$
2,3	$(-1/r_e)[4\cos\beta\sin\beta\ \sqrt{(5\cos^2\beta + 1)/(1 + \cos^2\beta)}\ ]\ \mu_X$
3,3	$(1/r_e^2)\{[16\cos^4\beta/(1+\cos^2\beta)+9\cos^2\beta+1][4\sin^2\beta\ \mu_X+\mu_Y]\}/(5\cos^2\beta+1)$
4,4	μ_Y
4,5	0
5,5	$(1/r_e^2)\ \mu_Y$
6,6	$(1/r_e^2)\ [4/(1 + \cos^2\beta)\ ]\ \mu_Y$
7,7	$2\sin^2\beta\ \mu_X + \mu_Y$
7,8	$(1/r_e)\ [2\sin\beta\ (\cos\beta - \rho)]\ \mu_X$
7,9	$(-1/r_e)(2\sqrt{2}\ \sin^3\beta/\sqrt{1 + \cos^2\beta})\ \mu_X$
8,8	$(1/r_e^2)[2(\rho-\cos\beta)^2\ \mu_X + \mu_Y + 2\ \rho^2\mu_Z]$
8,9	$(1/r_e^2)\ \sqrt{2}\ [2\sin^2\beta(\rho-\cos\beta)\ \mu_X + \cos\beta\ \mu_Y]\ /\ \sqrt{(1 + \cos^2\beta)}$
9,9	$(1/r_e^2)\{[4\sin^4\beta/(1 + \cos^2\beta)]\ \mu_X + 2\ \mu_Y\}$
1,10	0
2,10	0
3,10	0
10,10	0

The 9x9 submatrix shown in the upper left corner of the table 3 indicates the distribution of the G-, F-, and Σ-matrix elements.

Remarks:

- Owing to the molecular symmetry, the element $G_{4,5}$ is null so that necessarily $F_{4,5}$ and $\Sigma_{4,5} = 0$, for all XY_4Z groups with C_{4v} symmetry.
- With respect to blocking off, note that F' and F^* are related by the basic formula: $F^* = UF'\tilde{U}$. Any element F^*_{ij} can thus be written in the form of a linear combination as follows:

$$F^*_{ij} = \sum_{k=1}^{n} \sum_{l=1}^{n} (U_{ik}U_{jl})\ F'_{kl}$$

where n = order of F'-, F^*-, and U-matrices.

TABLE 5

F^*-MATRIX ELEMENTS

1,1	f_R
1,2	$2f_{rR}$
1,3	$2N_2 r_e f_{R\alpha} - 2N_1\sqrt{r_eR_e}\, f_{R\beta}$
2,2	$f_r + 2f_{rr} + f'_{rr}$
2,3	$2N_2\, r_e(f_{r\alpha} + f'_{r\alpha}) - N_1\sqrt{r_eR_e}\,(f_{r\beta} + 2f'_{r\beta} + f''_{r\beta})$
3,3	$N_2^2\, r_e^2\,(f_\alpha + 2f_{\alpha\alpha} + f'_{\alpha\alpha}) - 4N_1N_2 r_e\sqrt{r_eR_e}\,(f_{\alpha\beta} + f'_{\alpha\beta})$
	$+ N_1^2 r_e R_e\,(f_\beta + 2\, f_{\beta\beta} + f'_{\beta\beta})$
4,4	$f_r - 2\, f_{rr} + f'_{rr}$
4,5	$\sqrt{r_eR_e}\,(f_{r\beta} - 2\, f'_{r\beta} + f''_{r\beta})$
5,5	$r_eR_e\,(f_\beta - 2\, f_{\beta\beta} + f'_{\beta\beta})$
6,6	$r_e^2\,(f_\alpha - 2f_{\alpha\alpha} + f'_{\alpha\alpha})$
7,7	$f_r - f'_{rr}$
7,8	$\sqrt{r_eR_e}\,(f_{r\beta} - f''_{r\beta})$
7,9	$r_e\sqrt{2}\,(f_{r\alpha} - f'_{r\alpha})$
8,8	$r_eR_e\,(f_\beta - f'_{\beta\beta})$
8,9	$\sqrt{2}r_e\sqrt{r_eR_e}\,(f_{\alpha\beta} - f'_{\alpha\beta})$
9,9	$r_e^2\,(f_\alpha - f'_{\alpha\alpha})$
1,10	$2N_1 r_e\, f_{R\alpha} + 2N_2\sqrt{r_eR_e}\, f_{R\beta} \equiv 0$
2,10	$2N_1\, r_e(f_{r\alpha} + f'_{r\alpha}) + N_2\sqrt{r_eR_e}\,(f_{r\beta} + 2\, f'_{r\beta} + f''_{r\beta}) \equiv 0$
3,10	$N_1N_2 r_e^2\,(f_\alpha + 2f_{\alpha\alpha} + f'_{\alpha\alpha}) + 2(N_2^2 - N_1^2)\, r_e\sqrt{r_eR_e}\,(f_{\alpha\beta} + f'_{\alpha\beta})$
	$- N_1N_2\, r_eR_e\,(f_\beta + 2\, f_{\beta\beta} + f'_{\beta\beta}) \equiv 0$
10,10	$N_1^2\, r_e^2\,(f_\alpha + 2\, f_{\alpha\alpha} + f'_{\alpha\alpha}) + 4\, N_1N_2\, r_e\sqrt{r_eR_e}\,(f_{\alpha\beta} + f'_{\alpha\beta})$
	$+ N_2^2\, r_eR_e\,(f_\beta + 2\, f_{\beta\beta} + f'_{\beta\beta}) \equiv 0$

The F^*_{ij} elements may be non-null and are noted 'i,j' in table 3. They may also be nullified:

- when all the products $(U_{ik}U_{jl})$ are null. These elements are noted '0' in table 3;
- when the sum is null, without all the products $(U_{ik}U_{jl})$ being null. These elements are noted '0^+' in table 3.

Finally, the equations relating the force constants are those for which the products $(U_{ik}U_{jl})$ are not all null, namely, those which are related to the elements noted 'i,j' and '$0^{\dagger}$' in table 3.

For all groups which we investigated XY_4, XY_3Z_2, XY_6, XY_5Z_2 and XY_4Z (see references in 23), the number of equations previously defined is equal to the number of force constants (of the G.V.F.F.) of the group in question.Hence in every case we have as many equations as unknowns, and the resolution of such a system yields precisely the result of the blocking off. The solutions of the system of 20 equations with 20 unknowns(the force constants f) obtained for an XY_4Z group is shown in table 6.The expressions of σ are derived

TABLE 6

$$f_r = (1/4)F_{2,2} + (1/4)F_{4,4} + (1/2)F_{7,7}$$
$$f_{rr} = (1/4)F_{2,2} - (1/4)F_{4,4}$$
$$f'_{rr} = (1/4)F_{2,2} + (1/4)F_{4,4} - (1/2)F_{7,7}$$
$$r_e f_{r\alpha} = (N_2/4)F_{2,3} + (N_1/4)F_{2,10} + (1/\sqrt{8})F_{7,9}$$
$$r_e f'_{r\alpha} = (N_2/4)F_{2,3} + (N_1/4)F_{2,10} - (1/\sqrt{8})F_{7,9}$$
$$r_e^2 f_\alpha = (N_2^2/4)F_{3,3}+(N_1N_2/2)F_{3,10} + (1/4)F_{6,6} + (1/2)F_{9,9} + (N_1^2/4)F_{10,10}$$
$$r_e^2 f_{\alpha\alpha} = (N_2^2/4)F_{3,3}+(N_1N_2/2)F_{3,10} - (1/4)F_{6,6} + (N_1^2/4)F_{10,10}$$
$$r_e^2 f'_{\alpha\alpha} = (N_2^2/4)F_{3,3}+(N_1N_2/2)F_{3,10} + (1/4)F_{6,6} - (1/2)F_{9,9} + (N_1^2/4)F_{10,10}$$
$$f_{rR} = (1/2)F_{1,2}$$
$$\sqrt{r_eR_e}\, f_{r\beta} = -(N_1/4)F_{2,3} + (N_2/4)F_{2,10} + (1/4)F_{4,5} + (1/2)F_{7,8}$$
$$\sqrt{r_eR_e}\, f'_{r\beta} = -(N_1/4)F_{2,3} + (N_2/4)F_{2,10} - (1/4)F_{4,5}$$
$$\sqrt{r_eR_e}\, f''_{r\beta} = -(N_1/4)F_{2,3} + (N_2/4)F_{2,10} + (1/4)F_{4,5} - (1/2)F_{7,8}$$
$$r_e f_{R\alpha} = (N_2/2)F_{1,3} + (N_1/2)F_{1,10}$$
$$r_e\sqrt{r_eR_e}\, f_{\alpha\beta} = -(N_1N_2/4)F_{3,3} + [(N_2^2-N_1^2)/4]F_{3,10} + (1/\sqrt{8})F_{8,9} + (N_1N_2/4)F_{10,10}$$
$$r_e\sqrt{r_eR_e}\, f'_{\alpha\beta} = -(N_1N_2/4)F_{3,3} + [(N_2^2-N_1^2)/4]F_{3,10} - (1/\sqrt{8})F_{8,9} + (N_1N_2/4)F_{10,10}$$
$$f_R = F_{1,1}$$
$$\sqrt{r_eR_e}\, f_{R\beta} = -(N_1/2)F_{1,3} + (N_2/2)F_{1,10}$$
$$r_eR_e\, f_\beta = (N_1^2/4)F_{3,3} - (N_1N_2/2)F_{3,10} + (1/4)F_{5,5} + (1/2)F_{8,8} + (N_2^2/4)F_{10,10}$$
$$r_eR_e\, f_{\beta\beta} = (N_1^2/4)F_{3,3} - (N_1N_2/2)F_{3,10} - (1/4)F_{5,5} + (N_2^2/4)F_{10,10}$$
$$r_eR_e\, f'_{\beta\beta} = (N_1^2/4)F_{3,3} - (N_1N_2/2)F_{3,10} + (1/4)F_{5,5} - (1/2)F_{8,8} + (N_2^2/4)F_{10,10}$$

from those of f just as the elements of Σ'-are derived from those of $F^{\prime}$, and by replacing F by Σ .

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