中国科学院
应用化学研究所集刊

第十三集

科学出版社

1965年

中国科学院应用化学研究所集刊

第 十 三 集

编辑者　中 国 科 学 院
　　　　应用化学研究所集刊编审委员会

出版者　科 学 出 版 社
　　　　北京朝阳門内大街117号
　　　　北京市书刊出版业营业許可証出字第 061 号

印刷者　中 国 科 学 院 印 刷 厂

发行者　新华书店北京发行所发行
　　　　各 地 新 华 书 店 经 售

1965 年 2 月 第 一 版　　　开本：787×1092 1/16
1965 年 2 月 第一次印刷　　印张：6 3/8 插頁：1
印数：0001—3,200　　　　字数：144,000

統一书号：13031·2075

定 价： 1.10 元

本社书号：3171 · 13-4

中国科学院应用化学研究所集刊

第 十 三 集

目 录

綜 合 評 述

COLLECTED PAPERS OF THE INSTITUTE OF APPLIED CHEMISTRY, ACADEMIA SINICA

No. XIII

CONTENTS

CRITICAL REVIEW

多核自旋系統的核磁波譜分析

II. $A_2B_2X_m$ 和 $A_3B_2X_m$ 近似*

裘祖文　李立璞**　华士英**　俞琳华**

实驗已經証明，A_nBX_m ($n, m \leqslant 3$) 可以近似地概括相当多的化合物，最近 Corio[1] 已給出这一近似的普遍循环表达式．另一方面 $A_nB_2X_m$ ($n, m \leqslant 3$) 类化合物也很多，但由于 A_2B_2 系統的久期方程內就已出現 3×3 行列[2]，因此这一系統至今仍未討論过．事实上在 A_2B_2 系統中需要求的参数实际上只有 2 个 ($\delta = \omega_A - \omega_B$, J)，而它的 16 个能級中，有 13 个是可以列出具体解析形式的．因此，卽使在沒有全部解出久期行列式的情形下，仍然有可能得到所需要的参数[2]．同样的理由，在 A_3B_2 系統中，参数仍只有 2 个，而 32 个能級中有 26 个可以具体列出解析表达式．根据这样的考慮，本文列出了 $A_2B_2X_m$ 和 $A_3B_2X_m$ 的譜綫位置和跃迁強度表，并作了討論．为討論簡便起見，单核的核自旋都設为 1/2.

一、$A_2B_2X_m$ 近似

对于 $A_nB_2X_m$ 系統，下一条件满足:

$$|\delta_{AX}|\ |\delta_{BX}| \gg |\delta_{AB}|\ |J_{AB}|\ |J_{AX}|\ |J_{BX}|$$

設恆磁場方向为 Z 方向，核自旋哈密頓算符为:

$$\hat{\mathscr{H}} = -\{\omega_A \hat{I}_{AZ} + \omega_B \hat{I}_{BZ} + \omega_X \hat{I}_{XZ} + J_{AB}\mathbf{I}_A \cdot \mathbf{I}_B + J_{AX}\hat{I}_{AZ}\hat{I}_{XZ} + J_{BX}\hat{I}_{BZ}\hat{I}_{XZ}\}$$

式中 ω_G, $J_{GG'}$ 采用角頻率单位，为了写出算符 $\hat{\mathscr{H}}$ 的矩陣表象，通常选乘积函数 $A_{I_Am_A}B_{I_Bm_B}X_{I_Xm_X}$ 作为基函数，注意到算符 $\hat{I}_A^2$, $\hat{I}_B^2$, $\hat{I}_X^2$, $\hat{I}_{AZ}+\hat{I}_{BZ}$ 及 $\hat{I}_{XZ}$ 和 $\hat{\mathscr{H}}$ 可对易，因之量子数 I_A, I_B, I_X, $m_A + m_B$, m_X 及 $m \equiv \sum\limits_{A,B,X} m_G$ 都是好的量子数，换言之，只有当 $I'_A = I_A$, $I'_B = I_B$, $I'_X = I_X$, $m'_A + m'_B = m_A + m_B$, $m'_X = m_X$ 时，矩陣元 $\langle A_{I'_Am'_A} B_{I'_Bm'_B} X_{I'_Xm'_X} | \hat{\mathscr{H}} | A_{I_Am_A}B_{I_Bm_B}X_{I_Xm_X}\rangle$ 才可能不等于零．因之 $\hat{\mathscr{H}}$ 矩陣是由許多裂块矩陣所組成．今考慮 m_X 固定的裂块矩陣，对于 $A_2B_2X_m$ 系統，最多有 16 个乘积函数与之相对应（表 1）．表中 $G_{I_Gm_G}$ ($G = ABX$) 的具体形式为:

$$G_{1,1} = \alpha\alpha \qquad G_{1,-1} = \beta\beta$$

$$G_{1,0} = \frac{\alpha\beta + \beta\alpha}{\sqrt{2}} \qquad G_{0,0} = \frac{\alpha\beta - \beta\alpha}{\sqrt{2}} \tag{1}$$

显然，这个裂块矩陣实际上又是若干子矩陣所組成，其中 1X1 行列的子矩陣 9 个，2X2 行列的子矩陣 2 个，3X3 行列的子矩陣 1 个．对于 9 个 1X1 行列的子矩陣，其矩陣元就是

* 編审会于 1964 年 5 月 20 日收到.
** 长春化学学院光譜训练班 1963 年毕业同学.

表 1 $A_2B_2X_m$ 系統久期行列式的裂块矩陣

1X1	m	2X2	m	3X3	m
$A_{11}B_{11}X_{I_Xm_X}$	$2+m_X$	$A_{11}B_{10}X_{I_Xm_X}$	$1+m_X$	$A_{11}B_{1-1}X_{I_Xm_X}$	m_X
$A_{11}B_{00}X_{I_Xm_X}$	$1+m_X$	$A_{10}B_{11}X_{I_Xm_X}$		$A_{10}B_{10}X_{I_Xm_X}$	
$A_{00}B_{11}X_{I_Xm_X}$	$1+m_X$			$A_{1-1}B_{11}X_{I_Xm_X}$	
$A_{10}B_{00}X_{I_Xm_X}$	m_X	$A_{1-1}B_{10}X_{I_Xm_X}$	$-1+m_X$		
$A_{00}B_{10}X_{I_Xm_X}$	m_X	$A_{10}B_{1-1}X_{I_Xm_X}$			
$A_{00}B_{00}X_{I_Xm_X}$	m_X				
$A_{1-1}B_{00}X_{I_Xm_X}$	$-1+m_X$				
$A_{00}B_{1-1}X_{I_Xm_X}$	$-1+m_X$				
$A_{1-1}B_{1-1}X_{I_Xm_X}$	$-2+m_X$				

所需要的本征值,其一般公式为:

$$\langle A_{I_Am_A}B_{I_Bm_B}X_{I_Xm_X}|\hat{\mathscr{H}}|A_{I_Am_A}B_{I_Bm_B}X_{I_Xm_X}\rangle = = -\{m_A\omega_A + m_B\omega_B + m_X\omega_X + J_{AB}m_Am_B + J_{AX}m_Am_X + J_{BX}m_Bm_X\} \quad (2)$$

对于 2X2 行列的子矩陣, 其本征值和本征函数的求得需要解相应的二維久期行列式. 例如: 令

$$\phi_1 \equiv A_{11}B_{10}X_{I_Xm_X}; \quad \phi_2 = A_{10}B_{11}X_{I_Xm_X}$$

則久期行列式为

$$\begin{vmatrix} H_{11}-E & H_{12} \\ H_{12} & H_{22}-E \end{vmatrix} = 0 \quad (3)$$

式(3)中:

$$H_{11} = -\{\omega_A + m_X\omega_X + m_XJ_{AX}\}$$
$$H_{22} = -\{\omega_B + m_X\omega_X + m_XJ_{BX}\}$$
$$H_{12} \equiv \langle A_{11}B_{10}X_{I_Xm_X}|\hat{\mathscr{H}}|A_{10}B_{11}X_{I_Xm_X}\rangle = -J_{AB}$$

如果, 令 $H_{11}=\alpha+\beta$, $H_{22}=\alpha-\beta$, $H_{12}=\gamma$, 則展开式(3),得

$$E_\pm = \alpha \pm \sqrt{\beta^2+\gamma^2}$$

亦即

$$E_\pm = -\frac{1}{2}[(\omega_A+\omega_B) + 2m_X\omega_X + m_X(J_{AX}+J_{BX})] \pm \pm\frac{1}{2}\sqrt{[\delta + m_X(J_{AX}-J_{BX})]^2 + 4J_{AB}^2} \quad (4)$$

以后为簡写起見,令

$$\delta = \omega_A - \omega_B$$
$$R(m_X) = \sqrt{[\delta + m_X(J_{AX}-J_{BX})]^2 + 4J_{AB}^2}$$

对于本征函数的綫性組合系数,需要解下一联立方程式:

$$\begin{cases} C_1(\alpha+\beta-E) + C_2\gamma = 0 & \text{(i)} \\ C_1\gamma + C_2(\alpha-\beta-E) = 0 & \text{(ii)} \\ C_1^2 + C_2^2 = 1 & \text{(iii)} \end{cases} \quad (5)$$

式(5)中,方程 (i), (ii) 是綫性相关的.

从式 (i):

$$\frac{C_1}{C_2} = \frac{-\gamma}{\alpha+\beta-E}$$

設

$$E = E_- = \alpha - \frac{1}{2} R(m_X),$$

則

$$\frac{C_1}{C_2} = \frac{2J_{AB}}{-[\delta + m_X(J_{AX} - J_{BX})] + R(m_X)}$$

令

$$Q(m_X) \equiv \frac{2J_{AB}}{\delta + m_X(J_{AX} - J_{BX}) - R(m_X)}$$

則

$$\begin{cases} C_1 = -Q(m_X)C_2 \\ C_1^2 + C_2^2 = 1 \end{cases}$$

解之，得

$$C_1 = \frac{-Q(m_X)}{\sqrt{1 + Q^2(m_X)}}, \quad C_2 = \frac{1}{\sqrt{1 + Q^2(m_X)}}$$

因此对于能級

$$E_2 = E_- = -\frac{1}{2}[(\omega_A + \omega_B) + 2m_X\omega_X + m_X(J_{AX} + J_{BX})] - \frac{1}{2} R(m_X)$$

其本征函数为：

$$\psi_2 = [1 + Q^2(m_X)]^{-\frac{1}{2}}\{-Q(m_X)A_{11}B_{10}X_{I_Xm_X} + A_{10}B_{11}X_{I_Xm_X}\}$$

同理可得，对于能級

$$E_3 = E_+ = -\frac{1}{2}[(\omega_A + \omega_B) + 2m_X\omega_X + m_X(J_{AX} + J_{BX})] + \frac{1}{2} R(m_X)$$

其本征函数为：

$$\psi_3 = [1 + Q^2(m_X)]^{-\frac{1}{2}}\{A_{11}B_{10}X_{I_Xm_X} + Q(m_X)A_{10}B_{11}X_{I_Xm_X}\}$$

同样的方法可应用到求 E_7E_8，$\psi_7\psi_8$，其結果列于表 2． 对于 $A_2B_2X_m$ 系統，m_X 固定的裂块矩陣中还含有 $3X3$ 行列子矩陣，其形式为：

$$S = \begin{bmatrix} -\delta - m_X\omega_X + J_{AB} - m_X(J_{AX} - J_{BX}) & -J_{AB} & 0 \\ -J_{AB} & -m_X\omega_X & -J_{AB} \\ 0 & -J_{AB} & \delta - m_X\omega_X + J_{AB} + m_X(J_{AX} - J_{BX}) \end{bmatrix}$$

这个子矩陣的本征値和本征函数不能列出具体的解析表达式，今設 $\Omega_1 < \Omega_2 < \Omega_3$ 为矩陣 S 的本征值，$a = (a_{ij})$ 为 S 的归一化本征向量系数所做成的酉矩陣，即：

$$aSa^{-1} = (\Omega_i S_{ij}) \qquad i, j = 1, 2, 3$$

則 $A_2B_2X_m$ 的全部本征値、本征函数可形式地列于表 2．其中 13 个能級和本征函数是眞正有解析表达式的． 从本征値和本征函数表，我們便可以求出 $A_2B_2X_m$ 的跃迁頻率和跃迁強度的循环公式，从熟知的跃迁理論[1,2]知道，核磁共振选择定則为 $\Delta m = 1$，而共振綫的相对強度和矩陣元 $|\langle m| \sum_{A,B,X} I_G^+ |m-1\rangle|^2$ 成正比，此外注意到当 $J_{GG'}$ 一致地趋于零时，$Q(m_X) \to \infty$． 根据通常的命名法[1,2,3]我們称：对于 $\Delta m_G = 1, \Delta m_{G'} = 0$ 的跃迁为 G 类跃迁而 $\Delta m \equiv \sum_G \Delta m_G = 1$ 的跃迁为混合跃迁． 則我們就可以方便地将 $A_2B_2X_m$ 的全

表 2 $A_2B_2X_m$ 系統之本征函数、本征值

本征函数, Ψ		本征値, E	
Ψ_1	$A_{11}B_{11}X_{I_Xm_X}$	E_1	$-(\omega_A+\omega_B+J_{AB})-m_X(J_{AX}+J_{BX}+\omega_X)$
Ψ_2	$(1+Q^2)^{-1/2}\{A_{10}B_{11}X_{I_Xm_X}-QA_{11}B_{10}X_{I_Xm_X}\}$	E_2	$-\frac{1}{2}(\omega_A+\omega_B+R)-\frac{1}{2}m_X(2\omega_X+J_{AX}+J_{BX})$
Ψ_3	$(1+Q^2)^{-1/2}\{QA_{10}B_{11}X_{I_Xm_X}+A_{11}B_{10}X_{I_Xm_X}\}$	E_3	$-\frac{1}{2}(\omega_A+\omega_B-R)-\frac{1}{2}m_X(2\omega_X+J_{AX}+J_{BX})$
Ψ_4	$a_{11}A_{11}B_{1-1}X_{I_Xm_X}+a_{21}A_{10}B_{10}X_{I_Xm_X}+a_{31}A_{1-1}B_{11}X_{I_Xm_X}$	E_4	Ω_1
Ψ_5	$a_{12}A_{11}B_{1-1}X_{I_Xm_X}+a_{22}A_{10}B_{10}X_{I_Xm_X}+a_{32}A_{1-1}B_{11}X_{I_Xm_X}$	E_5	Ω_2
Ψ_6	$a_{13}A_{11}B_{1-1}X_{I_Xm_X}+a_{23}A_{10}B_{10}X_{I_Xm_X}+a_{33}A_{1-1}B_{11}X_{I_Xm_X}$	E_6	Ω_3
Ψ_7	$(1+Q^2)^{-1/2}\{QA_{1-1}B_{10}X_{I_Xm_X}+A_{10}B_{1-1}X_{I_Xm_X}\}$	E_7	$\frac{1}{2}(\omega_A+\omega_B+R)+\frac{1}{2}m_X(-2\omega_X+J_{AX}+J_{BX})$
Ψ_8	$(1+Q^2)^{-1/2}\{A_{1-1}B_{10}X_{I_Xm_X}-QA_{10}B_{1-1}X_{I_Xm_X}\}$	E_8	$\frac{1}{2}(\omega_A+\omega_B-R)+\frac{1}{2}m_X(-2\omega_X+J_{AX}+J_{BX})$
Ψ_9	$A_{1-1}B_{1-1}X_{I_Xm_X}$	E_9	$(\omega_A+\omega_B)-J_{AB}-m_X(\omega_X-J_{AX}-J_{BX})$
Ψ_{10}	$A_{11}B_{00}X_{I_Xm_X}$	E_{10}	$-\omega_A-m_X(\omega_X+J_{AX})$
Ψ_{11}	$A_{10}B_{00}X_{I_Xm_X}$	E_{11}	$-m_X\omega_X$
Ψ_{12}	$A_{1-1}B_{00}X_{I_Xm_X}$	E_{12}	$\omega_A-m_X(\omega_X-J_{AX})$
Ψ_{13}	$A_{00}B_{11}X_{I_Xm_X}$	E_{13}	$-\omega_B-m_X(\omega_X+J_{BX})$
Ψ_{14}	$A_{00}B_{10}X_{I_Xm_X}$	E_{14}	$-m_X\omega_X$
Ψ_{15}	$A_{00}B_{1-1}X_{I_Xm_X}$	E_{15}	$\omega_B-m_X(\omega_X-J_{BX})$
Ψ_{16}	$A_{00}B_{00}X_{I_Xm_X}$	E_{16}	$-m_X\omega_X$

部跃迁分成A类跃迁、B类跃迁、X类跃迁及混合跃迁四类，列于表 3—5. 其中由于A和B完全对称，B类跃迁完全是A类跃迁的反演，故不必再列. 兹举三例說明这些表是如何得来的.

表 3 $A_2B_2X_m$ 系統的A类跃迁强度及频率（B类与此对应）

A类跃迁($J_{GG'}\to 0$)	跃迁强度, I/g_{I_X}	频率
$A_{11}B_{11}X_{I_Xm_X}\to A_{10}B_{11}X_{I_Xm_X}$	$\frac{2(1+Q)^2}{1+Q^2}\cong 2\left(1-\frac{2J_{AB}}{R}\right)$	$\frac{1}{2}(\omega_A+\omega_B+R)+J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})$
$A_{10}B_{1-1}X_{I_Xm_X}\to A_{1-1}B_{1-1}X_{I_Xm_X}$	$\frac{2(1-Q)^2}{1+Q^2}\cong 2\left(1+\frac{2J_{AB}}{R}\right)$	$\frac{1}{2}(\omega_A+\omega_B+R)-J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})$
$A_{11}B_{10}X_{I_Xm_X}\to A_{10}B_{10}X_{I_Xm_X}$	$\frac{2[(a_{22}+a_{32})-Q(a_{12}+a_{22})]^2}{1+Q^2}$	$\Omega_2+\frac{1}{2}(\omega_A+\omega_B+R)+\frac{1}{2}m_X(2\omega_X+J_{AX}+J_{BX})$
$A_{10}B_{11}X_{I_Xm_X}\to A_{1-1}B_{11}X_{I_Xm_X}$	$\frac{2[(a_{13}+a_{23})+Q(a_{23}+a_{33})]^2}{1+Q^2}$	$\Omega_3+\frac{1}{2}(\omega_A+\omega_B-R)+\frac{1}{2}m_X(2\omega_X+J_{AX}+J_{BX})$
$A_{11}B_{1-1}X_{I_Xm_X}\to A_{10}B_{1-1}X_{I_Xm_X}$	$\frac{2[(a_{21}+a_{31})-Q(a_{11}+a_{21})]^2}{1+Q^2}$	$\frac{1}{2}(\omega_A+\omega_B-R)-\Omega_1+\frac{1}{2}m_X(-2\omega_X+J_{AX}+J_{BX})$
$A_{10}B_{10}X_{I_Xm_X}\to A_{1-1}B_{10}X_{I_Xm_X}$	$\frac{2[(a_{12}+a_{22})+Q(a_{22}+a_{32})]^2}{1+Q^2}$	$\frac{1}{2}(\omega_A+\omega_B+R)-\Omega_2+\frac{1}{2}m_X(-2\omega_X+J_{AX}+J_{BX})$
$A_{10}B_{00}X_{I_Xm_X}\to A_{1-1}B_{00}X_{I_Xm_X}$ $A_{11}B_{00}X_{I_Xm_X}\to A_{10}B_{00}X_{I_Xm_X}$	4	$\omega_A+m_XJ_{AX}$

表 4

X 类跃迁 ($J_{GG'} \to 0$)	跃迁強度, $I/g_{I_X}(I_X+m_X)(I_X-m_X+1)$	频率
$A_{11}B_{11}X_{I_Xm_X} \to A_{11}B_{11}X_{I_Xm_X-1}$	1	$\omega_X + (J_{AX} + J_{BX})$
$A_{11}B_{10}X_{I_Xm_X} \to A_{11}B_{10}X_{I_Xm_X-1}$	$(1+Q^2)^{-1}(1+Q'^2)^{-1}[1+QQ']^2$	$\frac{1}{2}(R-R') + \omega_X + \frac{1}{2}(J_{AX}+J_{BX})$
$A_{10}B_{11}X_{I_Xm_X} \to A_{10}B_{11}X_{I_Xm_X-1}$	$(1+Q^2)^{-1}(1+Q'^2)^{-1}[1+QQ']^2$	$\frac{1}{2}(R'-R) + \omega_X + \frac{1}{2}(J_{AX}+J_{BX})$
$A_{11}B_{1-1}X_{I_Xm_X} \to A_{11}B_{1-1}X_{I_Xm_X-1}$	$[a_{11}a'_{11} + a_{21}a'_{21} + a_{31}a'_{31}]^2$	$\Omega'_1 - \Omega_1$
$A_{10}B_{10}X_{I_Xm_X} \to A_{10}B_{10}X_{I_Xm_X-1}$	$[a_{12}a'_{12} + a_{22}a'_{22} + a_{32}a'_{32}]^2$	$\Omega'_2 - \Omega_2$
$A_{1-1}B_{11}X_{I_Xm_X} \to A_{1-1}B_{11}X_{I_Xm_X-1}$	$[a_{13}a'_{13} + a_{23}a'_{23} + a_{33}a'_{33}]^2$	$\Omega'_3 - \Omega_3$
$A_{1-1}B_{10}X_{I_Xm_X} \to A_{1-1}B_{10}X_{I_Xm_X-1}$	$(1+Q^2)^{-1}(1+Q'^2)^{-1}[1+QQ']^2$	$\frac{1}{2}(R'-R) + \omega_X - \frac{1}{2}(J_{AX}+J_{BX})$
$A_{10}B_{1-1}X_{I_Xm_X} \to A_{10}B_{1-1}X_{I_Xm_X-1}$	$(1+Q^2)^{-1}(1+Q'^2)^{-1}[1+QQ']^2$	$\frac{R}{2} - \frac{R'}{2} + \omega_X - \frac{1}{2}(J_{AX}+J_{BX})$
$A_{1-1}B_{1-1}X_{I_Xm_X} \to A_{1-1}B_{1-1}X_{I_Xm_X-1}$	1	$\omega_X - (J_{AX}+J_{BX})$
$A_{11}B_{00}X_{I_Xm_X} \to A_{11}B_{00}X_{I_Xm_X-1}$	1	$\omega_X + J_{AX}$
$A_{00}B_{1-1}X_{I_Xm_X} \to A_{00}B_{1-1}X_{I_Xm_X-1}$	1	$\omega_X - J_{BX}$
$A_{1-1}B_{00}X_{I_Xm_X} \to A_{1-1}B_{00}X_{I_Xm_X-1}$	1	$\omega_X - J_{AX}$
$A_{00}B_{11}X_{I_Xm_X} \to A_{00}B_{11}X_{I_Xm_X-1}$	1	$\omega_X + J_{BX}$
$A_{00}B_{10}X_{I_Xm_X} \to A_{00}B_{10}X_{I_Xm_X-1}$ $A_{00}B_{00}X_{I_Xm_X} \to A_{00}B_{00}X_{I_Xm_X-1}$ $A_{10}B_{00}X_{I_Xm_X} \to A_{10}B_{00}X_{I_Xm_X-1}$	3	ω_X

[例 1]　$E_3 \to E_1$ 显然是允許跃迁 ($\Delta m = 1$). 从表 2 可得:

$$\Delta E = E_3 - E_1 = \frac{1}{2}(\omega_A + \omega_B + R) + J_{AB} + \frac{1}{2} m_X (J_{AX} + J_{BX}).$$

其相对強度为:

$$|\langle \psi_1 | I^+ | \psi_3 \rangle|^2 = |\langle A_{11}B_{11}X_{I_Xm_X} | I_A^+ + I_B^+ + + I_X^+ | (1+Q^2)^{-\frac{1}{2}} \{ Q A_{10}B_{11}X_{I_Xm_X} + A_{11}B_{10}X_{I_Xm_X} \} \rangle|^2 = = (1+Q^2)^{-1}\{2(1+Q)^2\} \equiv 2\left(1 - \frac{2J_{AB}}{R}\right)$$

当 $Q \to \infty$ 时, $\psi_3 \to A_{10}B_{11}X_{I_Xm_X}$, 因此这个跃迁为 A 类跃迁.

[例 2]　$\psi_3(m_X) \to \psi_3(m_X - 1)$, 由于 $\Delta m_X = 1$, 故亦为允許跃迁, 且显然是 X 类跃迁, 其相对強度为:

$$\left| \left\langle \frac{1}{\sqrt{1+Q^2(m_X)}} \{ Q(m_X) A_{10}B_{11}X_{I_Xm_X} + A_{11}B_{10}X_{I_Xm_X} \} \right| I^+ \left| \frac{1}{\sqrt{1+Q^2(m_X-1)}} \cdot \right.\right.$$
$$\left.\left. \cdot \{ Q(m_X-1) A_{10}B_{11}X_{I_Xm_X-1} + A_{11}B_{10}X_{I_Xm_X-1} \} \right\rangle \right|^2 =$$
$$= \frac{1}{[1+Q^2(m_X)][1+Q^2(m_X-1)]} [1 + Q(m_X)Q(m_X-1)]^2 \cdot$$
$$\cdot (I_X - m_X + 1)(I_X + m_X)$$

表 5

混合跃迁 ($J_{GG'} \to 0$)	跃迁强度，I/g_{I_X}	频率
$A_{11}B_{10}X_{I_Xm_X} \to A_{1-1}B_{11}X_{I_Xm_X}$	$(1+Q^2)^{-1}2[(a_{23}+a_{33})-Q(a_{13}+a_{23})]^2$	$\frac{1}{2}(\omega_A+\omega_B+R)+\Omega_3+\frac{1}{2}m_X[2\omega_X+J_{AX}+J_{BX}]$
$A_{11}B_{1-1}X_{I_Xm_X} \to A_{1-1}B_{10}X_{I_Xm_X}$	$(1+Q^2)^{-1}2[(a_{21}+a_{11})+Q(a_{21}+a_{31})]^2$	$\frac{1}{2}(\omega_A+\omega_B+R)-\Omega_1+\frac{1}{2}m_X[-2\omega_X+J_{AX}+J_{BX}]$
$A_{1-1}B_{11}X_{I_Xm_X} \to A_{10}B_{1-1}X_{I_Xm_X}$	$(1+Q^2)^{-1}2[(a_{23}+a_{33})-Q(a_{13}+a_{23})]^2$	$\frac{1}{2}(\omega_A+\omega_B-R)-\Omega_3+\frac{1}{2}m_X[-2\omega_X+J_{AX}+J_{BX}]$
$A_{10}B_{11}X_{I_Xm_X} \to A_{11}B_{1-1}X_{I_Xm_X}$	$(1+Q^2)^{-1}2[(a_{21}+a_{11})+Q(a_{21}+a_{31})]^2$	$\frac{1}{2}(\omega_A+\omega_B-R)+\Omega_1+\frac{1}{2}m_X[2\omega_X+J_{AX}+J_{BX}]$

混合跃迁 ($J_{GG'} \to 0$)	跃迁强度，$I/g_{I_X}(I_X+m_X)(I_X-m_X+1)$	频率
$A_{11}B_{10}X_{I_Xm_X} \to A_{10}B_{11}X_{I_Xm_X-1}$	$(1+Q^2)^{-1}(1+Q'^2)^{-1}[Q'-Q]^2$	$\frac{1}{2}(R+R')+\omega_X+\frac{1}{2}(J_{AX}+J_{BX})$
$A_{10}B_{11}X_{I_Xm_X} \to A_{11}B_{10}X_{I_Xm_X-1}$	$(1+Q^2)^{-1}(1+Q'^2)^{-1}[Q-Q']^2$	$-\frac{1}{2}(R+R')+\omega_X+\frac{1}{2}(J_{AX}+J_{BX})$
$A_{11}B_{1-1}X_{I_Xm_X} \to A_{10}B_{10}X_{I_Xm_X-1}$	$[a_{11}a'_{12}+a_{21}a'_{22}+a_{31}a'_{32}]^2$	$\Omega'_2-\Omega_1$
$A_{11}B_{1-1}X_{I_Xm_X} \to A_{1-1}B_{11}X_{I_Xm_X-1}$	$[a_{11}a'_{13}+a_{21}a'_{23}+a_{31}a'_{33}]^2$	$\Omega'_3-\Omega_1$
$A_{10}B_{10}X_{I_Xm_X} \to A_{11}B_{1-1}X_{I_Xm_X-1}$	$[a_{12}a'_{11}+a_{22}a'_{21}+a_{32}a'_{31}]^2$	$\Omega'_1-\Omega_2$
$A_{10}B_{10}X_{I_Xm_X} \to A_{1-1}B_{11}X_{I_Xm_X-1}$	$[a_{12}a'_{13}+a_{22}a'_{23}+a_{32}a'_{33}]^2$	$\Omega'_3-\Omega_2$
$A_{1-1}B_{11}X_{I_Xm_X} \to A_{11}B_{1-1}X_{I_Xm_X-1}$	$[a_{13}a'_{11}+a_{23}a'_{21}+a_{33}a'_{31}]^2$	$\Omega'_1-\Omega_3$
$A_{1-1}B_{11}X_{I_Xm_X} \to A_{10}B_{10}X_{I_Xm_X-1}$	$[a_{13}a'_{12}+a_{23}a'_{22}+a_{33}a'_{32}]^2$	$\Omega'_2-\Omega_3$
$A_{1-1}B_{10}X_{I_Xm_X} \to A_{10}B_{1-1}X_{I_Xm_X-1}$	$(1+Q^2)^{-1}(1+Q'^2)^{-1}[Q-Q']^2$	$-\frac{1}{2}(R+R')+\omega_X-\frac{1}{2}(J_{AX}+J_{BX})$
$A_{10}B_{1-1}X_{I_Xm_X} \to A_{1-1}B_{10}X_{I_Xm_X-1}$	$(1+Q^2)(1+Q'^2)[Q'-Q]^2$	$\frac{1}{2}(R+R')+\omega_X-\frac{1}{2}(J_{AX}+J_{BX})$

在表 3—5 中为簡便起見，令

$$R \equiv R(m_X), \qquad R' \equiv R(m_X - 1)$$

$$Q \equiv Q(m_X), \qquad Q' \equiv Q(m_X - 1)$$

[例 3] $\psi_3(m_X) \to \psi_2(m_X - 1)$，其相对強度为：

$$\left|\left\langle \frac{1}{\sqrt{1+Q^2(m_X)}} \{Q(m_X) A_{10}B_{11}X_{I_X m_X} + A_{11}B_{10}X_{I_X m_X}\} \right| I^+ \left| \frac{1}{\sqrt{1+Q^2(m_X-1)}} \cdot \right.\right.$$

$$\left.\left. \cdot \{A_{10}B_{11}X_{I_X m_X - 1} - Q(m_X-1)A_{11}B_{10}X_{I_X m_X - 1}\} \right\rangle\right|^2 =$$

$$= \frac{1}{[1+Q^2(m_X)][1+Q^2(m_X-1)]} \{Q(m_X) - Q(m_X-1)\}^2 \cdot$$

$$\cdot (I_X - m_X + 1)(I_X + m_X)$$

注意当 $Q(m_X)$，$Q'(m_X-1) \to \infty$ 时，当相当于：$A_{10}B_{11}X_{I_X m_X} \to A_{11}B_{10}X_{I_X m_X - 1}$，故是混合跃迁.

从表 2—5 可知，$A_2B_2X_m$ 有下列特征及关系式.

1. 在 X 跃迁中，$X(14)$ 最強，其位置恰为 ω_X. 有 6 条強度恰为最強綫 1/3 的譜綫对称地分布在 $X(14)$ 二側，并且：

$$X(1) - X(9) = 2(J_{AX} + J_{BX})$$

$$X(10) - X(12) = 2J_{AX}$$

$$X(11) - X(13) = 2J_{BX}$$

此外 $X(2)$，$X(3)$，$X(7)$，$X(8)$ 四綫強度相同. 而且：

$$X(2) - X(3) = X(8) - X(7) = R - R'$$

$$X(2) - X(8) = X(3) - X(7) = J_{AX} + J_{BX}$$

根据經相似变换后矩陣迹不变的性质，还知：

$$X(4) + X(5) + X(6) = 3\omega_X$$

2. 在 A，B 类跃迁中，B 类跃迁是 A 类跃迁的反演，反演中心为 $\frac{1}{2}(\omega_A + \omega_B) + \frac{1}{2} m_X(J_{AX} + J_{BX})$. $A(7)$，$B(7)$ 的強度为一恆数，因此在辨認了 $X(14)$ 后可以帮助找 $A(7)$，$B(7)$，并且：

$$A(7) - B(7) = \delta + m_X(J_{AX} - J_{BX})$$

$$A(1) - A(2) = 2J_{AB}$$

$$A(1) - B(1) = R + 2J_{AB}$$

$$A(2) - B(2) = R - 2J_{AB}$$

$A(1)$，$A(2)$ 強度之和等于 $A(7)$ 的強度.

3. 当 $J_{GG'} \to 0$ 时，所有混合跃迁綫的強度都一致地趋于零，在一般情形下，混合跃迁強度也很弱，这就在一定程度上減少波譜的复杂性，对譜分析有利.

二、$A_3B_2X_m$ 近似

对于 $A_3B_2X_m$ 系統，m_X 固定的裂块矩陣也是由若干子矩陣所組成（表 6）. 其中 1X1

表 6

1X1	m	2X2	m	3X3	m
$A_{3/2\ 3/2}B_{11}X_{I_Xm_X}$	$5/2+m_X$	$A_{3/2\ 3/2}B_{10}X_{I_Xm_X}$	$\frac{3}{2}+m_X$	$A_{3/2\ 3/2}B_{1-1}X_{I_Xm_X}$	$1/2+m_X$
$A_{3/2\ 3/2}B_{00}X_{I_Xm_X}$	$3/2+m_X$	$A_{3/2\ 1/2}B_{11}X_{I_Xm_X}$		$A_{3/2\ 1/2}B_{10}X_{I_Xm_X}$	
$A_{1/2\ 1/2}B_{11}X_{I_Xm_X}$	$3/2+m_X$	$A_{1/2\ 1/2}B_{10}X_{I_Xm_X}$	$\frac{1}{2}+m_X$	$A_{3/2\ -1/2}B_{11}X_{I_Xm_X}$	
$A^*_{1/2\ 1/2}B_{11}X_{I_Xm_X}$	$3/2+m_X$	$A_{1/2\ -1/2}B_{11}X_{I_Xm_X}$		$A_{3/2\ -3/2}B_{11}X_{I_Xm_X}$	$-1/2+m_X$
$A_{3/2\ 1/2}B_{00}X_{I_Xm_X}$	$1/2+m_X$	$A^*_{1/2\ 1/2}B_{10}X_{I_Xm_X}$	$\frac{1}{2}+m_X$	$A_{3/2\ -1/2}B_{10}X_{I_Xm_X}$	
$A_{1/2\ 1/2}B_{00}X_{I_Xm_X}$	$1/2+m_X$	$A^*_{1/2\ -1/2}B_{11}X_{I_Xm_X}$		$A_{3/2\ 1/2}B_{1-1}X_{I_Xm_X}$	
$A^*_{1/2\ 1/2}B_{00}X_{I_Xm_X}$	$1/2+m_X$	$A_{1/2\ 1/2}B_{1-1}X_{I_Xm_X}$	$-\frac{1}{2}+m_X$		
$A_{1/2\ -1/2}B_{00}X_{I_Xm_X}$	$-1/2+m_X$	$A_{1/2\ -1/2}B_{10}X_{I_Xm_X}$			
$A^*_{1/2\ -1/2}B_{00}X_{I_Xm_X}$	$-1/2+m_X$	$A^*_{1/2\ 1/2}B_{1-1}X_{I_Xm_X}$	$-\frac{1}{2}+m_X$		
$A_{3/2\ -1/2}B_{00}X_{I_Xm_X}$	$-1/2+m_X$	$A^*_{1/2\ -1/2}B_{10}X_{I_Xm_X}$			
$A_{1/2\ -1/2}B_{1-1}X_{I_Xm_X}$	$-3/2+m_X$	$A_{3/2\ -1/2}B_{1-1}X_{I_Xm_X}$	$-\frac{3}{2}+m_X$		
$A^*_{1/2\ -1/2}B_{1-1}X_{I_Xm_X}$	$-3/2+m_X$	$A_{3/2\ -3/2}B_{10}X_{I_Xm_X}$			
$A_{3/2\ -3/2}B_{00}X_{I_Xm_X}$	$-3/2+m_X$				
$A_{3/2\ -3/2}B_{1-1}X_{I_Xm_X}$	$-5/2+m_X$				

子矩陣 14 个,2X2 子矩陣 6 个, 及 3X3 子矩陣 2 个. 因此有 26 个本征值,本征函数可具体解出. 表中 G_3 系統的 $G_{I_Gm_G}$ 的具体形式为:

$$G_{\frac{3}{2},\frac{3}{2}}=\alpha\alpha\alpha \qquad G_{\frac{1}{2},\frac{1}{2}}=\frac{1}{\sqrt{6}}(\alpha\alpha\beta+\alpha\beta\alpha-2\beta\alpha\alpha)$$

$$G_{\frac{3}{2},\frac{1}{2}}=\frac{1}{\sqrt{3}}(\alpha\alpha\beta+\alpha\beta\alpha+\beta\alpha\alpha) \qquad G_{\frac{1}{2},\frac{-1}{2}}=\frac{1}{\sqrt{6}}(\beta\beta\alpha+\beta\alpha\beta-2\alpha\beta\beta)$$

$$G_{\frac{3}{2},\frac{-1}{2}}=\frac{1}{\sqrt{3}}(\beta\beta\alpha+\beta\alpha\beta+\alpha\beta\beta) \qquad G^*_{\frac{1}{2},\frac{1}{2}}=\frac{1}{\sqrt{2}}(\alpha\alpha\beta-\alpha\beta\alpha)$$

$$G_{\frac{3}{2},\frac{-3}{2}}=\beta\beta\beta \qquad G^*_{\frac{1}{2},\frac{-1}{2}}=\frac{1}{\sqrt{2}}(\beta\beta\alpha-\beta\alpha\beta)$$

二个 3X3 子矩陣具体形式为:

$$S^{\pm}=\begin{bmatrix} \begin{matrix}\mp\frac{3}{2}\omega_A\pm\omega_B+\frac{3}{2}J_{AB}\\ -m_X\omega_X\mp m_X\left(\frac{3}{2}J_{AX}-J_{BX}\right)\end{matrix} & -\sqrt{\frac{3}{2}}J_{AB} & 0 \\ -\sqrt{\frac{3}{2}}J_{AB} & \mp\frac{1}{2}\omega_A-m_X\left(\omega_X\pm\frac{1}{2}J_{AX}\right) & -\sqrt{2}J_{AB} \\ 0 & -\sqrt{2}J_{AB} & \begin{matrix}\pm\frac{1}{2}\omega_A\mp\omega_B+\frac{1}{2}J_{AB}\\ -m_X\omega_X\pm m_X\left(\frac{1}{2}J_{AX}-J_{BX}\right)\end{matrix} \end{bmatrix}$$

設 $\Omega_1<\Omega_2<\Omega_3$, $\Omega_4<\Omega_5<\Omega_6$ 依次为 S^+, S^- 的本征值, $a=(a_{ij})$, $b=(b_{ij})$ 依次为 S^+, S^- 归一化本征向量系数做成的酉矩陣,即:

$$aS^+a^{-1}=(\Omega_i\delta_{ij}) \qquad (i,\ j=123)$$

$$bS^-b^{-1}=(\Omega_k\delta_{kl}) \qquad (k,\ l=456)$$

則 $A_3B_2X_m$ 的全部本征值，本征函数可形式地列于表 7． 在表 7—11 中，我們采用下列簡写符号：

$$R_1(m_X) = \sqrt{\left[\delta - \frac{1}{2} J_{AB} + m_X(J_{AX} - J_{BX})\right]^2 + 6J_{AB}^2}$$

$$R_2(m_X) = \sqrt{\left[\delta + \frac{1}{2} J_{AB} + m_X(J_{AX} - J_{BX})\right]^2 + 6J_{AB}^2}$$

$$R_3(m_X) = \sqrt{\left[\delta + \frac{1}{2} J_{AB} + m_X(J_{AX} - J_{BX})\right]^2 + 2J_{AB}^2}$$

$$R_4(m_X) = \sqrt{\left[\delta - \frac{1}{2} J_{AB} + m_X(J_{AX} - J_{BX})\right]^2 + 2J_{AB}^2}$$

$$Q_1(m_X) = \frac{\sqrt{6}\,J_{AB}}{\delta - \frac{1}{2} J_{AB} + m_X(J_{AX} - J_{BX}) - R_1(m_X)}$$

$$Q_2(m_X) = \frac{-\sqrt{6}\,J_{AB}}{\delta + \frac{1}{2} J_{AB} + m_X(J_{AX} - J_{BX}) + R_2(m_X)}$$

$$Q_3(m_X) = \frac{\sqrt{2}\,J_{AB}}{\delta + \frac{1}{2} J_{AB} + m_X(J_{AX} - J_{BX}) - R_3(m_X)}$$

$$Q_4(m_X) = \frac{-\sqrt{2}\,J_{AB}}{\delta - \frac{1}{2} J_{AB} + m_X(J_{AX} - J_{BX}) + R_4(m_X)}$$

表 7 $A_3B_2X_m$ 系統本征值和本征函数

本征函数，Ψ		本征值，E	
Ψ_1	$A_{3/2\ 3/2}B_{11}X_{I_Xm_X}$	E_1	$-\frac{3}{2}\omega_A-\omega_B-\frac{3}{2}J_{AB}-m_X\left(\omega_X+\frac{3}{2}J_{AX}+J_{BX}\right)$
Ψ_2	$(Q_1^2+1)^{-1/2}[-Q_1A_{3/2\ 3/2}B_{10}X_{I_Xm_X}+A_{3/2\ 1/2}B_{11}X_{I_Xm_X}]$	E_2	$-\omega_A-\frac{1}{2}\omega_B-\frac{1}{4}J_{AB}-m_X\left(\omega_X+J_{AX}+\frac{1}{2}J_{BX}\right)-\frac{R_1}{2}$
Ψ_3	$(Q_1^2+1)^{-1/2}[A_{3/2\ 3/2}B_{10}X_{I_Xm_X}+Q_1A_{3/2\ 1/2}B_{11}X_{I_Xm_X}]$	E_3	$-\omega_A-\frac{1}{2}\omega_B-\frac{1}{4}J_{AB}-m_X\left(\omega_X+J_{AX}+\frac{1}{2}J_{BX}\right)+\frac{R_1}{2}$
Ψ_4	$a_{11}A_{3/2\ 3/2}B_{1-1}X_{I_Xm_X}+a_{21}A_{3/2\ 1/2}B_{10}X_{I_Xm_X}+$ $+a_{31}A_{3/2\ -1/2}B_{11}X_{I_Xm_X}$	E_4	Ω_1
Ψ_5	$a_{12}A_{3/2\ 3/2}B_{1-1}X_{I_Xm_X}+a_{22}A_{3/2\ 1/2}B_{10}X_{I_Xm_X}+$ $+a_{32}A_{3/2\ -1/2}B_{11}X_{I_Xm_X}$	E_5	Ω_2
Ψ_6	$a_{13}A_{3/2\ 3/2}B_{1-1}X_{I_Xm_X}+a_{23}A_{3/2\ 1/2}B_{10}X_{I_Xm_X}+$ $+a_{33}A_{3/2\ -1/2}B_{11}X_{I_Xm_X}$	E_6	Ω_3
Ψ_7	$b_{11}A_{3/2\ -3/2}B_{11}X_{I_Xm_X}+b_{21}A_{3/2\ -1/2}B_{10}X_{I_Xm_X}+$ $+b_{31}A_{3/2\ 1/2}B_{1-1}X_{I_Xm_X}$	E_7	Ω_4

（續 表 7）

本 征 函 数，Ψ		本 征 值，E	
Ψ_8	$b_{12}A_{3/2\,-3/2}B_{11}X_{I_X m_X}+b_{22}A_{3/2\,-1/2}B_{10}X_{I_X m_X}+$ $+\,b_{32}A_{3/2\,1/2}B_{1-1}X_{I_X m_X}$	E_8	Ω_5
Ψ_9	$b_{13}A_{3/2\,-3/2}B_{11}X_{I_X m_X}+b_{23}A_{3/2\,-1/2}B_{10}X_{I_X m_X}+$ $+\,b_{33}A_{3/2\,1/2}B_{1-1}X_{I_X m_X}$	E_9	Ω_6
Ψ_{10}	$(Q_2^2+1)^{-1/2}[A_{3/2\,-1/2}B_{1-1}X_{I_X m_X}-Q_2A_{3/2\,-3/2}B_{10}X_{I_X m_X}]$	E_{10}	$\omega_A+\frac{1}{2}\omega_B-\frac{1}{4}J_{AB}-m_X\left(\omega_X-J_{AX}-\right.$ $\left.-\frac{1}{2}J_{BX}\right)-\frac{R_2}{2}$
Ψ_{11}	$(Q_2^2+1)^{-1/2}[Q_2A_{3/2\,-1/2}B_{1-1}X_{I_X m_X}+A_{3/2\,-3/2}B_{10}X_{I_X m_X}]$	E_{11}	$\omega_A+\frac{1}{2}\omega_B-\frac{1}{4}J_{AB}-m_X\left(\omega_X-J_{AX}-\right.$ $\left.-\frac{1}{2}J_{BX}\right)+\frac{R_2}{2}$
Ψ_{12}	$A_{3/2\,-3/2}B_{1-1}X_{I_X m_X}$	E_{12}	$\frac{3}{2}\omega_A+\omega_B-\frac{3}{2}J_{AB}-m_X\left(\omega_X-\frac{3}{2}J_{AX}-J_{BX}\right)$
Ψ_{13}	$A_{3/2\,3/2}B_{00}X_{I_X m_X}$	E_{13}	$-\frac{3}{2}\omega_A-m_X\left(\omega_X+\frac{3}{2}J_{AX}\right)$
Ψ_{14}	$A_{3/2\,1/2}B_{00}X_{I_X m_X}$	E_{14}	$-\frac{1}{2}\omega_A-m_X\left(\omega_X+\frac{1}{2}J_{AX}\right)$
Ψ_{15}	$A_{3/2\,-1/2}B_{00}X_{I_X m_X}$	E_{15}	$\frac{1}{2}\omega_A-m_X\left(\omega_X-\frac{1}{2}J_{AX}\right)$
Ψ_{16}	$A_{3/2\,-3/2}B_{00}X_{I_X m_X}$	E_{16}	$\frac{3}{2}\omega_A-m_X\left(\omega_X-\frac{3}{2}J_{AX}\right)$
Ψ_{17}	$A_{1/2\,1/2}B_{11}X_{I_X m_X}$	E_{17}	$-\frac{1}{2}\omega_A-\omega_B-\frac{1}{2}J_{AB}-m_X\left(\omega_X+\frac{1}{2}J_{AX}+J_{BX}\right)$
Ψ_{18}	$(Q_3^2+1)^{-1/2}[-Q_3A_{1/2\,1/2}B_{10}X_{I_X m_X}+$ $+\,A_{1/2\,-1/2}B_{11}X_{I_X m_X}]$	E_{18}	$-\frac{1}{2}\omega_B+\frac{J_{AB}}{4}-m_X\left(\omega_X+\frac{1}{2}J_{BX}\right)-\frac{R_3}{2}$
Ψ_{19}	$(Q_3^2+1)^{-1/2}[A_{1/2\,1/2}B_{10}X_{I_X m_X}+Q_3A_{1/2\,-1/2}B_{11}X_{I_X m_X}]$	E_{19}	$-\frac{1}{2}\omega_B+\frac{J_{AB}}{4}-m_X\left(\omega_X+\frac{1}{2}J_{BX}\right)+\frac{R_3}{2}$
Ψ_{20}	$(Q_4^2+1)^{-1/2}[A_{1/2\,1/2}B_{1-1}X_{I_X m_X}-Q_4A_{1/2\,-1/2}B_{10}X_{I_X m_X}]$	E_{20}	$\frac{1}{2}\omega_B+\frac{J_{AB}}{4}-m_X\left(\omega_X-\frac{1}{2}J_{BX}\right)-\frac{R_4}{2}$
Ψ_{21}	$(Q_4^2+1)^{-1/2}[Q_4A_{1/2\,1/2}B_{1-1}X_{I_X m_X}+A_{1/2\,-1/2}B_{10}X_{I_X m_X}]$	E_{21}	$\frac{1}{2}\omega_B+\frac{J_{AB}}{4}-m_X\left(\omega_X-\frac{1}{2}J_{BX}\right)+\frac{R_4}{2}$
Ψ_{22}	$A_{1/2\,-1/2}B_{1-1}X_{I_X m_X}$	E_{22}	$\frac{1}{2}\omega_A+\omega_B-\frac{1}{2}J_{AB}-m_X\left(\omega_X-\frac{1}{2}J_{AX}-J_{BX}\right)$
Ψ_{23}	$A_{1/2\,1/2}B_{00}X_{I_X m_X}$	E_{23}	$-\frac{1}{2}\omega_A-m_X\left(\omega_X+\frac{1}{2}J_{AX}\right)$
Ψ_{24}	$A_{1/2\,-1/2}B_{00}X_{I_X m_X}$	E_{24}	$\frac{1}{2}\omega_A-m_X\left(\omega_X-\frac{1}{2}J_{AX}\right)$
Ψ_{25}	$A^*_{1/2\,1/2}B_{11}X_{I_X m_X}$	E_{25}	$-\frac{1}{2}\omega_A-\omega_B-\frac{1}{2}J_{AB}-m_X\left(\omega_X+\right.$ $\left.+\frac{1}{2}J_{AX}+J_{BX}\right)$
Ψ_{26}	$(Q_3^2+1)^{-1/2}[-Q_3A^*_{1/2\,1/2}B_{10}X_{I_X m_X}+$ $+\,A^*_{1/2\,-1/2}B_{11}X_{I_X m_X}]$	E_{26}	$-\frac{1}{2}\omega_B+\frac{J_{AB}}{4}-m_X\left(\omega_X+\frac{1}{2}J_{BX}\right)-\frac{R_3}{2}$
Ψ_{27}	$(Q_3^2+1)^{-1/2}[A^*_{1/2\,1/2}B_{10}X_{I_X m_X}+Q_3A^*_{1/2\,-1/2}B_{11}X_{I_X m_X}]$	E_{27}	$-\frac{1}{2}\omega_B+\frac{J_{AB}}{4}-m_X\left(\omega_X+\frac{1}{2}J_{BX}\right)+\frac{R_3}{2}$
Ψ_{28}	$(Q_4^2+1)^{-1/2}[A^*_{1/2\,1/2}B_{1-1}X_{I_X m_X}-Q_4A^*_{1/2\,-1/2}B_{10}X_{I_X m_X}]$	E_{28}	$\frac{1}{2}\omega_B+\frac{J_{AB}}{2}-m_X\left(\omega_X-\frac{1}{2}J_{BX}\right)-\frac{R_4}{2}$
Ψ_{29}	$(Q_4^2+1)^{-1/2}[Q_4A^*_{1/2\,1/2}B_{1-1}X_{I_X m_X}+A^*_{1/2\,-1/2}B_{10}X_{I_X m_X}]$	E_{29}	$\frac{1}{2}\omega_B+\frac{J_{AB}}{2}-m_X\left(\omega_X-\frac{1}{2}J_{BX}\right)+\frac{R_4}{2}$
Ψ_{30}	$A^*_{1/2\,-1/2}B_{1-1}X_{I_X m_X}$	E_{30}	$\frac{1}{2}\omega_A+\omega_B-\frac{1}{2}J_{AB}-m_X\left(\omega_X-\right.$ $\left.-\frac{1}{2}J_{AX}-J_{BX}\right)$
Ψ_{31}	$A^*_{1/2\,1/2}B_{00}X_{I_X m_X}$	E_{31}	$-\frac{1}{2}\omega_A-m_X\left(\omega_X+\frac{1}{2}J_{AX}\right)$
Ψ_{32}	$A^*_{1/2\,-1/2}B_{00}X_{I_X m_X}$	E_{32}	$\frac{1}{2}\omega_A-m_X\left(\omega_X-\frac{1}{2}J_{AX}\right)$

表8　$A_3B_2X_m$ 系統的 A 类跃迁强度及頻率

	A 类跃迁 ($J_{GG'} \to 0$)	跃迁强度，I/g_{I_X}	頻率
1	$A_{3/2\,3/2}B_{11}X_{I_Xm_X} \to A_{3/2\,1/2}B_{11}X_{I_Xm_X}$	$\frac{(\sqrt{2}+\sqrt{3}\,Q_1)^2}{1+Q_1^2}$	$\frac{1}{2}(\omega_A+\omega_B)+\frac{5}{4}J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})+\frac{R_1}{2}$
2	$A_{1/2\,1/2}B_{11}X_{I_Xm_X} \to A_{1/2\,-1/2}B_{11}X_{I_Xm_X}$ $A^*_{1/2\,1/2}B_{11}X_{I_Xm_X} \to A^*_{1/2\,-1/2}B_{11}X_{I_Xm_X}$	$\frac{2(Q_3+\sqrt{2})^2}{1+Q_3^2}$	$\frac{1}{2}(\omega_A+\omega_B)+\frac{3}{4}J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})+\frac{R_3}{2}$
3	$A_{3/2\,-1/2}B_{1-1}X_{I_Xm_X} \to A_{3/2\,-3/2}B_{1-1}X_{I_Xm_X}$	$\frac{(\sqrt{2}\,Q_2-\sqrt{3})^2}{1+Q_2^2}$	$\frac{1}{2}(\omega_A+\omega_B)-\frac{5}{4}J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})+\frac{R_2}{2}$
4	$A_{1/2\,1/2}B_{10}X_{I_Xm_X} \to A_{1/2\,-1/2}B_{10}X_{I_Xm_X}$ $A^*_{1/2\,1/2}B_{10}X_{I_Xm_X} \to A^*_{1/2\,-1/2}B_{10}X_{I_Xm_X}$	$\frac{2[Q_3+\sqrt{2}(Q_4Q_3-1)]^2}{(1+Q_3^2)(1+Q_4^2)}$	$\omega_B+m_XJ_{BX}+\frac{R_4}{2}+\frac{R_3}{2}$
5	$A_{1/2\,1/2}B_{1-1}X_{I_Xm_X} \to A_{1/2\,-1/2}B_{1-1}X_{I_Xm_X}$ $A^*_{1/2\,1/2}B_{1-1}X_{I_Xm_X} \to A^*_{1/2\,-1/2}B_{1-1}X_{I_Xm_X}$	$\frac{2(\sqrt{2}\,Q_4-1)^2}{1+Q_4^2}$	$\frac{1}{2}(\omega_A+\omega_B)-\frac{3}{4}J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})+\frac{R_4}{2}$
6	$A_{3/2\,3/2}B_{00}X_{I_Xm_X} \to A_{3/2\,1/2}B_{00}X_{I_Xm_X}$ $A_{3/2\,1/2}B_{00}X_{I_Xm_X} \to A_{3/2\,-1/2}B_{00}X_{I_Xm_X}$ $A_{3/2\,-1/2}B_{00}X_{I_Xm_X} \to A_{3/2\,-3/2}B_{00}X_{I_Xm_X}$ $A_{1/2\,1/2}B_{00}X_{I_Xm_X} \to A_{1/2\,-1/2}B_{00}X_{I_Xm_X}$ $A^*_{1/2\,1/2}B_{00}X_{I_Xm_X} \to A^*_{1/2\,-1/2}B_{00}X_{I_Xm_X}$	12	$\omega_A+m_XJ_{AX}$
7	$A_{3/2\,1/2}B_{11}X_{I_Xm_X} \to A_{3/2\,-1/2}B_{11}X_{I_Xm_X}$	$\frac{[\sqrt{2}\,a_{13}+(\sqrt{3}+\sqrt{2}\,Q_1)a_{23}+2Q_1a_{33}]^2}{1+Q_1^2}$	$\Omega_3+\omega_A+\frac{1}{2}\omega_B+\frac{1}{4}J_{AB}+m_X\left(\omega_X+J_{AX}+\frac{1}{2}J_{BX}\right)-\frac{R_1}{2}$
8	$A_{3/2\,3/2}B_{10}X_{I_Xm_X} \to A_{3/2\,1/2}B_{10}X_{I_Xm_X}$	$\frac{[\sqrt{2}Q_1a_{12}+(\sqrt{3}\,Q_1-\sqrt{2})a_{22}-2a_{32}]^2}{1+Q_1^2}$	$\Omega_2+\omega_A+\frac{1}{2}\omega_B+\frac{1}{4}J_{AB}+m_X\left(\omega_X+J_{AX}+\frac{1}{2}J_{BX}\right)+\frac{R_1}{2}$
9	$A_{3/2\,3/2}B_{1-1}X_{I_Xm_X} \to A_{3/2\,1/2}B_{1-1}X_{I_Xm_X}$	$[\sqrt{3}\,a_{31}b_{13}+(2a_{21}+\sqrt{2}\,a_{31})b_{23}+$ $+(\sqrt{3}\,a_{11}+\sqrt{2}\,a_{21})b_{33}]^2$	$\Omega_6-\Omega_1$
10	$A_{3/2\,1/2}B_{10}X_{I_Xm_X} \to A_{3/2\,-1/2}B_{10}X_{I_Xm_X}$	$[\sqrt{3}\,a_{32}b_{12}+(2a_{22}+\sqrt{2}\,a_{32})b_{22}+$ $+(\sqrt{3}\,a_{12}+\sqrt{2}\,a_{22})b_{32}]^2$	$\Omega_5-\Omega_2$
11	$A_{3/2\,-1/2}B_{11}X_{I_Xm_X} \to A_{3/2\,-3/2}B_{11}X_{I_Xm_X}$	$[\sqrt{3}\,a_{33}b_{11}+(2a_{23}+\sqrt{2}\,a_{33})b_{21}+$ $+(\sqrt{3}\,a_{13}+\sqrt{2}\,a_{23})b_{31}]^2$	$\Omega_4-\Omega_3$
12	$A_{3/2\,-1/2}B_{10}X_{I_Xm_X} \to A_{3/2\,-3/2}B_{10}X_{I_Xm_X}$	$\frac{[\sqrt{2}\,b_{12}+(\sqrt{3}+\sqrt{2}\,Q_2)b_{22}+2Q_2b_{32}]^2}{1+Q_2^2}$	$\omega_A+\frac{1}{2}\omega_B-\frac{1}{4}J_{AB}+m_X\left(J_{AX}+\frac{1}{2}J_{BX}-\omega_X\right)+\frac{R_2}{2}-\Omega_5$
13	$A_{3/2\,1/2}B_{1-1}X_{I_Xm_X} \to A_{3/2\,-1/2}B_{1-1}X_{I_Xm_X}$	$\frac{[\sqrt{2}\,Q_2b_{13}+(\sqrt{3}\,Q_2-\sqrt{2})b_{23}-2b_{33}]^2}{1+Q_2^2}$	$\omega_A+\frac{1}{2}\omega_B-\frac{1}{4}J_{AB}+m_X\left(J_{AX}+\frac{1}{2}J_{BX}-\omega_X\right)-\frac{R_2}{2}-\Omega_6$

表 9　$A_3B_2X_m$ 系統的 B 类跃迁强度及頻率

	B 类跃迁 ($J_{GG'}\to 0$)	跃迁强度, I/g_{I_X}	頻率
1	$A_{3/2\ 3/2}B_{11}X_{I_Xm_X}\to A_{3/2\ 3/2}B_{10}X_{I_Xm_X}$	$\frac{(\sqrt{2}Q_1-\sqrt{3})^2}{1+Q_1^2}$	$\frac{1}{2}(\omega_A+\omega_B)+\frac{5}{4}J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})-\frac{R_1}{2}$
2	$A_{1/2\ 1/2}B_{11}X_{I_Xm_X}\to A_{1/2\ 1/2}B_{10}X_{I_Xm_X}$ $A^*_{1/2\ 1/2}B_{11}X_{I_Xm_X}\to A^*_{1/2\ 1/2}B_{10}X_{I_Xm_X}$	$\frac{2(\sqrt{2}Q_3-1)^2}{1+Q_3^2}$	$\frac{1}{2}(\omega_A+\omega_B)+\frac{3}{4}J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})-\frac{R_3}{2}$
3	$A_{3/2\ -3/2}B_{10}X_{I_Xm_X}\to A_{3/2\ -3/2}B_{1-1}X_{I_Xm_X}$	$\frac{(\sqrt{2}+\sqrt{3}Q_2)^2}{1+Q_2^2}$	$\frac{1}{2}(\omega_A+\omega_B)-\frac{5}{4}J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})-\frac{R_2}{2}$
4	$A_{1/2\ -1/2}B_{11}X_{I_Xm_X}\to A_{1/2\ -1/2}B_{10}X_{I_Xm_X}$ $A^*_{1/2\ -1/2}B_{11}X_{I_Xm_X}\to A^*_{1/2\ -1/2}B_{10}X_{I_Xm_X}$	$\frac{2[1+\sqrt{2}(Q_3+Q_4)]^2}{(1+Q_3^2)(1+Q_4^2)}$	$\omega_B+m_XJ_{BX}+\frac{R_4}{2}-\frac{R_3}{2}$
5	$A_{1/2\ 1/2}B_{10}X_{I_Xm_X}\to A_{1/2\ 1/2}B_{1-1}X_{I_Xm_X}$ $A^*_{1/2\ 1/2}B_{10}X_{I_Xm_X}\to A^*_{1/2\ 1/2}B_{1-1}X_{I_Xm_X}$	$\frac{2[(Q_3-\sqrt{2})Q_4-\sqrt{2}Q_3]^2}{(1+Q_3^2)(1+Q_4^2)}$	$\omega_B+m_XJ_{BX}-\frac{R_4}{2}+\frac{R_3}{2}$
6	$A_{1/2\ -1/2}B_{10}X_{I_Xm_X}\to A_{1/2\ -1/2}B_{1-1}X_{I_Xm_X}$ $A^*_{1/2\ -1/2}B_{10}X_{I_Xm_X}\to A^*_{1/2\ -1/2}B_{1-1}X_{I_Xm_X}$	$\frac{2(Q_4+\sqrt{2})^2}{1+Q_4^2}$	$\frac{1}{2}(\omega_A+\omega_B)-\frac{3}{4}J_{AB}+\frac{1}{2}m_X(J_{AX}+J_{BX})-\frac{R_4}{2}$
7	$A_{3/2\ 3/2}B_{10}X_{I_Xm_X}\to A_{3/2\ 3/2}B_{1-1}X_{I_Xm_X}$	$\frac{[\sqrt{2}Q_1a_{11}+(\sqrt{3}Q_1-\sqrt{2})a_{21}-2a_{31}]^2}{1+Q_1^2}$	$\left(\omega_A+\frac{1}{2}\omega_B\right)+\frac{1}{4}J_{AB}+m_X\left(\omega_X+J_{AX}+\frac{1}{2}J_{BX}\right)+\frac{R_1}{2}+\Omega_1$
8	$A_{3/2\ 1/2}B_{11}X_{I_Xm_X}\to A_{3/2\ 1/2}B_{10}X_{I_Xm_X}$	$\frac{[\sqrt{2}a_{12}+(\sqrt{3}+\sqrt{2}Q_1)a_{22}+2Q_1a_{32}]^2}{1+Q_1^2}$	$\left(\omega_A+\frac{1}{2}\omega_B\right)+\frac{1}{4}J_{AB}+m_X\left(\omega_X+J_{AX}+\frac{1}{2}J_{BX}\right)-\frac{R}{2}+\Omega_2$
9	$A_{3/2\ -3/2}B_{11}X_{I_Xm_X}\to A_{3/2\ -3/2}B_{10}X_{I_Xm_X}$	$\frac{[\sqrt{2}b_{11}+(\sqrt{3}+\sqrt{2}Q_2)b_{21}+2Q_2b_{31}]^2}{1+Q_2^2}$	$\left(\omega_A+\frac{1}{2}\omega_B\right)-\frac{1}{4}J_{AB}+m_X\left(-\omega_X+J_{AX}+\frac{1}{2}J_{BX}\right)+\frac{R_2}{2}-\Omega_4$
10	$A_{3/2\ -1/2}B_{10}X_{I_Xm_X}\to A_{3/2\ -1/2}B_{1-1}X_{I_Xm_X}$	$\frac{[\sqrt{2}Q_2b_{12}+(\sqrt{3}Q_2-\sqrt{2})b_{22}-2b_{32}]^2}{1+Q_2^2}$	$\left(\omega_A+\frac{1}{2}\omega_B\right)-\frac{1}{4}J_{AB}+m_X\left(J_{AX}+\frac{1}{2}J_{BX}-\omega_X\right)-\frac{R_2}{2}-\Omega_5$
11	$A_{3/2\ -1/2}B_{11}X_{I_Xm_X}\to A_{3/2\ -1/2}B_{10}X_{I_Xm_X}$	$[\sqrt{3}a_{33}b_{12}+(2a_{23}+\sqrt{2}a_{33})b_{22}+$ $+(\sqrt{3}a_{13}+\sqrt{2}a_{23})b_{32}]^2$	$\Omega_5-\Omega_3$
12	$A_{3/2\ 1/2}B_{10}X_{I_Xm_X}\to A_{3/2\ 1/2}B_{1-1}X_{I_Xm_X}$	$[\sqrt{3}a_{32}b_{13}+(2a_{22}+\sqrt{2}a_{32})b_{23}+$ $+(\sqrt{3}a_{12}+\sqrt{2}a_{22})b_{33}]^2$	$\Omega_6-\Omega_2$

表 10 $A_3B_2X_m$ 系统的 X 类跃迁强度及频率

	X 类跃迁 ($J_{GG'}\to 0$)	跃迁强度，I/g_{I_X}	频率
1	$A_{3/2\,3/2}B_{11}X_{I_Xm_X}\to A_{3/2\,3/2}B_{11}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)$	$\omega_X+\frac{3}{2}J_{AX}+J_{BX}$
2	$A_{3/2\,-3/2}B_{1-1}X_{I_Xm_X}\to A_{3/2\,-3/2}B_{1-1}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)$	$\omega_X-\frac{3}{2}J_{AX}-J_{BX}$
3	$A_{3/2\,3/2}B_{10}X_{I_Xm_X}\to A_{3/2\,3/2}B_{10}X_{I_Xm_X-1}$	$\frac{(I_X+m_X)(I_X-m_X+1)[Q_1Q_1'+1]^2}{(1+Q_1^2)(1+Q_1'^2)}$	$\omega_X+J_{AX}+\frac{1}{2}J_{BX}-\frac{R_1'}{2}+\frac{R_1}{2}$
4	$A_{3/2\,1/2}B_{11}X_{I_Xm_X}\to A_{3/2\,1/2}B_{11}X_{I_Xm_X-1}$	$\frac{(I_X+m_X)(I_X-m_X+1)[1+Q_1Q_1']^2}{(1+Q_1^2)(1+Q_1'^2)}$	$\omega_X+J_{AX}+\frac{1}{2}J_{BX}+\frac{R_1'}{2}-\frac{R_1}{2}$
5	$A_{3/2\,3/2}B_{1-1}X_{I_Xm_X}\to A_{3/2\,3/2}B_{1-1}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)[a_{11}a_{11}'+$ $+a_{21}a_{21}'+a_{31}a_{31}']^2$	$\Omega_1'-\Omega_1$
6	$A_{3/2\,1/2}B_{10}X_{I_Xm_X}\to A_{3/2\,1/2}B_{10}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)[a_{12}a_{12}'+$ $+a_{22}a_{22}'+a_{32}a_{32}']^2$	$\Omega_2'-\Omega_2$
7	$A_{3/2\,-1/2}B_{11}X_{I_Xm_X}\to A_{3/2\,-1/2}B_{11}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)[a_{13}a_{13}'+$ $+a_{23}a_{23}'+a_{33}a_{33}']^2$	$\Omega_3'-\Omega_3$
8	$A_{3/2\,-3/2}B_{11}X_{I_Xm_X}\to A_{3/2\,-3/2}B_{11}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)[b_{11}b_{11}'+$ $+b_{21}b_{21}'+b_{31}b_{31}']^2$	$\Omega_4'-\Omega_4$
9	$A_{3/2\,-1/2}B_{10}X_{I_Xm_X}\to A_{3/2\,-1/2}B_{10}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)[b_{12}b_{12}'+$ $+b_{22}b_{22}'+b_{32}b_{32}']^2$	$\Omega_5'-\Omega_5$
10	$A_{3/2\,1/2}B_{1-1}X_{I_Xm_X}\to A_{3/2\,1/2}B_{1-1}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)[b_{13}b_{13}'+$ $+b_{23}b_{23}'+b_{33}b_{33}']^2$	$\Omega_6'-\Omega_6$
11	$A_{3/2\,-1/2}B_{1-1}X_{I_Xm_X}\to A_{3/2\,-1/2}B_{1-1}X_{I_Xm_X-1}$	$\frac{(I_X+m_X)(I_X-m_X+1)[1+Q_2Q_2']^2}{(1+Q_2^2)(1+Q_2'^2)}$	$\omega_X-J_{AX}-\frac{1}{2}J_{BX}-\frac{R_2'}{2}+\frac{R_2}{2}$
12	$A_{3/2\,-3/2}B_{10}X_{I_Xm_X}\to A_{3/2\,-3/2}B_{10}X_{I_Xm_X-1}$	$\frac{(I_X+m_X)(I_X-m_X+1)[1+Q_2Q_2']^2}{(1+Q_2^2)(1+Q_2'^2)}$	$\omega_X-J_{AX}-\frac{1}{2}J_{BX}+\frac{R_2'}{2}-\frac{R_2}{2}$
13	$A_{3/2\,3/2}B_{00}X_{I_Xm_X}\to A_{3/2\,3/2}B_{00}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)$	$\omega_X+\frac{3}{2}J_{AX}$
14	$A_{3/2\,-3/2}B_{00}X_{I_Xm_X}\to A_{3/2\,-3/2}B_{00}X_{I_Xm_X-1}$	$(I_X+m_X)(I_X-m_X+1)$	$\omega_X-\frac{3}{2}J_{AX}$
15	$A_{1/2\,1/2}B_{11}X_{I_Xm_X}\to A_{1/2\,1/2}B_{11}X_{I_Xm_X-1}$ $A_{1/2\,1/2}^*B_{11}X_{I_Xm_X}\to A_{1/2\,1/2}^*B_{11}X_{I_Xm_X-1}$	$2(I_X+m_X)(I_X-m_X+1)$	$\omega_X+\frac{1}{2}J_{AX}+J_{BX}$
16	$A_{1/2\,-1/2}B_{1-1}X_{I_Xm_X}\to A_{1/2\,-1/2}B_{1-1}X_{I_Xm_X-1}$ $A_{1/2\,-1/2}^*B_{1-1}X_{I_Xm_X}\to A_{1/2\,-1/2}^*B_{1-1}X_{I_Xm_X-1}$	$2(I_X+m_X)(I_X-m_X+1)$	$\omega_X-\frac{1}{2}J_{AX}-J_{BX}$
17	$A_{1/2\,1/2}B_{10}X_{I_Xm_X}\to A_{1/2\,+1/2}B_{10}X_{I_Xm_X-1}$ $A_{1/2\,1/2}^*B_{10}X_{I_Xm_X}\to A_{1/2\,1/2}^*B_{10}X_{I_Xm_X-1}$	$\frac{2(I_X+m_X)(I_X-m_X+1)[1+Q_3Q_3']^2}{(1+Q_3^2)(1+Q_3'^2)}$	$\omega_X+\frac{1}{2}J_{BX}-\frac{R_3'}{2}+\frac{R_3}{2}$
18	$A_{1/2\,-1/2}B_{11}X_{I_Xm_X}\to A_{1/2\,-1/2}B_{11}X_{I_Xm_X-1}$ $A_{1/2\,-1/2}^*B_{11}X_{I_Xm_X}\to A_{1/2\,-1/2}^*B_{11}X_{I_Xm_X-1}$	$\frac{2(I_X+m_X)(I_X-m_X+1)[1+Q_3Q_3']^2}{(1+Q_3^2)(1+Q_3'^2)}$	$\omega_X+\frac{1}{2}J_{BX}+\frac{R_3'}{2}-\frac{R_3}{2}$
19	$A_{1/2\,1/2}B_{1-1}X_{I_Xm_X}\to A_{1/2\,1/2}B_{1-1}X_{I_Xm_X-1}$ $A_{1/2\,1/2}^*B_{1-1}X_{I_Xm_X}\to A_{1/2\,1/2}^*B_{1-1}X_{I_Xm_X-1}$	$\frac{2(I_X+m_X)(I_X-m_X+1)[1+Q_4Q_4']^2}{(1+Q_4^2)(1+Q_4'^2)}$	$\omega_X-\frac{1}{2}J_{BX}-\frac{R_4'}{2}+\frac{R_4}{2}$
20	$A_{1/2\,-1/2}B_{10}X_{I_Xm_X}\to A_{1/2\,-1/2}B_{10}X_{I_Xm_X-1}$ $A_{1/2\,-1/2}^*B_{10}X_{I_Xm_X}\to A_{1/2\,-1/2}^*B_{10}X_{I_Xm_X-1}$	$\frac{2(I_X+m_X)(I_X-m_X+1)[1+Q_4Q_4']^2}{(1+Q_4^2)(1+Q_4'^2)}$	$\omega_X-\frac{1}{2}J_{BX}+\frac{R_4'}{2}-\frac{R_4}{2}$
21	$A_{3/2\,1/2}B_{00}X_{I_Xm_X}\to A_{3/2\,1/2}B_{00}X_{I_Xm_X-1}$ $A_{1/2\,1/2}B_{00}X_{I_Xm_X}\to A_{1/2\,1/2}B_{00}X_{I_Xm_X-1}$ $A_{1/2\,1/2}^*B_{00}X_{I_Xm_X}\to A_{1/2\,1/2}^*B_{00}X_{I_Xm_X-1}$	$3(I_X+m_X)(I_X-m_X+1)$	$\omega_X+\frac{1}{2}J_{AX}$
22	$A_{1/2\,-1/2}B_{00}X_{I_Xm_X}\to A_{1/2\,-1/2}B_{00}X_{I_Xm_X-1}$ $A_{1/2\,-1/2}^*B_{00}X_{I_Xm_X}\to A_{1/2\,-1/2}^*B_{00}X_{I_Xm_X-1}$ $A_{3/2\,-1/2}B_{00}X_{I_Xm_X}\to A_{3/2\,-1/2}B_{00}X_{I_Xm_X-1}$	$3(I_X+m_X)(I_X-m_X+1)$	$\omega_X-\frac{1}{2}J_{AX}$