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Appendix Tables

Appendix 1

$$\Psi_1 = \Psi_{200}\bar{\Psi}_{200},\ \Psi_2 = \Psi_{200}\bar{\Psi}_{31-1},\ \Psi_3 = \Psi_{200}\bar{\Psi}_{310},\ \Psi_4 = \Psi_{200}\bar{\Psi}_{311},\ \Psi_5 = \Psi_{31-1}\bar{\Psi}_{200},\ \Psi_6 = \Psi_{310}\bar{\Psi}_{200},$$

$$\Psi_7 = \Psi_{311}\bar{\Psi}_{200},\ \Psi_8 = \Psi_{31-1}\bar{\Psi}_{31-1},\ \Psi_9 = \frac{1}{\sqrt{2}}\left(\Psi_{31-1}\bar{\Psi}_{31-0} + \Psi_{310}\bar{\Psi}_{31-1}\right)$$

$$,\ \Psi_{10} = \frac{1}{\sqrt{6}}\left(\Psi_{31-1}\bar{\Psi}_{311} + 2\Psi_{310}\bar{\Psi}_{310} + \Psi_{311}\bar{\Psi}_{31-1}\right),\ \Psi_{11} = \frac{1}{\sqrt{2}}\left(\Psi_{310}\bar{\Psi}_{311} + \Psi_{311}\bar{\Psi}_{310}\right),\ \Psi_{12} = \Psi_{311}\bar{\Psi}_{311}$$

$$,\ \Psi_{13} = \frac{1}{\sqrt{2}}\left(\Psi_{310}\bar{\Psi}_{31-1} - \Psi_{31-1}\bar{\Psi}_{310}\right),\ \Psi_{14} = \frac{1}{\sqrt{2}}\left(\Psi_{311}\bar{\Psi}_{31-1} - \Psi_{31-1}\bar{\Psi}_{311}\right),\ \Psi_{15} = \frac{1}{\sqrt{2}}\left(\Psi_{311}\bar{\Psi}_{310} - \Psi_{310}\bar{\Psi}_{311}\right),$$

$$\Psi_{16} = \frac{1}{\sqrt{3}}\left(\Psi_{31-1}\bar{\Psi}_{311} - \Psi_{310}\bar{\Psi}_{310} + \Psi_{311}\bar{\Psi}_{31-1}\right)$$

Appendix 2

$$\mathbf{P_{1A}} = 4X(E_1\mathbf{i} + E_2\mathbf{j} + E_3\mathbf{k}),\ \mathbf{P_{2A}} = (XE_1 + YE_2)\mathbf{i} + (YE_1 + XE_2)\mathbf{j} + 2XE_3\mathbf{k},\ \mathbf{P_{3A}} = 2X(E_1\mathbf{i} + E_2\mathbf{j})$$

, $\mathbf{P_{4A}} = (XE_1 + YE_2)\mathbf{i} + (-YE_1 + XE_2)\mathbf{j} + 2XE_3\mathbf{k}$, {$\mathbf{P_{5A}} = \mathbf{P_{2A}}$, $\mathbf{P_{6A}} = \mathbf{P_{3A}}$, $\mathbf{P_{7A}} = \mathbf{P_{4A}}$,}=Degenerates states,

$$\mathbf{P_{8A}} = -2\left[\left(XE_1 - YE_2\right)\mathbf{i} + \left(-YE_1 + XE_2\right)\mathbf{j}\right],\ \mathbf{P_{9A}} = \left(-XE_1 - YE_2\right)\mathbf{i} + (YE_1 - XE_2)\mathbf{j} - 2XE_3\mathbf{k}$$

$$,\ \mathbf{P_{10A}} = -2X(E_1\mathbf{i} + E_2\mathbf{j} + 4E_3\mathbf{k})/3,\ \mathbf{P_{11A}} = \left(-XE_1 + YE_2\right)\mathbf{i} + (-YE_1 - XE_2)\mathbf{j} - 2XE_3\mathbf{k}$$

$$,\ \mathbf{P_{12A}} = -2\left[\left(XE_1 - YE_2\right)\mathbf{i} + \left(YE_1 + XE_2\right)\mathbf{j}\right],\ \mathbf{P_{13A}} = \left(-XE_1 + YE_2\right)\mathbf{i} + (YE_1 - XE_2)\mathbf{j} - 2XE_3\mathbf{k},$$

$$\mathbf{P_{14A}} = -2X(E_1\mathbf{i} + E_2\mathbf{j}),\ \mathbf{P_{15A}} = \left(-XE_1 + YE_2\right)\mathbf{i} + (-YE_1 - XE_2)\mathbf{j} - 2XE_3\mathbf{k},\ \mathbf{P_{16A}} = -4X\left(E_1\mathbf{i} + E_2\mathbf{j} + E_3\mathbf{k}\right)/3$$

with

$$X = \frac{d^2\omega_0\left[\cos\omega_0 t - \cos\omega t\right]}{3\hbar\left[\omega^2 - \omega_0^2\right]},\ Y = \frac{d^2\omega_0\left[\omega_0\sin\omega_0 t - \omega\sin\omega t\right]}{3\hbar\left[\omega^2 - \omega_0^2\right]},\ d = -e\int_0^\infty R_{20}R_{31}r^3 dr$$

R_{20}, R_{31} are the radial functions, *e* represents the charge of a positron, and $\omega_0=\omega_2-\omega_1$, $\omega^2 \neq \omega_0^2$.

Appendix 3

Of the equation 37 the irreducible representation is $\Gamma_\pi = 2A_2 + 3B_2$, using the notation $N_1 = \phi_1, C_2 = \phi_2,\ C_3 = \phi_3,\ C_4 = \phi_4, C_5 = \phi_5$ and using the relationship projection operator

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$$\hat{\mathrm{P}}^{j} = \frac{l_j}{h}\sum_{R}\chi(R)^{j}\hat{R}$$

Where l_j represents the dimension of the group, we have:

$$\Psi_1^{A_2} = \frac{1}{\sqrt{2}}(\phi_2 - \phi_5)$$

$$\Psi_2^{A_2} = \frac{1}{\sqrt{2}}(\phi_3 - \phi_4)$$

$$\Psi_3^{B_2} = \phi_1$$

$$\Psi_4^{B_2} = \frac{1}{\sqrt{2}}(\phi_2 - \phi_5)$$

$$\Psi_5^{B_2} = \frac{1}{\sqrt{2}}(\phi_3 - \phi_4)$$