

Spin-orbitals, terms, and wave functions for two-electrons in the 32 crystallographic point groups

Compiled and computed by Juan Lizarazo

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This tables collect symbolic expressions for the terms of two-electrons under the point group symmetry of the 32 crystallographic point groups.

In the expressions for the wave functions for the various terms under each group the vertical bars denote determinantal states of the two enclosed spin-orbital symbols. If the symbol for a spin orbital is decorated with a top bar that denotes that it has spin down, if not decorated thus then it has spin up. The different wave functions are grouped under headings in red that denote the origin of the wave functions that follow, in the sense of which two irreducible representations gave way to them. Each term may contain more than one basis for the irreducible representation of the term, if this is the case then the several bases can be identified as grouping of wave functions under the same red heading, with the same value for M and a full collection of component symbols for the irreducible representation of the term.

The provided expressions for the wave functions are eigenvectors of S^2 , S_z , and together with the adequate other wave functions in the term form bases for the corresponding irreducible representation. The "z-axis" here may be taken as any axis that is convenient to choose according to the symmetries of the different groups.

For the electronic access to these tables, an electronic version is provided in the GitHub repository for `qdef` in the file `./Data/2e-terms.pkl`. It consists of a python dictionary whose keys are labels for the different groups, and whose values are `qdefcore.Term` objects that include symbolic expressions for the wave functions as well as additional information for the corresponding term.

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1 Spin-orbitals

	$ \alpha_u \overline{\alpha}_u $	$B_{1u} \cdot B_{1u} :$
Group C_1	$B_g \cdot B_g :$	$ \beta_u \overline{\beta}_u $
$A \cdot A :$	$ \beta_g \overline{\beta}_g $	$B_{2u} \cdot B_{2u} :$
$ \alpha \overline{\alpha} $		$ \gamma_u \overline{\gamma}_u $
		$A_{1u} \cdot A_{1u} :$
Group C_i	$A_1 \cdot A_1 :$	$ \alpha_u \overline{\alpha}_u $
$A_g \cdot A_g :$	$ \alpha \overline{\alpha} $	$B_{3g} \cdot B_{3g} :$
$ \alpha_g \overline{\alpha}_g $	$B_1 \cdot B_1 :$	$ \zeta_g \overline{\zeta}_g $
$A_u \cdot A_u :$	$ \beta \overline{\beta} $	$B_{1g} \cdot B_{1g} :$
$ \alpha_u \overline{\alpha}_u $	$B_2 \cdot B_2 :$	$ \beta_g \overline{\beta}_g $
	$ \gamma \overline{\gamma} $	$B_{2g} \cdot B_{2g} :$
Group C_2	$B_3 \cdot B_3 :$	$ \gamma_g \overline{\gamma}_g $
$A \cdot A :$	$ \zeta \overline{\zeta} $	
$ \alpha \overline{\alpha} $		Group C_4
$B \cdot B :$	Group C_{2v}	$A \cdot A :$
$ \beta \overline{\beta} $	$A_1 \cdot A_1 :$	$ \alpha \overline{\alpha} $
	$B_2 \cdot B_2 :$	$E^1 \cdot E^1 :$
Group C_s	$ \alpha \overline{\alpha} $	$ \gamma \overline{\gamma} $
$A' \cdot A' :$	$ \zeta \overline{\zeta} $	$E^2 \cdot E^2 :$
$ \alpha \overline{\alpha} $	$B_1 \cdot B_1 :$	$ \zeta \overline{\zeta} $
$A'' \cdot A'' :$	$ \gamma \overline{\gamma} $	$B \cdot B :$
$ \beta \overline{\beta} $	$A_2 \cdot A_2 :$	$ \beta \overline{\beta} $
	$ \beta \overline{\beta} $	
Group C_{2h}		Group S_4
$A_g \cdot A_g :$	Group D_{2h}	$A \cdot A :$
$ \alpha_g \overline{\alpha}_g $	$A_{1g} \cdot A_{1g} :$	$ \alpha \overline{\alpha} $
$B_u \cdot B_u :$	$ \alpha_g \overline{\alpha}_g $	$E^1 \cdot E^1 :$
$ \beta_u \overline{\beta}_u $	$B_{3u} \cdot B_{3u} :$	$ \gamma \overline{\gamma} $
$A_u \cdot A_u :$	$ \zeta_u \overline{\zeta}_u $	$E^2 \cdot E^2 :$

$B \cdot B :$	$ \eta\bar{\eta} , \eta\mu , \eta\bar{\mu} , \bar{\eta}\mu , \bar{\eta}\bar{\mu} , \mu\bar{\mu} $	$B_{2g} \cdot B_{2g} :$
$ \beta\bar{\beta} $		$ \zeta_g\bar{\zeta}_g $
<hr/>	<hr/>	<hr/>
Group C_{4v}		$A_{2u} \cdot A_{2u} :$
$A_1 \cdot A_1 :$	$ \alpha\bar{\alpha} $	$ \beta_u\bar{\beta}_u $
$A_2 \cdot A_2 :$	$ \beta\bar{\beta} $	$B_{2u} \cdot B_{2u} :$
$B_2 \cdot B_2 :$	$ \zeta\bar{\zeta} $	$B_{1u} \cdot B_{1u} :$
$B_1 \cdot B_1 :$	$ \gamma\bar{\gamma} $	$A_{1u} \cdot A_{1u} :$
$E \cdot E :$		$ \alpha_u\bar{\alpha}_u $
<hr/>	<hr/>	$B_{1g} \cdot B_{1g} :$
$ \eta\bar{\eta} , \eta\mu , \eta\bar{\mu} , \bar{\eta}\mu , \bar{\eta}\bar{\mu} , \mu\bar{\mu} $		$ \gamma_g\bar{\gamma}_g $
$ \gamma_5\bar{\gamma}_5 $		$E_u \cdot E_u :$
<hr/>	<hr/>	$E_g \cdot E_g :$
Group D_{2d}		$ \eta_g\bar{\eta}_g , \eta_g\mu_g , \eta_g\bar{\mu}_g , \bar{\eta}_g\mu_g ,$
$A_1 \cdot A_1 :$	$ \alpha\bar{\alpha} $	$ \overline{ \eta_g\mu_g }, \mu_g\bar{\mu}_g $
$A_2 \cdot A_2 :$	$ \beta\bar{\beta} $	<hr/>
$B_1 \cdot B_1 :$	$ \zeta\bar{\zeta} $	Group C_3
$B_2 \cdot B_2 :$	$ \gamma\bar{\gamma} $	$A \cdot A :$
$E \cdot E :$		$ \alpha\bar{\alpha} $
<hr/>	<hr/>	$E^1 \cdot E^1 :$
Group D_4		$ \beta\bar{\beta} $
$A_1 \cdot A_1 :$	$ \zeta\bar{\zeta} $	$E^2 \cdot E^2 :$
$ \alpha\bar{\alpha} $	$E \cdot E :$	$ \gamma\bar{\gamma} $
$A_2 \cdot A_2 :$	$ \eta\bar{\eta} , \eta\mu , \eta\bar{\mu} , \bar{\eta}\mu , \bar{\eta}\bar{\mu} , \mu\bar{\mu} $	<hr/>
$ \beta\bar{\beta} $		Group S_6
<hr/>	<hr/>	$A_g \cdot A_g :$
$B_2 \cdot B_2 :$	Group D_{4h}	$ \alpha_g\bar{\alpha}_g $
$ \zeta\bar{\zeta} $	$A_{1g} \cdot A_{1g} :$	$A_u \cdot A_u :$
$B_1 \cdot B_1 :$	$ \alpha_g\bar{\alpha}_g $	$ \alpha_u\bar{\alpha}_u $
$ \gamma\bar{\gamma} $	$A_{2g} \cdot A_{2g} :$	$E_u^1 \cdot E_u^1 :$
$E \cdot E :$	$ \beta_g\bar{\beta}_g $	$ \beta_u\bar{\beta}_u $

$E_u^2 \cdot E_u^2 :$	$ \beta_g \overline{\beta_g} $	$ \mu \overline{\mu} $
$ \gamma_u \overline{\gamma_u} $	$E_g \cdot E_g :$	$E'^1 \cdot E'^1 :$
$E_g^2 \cdot E_g^2 :$	$ \gamma_g \overline{\gamma_g} , \gamma_g \zeta_g , \gamma_g \overline{\zeta_g} , \overline{\gamma_g} \zeta_g , \overline{\gamma_g} \overline{\zeta_g} ,$ $ \zeta_g \overline{\zeta_g} $	$ \eta \overline{\eta} $
$ \gamma_g \overline{\gamma_g} $		
$E_g^1 \cdot E_g^1 :$	$E_u \cdot E_u :$	Group C_{6h}
$ \beta_g \overline{\beta_g} $	$ \gamma_u \overline{\gamma_u} , \gamma_u \zeta_u , \gamma_u \overline{\zeta_u} , \overline{\gamma_u} \zeta_u ,$ $ \overline{\gamma_u} \overline{\zeta_u} , \zeta_u \overline{\zeta_u} $	$\Gamma^1 \cdot \Gamma^1 :$ $ \gamma_4 \overline{\gamma_4} $
		$\Gamma^2 \cdot \Gamma^2 :$
Group D_3	Group C_6	
$A_1 \cdot A_1 :$	$A \cdot A :$	$ \gamma_5 \overline{\gamma_5} $
$ \alpha \overline{\alpha} $	$ \alpha \overline{\alpha} $	$\Gamma^3 \cdot \Gamma^3 :$ $ \gamma_6 \overline{\gamma_6} $
$A_2 \cdot A_2 :$	$B \cdot B :$	$\Gamma^4 \cdot \Gamma^4 :$
$ \beta \overline{\beta} $	$ \beta \overline{\beta} $	$ \gamma_7 \overline{\gamma_7} $
$E \cdot E :$	$E'^1 \cdot E'^1 :$	$\Gamma^5 \cdot \Gamma^5 :$ $ \gamma_8 \overline{\gamma_8} $
$ \gamma \overline{\gamma} , \gamma \zeta , \gamma \overline{\zeta} , \overline{\gamma} \zeta , \overline{\gamma} \overline{\zeta} , \zeta \overline{\zeta} $	$E'^2 \cdot E'^2 :$	$\Gamma^6 \cdot \Gamma^6 :$
Group C_{3v}	$ \mu \overline{\mu} $	$ \gamma_9 \overline{\gamma_9} $
$A_1 \cdot A_1 :$	$E''^2 \cdot E''^2 :$	$\Gamma^7 \cdot \Gamma^7 :$
$ \alpha \overline{\alpha} $	$ \zeta \overline{\zeta} $	$ \gamma_{10} \overline{\gamma_{10}} $
$A_2 \cdot A_2 :$	$E''^1 \cdot E''^1 :$	$\Gamma^8 \cdot \Gamma^8 :$
$ \beta \overline{\beta} $	$ \gamma \overline{\gamma} $	$ \gamma_{11} \overline{\gamma_{11}} $
$E \cdot E :$		$\Gamma^9 \cdot \Gamma^9 :$
$ \gamma \overline{\gamma} , \gamma \zeta , \gamma \overline{\zeta} , \overline{\gamma} \zeta , \overline{\gamma} \overline{\zeta} , \zeta \overline{\zeta} $		$ \gamma_{12} \overline{\gamma_{12}} $
		$\Gamma^{10} \cdot \Gamma^{10} :$
Group D_{3d}	Group C_{3h}	
$A_{1g} \cdot A_{1g} :$	$A' \cdot A' :$	$ \gamma_1 \overline{\gamma_1} $
$ \alpha_g \overline{\alpha_g} $	$ \alpha \overline{\alpha} $	$\Gamma^{11} \cdot \Gamma^{11} :$
$A_{1u} \cdot A_{1u} :$	$A'' \cdot A'' :$	$ \gamma_2 \overline{\gamma_2} $
$ \alpha_u \overline{\alpha_u} $	$ \beta \overline{\beta} $	$\Gamma^{12} \cdot \Gamma^{12} :$ $ \gamma_3 \overline{\gamma_3} $
$A_{2u} \cdot A_{2u} :$	$E''^2 \cdot E''^2 :$	
$ \beta_u \overline{\beta_u} $	$ \zeta \overline{\zeta} $	
$A_{2g} \cdot A_{2g} :$	$E''^1 \cdot E''^1 :$	Group D_6
	$ \gamma \overline{\gamma} $	$A_1 \cdot A_1 :$
	$E'^2 \cdot E'^2 :$	$ \alpha \overline{\alpha} $

$B_1 \cdot B_1 :$	$ \gamma\bar{\gamma} $	$ \eta_g\bar{\eta}_g , \eta_g\mu_g , \eta_g\bar{\mu}_g , \bar{\eta}_g\mu_g ,$
$ \gamma\bar{\gamma} $	$A'_2 \cdot A'_2 :$	$ \bar{\eta}_g\mu_g , \mu_g\bar{\mu}_g $
$B_2 \cdot B_2 :$	$ \beta\bar{\beta} $	$E_{2u} \cdot E_{2u} :$
$ \zeta\bar{\zeta} $	$E' \cdot E' :$	$ \nu_u\bar{\nu}_u , \nu_u\xi_u , \nu_u\bar{\xi}_u , \bar{\nu}_u\xi_u ,$
$A_2 \cdot A_2 :$	$ \eta\bar{\eta} , \eta\mu , \eta\bar{\mu} , \bar{\eta}\mu , \bar{\eta}\bar{\mu} , \mu\bar{\mu} $	$ \bar{\nu}_u\xi_u , \xi_u\bar{\xi}_u $
$ \beta\bar{\beta} $	$E'' \cdot E'' :$	<hr/>
$E_2 \cdot E_2 :$	$ \nu\bar{\nu} , \nu\xi , \nu\bar{\xi} , \bar{\nu}\xi , \bar{\nu}\bar{\xi} , \xi\bar{\xi} $	Group T
$ \nu\bar{\nu} , \nu\xi , \nu\bar{\xi} , \bar{\nu}\xi , \bar{\nu}\bar{\xi} , \xi\bar{\xi} $	<hr/>	$A \cdot A :$
$E_1 \cdot E_1 :$	$ \alpha\bar{\alpha} $	$ \alpha\bar{\alpha} $
$ \eta\bar{\eta} , \eta\mu , \eta\bar{\mu} , \bar{\eta}\mu , \bar{\eta}\bar{\mu} , \mu\bar{\mu} $	$Group D_{6h}$	$E^1 \cdot E^1 :$
<hr/>	$A_{1g} \cdot A_{1g} :$	$ \beta\bar{\beta} $
Group C_{6v}	$ \alpha_g\bar{\alpha}_g $	$E^2 \cdot E^2 :$
$A_1 \cdot A_1 :$	$A_{2u} \cdot A_{2u} :$	$ \gamma\bar{\gamma} $
$ \alpha\bar{\alpha} $	$ \beta_u\bar{\beta}_u $	$T \cdot T :$
$B_2 \cdot B_2 :$	$A_{1u} \cdot A_{1u} :$	$ \zeta\bar{\zeta} , \zeta\eta , \zeta\bar{\eta} , \bar{\zeta}\eta , \bar{\zeta}\bar{\eta} , \zeta\mu ,$
$ \zeta\bar{\zeta} $	$ \alpha_u\bar{\alpha}_u $	$ \zeta\bar{\mu} , \zeta\mu , \bar{\zeta}\mu , \eta\bar{\eta} , \eta\mu , \eta\bar{\mu} ,$
$B_1 \cdot B_1 :$	$B_{1g} \cdot B_{1g} :$	$ \bar{\eta}\mu , \bar{\eta}\bar{\mu} , \mu\bar{\mu} $
$ \gamma\bar{\gamma} $	$ \gamma_g\bar{\gamma}_g $	<hr/>
$A_2 \cdot A_2 :$	$B_{2g} \cdot B_{2g} :$	Group T_h
$ \beta\bar{\beta} $	$ \zeta_g\bar{\zeta}_g $	$A_g \cdot A_g :$
$E_2 \cdot E_2 :$	$B_{1u} \cdot B_{1u} :$	$ \alpha_g\bar{\alpha}_g $
$ \nu\bar{\nu} , \nu\xi , \nu\bar{\xi} , \bar{\nu}\xi , \bar{\nu}\bar{\xi} , \xi\bar{\xi} $	$ \gamma_u\bar{\gamma}_u $	$A_u \cdot A_u :$
$E_1 \cdot E_1 :$	$B_{2u} \cdot B_{2u} :$	$ \alpha_u\bar{\alpha}_u $
$ \eta\bar{\eta} , \eta\mu , \eta\bar{\mu} , \bar{\eta}\mu , \bar{\eta}\bar{\mu} , \mu\bar{\mu} $	$ \zeta_u\bar{\zeta}_u $	$E_u^1 \cdot E_u^1 :$
<hr/>	$A_{2g} \cdot A_{2g} :$	$ \beta_u\bar{\beta}_u $
Group D_{3h}	$ \beta_g\bar{\beta}_g $	$E_u^2 \cdot E_u^2 :$
$A'_1 \cdot A'_1 :$	$E_{2g} \cdot E_{2g} :$	$ \gamma_u\bar{\gamma}_u $
$ \alpha\bar{\alpha} $	$ \nu_g\bar{\nu}_g , \nu_g\xi_g , \nu_g\bar{\xi}_g , \bar{\nu}_g\xi_g , \bar{\nu}_g\bar{\xi}_g ,$	$E_g^2 \cdot E_g^2 :$
$A''_2 \cdot A''_2 :$	$ \xi_g\bar{\xi}_g $	$ \gamma_g\bar{\gamma}_g $
$ \zeta\bar{\zeta} $	$E_{1u} \cdot E_{1u} :$	$E_g^1 \cdot E_g^1 :$
$A''_1 \cdot A''_1 :$	$ \eta_u\bar{\eta}_u , \eta_u\mu_u , \eta_u\bar{\mu}_u , \bar{\eta}_u\mu_u ,$	$ \beta_g\bar{\beta}_g $
	$ \bar{\eta}_u\mu_u , \mu_u\bar{\mu}_u $	<hr/>
	$E_{1g} \cdot E_{1g} :$	$T_g \cdot T_g :$

$ \zeta_g \overline{\zeta_g} , \zeta_g \eta_g , \zeta_g \overline{\eta_g} , \overline{\zeta_g} \eta_g , \overline{\zeta_g} \overline{\eta_g} ,$ $ \zeta_g \mu_g , \zeta_g \overline{\mu_g} , \zeta_g \mu_g , \zeta_g \overline{\mu_g} ,$ $ \eta_g \overline{\eta_g} , \eta_g \mu_g , \eta_g \overline{\mu_g} , \overline{\eta_g} \mu_g ,$ $ \overline{\eta_g} \mu_g , \mu_g \overline{\mu_g} $	$A_1 \cdot A_1 :$ $ \alpha \overline{\alpha} $ $A_2 \cdot A_2 :$ $ \beta \overline{\beta} $	$E_u \cdot E_u :$ $ \gamma_u \overline{\gamma_u} , \gamma_u \zeta_u , \gamma_u \overline{\zeta_u} , \overline{\gamma_u} \zeta_u ,$ $ \overline{\gamma_u} \overline{\zeta_u} , \zeta_u \overline{\zeta_u} $
$T_u \cdot T_u :$ $ \zeta_u \overline{\zeta_u} , \zeta_u \eta_u , \zeta_u \overline{\eta_u} , \overline{\zeta_u} \eta_u ,$ $ \zeta_u \overline{\eta_u} , \zeta_u \mu_u , \zeta_u \overline{\mu_u} , \overline{\zeta_u} \mu_u ,$ $ \zeta_u \overline{\mu_u} , \eta_u \overline{\eta_u} , \eta_u \mu_u , \eta_u \overline{\mu_u} ,$ $ \overline{\eta_u} \mu_u , \eta_u \overline{\mu_u} , \mu_u \overline{\mu_u} $	$E \cdot E :$ $ \gamma \overline{\gamma} , \gamma \zeta , \gamma \overline{\zeta} , \overline{\gamma} \zeta , \zeta \overline{\zeta} $	$E_g \cdot E_g :$ $ \gamma_g \overline{\gamma_g} , \gamma_g \zeta_g , \gamma_g \overline{\zeta_g} , \overline{\gamma_g} \zeta_g , \overline{\gamma_g} \overline{\zeta_g} ,$ $ \zeta_g \overline{\zeta_g} $
<hr/>	$T_2 \cdot T_2 :$ $ \xi \overline{\xi} , \xi \phi , \xi \overline{\phi} , \overline{\xi} \phi , \overline{\xi} \overline{\phi} , \xi \chi ,$ $ \xi \overline{\chi} , \xi \chi , \xi \overline{\chi} , \phi \overline{\phi} , \phi \chi , \phi \overline{\chi} ,$ $ \phi \chi , \phi \overline{\chi} , \chi \overline{\chi} $	$T_{1g} \cdot T_{1g} :$ $ \eta_g \overline{\eta_g} , \eta_g \mu_g , \eta_g \overline{\mu_g} , \overline{\eta_g} \mu_g ,$ $ \overline{\eta_g} \mu_g , \eta_g \nu_g , \eta_g \overline{\nu_g} , \overline{\eta_g} \nu_g ,$ $ \overline{\eta_g} \nu_g , \mu_g \overline{\mu_g} , \mu_g \nu_g , \mu_g \overline{\nu_g} ,$ $ \overline{\mu_g} \nu_g , \overline{\mu_g} \overline{\nu_g} , \nu_g \overline{\nu_g} $
$\text{Group } O$ $A_1 \cdot A_1 :$ $ \alpha \overline{\alpha} $ $A_2 \cdot A_2 :$ $ \beta \overline{\beta} $ $E \cdot E :$ $ \gamma \overline{\gamma} , \gamma \zeta , \gamma \overline{\zeta} , \overline{\gamma} \zeta , \zeta \overline{\zeta} $	$T_1 \cdot T_1 :$ $ \eta \overline{\eta} , \eta \mu , \eta \overline{\mu} , \overline{\eta} \mu , \overline{\eta} \overline{\mu} , \eta \nu ,$ $ \eta \overline{\nu} , \eta \nu , \eta \overline{\nu} , \mu \overline{\mu} , \mu \nu , \mu \overline{\nu} ,$ $ \overline{\mu} \nu , \overline{\mu} \overline{\nu} , \nu \overline{\nu} $	$T_{2g} \cdot T_{2g} :$ $ \xi_g \overline{\xi_g} , \xi_g \phi_g , \xi_g \overline{\phi_g} , \overline{\xi_g} \phi_g ,$ $ \xi_g \overline{\phi_g} , \xi_g \chi_g , \xi_g \overline{\chi_g} , \overline{\xi_g} \chi_g ,$ $ \xi_g \overline{\chi_g} , \phi_g \overline{\phi_g} , \phi_g \chi_g , \phi_g \overline{\chi_g} ,$ $ \phi_g \chi_g , \phi_g \overline{\chi_g} , \chi_g \overline{\chi_g} $
<hr/>	$\text{Group } O_h$ $A_{1g} \cdot A_{1g} :$ $ \alpha_g \overline{\alpha_g} $ $A_{2u} \cdot A_{2u} :$ $ \beta_u \overline{\beta_u} $	$T_{1u} \cdot T_{1u} :$ $ \eta_u \overline{\eta_u} , \eta_u \mu_u , \eta_u \overline{\mu_u} , \overline{\eta_u} \mu_u ,$ $ \eta_u \overline{\mu_u} , \eta_u \nu_u , \eta_u \overline{\nu_u} , \overline{\eta_u} \nu_u ,$ $ \overline{\eta_u} \nu_u , \mu_u \overline{\mu_u} , \mu_u \nu_u , \mu_u \overline{\nu_u} ,$ $ \overline{\mu_u} \nu_u , \overline{\mu_u} \overline{\nu_u} , \nu_u \overline{\nu_u} $
$T_1 \cdot T_1 :$ $ \eta \overline{\eta} , \eta \mu , \eta \overline{\mu} , \overline{\eta} \mu , \overline{\eta} \overline{\mu} , \eta \nu ,$ $ \eta \overline{\nu} , \eta \nu , \eta \overline{\nu} , \mu \overline{\mu} , \mu \nu , \mu \overline{\nu} ,$ $ \overline{\mu} \nu , \overline{\mu} \overline{\nu} , \nu \overline{\nu} $	$A_{1u} \cdot A_{1u} :$ $ \alpha_u \overline{\alpha_u} $ $A_{2g} \cdot A_{2g} :$ $ \beta_g \overline{\beta_g} $	$T_{2u} \cdot T_{2u} :$ $ \xi_u \overline{\xi_u} , \xi_u \phi_u , \xi_u \overline{\phi_u} , \overline{\xi_u} \phi_u ,$ $ \xi_u \overline{\phi_u} , \xi_u \chi_u , \xi_u \overline{\chi_u} , \overline{\xi_u} \chi_u ,$ $ \xi_u \overline{\chi_u} , \phi_u \overline{\phi_u} , \phi_u \chi_u , \phi_u \overline{\chi_u} ,$ $ \phi_u \chi_u , \phi_u \overline{\chi_u} , \chi_u \overline{\chi_u} $
<hr/>	$\text{Group } T_d$	

2 Terms and wave functions

2.1 Group C_1

Component labels

$$A : \{\alpha\}$$

2.1.1 1A

$$\color{red}a^2$$

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_1(a^2, ^1A, M=0, \alpha) = -|\overline{\alpha}\alpha|$$

2.2 Group C_i

Component labels

$$A_g : \{\alpha_g\} \longrightarrow A_u : \{\alpha_u\}$$

2.2.1 1A_g

$$\boxed{\Delta E = -\langle \alpha_g\alpha_g || \alpha_u\alpha_u \rangle + \langle \alpha_g\alpha_u || \alpha_g\alpha_u \rangle}$$

$$\color{red}a_g^2$$

$$\boxed{\Delta E = \langle \alpha_g\alpha_g || \alpha_g\alpha_g \rangle}$$

$$\Psi_1(a_g^2, ^1A_g, M=0, \alpha_g) = -|\overline{\alpha_g}\alpha_g|$$

$$\Psi_1(a_g a_u, ^3A_u, M=-1, \alpha_u) = |\overline{\alpha_g}\alpha_u|$$

$$\Psi_2(a_g a_u, ^3A_u, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\alpha_g}\alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\alpha_u}|}{2}$$

$$\Psi_3(a_g a_u, ^3A_u, M=1, \alpha_u) = |\alpha_g\alpha_u|$$

$$\color{red}a_u^2$$

$$\boxed{\Delta E = \langle \alpha_u\alpha_u || \alpha_u\alpha_u \rangle}$$

$$\Psi_2(a_u^2, ^1A_g, M=0, \alpha_g) = -|\overline{\alpha_u}\alpha_u|$$

2.2.3 1A_u

$$\color{red}a_g a_u$$

$$\boxed{\Delta E = \langle \alpha_g\alpha_g || \alpha_u\alpha_u \rangle + \langle \alpha_g\alpha_u || \alpha_g\alpha_u \rangle}$$

2.2.2 3A_u

$$\Psi_1(a_g a_u, ^1A_u, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\alpha_u}|}{2}$$

2.3 Group C_2

Component labels

$$A : \{\alpha\} \longrightarrow B : \{\beta\}$$

2.3.1 1A a^2

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_1(a^2, {}^1A, M=0, \alpha) = -|\bar{\alpha}\alpha|$$

 b^2

$$\boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle}$$

$$\Psi_2(b^2, {}^1A, M=0, \alpha) = -|\bar{\beta}\beta|$$

2.3.2 3B ab

$$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(ab, {}^3B, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$\Psi_2(ab, {}^3B, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(ab, {}^3B, M=1, \beta) = |\alpha\beta|$$

2.3.3 1B ab

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(ab, {}^1B, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

2.4 Group C_s Component labels

$$A' : \{\alpha\} \longrightarrow A'' : \{\beta\}$$

$$\left(a'' \right)^2$$
2.4.1 ${}^1A'$

$$\boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle}$$

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_2(\left(a' \right)^2, {}^1A', M=0, \alpha) = -|\bar{\beta}\beta|$$

$$\Psi_1(\left(a' \right)^2, {}^1A', M=0, \alpha) = -|\bar{\alpha}\alpha|$$

2.4.2 ${}^3A''$ $a' a''$

$$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a' a'', {}^3A'', M=-1, \beta) = |\overline{\alpha}\overline{\beta}|$$

$$\Psi_2(a' a'', {}^3A'', M=0, \beta) = \frac{\sqrt{2}|\overline{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\overline{\beta}|}{2}$$

$$\Psi_3(a' a'', {}^3A'', M=1, \beta) = |\alpha\beta|$$

2.4.3 ${}^1A''$ $a' a''$

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a' a'', {}^1A'', M=0, \beta) = -\frac{\sqrt{2}|\overline{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\overline{\beta}|}{2}$$

2.5 Group C_{2h} Component labels

$$A_g : \{\alpha_g\} \longrightarrow B_u : \{\beta_u\} \longrightarrow A_u : \{\alpha_u\} \longrightarrow B_g : \{\beta_g\}$$

$$\Psi_2(a_g b_u, {}^3B_u, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\alpha}_g \beta_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta}_u|}{2}$$

2.5.1 1A_g a_g^2

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \alpha_g \alpha_g \rangle}$$

 $a_u b_g$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \beta_g \beta_g \rangle + \langle \alpha_u \beta_g || \alpha_u \beta_g \rangle}$$

$$\Psi_1(a_g^2, {}^1A_g, M=0, \alpha_g) = -|\overline{\alpha}_g \alpha_g|$$

$$\Psi_4(a_u b_g, {}^3B_u, M=-1, \beta_u) = |\overline{\alpha}_u \overline{\beta}_g|$$

 b_u^2

$$\boxed{\Delta E = \langle \beta_u \beta_u || \beta_u \beta_u \rangle}$$

$$\Psi_5(a_u b_g, {}^3B_u, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\alpha}_u \beta_g|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\beta}_g|}{2}$$

$$\Psi_6(a_u b_g, {}^3B_u, M=1, \beta_u) = |\alpha_u \beta_g|$$

$$\Psi_2(b_u^2, {}^1A_g, M=0, \alpha_g) = -|\overline{\beta}_u \beta_u|$$

 a_u^2

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \alpha_u \alpha_u \rangle}$$

2.5.3 1B_u $a_g b_u$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_u \beta_u \rangle + \langle \alpha_g \beta_u || \alpha_g \beta_u \rangle}$$

$$\Psi_3(a_u^2, {}^1A_g, M=0, \alpha_g) = -|\overline{\alpha}_u \alpha_u|$$

 b_g^2

$$\boxed{\Delta E = \langle \beta_g \beta_g || \beta_g \beta_g \rangle}$$

 $a_g b_u$

$$\Psi_1(a_g b_u, {}^1B_u, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\alpha}_g \beta_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta}_u|}{2}$$

 $a_u b_g$ **2.5.2** 3B_u

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \beta_g \beta_g \rangle + \langle \alpha_u \beta_g || \alpha_u \beta_g \rangle}$$

 $a_g b_u$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \beta_u \beta_u \rangle + \langle \alpha_g \beta_u || \alpha_g \beta_u \rangle}$$

$$\Psi_2(a_u b_g, {}^1B_u, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\alpha}_u \beta_g|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\beta}_g|}{2}$$

$$\Psi_1(a_g b_u, {}^3B_u, M=-1, \beta_u) = |\overline{\alpha}_g \overline{\beta}_u|$$

2.5.4 3A_u **2.5.6** 3B_g $a_g a_u$ $a_g b_g$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_g a_u, ^3A_u, M=-1, \alpha_u) = |\overline{\alpha_g} \overline{\alpha_u}|$$

$$\Psi_1(a_g b_g, ^3B_g, M=-1, \beta_g) = |\overline{\alpha_g} \overline{\beta_g}|$$

$$\Psi_2(a_g a_u, ^3A_u, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\alpha_g} \alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\alpha_u}|}{2}$$

$$\Psi_2(a_g b_g, ^3B_g, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\alpha_g} \beta_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_g}|}{2}$$

$$\Psi_3(a_g a_u, ^3A_u, M=1, \alpha_u) = |\alpha_g \alpha_u|$$

$$\Psi_3(a_g b_g, ^3B_g, M=1, \beta_g) = |\alpha_g \beta_g|$$

 $b_g b_u$ $a_u b_u$

$$\boxed{\Delta E = \langle \beta_u \beta_g || \beta_u \beta_g \rangle - \langle \beta_u \beta_u || \beta_g \beta_g \rangle}$$

$$\boxed{\Delta E = \langle \beta_u \alpha_u || \beta_u \alpha_u \rangle - \langle \beta_u \beta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_4(b_g b_u, ^3A_u, M=-1, \alpha_u) = |\overline{\beta_u} \overline{\beta_g}|$$

$$\Psi_4(a_u b_u, ^3B_g, M=-1, \beta_g) = |\overline{\beta_u} \overline{\alpha_u}|$$

$$\Psi_5(b_g b_u, ^3A_u, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\beta_u} \beta_g|}{2} + \frac{\sqrt{2}|\beta_u \overline{\beta_g}|}{2}$$

$$\Psi_5(a_u b_u, ^3B_g, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\beta_u} \alpha_u|}{2} + \frac{\sqrt{2}|\beta_u \overline{\alpha_u}|}{2}$$

$$\Psi_6(b_g b_u, ^3A_u, M=1, \alpha_u) = |\beta_u \beta_g|$$

$$\Psi_6(a_u b_u, ^3B_g, M=1, \beta_g) = |\beta_u \alpha_u|$$

2.5.5 1A_u **2.5.7** 1B_g $a_g a_u$ $a_g b_g$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_g a_u, ^1A_u, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\alpha_g} \alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\alpha_u}|}{2}$$

$$\Psi_1(a_g b_g, ^1B_g, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\alpha_g} \beta_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_g}|}{2}$$

 $b_g b_u$ $a_u b_u$

$$\boxed{\Delta E = \langle \beta_u \beta_g || \beta_u \beta_g \rangle + \langle \beta_u \beta_u || \beta_g \beta_g \rangle}$$

$$\boxed{\Delta E = \langle \beta_u \alpha_u || \beta_u \alpha_u \rangle + \langle \beta_u \beta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_2(b_g b_u, ^1A_u, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\beta_u} \beta_g|}{2} + \frac{\sqrt{2}|\beta_u \overline{\beta_g}|}{2}$$

$$\Psi_2(a_u b_u, ^1B_g, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\beta_u} \alpha_u|}{2} + \frac{\sqrt{2}|\beta_u \overline{\alpha_u}|}{2}$$

2.6 Group D_2 Component labels

$$A_1 : \{\alpha\} \text{ --- } B_1 : \{\beta\} \text{ --- } B_2 : \{\gamma\} \text{ --- } B_3 : \{\zeta\}$$

 b_1^2

$$\boxed{\Delta E = \langle \beta \beta || \beta \beta \rangle}$$

2.6.1 1A_1

$$\Psi_2(b_1^2, ^1A_1, M=0, \alpha) = -|\overline{\beta} \beta|$$

 a_1^2 b_2^2

$$\boxed{\Delta E = \langle \alpha \alpha || \alpha \alpha \rangle}$$

$$\boxed{\Delta E = \langle \gamma \gamma || \gamma \gamma \rangle}$$

$$\Psi_1(a_1^2, ^1A_1, M=0, \alpha) = -|\overline{\alpha} \alpha|$$

$$\Psi_3(b_2^2, ^1A_1, M=0, \alpha) = -|\overline{\gamma} \gamma|$$

b_3^2

$\boxed{\Delta E = \langle \zeta \zeta || \zeta \zeta \rangle}$

$\Psi_4(b_3^2, {}^1A_1, M=0, \alpha) = -|\bar{\zeta} \zeta|$

2.6.2 3B_1

$a_1 b_1$

$\boxed{\Delta E = -\langle \alpha \alpha || \beta \beta \rangle + \langle \alpha \beta || \alpha \beta \rangle}$

$\Psi_1(a_1 b_1, {}^3B_1, M=-1, \beta) = |\bar{\alpha} \bar{\beta}|$

$\Psi_2(a_1 b_1, {}^3B_1, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha} \beta|}{2} + \frac{\sqrt{2}|\alpha \bar{\beta}|}{2}$

$\Psi_3(a_1 b_1, {}^3B_1, M=1, \beta) = |\alpha \beta|$

$b_2 b_3$

$\boxed{\Delta E = -\langle \gamma \gamma || \zeta \zeta \rangle + \langle \gamma \zeta || \gamma \zeta \rangle}$

$\Psi_4(b_2 b_3, {}^3B_1, M=-1, \beta) = |\bar{\gamma} \bar{\zeta}|$

$\Psi_5(b_2 b_3, {}^3B_1, M=0, \beta) = \frac{\sqrt{2}|\bar{\gamma} \zeta|}{2} + \frac{\sqrt{2}|\gamma \bar{\zeta}|}{2}$

$\Psi_6(b_2 b_3, {}^3B_1, M=1, \beta) = |\gamma \zeta|$

2.6.3 1B_1

$a_1 b_1$

$\boxed{\Delta E = \langle \alpha \alpha || \beta \beta \rangle + \langle \alpha \beta || \alpha \beta \rangle}$

$\Psi_1(a_1 b_1, {}^1B_1, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha} \beta|}{2} + \frac{\sqrt{2}|\alpha \bar{\beta}|}{2}$

$b_2 b_3$

$\boxed{\Delta E = \langle \gamma \gamma || \zeta \zeta \rangle + \langle \gamma \zeta || \gamma \zeta \rangle}$

$\Psi_2(b_2 b_3, {}^1B_1, M=0, \beta) = -\frac{\sqrt{2}|\bar{\gamma} \zeta|}{2} + \frac{\sqrt{2}|\gamma \bar{\zeta}|}{2}$

2.6.4 3B_2

$a_1 b_2$

$\boxed{\Delta E = -\langle \alpha \alpha || \gamma \gamma \rangle + \langle \alpha \gamma || \alpha \gamma \rangle}$

$\Psi_1(a_1 b_2, {}^3B_2, M=-1, \gamma) = |\bar{\alpha} \bar{\gamma}|$

$\Psi_2(a_1 b_2, {}^3B_2, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha} \gamma|}{2} + \frac{\sqrt{2}|\alpha \bar{\gamma}|}{2}$

$\Psi_3(a_1 b_2, {}^3B_2, M=1, \gamma) = |\alpha \gamma|$

$b_1 b_3$

$\boxed{\Delta E = -\langle \beta \beta || \zeta \zeta \rangle + \langle \beta \zeta || \beta \zeta \rangle}$

$\Psi_4(b_1 b_3, {}^3B_2, M=-1, \gamma) = |\bar{\beta} \bar{\zeta}|$

$\Psi_5(b_1 b_3, {}^3B_2, M=0, \gamma) = \frac{\sqrt{2}|\bar{\beta} \zeta|}{2} + \frac{\sqrt{2}|\beta \bar{\zeta}|}{2}$

$\Psi_6(b_1 b_3, {}^3B_2, M=1, \gamma) = |\beta \zeta|$

2.6.5 1B_2

$a_1 b_2$

$\boxed{\Delta E = \langle \alpha \alpha || \gamma \gamma \rangle + \langle \alpha \gamma || \alpha \gamma \rangle}$

$\Psi_1(a_1 b_2, {}^1B_2, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha} \gamma|}{2} + \frac{\sqrt{2}|\alpha \bar{\gamma}|}{2}$

$b_1 b_3$

$\boxed{\Delta E = \langle \beta \beta || \zeta \zeta \rangle + \langle \beta \zeta || \beta \zeta \rangle}$

$\Psi_2(b_1 b_3, {}^1B_2, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\beta} \zeta|}{2} + \frac{\sqrt{2}|\beta \bar{\zeta}|}{2}$

2.6.6 3B_3

$a_1 b_3$

$\boxed{\Delta E = -\langle \alpha \alpha || \zeta \zeta \rangle + \langle \alpha \zeta || \alpha \zeta \rangle}$

$\Psi_1(a_1 b_3, {}^3B_3, M=-1, \zeta) = |\bar{\alpha} \bar{\zeta}|$

$\Psi_2(a_1 b_3, {}^3B_3, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha} \zeta|}{2} + \frac{\sqrt{2}|\alpha \bar{\zeta}|}{2}$

$\Psi_3(a_1 b_3, {}^3B_3, M=1, \zeta) = |\alpha \zeta|$

$b_1 b_2$

$\boxed{\Delta E = -\langle \beta \beta || \gamma \gamma \rangle + \langle \beta \gamma || \beta \gamma \rangle}$

$\Psi_4(b_1 b_2, {}^3B_3, M=-1, \zeta) = |\bar{\beta} \bar{\gamma}|$

$\Psi_5(b_1 b_2, {}^3B_3, M=0, \zeta) = \frac{\sqrt{2}|\bar{\beta} \gamma|}{2} + \frac{\sqrt{2}|\beta \bar{\gamma}|}{2}$

$\Psi_6(b_1 b_2, {}^3B_3, M=1, \zeta) = |\beta \gamma|$

2.6.7 1B_3 $a_1 b_2$ $a_1 b_3$

$$\boxed{\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\boxed{\Delta E = \langle \beta\beta || \gamma\gamma \rangle + \langle \beta\gamma || \beta\gamma \rangle}$$

$$\Psi_1(a_1 b_3, ^1B_3, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_2(b_1 b_2, ^1B_3, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

2.7 Group C_{2v} Component labels

$$A_1 : \{\alpha\} \longrightarrow B_2 : \{\zeta\} \longrightarrow B_1 : \{\gamma\} \longrightarrow A_2 : \{\beta\}$$

 $a_2 b_1$ **2.7.1** 1A_1 a_1^2

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_4(a_2 b_1, ^3B_2, M=-1, \zeta) = |\bar{\gamma}\bar{\beta}|$$

$$\Psi_5(a_2 b_1, ^3B_2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

$$\Psi_6(a_2 b_1, ^3B_2, M=1, \zeta) = |\gamma\beta|$$

$$\Psi_1(a_1^2, ^1A_1, M=0, \alpha) = -|\bar{\alpha}\alpha|$$

 b_2^2

$$\boxed{\Delta E = \langle \zeta\zeta || \zeta\zeta \rangle}$$

2.7.3 1B_2 $a_1 b_2$ b_1^2

$$\boxed{\Delta E = \langle \gamma\gamma || \gamma\gamma \rangle}$$

$$\boxed{\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1 b_2, ^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_3(b_1^2, ^1A_1, M=0, \alpha) = -|\bar{\gamma}\gamma|$$

 $a_2 b_1$ a_2^2

$$\boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle}$$

$$\boxed{\Delta E = \langle \beta\beta || \gamma\beta \rangle + \langle \gamma\gamma || \beta\beta \rangle}$$

$$\Psi_2(a_2 b_1, ^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

$$\Psi_4(a_2^2, ^1A_1, M=0, \alpha) = -|\bar{\beta}\beta|$$

2.7.4 3B_1 $a_1 b_1$ $a_1 b_2$

$$\boxed{\Delta E = -\langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\boxed{\Delta E = -\langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle}$$

2.7.2 3B_2

$$\Psi_1(a_1 b_1, ^3B_1, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

$$\Psi_2(a_1 b_1, ^3B_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(a_1 b_1, ^3B_1, M=1, \gamma) = |\alpha\gamma|$$

 $a_2 b_2$

$$\begin{aligned} \Psi_1(a_1 b_2, ^3B_2, M=-1, \zeta) &= |\bar{\alpha}\bar{\zeta}| \\ \Psi_2(a_1 b_2, ^3B_2, M=0, \zeta) &= \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2} \\ \Psi_3(a_1 b_2, ^3B_2, M=1, \zeta) &= |\alpha\zeta| \end{aligned}$$

$$\begin{aligned} \Delta E &= \langle \zeta\beta || \zeta\beta \rangle - \langle \zeta\zeta || \beta\beta \rangle \\ \Psi_4(a_1 a_2, {}^3A_2, M=-1, \gamma) &= |\bar{\zeta}\bar{\beta}| \\ \Psi_5(a_2 b_2, {}^3B_1, M=0, \gamma) &= \frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2} \\ \Psi_6(a_2 b_2, {}^3B_1, M=1, \gamma) &= |\zeta\beta| \\ \Delta E &= \langle \zeta\gamma || \zeta\gamma \rangle - \langle \zeta\zeta || \gamma\gamma \rangle \end{aligned}$$

2.7.5 1B_1 $a_1 b_1$

$$\Psi_1(a_1 b_1, {}^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

 $a_2 b_2$

$$\Delta E = \langle \zeta\beta || \zeta\beta \rangle + \langle \zeta\zeta || \beta\beta \rangle$$

$$\Psi_2(a_2 b_2, {}^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2}$$

2.7.6 3A_2 $a_1 a_2$

$$\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle$$

$$\begin{aligned} \Psi_4(b_1 b_2, {}^3A_2, M=-1, \beta) &= |\bar{\zeta}\bar{\gamma}| \\ \Psi_5(b_1 b_2, {}^3A_2, M=0, \beta) &= \frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2} \\ \Psi_6(b_1 b_2, {}^3A_2, M=1, \beta) &= |\zeta\gamma| \end{aligned}$$

2.7.7 1A_2 $a_1 a_2$

$$\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle$$

$$\Psi_1(a_1 a_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

 $b_1 b_2$

$$\Delta E = \langle \zeta\gamma || \zeta\gamma \rangle + \langle \zeta\zeta || \gamma\gamma \rangle$$

$$\Psi_2(b_1 b_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

2.8 Group D_{2h} Component labels

$$\begin{aligned} A_{1g} : \{\alpha_g\} &\longrightarrow B_{3u} : \{\zeta_u\} \longrightarrow B_{1u} : \{\beta_u\} \longrightarrow B_{2u} : \{\gamma_u\} \longrightarrow A_{1u} : \{\alpha_u\} \longrightarrow B_{3g} : \{\zeta_g\} \longrightarrow \\ &B_{1g} : \{\beta_g\} \longrightarrow B_{2g} : \{\gamma_g\} \end{aligned}$$

2.8.1 ${}^1A_{1g}$ a_{1g}^2

$$\Delta E = \langle \alpha_g \alpha_g || \alpha_g \alpha_g \rangle$$

$$\Psi_1(a_{1g}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\overline{\alpha_g} \alpha_g|$$

 b_{3u}^2

$$\Delta E = \langle \zeta_u \zeta_u || \zeta_u \zeta_u \rangle$$

$$\Psi_2(b_{3u}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\overline{\zeta_u} \zeta_u|$$

$$\Psi_3(b_{1u}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\overline{\beta_u} \beta_u|$$

 b_{2u}^2

$$\Delta E = \langle \gamma_u \gamma_u || \gamma_u \gamma_u \rangle$$

$$\Psi_4(b_{2u}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\overline{\gamma_u} \gamma_u|$$

 a_{1u}^2

$$\Delta E = \langle \alpha_u \alpha_u || \alpha_u \alpha_u \rangle$$

$$\Psi_5(a_{1u}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\overline{\alpha_u}\alpha_u|$$

$$\boxed{\Delta E = \langle \zeta_g \zeta_g || \zeta_g \zeta_g \rangle}$$

$$\Psi_6(b_{3g}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\overline{\zeta_g}\zeta_g|$$

$$\boxed{\Delta E = \langle \beta_g \beta_g || \beta_g \beta_g \rangle}$$

$$\Psi_7(b_{1g}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\overline{\beta_g}\beta_g|$$

$$\boxed{\Delta E = \langle \gamma_g \gamma_g || \gamma_g \gamma_g \rangle}$$

$$\Psi_8(b_{2g}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\overline{\gamma_g}\gamma_g|$$

2.8.2 ${}^3B_{3u}$

$$a_{1g}b_{3u}$$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u || \alpha_g \zeta_u \rangle}$$

$$\Psi_1(a_{1g}b_{3u}, {}^3B_{3u}, M=-1, \zeta_u) = |\overline{\alpha_g}\zeta_u|$$

$$\Psi_2(a_{1g}b_{3u}, {}^3B_{3u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_g}\zeta_u|}{2} + \frac{\sqrt{2}|\alpha_g\zeta_u|}{2}$$

$$\Psi_3(a_{1g}b_{3u}, {}^3B_{3u}, M=1, \zeta_u) = |\alpha_g\zeta_u|$$

$$b_{1u}b_{2g}$$

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \gamma_g \gamma_g \rangle + \langle \beta_u \gamma_g || \beta_u \gamma_g \rangle}$$

$$\Psi_4(b_{1u}b_{2g}, {}^3B_{3u}, M=-1, \zeta_u) = |\overline{\beta_u}\gamma_g|$$

$$\Psi_5(b_{1u}b_{2g}, {}^3B_{3u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\beta_u}\gamma_g|}{2} + \frac{\sqrt{2}|\beta_u\gamma_g|}{2}$$

$$\Psi_6(b_{1u}b_{2g}, {}^3B_{3u}, M=1, \zeta_u) = |\beta_u\gamma_g|$$

$$b_{1g}b_{2u}$$

$$\boxed{\Delta E = \langle \gamma_u \beta_g || \gamma_u \beta_g \rangle - \langle \gamma_u \gamma_u || \beta_g \beta_g \rangle}$$

$$\Psi_7(b_{1g}b_{2u}, {}^3B_{3u}, M=-1, \zeta_u) = |\overline{\gamma_u}\beta_g|$$

$$\Psi_8(b_{1g}b_{2u}, {}^3B_{3u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\gamma_u}\beta_g|}{2} + \frac{\sqrt{2}|\gamma_u\beta_g|}{2}$$

$$\Psi_9(b_{1g}b_{2u}, {}^3B_{3u}, M=1, \zeta_u) = |\gamma_u\beta_g|$$

$$a_{1u}b_{3g}$$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \zeta_g \zeta_g \rangle + \langle \alpha_u \zeta_g || \alpha_u \zeta_g \rangle}$$

$$\Psi_{10}(a_{1u}b_{3g}, {}^3B_{3u}, M=-1, \zeta_u) = |\overline{\alpha_u}\zeta_g|$$

$$\Psi_{11}(a_{1u}b_{3g}, {}^3B_{3u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_u}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_u\zeta_g|}{2}$$

$$\Psi_{12}(a_{1u}b_{3g}, {}^3B_{3u}, M=1, \zeta_u) = |\alpha_u\zeta_g|$$

2.8.3 ${}^1B_{3u}$

$$a_{1g}b_{3u}$$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u || \alpha_g \zeta_u \rangle}$$

$$\Psi_1(a_{1g}b_{3u}, {}^1B_{3u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\zeta_u|}{2} + \frac{\sqrt{2}|\alpha_g\zeta_u|}{2}$$

$$b_{1u}b_{2g}$$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \gamma_g \gamma_g \rangle + \langle \beta_u \gamma_g || \beta_u \gamma_g \rangle}$$

$$\Psi_2(b_{1u}b_{2g}, {}^1B_{3u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\beta_u}\gamma_g|}{2} + \frac{\sqrt{2}|\beta_u\gamma_g|}{2}$$

$$b_{1g}b_{2u}$$

$$\boxed{\Delta E = \langle \gamma_u \beta_g || \gamma_u \beta_g \rangle + \langle \gamma_u \gamma_u || \beta_g \beta_g \rangle}$$

$$\Psi_3(b_{1g}b_{2u}, {}^1B_{3u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\gamma_u}\beta_g|}{2} + \frac{\sqrt{2}|\gamma_u\beta_g|}{2}$$

$$a_{1u}b_{3g}$$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \zeta_g \zeta_g \rangle + \langle \alpha_u \zeta_g || \alpha_u \zeta_g \rangle}$$

$$\Psi_4(a_{1u}b_{3g}, {}^1B_{3u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_u\zeta_g|}{2}$$

2.8.4 ${}^3B_{1u}$

$$a_{1g}b_{1u}$$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \beta_u \beta_u \rangle + \langle \alpha_g \beta_u || \alpha_g \beta_u \rangle}$$

$$\Psi_1(a_{1g}b_{1u}, {}^3B_{1u}, M=-1, \beta_u) = |\overline{\alpha_g}\beta_u|$$

$$\Psi_2(a_{1g}b_{1u}, {}^3B_{1u}, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\alpha_g}\beta_u|}{2} + \frac{\sqrt{2}|\alpha_g\beta_u|}{2}$$

$$\Psi_3(a_{1g}b_{1u}, {}^3B_{1u}, M=1, \beta_u) = |\alpha_g\beta_u|$$

$$b_{2g}b_{3u}$$

$$\boxed{\Delta E = \langle \zeta_u \gamma_g || \zeta_u \gamma_g \rangle - \langle \zeta_u \zeta_u || \gamma_g \gamma_g \rangle}$$

$$\Psi_4(b_{2g}b_{3u}, {}^3B_{1u}, M=-1, \beta_u) = |\overline{\zeta_u}\gamma_g|$$

$$\Psi_5(b_{2g}b_{3u}, {}^3B_{1u}, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\zeta_u}\gamma_g|}{2} + \frac{\sqrt{2}|\zeta_u\gamma_g|}{2}$$

$$\Psi_6(b_{2g}b_{3u}, {}^3B_{1u}, M=1, \beta_u) = |\zeta_u\gamma_g|$$

$$b_{2u}b_{3g}$$

$$\boxed{\Delta E = -\langle \gamma_u \gamma_u || \zeta_g \zeta_g \rangle + \langle \gamma_u \zeta_g || \gamma_u \zeta_g \rangle}$$

$$\Psi_7(b_{2u}b_{3g}, {}^3B_{1u}, M=-1, \beta_u) = |\overline{\gamma_u}\zeta_g|$$

$$\Psi_8(b_{2u}b_{3g}, {}^3B_{1u}, M=0, \beta_u) = \frac{\sqrt{2}|\gamma_u\zeta_g|}{2} + \frac{\sqrt{2}|\gamma_u\bar{\zeta}_g|}{2}$$

$$\Psi_9(b_{2u}b_{3g}, {}^3B_{1u}, M=1, \beta_u) = |\gamma_u\zeta_g|$$

a_{1u}b_{1g}

$$\boxed{\Delta E = -\langle \alpha_u\alpha_u || \beta_g\beta_g \rangle + \langle \alpha_u\beta_g || \alpha_u\beta_g \rangle}$$

$$\Psi_{10}(a_{1u}b_{1g}, {}^3B_{1u}, M=-1, \beta_u) = |\overline{\alpha_u}\overline{\beta_g}|$$

$$\Psi_{11}(a_{1u}b_{1g}, {}^3B_{1u}, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\alpha_u}\beta_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\beta_g}|}{2}$$

$$\Psi_{12}(a_{1u}b_{1g}, {}^3B_{1u}, M=1, \beta_u) = |\alpha_u\beta_g|$$

2.8.5 ¹B_{1u}*a_{1g}b_{1u}*

$$\boxed{\Delta E = \langle \alpha_g\alpha_g || \beta_u\beta_u \rangle + \langle \alpha_g\beta_u || \alpha_g\beta_u \rangle}$$

$$\Psi_1(a_{1g}b_{1u}, {}^1B_{1u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\beta_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\beta_u}|}{2}$$

b_{2g}b_{3u}

$$\boxed{\Delta E = \langle \zeta_u\gamma_g || \zeta_u\gamma_g \rangle + \langle \zeta_u\zeta_u || \gamma_g\gamma_g \rangle}$$

$$\Psi_2(b_{2g}b_{3u}, {}^1B_{1u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\zeta_u}\gamma_g|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\gamma_g}|}{2}$$

b_{2u}b_{3g}

$$\boxed{\Delta E = \langle \gamma_u\gamma_u || \zeta_g\zeta_g \rangle + \langle \gamma_u\zeta_g || \gamma_u\zeta_g \rangle}$$

$$\Psi_3(b_{2u}b_{3g}, {}^1B_{1u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\gamma_u}\zeta_g|}{2} + \frac{\sqrt{2}|\gamma_u\overline{\zeta_g}|}{2}$$

a_{1u}b_{1g}

$$\boxed{\Delta E = \langle \alpha_u\alpha_u || \beta_g\beta_g \rangle + \langle \alpha_u\beta_g || \alpha_u\beta_g \rangle}$$

$$\Psi_4(a_{1u}b_{1g}, {}^1B_{1u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\beta_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\beta_g}|}{2}$$

2.8.6 ³B_{2u}*a_{1g}b_{2u}*

$$\boxed{\Delta E = -\langle \alpha_g\alpha_g || \gamma_u\gamma_u \rangle + \langle \alpha_g\gamma_u || \alpha_g\gamma_u \rangle}$$

$$\Psi_1(a_{1g}b_{2u}, {}^3B_{2u}, M=-1, \gamma_u) = |\overline{\alpha_g}\gamma_u|$$

$$\Psi_2(a_{1g}b_{2u}, {}^3B_{2u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_g}\gamma_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\gamma_u}|}{2}$$

$$\Psi_3(a_{1g}b_{2u}, {}^3B_{2u}, M=1, \gamma_u) = |\alpha_g\gamma_u|$$

b_{1g}b_{3u}

$$\boxed{\Delta E = \langle \zeta_u\beta_g || \zeta_u\beta_g \rangle - \langle \zeta_u\zeta_u || \beta_g\beta_g \rangle}$$

$$\Psi_4(b_{1g}b_{3u}, {}^3B_{2u}, M=-1, \gamma_u) = |\overline{\zeta_u}\beta_g|$$

$$\Psi_5(b_{1g}b_{3u}, {}^3B_{2u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\zeta_u}\beta_g|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\beta_g}|}{2}$$

$$\Psi_6(b_{1g}b_{3u}, {}^3B_{2u}, M=1, \gamma_u) = |\zeta_u\beta_g|$$

b_{1u}b_{3g}

$$\boxed{\Delta E = -\langle \beta_u\beta_u || \zeta_g\zeta_g \rangle + \langle \beta_u\zeta_g || \beta_u\zeta_g \rangle}$$

$$\Psi_7(b_{1u}b_{3g}, {}^3B_{2u}, M=-1, \gamma_u) = |\overline{\beta_u}\zeta_g|$$

$$\Psi_8(b_{1u}b_{3g}, {}^3B_{2u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\beta_u}\zeta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\zeta_g}|}{2}$$

$$\Psi_9(b_{1u}b_{3g}, {}^3B_{2u}, M=1, \gamma_u) = |\beta_u\zeta_g|$$

a_{1u}b_{2g}

$$\boxed{\Delta E = -\langle \alpha_u\alpha_u || \gamma_g\gamma_g \rangle + \langle \alpha_u\gamma_g || \alpha_u\gamma_g \rangle}$$

$$\Psi_{10}(a_{1u}b_{2g}, {}^3B_{2u}, M=-1, \gamma_u) = |\overline{\alpha_u}\gamma_g|$$

$$\Psi_{11}(a_{1u}b_{2g}, {}^3B_{2u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_u}\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\gamma_g}|}{2}$$

$$\Psi_{12}(a_{1u}b_{2g}, {}^3B_{2u}, M=1, \gamma_u) = |\alpha_u\gamma_g|$$

2.8.7 ¹B_{2u}*a_{1g}b_{2u}*

$$\boxed{\Delta E = \langle \alpha_g\alpha_g || \gamma_u\gamma_u \rangle + \langle \alpha_g\gamma_u || \alpha_g\gamma_u \rangle}$$

$$\Psi_1(a_{1g}b_{2u}, {}^1B_{2u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\gamma_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\gamma_u}|}{2}$$

b_{1g}b_{3u}

$$\boxed{\Delta E = \langle \zeta_u\beta_g || \zeta_u\beta_g \rangle + \langle \zeta_u\zeta_u || \beta_g\beta_g \rangle}$$

$$\Psi_2(b_{1g}b_{3u}, {}^1B_{2u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\zeta_u}\beta_g|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\beta_g}|}{2}$$

b_{1u}b_{3g}

$$\boxed{\Delta E = \langle \beta_u\beta_u || \zeta_g\zeta_g \rangle + \langle \beta_u\zeta_g || \beta_u\zeta_g \rangle}$$

$$\Psi_3(b_{1u}b_{3g}, {}^1B_{2u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\beta_u}\zeta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\zeta_g}|}{2}$$

a_{1u}b_{2g}

$$\boxed{\Delta E = \langle \alpha_u\alpha_u || \gamma_g\gamma_g \rangle + \langle \alpha_u\gamma_g || \alpha_u\gamma_g \rangle}$$

$$\Psi_4(a_{1u}b_{2g}, {}^1B_{2u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\gamma_g}|}{2}$$

2.8.8 $^3A_{1u}$ $a_{1g}a_{1u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_{1g}a_{1u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\alpha_g \alpha_u}|$$

$$\Psi_2(a_{1g}a_{1u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\alpha_g \alpha_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\alpha_u}|}{2}$$

$$\Psi_3(a_{1g}a_{1u}, ^3A_{1u}, M=1, \alpha_u) = |\alpha_g \alpha_u|$$

 $b_{3g}b_{3u}$

$$\boxed{\Delta E = \langle \zeta_u \zeta_g || \zeta_u \zeta_g \rangle - \langle \zeta_u \zeta_u || \zeta_g \zeta_g \rangle}$$

$$\Psi_4(b_{3g}b_{3u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\zeta_u \zeta_g}|$$

$$\Psi_5(b_{3g}b_{3u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\zeta_u \zeta_g}|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\zeta_g}|}{2}$$

$$\Psi_6(b_{3g}b_{3u}, ^3A_{1u}, M=1, \alpha_u) = |\zeta_u \zeta_g|$$

 $b_{1g}b_{1u}$

$$\boxed{\Delta E = \langle \beta_u \beta_g || \beta_u \beta_g \rangle - \langle \beta_u \beta_u || \beta_g \beta_g \rangle}$$

$$\Psi_7(b_{1g}b_{1u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\beta_u \beta_g}|$$

$$\Psi_8(b_{1g}b_{1u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\beta_u \beta_g}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\beta_g}|}{2}$$

$$\Psi_9(b_{1g}b_{1u}, ^3A_{1u}, M=1, \alpha_u) = |\beta_u \beta_g|$$

 $b_{2g}b_{2u}$

$$\boxed{\Delta E = \langle \gamma_u \gamma_g || \gamma_u \gamma_g \rangle - \langle \gamma_u \gamma_u || \gamma_g \gamma_g \rangle}$$

$$\Psi_{10}(b_{2g}b_{2u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\gamma_u \gamma_g}|$$

$$\Psi_{11}(b_{2g}b_{2u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\gamma_u \gamma_g}|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\gamma_g}|}{2}$$

$$\Psi_{12}(b_{2g}b_{2u}, ^3A_{1u}, M=1, \alpha_u) = |\gamma_u \gamma_g|$$

2.8.9 $^1A_{1u}$ $a_{1g}a_{1u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_{1g}a_{1u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\alpha_g \alpha_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\alpha_u}|}{2}$$

 $b_{3g}b_{3u}$

$$\boxed{\Delta E = \langle \zeta_u \zeta_g || \zeta_u \zeta_g \rangle + \langle \zeta_u \zeta_u || \zeta_g \zeta_g \rangle}$$

$$\Psi_2(b_{3g}b_{3u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\zeta_u \zeta_g}|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\zeta_g}|}{2}$$

 $b_{1g}b_{1u}$

$$\boxed{\Delta E = \langle \beta_u \beta_g || \beta_u \beta_g \rangle + \langle \beta_u \beta_u || \beta_g \beta_g \rangle}$$

 $b_{2g}b_{2u}$

$$\boxed{\Delta E = \langle \gamma_u \gamma_g || \gamma_u \gamma_g \rangle + \langle \gamma_u \gamma_u || \gamma_g \gamma_g \rangle}$$

$$\Psi_4(b_{2g}b_{2u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\gamma_u \gamma_g}|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\gamma_g}|}{2}$$

2.8.10 $^3B_{3g}$ $a_{1g}b_{3g}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \zeta_g \zeta_g \rangle + \langle \alpha_g \zeta_g || \alpha_g \zeta_g \rangle}$$

$$\Psi_1(a_{1g}b_{3g}, ^3B_{3g}, M=-1, \zeta_g) = |\overline{\alpha_g \zeta_g}|$$

$$\Psi_2(a_{1g}b_{3g}, ^3B_{3g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\alpha_g \zeta_g}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\zeta_g}|}{2}$$

$$\Psi_3(a_{1g}b_{3g}, ^3B_{3g}, M=1, \zeta_g) = |\alpha_g \zeta_g|$$

 $a_{1u}b_{3u}$

$$\boxed{\Delta E = \langle \zeta_u \alpha_u || \zeta_u \alpha_u \rangle - \langle \zeta_u \zeta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_4(a_{1u}b_{3u}, ^3B_{3g}, M=-1, \zeta_g) = |\overline{\zeta_u \alpha_u}|$$

$$\Psi_5(a_{1u}b_{3u}, ^3B_{3g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\zeta_u \alpha_u}|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\alpha_u}|}{2}$$

$$\Psi_6(a_{1u}b_{3u}, ^3B_{3g}, M=1, \zeta_g) = |\zeta_u \alpha_u|$$

 $b_{1u}b_{2u}$

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \gamma_u \gamma_u \rangle + \langle \beta_u \gamma_u || \beta_u \gamma_u \rangle}$$

$$\Psi_7(b_{1u}b_{2u}, ^3B_{3g}, M=-1, \zeta_g) = |\overline{\beta_u \gamma_u}|$$

$$\Psi_8(b_{1u}b_{2u}, ^3B_{3g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_u \gamma_u}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\gamma_u}|}{2}$$

$$\Psi_9(b_{1u}b_{2u}, ^3B_{3g}, M=1, \zeta_g) = |\beta_u \gamma_u|$$

 $b_{1g}b_{2g}$

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \gamma_g \gamma_g \rangle + \langle \beta_g \gamma_g || \beta_g \gamma_g \rangle}$$

$$\Psi_{10}(b_{1g}b_{2g}, ^3B_{3g}, M=-1, \zeta_g) = |\overline{\beta_g \gamma_g}|$$

$$\Psi_{11}(b_{1g}b_{2g}, ^3B_{3g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_g \gamma_g}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\gamma_g}|}{2}$$

$$\Psi_{12}(b_{1g}b_{2g}, ^3B_{3g}, M=1, \zeta_g) = |\beta_g \gamma_g|$$

2.8.11 $^1B_{3g}$

$a_{1g}b_{3g}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \zeta_g \zeta_g \rangle + \langle \alpha_g \zeta_g || \alpha_g \zeta_g \rangle}$$

$$\Psi_1(a_{1g}b_{3g}, ^1B_{3g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\zeta_g}|}{2}$$

$a_{1u}b_{3u}$

$$\boxed{\Delta E = \langle \zeta_u \alpha_u || \zeta_u \alpha_u \rangle + \langle \zeta_u \zeta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_2(a_{1u}b_{3u}, ^1B_{3g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\zeta_u}\alpha_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\alpha_u}|}{2}$$

$b_{1u}b_{2u}$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \gamma_u \gamma_u \rangle + \langle \beta_u \gamma_u || \beta_u \gamma_u \rangle}$$

$$\Psi_3(b_{1u}b_{2u}, ^1B_{3g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\beta_u}\gamma_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\gamma_u}|}{2}$$

$b_{1g}b_{2g}$

$$\boxed{\Delta E = \langle \beta_g \beta_g || \gamma_g \gamma_g \rangle + \langle \beta_g \gamma_g || \beta_g \gamma_g \rangle}$$

$$\Psi_4(b_{1g}b_{2g}, ^1B_{3g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\beta_g}\gamma_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\gamma_g}|}{2}$$

2.8.12 $^3B_{1g}$

$a_{1g}b_{1g}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_{1g}b_{1g}, ^3B_{1g}, M=-1, \beta_g) = |\overline{\alpha_g}\overline{\beta_g}|$$

$$\Psi_2(a_{1g}b_{1g}, ^3B_{1g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\alpha_g}\beta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\beta_g}|}{2}$$

$$\Psi_3(a_{1g}b_{1g}, ^3B_{1g}, M=1, \beta_g) = |\alpha_g\beta_g|$$

$b_{2u}b_{3u}$

$$\boxed{\Delta E = \langle \zeta_u \gamma_u || \zeta_u \gamma_u \rangle - \langle \zeta_u \zeta_u || \gamma_u \gamma_u \rangle}$$

$$\Psi_4(b_{2u}b_{3u}, ^3B_{1g}, M=-1, \beta_g) = |\overline{\zeta_u}\overline{\gamma_u}|$$

$$\Psi_5(b_{2u}b_{3u}, ^3B_{1g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\zeta_u}\gamma_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\gamma_u}|}{2}$$

$$\Psi_6(b_{2u}b_{3u}, ^3B_{1g}, M=1, \beta_g) = |\zeta_u\gamma_u|$$

$a_{1u}b_{1u}$

$$\boxed{\Delta E = \langle \beta_u \alpha_u || \beta_u \alpha_u \rangle - \langle \beta_u \beta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_7(a_{1u}b_{1u}, ^3B_{1g}, M=-1, \beta_g) = |\overline{\beta_u}\overline{\alpha_u}|$$

$$\Psi_8(a_{1u}b_{1u}, ^3B_{1g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\beta_u}\alpha_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\alpha_u}|}{2}$$

$$\Psi_9(a_{1u}b_{1u}, ^3B_{1g}, M=1, \beta_g) = |\beta_u\alpha_u|$$

$b_{2g}b_{3g}$

$$\boxed{\Delta E = \langle \zeta_g \gamma_g || \zeta_g \gamma_g \rangle - \langle \zeta_g \zeta_g || \gamma_g \gamma_g \rangle}$$

$$\Psi_{10}(b_{2g}b_{3g}, ^3B_{1g}, M=-1, \beta_g) = |\overline{\zeta_g}\overline{\gamma_g}|$$

$$\Psi_{11}(b_{2g}b_{3g}, ^3B_{1g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\zeta_g}\gamma_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\gamma_g}|}{2}$$

$$\Psi_{12}(b_{2g}b_{3g}, ^3B_{1g}, M=1, \beta_g) = |\zeta_g\gamma_g|$$

2.8.13 $^1B_{1g}$

$a_{1g}b_{1g}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_{1g}b_{1g}, ^1B_{1g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\beta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\beta_g}|}{2}$$

$b_{2u}b_{3u}$

$$\boxed{\Delta E = \langle \zeta_u \gamma_u || \zeta_u \gamma_u \rangle + \langle \zeta_u \zeta_u || \gamma_u \gamma_u \rangle}$$

$$\Psi_2(b_{2u}b_{3u}, ^1B_{1g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\zeta_u}\gamma_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\gamma_u}|}{2}$$

$a_{1u}b_{1u}$

$$\boxed{\Delta E = \langle \beta_u \alpha_u || \beta_u \alpha_u \rangle + \langle \beta_u \beta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_3(a_{1u}b_{1u}, ^1B_{1g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\beta_u}\alpha_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\alpha_u}|}{2}$$

$b_{2g}b_{3g}$

$$\boxed{\Delta E = \langle \zeta_g \gamma_g || \zeta_g \gamma_g \rangle + \langle \zeta_g \zeta_g || \gamma_g \gamma_g \rangle}$$

$$\Psi_4(b_{2g}b_{3g}, ^1B_{1g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\zeta_g}\gamma_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\gamma_g}|}{2}$$

2.8.14 $^3B_{2g}$

$a_{1g}b_{2g}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \gamma_g \gamma_g \rangle + \langle \alpha_g \gamma_g || \alpha_g \gamma_g \rangle}$$

$$\Psi_1(a_{1g}b_{2g}, ^3B_{2g}, M=-1, \gamma_g) = |\overline{\alpha_g}\overline{\gamma_g}|$$

$$\Psi_2(a_{1g}b_{2g}, ^3B_{2g}, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\alpha_g}\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\gamma_g}|}{2}$$

$$\Psi_3(a_{1g}b_{2g}, ^3B_{2g}, M=1, \gamma_g) = |\alpha_g\gamma_g|$$

$b_{1u}b_{3u}$

$$\boxed{\Delta E = \langle \zeta_u \beta_u || \zeta_u \beta_u \rangle - \langle \zeta_u \zeta_u || \beta_u \beta_u \rangle}$$

$$\Psi_4(b_{1u}b_{3u}, ^3B_{2g}, M=-1, \gamma_g) = |\overline{\zeta_u}\overline{\beta_u}|$$

$$\Psi_5(b_{1u}b_{3u}, ^3B_{2g}, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\zeta_u}\beta_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\beta_u}|}{2}$$

$$\Psi_6(b_{1u}b_{3u}, {}^3B_{2g}, M=1, \gamma_g) = |\zeta_u\beta_u|$$

a_{1u}b_{2u}

$$\boxed{\Delta E = \langle \gamma_u \alpha_u || \gamma_u \alpha_u \rangle - \langle \gamma_u \gamma_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_7(a_{1u}b_{2u}, {}^3B_{2g}, M=-1, \gamma_g) = |\overline{\gamma_u \alpha_u}|$$

$$\Psi_8(a_{1u}b_{2u}, {}^3B_{2g}, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\gamma_u \alpha_u}|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\alpha_u}|}{2}$$

$$\Psi_9(a_{1u}b_{2u}, {}^3B_{2g}, M=1, \gamma_g) = |\gamma_u \alpha_u|$$

b_{1g}b_{3g}

$$\boxed{\Delta E = \langle \zeta_g \beta_g || \zeta_g \beta_g \rangle - \langle \zeta_g \zeta_g || \beta_g \beta_g \rangle}$$

$$\Psi_{10}(b_{1g}b_{3g}, {}^3B_{2g}, M=-1, \gamma_g) = |\overline{\zeta_g \beta_g}|$$

$$\Psi_{11}(b_{1g}b_{3g}, {}^3B_{2g}, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\zeta_g \beta_g}|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\beta_g}|}{2}$$

$$\Psi_{12}(b_{1g}b_{3g}, {}^3B_{2g}, M=1, \gamma_g) = |\zeta_g \beta_g|$$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \gamma_g \gamma_g \rangle + \langle \alpha_g \gamma_g || \alpha_g \gamma_g \rangle}$$

$$\Psi_1(a_{1g}b_{2g}, {}^1B_{2g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\alpha_g} \gamma_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\gamma_g}|}{2}$$

b_{1u}b_{3u}

$$\boxed{\Delta E = \langle \zeta_u \beta_u || \zeta_u \beta_u \rangle + \langle \zeta_u \zeta_u || \beta_u \beta_u \rangle}$$

$$\Psi_2(b_{1u}b_{3u}, {}^1B_{2g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\zeta_u} \beta_u|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\beta_u}|}{2}$$

a_{1u}b_{2u}

$$\boxed{\Delta E = \langle \gamma_u \alpha_u || \gamma_u \alpha_u \rangle + \langle \gamma_u \gamma_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_3(a_{1u}b_{2u}, {}^1B_{2g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\gamma_u} \alpha_u|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\alpha_u}|}{2}$$

b_{1g}b_{3g}

$$\boxed{\Delta E = \langle \zeta_g \beta_g || \zeta_g \beta_g \rangle + \langle \zeta_g \zeta_g || \beta_g \beta_g \rangle}$$

$$\Psi_4(b_{1g}b_{3g}, {}^1B_{2g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\zeta_g} \beta_g|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\beta_g}|}{2}$$

2.8.15 ${}^1B_{2g}$

a_{1g}b_{2g}

$$\boxed{\Delta E = \langle \zeta_g \beta_g || \zeta_g \beta_g \rangle + \langle \zeta_g \zeta_g || \beta_g \beta_g \rangle}$$

2.9 Group C_4

Component labels

$$A : \{\alpha\} \longrightarrow E^1 : \{\gamma\} \longrightarrow E^2 : \{\zeta\} \longrightarrow B : \{\beta\}$$

2.9.2 ${}^3E^1$

2.9.1 1A

ae¹

a²

$$\boxed{\Delta E = \langle \alpha \gamma || \alpha \gamma \rangle}$$

$$\boxed{\Delta E = \langle \alpha \alpha || \alpha \alpha \rangle}$$

$$\Psi_1(a^2, {}^1A, M=0, \alpha) = -|\overline{\alpha} \alpha|$$

e¹e²

$$\Psi_1(ae^1, {}^3E^1, M=-1, \gamma) = |\overline{\alpha} \gamma|$$

$$\Psi_2(ae^1, {}^3E^1, M=0, \gamma) = \frac{\sqrt{2}|\overline{\alpha} \gamma|}{2} + \frac{\sqrt{2}|\alpha \overline{\gamma}|}{2}$$

$$\Psi_3(ae^1, {}^3E^1, M=1, \gamma) = |\alpha \gamma|$$

be²

$$\boxed{\Delta E = \langle \zeta \beta || \zeta \beta \rangle}$$

$$\boxed{\Delta E = \langle \gamma \gamma || \zeta \zeta \rangle + \langle \gamma \zeta || \gamma \zeta \rangle}$$

$$\Psi_2(e^1e^2, {}^1A, M=0, \alpha) = -\frac{\sqrt{2}|\overline{\gamma} \zeta|}{2} + \frac{\sqrt{2}|\gamma \overline{\zeta}|}{2}$$

b²

$$\Psi_4(be^2, {}^3E^1, M=-1, \gamma) = |\overline{\zeta} \beta|$$

$$\boxed{\Delta E = \langle \beta \beta || \beta \beta \rangle}$$

$$\Psi_5(be^2, {}^3E^1, M=0, \gamma) = \frac{\sqrt{2}|\overline{\zeta} \beta|}{2} + \frac{\sqrt{2}|\zeta \overline{\beta}|}{2}$$

$$\Psi_6(be^2, {}^3E^1, M=1, \gamma) = |\zeta \beta|$$

$$\Psi_3(b^2, {}^1A, M=0, \alpha) = -|\overline{\beta} \beta|$$

2.9.3 $^1E^1$ **2.9.6** 3B *ae¹*

$$\boxed{\Delta E = \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(ae^1, ^1E^1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

be²

$$\boxed{\Delta E = \langle \zeta\beta || \zeta\beta \rangle}$$

$$\Psi_2(be^2, ^1E^1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2}$$

ab

$$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(ab, ^3B, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$\Psi_2(ab, ^3B, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(ab, ^3B, M=1, \beta) = |\alpha\beta|$$

2.9.4 $^3E^2$ **2.9.7** 1B *ae²*

$$\boxed{\Delta E = \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(ae^2, ^3E^2, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}|$$

$$\Psi_2(ae^2, ^3E^2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_3(ae^2, ^3E^2, M=1, \zeta) = |\alpha\zeta|$$

be¹

$$\boxed{\Delta E = \langle \gamma\beta || \gamma\beta \rangle}$$

$$\Psi_4(be^1, ^3E^2, M=-1, \zeta) = |\bar{\gamma}\bar{\beta}|$$

$$\Psi_5(be^1, ^3E^2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

$$\Psi_6(be^1, ^3E^2, M=1, \zeta) = |\gamma\beta|$$

ab

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(ab, ^1B, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$(e^1)^2$$

$$\boxed{\Delta E = \langle \gamma\gamma || \gamma\gamma \rangle}$$

$$\Psi_2((e^1)^2, ^1B, M=0, \beta) = -|\bar{\gamma}\gamma|$$

$$(e^2)^2$$

$$\boxed{\Delta E = \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\Psi_3((e^2)^2, ^1B, M=0, \beta) = -|\bar{\zeta}\zeta|$$

2.9.5 $^1E^2$ *ae²*

$$\boxed{\Delta E = \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(ae^2, ^1E^2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

be¹

$$\boxed{\Delta E = \langle \gamma\beta || \gamma\beta \rangle}$$

$$\Psi_2(be^1, ^1E^2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

2.9.8 3A *e¹e²*

$$\boxed{\Delta E = -\langle \gamma\gamma || \zeta\zeta \rangle + \langle \gamma\zeta || \gamma\zeta \rangle}$$

$$\Psi_1(e^1e^2, ^3A, M=-1, \alpha) = |\bar{\gamma}\bar{\zeta}|$$

$$\Psi_2(e^1e^2, ^3A, M=0, \alpha) = \frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\gamma\bar{\zeta}|}{2}$$

$$\Psi_3(e^1e^2, ^3A, M=1, \alpha) = |\gamma\zeta|$$

2.10 Group S_4 Component labels

$$A : \{\alpha\} \longrightarrow E^1 : \{\gamma\} \longrightarrow E^2 : \{\zeta\} \longrightarrow B : \{\beta\}$$

2.10.1 1A a^2

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_1(a^2, {}^1A, M=0, \alpha) = -|\bar{\alpha}\alpha|$$

 $e^1 e^2$

$$\boxed{\Delta E = \langle \gamma\gamma || \zeta\zeta \rangle + \langle \gamma\zeta || \gamma\zeta \rangle}$$

$$\Psi_2(e^1 e^2, {}^1A, M=0, \alpha) = -\frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\gamma\bar{\zeta}|}{2}$$

 b^2

$$\boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle}$$

$$\Psi_3(b^2, {}^1A, M=0, \alpha) = -|\bar{\beta}\beta|$$

2.10.2 ${}^3E^1$ ae^1

$$\boxed{\Delta E = \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(ae^1, {}^3E^1, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

$$\Psi_2(ae^1, {}^3E^1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(ae^1, {}^3E^1, M=1, \gamma) = |\alpha\gamma|$$

 be^2

$$\boxed{\Delta E = \langle \zeta\beta || \zeta\beta \rangle}$$

$$\Psi_4(be^2, {}^3E^1, M=-1, \gamma) = |\bar{\zeta}\beta|$$

$$\Psi_5(be^2, {}^3E^1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2}$$

$$\Psi_6(be^2, {}^3E^1, M=1, \gamma) = |\zeta\beta|$$

2.10.3 ${}^1E^1$ ae^1

$$\boxed{\Delta E = \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(ae^1, {}^1E^1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

 be^2

$$\boxed{\Delta E = \langle \zeta\beta || \zeta\beta \rangle}$$

$$\Psi_2(be^2, {}^1E^1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2}$$

2.10.4 ${}^3E^2$ ae^2

$$\boxed{\Delta E = \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(ae^2, {}^3E^2, M=-1, \zeta) = |\bar{\alpha}\zeta|$$

$$\Psi_2(ae^2, {}^3E^2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_3(ae^2, {}^3E^2, M=1, \zeta) = |\alpha\zeta|$$

 be^1

$$\boxed{\Delta E = \langle \gamma\beta || \gamma\beta \rangle}$$

$$\Psi_4(be^1, {}^3E^2, M=-1, \zeta) = |\bar{\gamma}\beta|$$

$$\Psi_5(be^1, {}^3E^2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

$$\Psi_6(be^1, {}^3E^2, M=1, \zeta) = |\gamma\beta|$$

$$\Psi_1(ae^1, {}^3E^1, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

2.10.5 ${}^1E^2$ ae^2

$$\boxed{\Delta E = \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(ae^2, {}^1E^2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

 be^1

$$\boxed{\Delta E = \langle \gamma\beta || \gamma\beta \rangle}$$

$$\Psi_2(be^1, {}^1E^2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

<p>2.10.6 3B</p> <p style="text-align: center;"><i>ab</i></p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = -\langle \alpha\alpha \beta\beta \rangle + \langle \alpha\beta \alpha\beta \rangle$ </div> <p style="text-align: center;">$\Psi_1(ab, {}^3B, M=1, \beta) = \overline{\alpha}\overline{\beta}$</p> <p style="text-align: center;">$\Psi_2(ab, {}^3B, M=0, \beta) = \frac{\sqrt{2} \overline{\alpha}\beta }{2} + \frac{\sqrt{2} \alpha\overline{\beta} }{2}$</p> <p style="text-align: center;">$\Psi_3(ab, {}^3B, M=1, \beta) = \alpha\beta$</p>	<p style="text-align: right;">$(e^1)^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \zeta\zeta \zeta\zeta \rangle$ </div> <p style="text-align: right;">$\Psi_2((e^1)^2, {}^1B, M=0, \beta) = - \overline{\gamma}\gamma$</p> <p style="text-align: right;">$(e^2)^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \zeta\zeta \zeta\zeta \rangle$ </div> <p style="text-align: right;">$\Psi_3((e^2)^2, {}^1B, M=0, \beta) = - \overline{\zeta}\zeta$</p>
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<p>2.10.7 1B</p> <p style="text-align: center;"><i>ab</i></p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \alpha\alpha \beta\beta \rangle + \langle \alpha\beta \alpha\beta \rangle$ </div> <p style="text-align: center;">$\Psi_1(ab, {}^1B, M=0, \beta) = -\frac{\sqrt{2} \overline{\alpha}\beta }{2} + \frac{\sqrt{2} \alpha\overline{\beta} }{2}$</p> <p style="text-align: center;">$(e^1)^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma\gamma \gamma\gamma \rangle$ </div>	<p>2.10.8 3A</p> <p style="text-align: center;">$e^1 e^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = -\langle \gamma\gamma \zeta\zeta \rangle + \langle \gamma\zeta \gamma\zeta \rangle$ </div> <p style="text-align: center;">$\Psi_1(e^1 e^2, {}^3A, M=-1, \alpha) = \overline{\gamma}\overline{\zeta}$</p> <p style="text-align: center;">$\Psi_2(e^1 e^2, {}^3A, M=0, \alpha) = \frac{\sqrt{2} \overline{\gamma}\zeta }{2} + \frac{\sqrt{2} \gamma\overline{\zeta} }{2}$</p> <p style="text-align: center;">$\Psi_3(e^1 e^2, {}^3A, M=1, \alpha) = \gamma\zeta$</p>
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<p>2.11 Group C_{4h}</p> <p style="text-align: center;"><u>Component labels</u></p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Gamma^1 : \{\gamma_1\} \longrightarrow \Gamma^2 : \{\gamma_2\} \longrightarrow \Gamma^3 : \{\gamma_3\} \longrightarrow \Gamma^4 : \{\gamma_4\} \longrightarrow \Gamma^5 : \{\gamma_5\} \longrightarrow \Gamma^6 : \{\gamma_6\} \longrightarrow \Gamma^7 : \{\gamma_7\} \longrightarrow \Gamma^8 : \{\gamma_8\}$ </div>	<p style="text-align: center;">$(\gamma^5)^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma_5\gamma_5 \gamma_5\gamma_5 \rangle$ </div>
<p>2.11.1 ${}^1\Gamma^1$</p> <p style="text-align: center;">$(\gamma^1)^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma_1\gamma_1 \gamma_1\gamma_1 \rangle$ </div> <p style="text-align: center;">$\Psi_4((\gamma^5)^2, {}^1\Gamma^1, M=0, \gamma_1) = - \overline{\gamma_5}\gamma_5$</p>	<p style="text-align: center;">$\gamma^6\gamma^7$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma_6\gamma_6 \gamma_7\gamma_7 \rangle + \langle \gamma_6\gamma_7 \gamma_6\gamma_7 \rangle$ </div> <p style="text-align: center;">$\Psi_5(\gamma^6\gamma^7, {}^1\Gamma^1, M=0, \gamma_1) = -\frac{\sqrt{2} \overline{\gamma_6}\gamma_7 }{2} + \frac{\sqrt{2} \gamma_6\overline{\gamma_7} }{2}$</p>
<p style="text-align: center;">$\gamma^2\gamma^3$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma_2\gamma_2 \gamma_3\gamma_3 \rangle + \langle \gamma_2\gamma_3 \gamma_2\gamma_3 \rangle$ </div> <p style="text-align: center;">$\Psi_2(\gamma^2\gamma^3, {}^1\Gamma^1, M=0, \gamma_1) = -\frac{\sqrt{2} \overline{\gamma_2}\gamma_3 }{2} + \frac{\sqrt{2} \gamma_2\overline{\gamma_3} }{2}$</p> <p style="text-align: center;">$(\gamma^4)^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma_4\gamma_4 \gamma_4\gamma_4 \rangle$ </div> <p style="text-align: center;">$\Psi_3((\gamma^4)^2, {}^1\Gamma^1, M=0, \gamma_1) = - \overline{\gamma_4}\gamma_4$</p>	<p style="text-align: center;">$(\gamma^8)^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma_8\gamma_8 \gamma_8\gamma_8 \rangle$ </div> <p style="text-align: center;">$\Psi_6((\gamma^8)^2, {}^1\Gamma^1, M=0, \gamma_1) = - \overline{\gamma_8}\gamma_8$</p>

2.11.2 $^3\Gamma^2$

$$\Psi_3(\gamma^4\gamma^7, ^1\Gamma^2, M=0, \gamma_2) = -\frac{\sqrt{2}|\bar{\gamma}_4\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_4\bar{\gamma}_7|}{2}$$

$$\gamma^1\gamma^2$$

$$\boxed{\Delta E = \langle \gamma_1\gamma_2 || \gamma_1\gamma_2 \rangle}$$

$$\gamma^5\gamma^6$$

$$\boxed{\Delta E = \langle \gamma_5\gamma_6 || \gamma_5\gamma_6 \rangle}$$

$$\Psi_1(\gamma^1\gamma^2, ^3\Gamma^2, M=-1, \gamma_2) = |\bar{\gamma}_1\gamma_2|$$

$$\Psi_2(\gamma^1\gamma^2, ^3\Gamma^2, M=0, \gamma_2) = \frac{\sqrt{2}|\bar{\gamma}_1\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_1\bar{\gamma}_2|}{2}$$

$$\Psi_3(\gamma^1\gamma^2, ^3\Gamma^2, M=1, \gamma_2) = |\gamma_1\gamma_2|$$

$$\gamma^3\gamma^8$$

$$\boxed{\Delta E = \langle \gamma_3\gamma_8 || \gamma_3\gamma_8 \rangle}$$

2.11.4 $^3\Gamma^3$

$$\gamma^1\gamma^3$$

$$\boxed{\Delta E = \langle \gamma_1\gamma_3 || \gamma_1\gamma_3 \rangle}$$

$$\Psi_4(\gamma^3\gamma^8, ^3\Gamma^2, M=-1, \gamma_2) = |\bar{\gamma}_3\gamma_8|$$

$$\Psi_5(\gamma^3\gamma^8, ^3\Gamma^2, M=0, \gamma_2) = \frac{\sqrt{2}|\bar{\gamma}_3\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_3\bar{\gamma}_8|}{2}$$

$$\Psi_6(\gamma^3\gamma^8, ^3\Gamma^2, M=1, \gamma_2) = |\gamma_3\gamma_8|$$

$$\gamma^4\gamma^7$$

$$\boxed{\Delta E = \langle \gamma_4\gamma_7 || \gamma_4\gamma_7 \rangle}$$

$$\Psi_1(\gamma^1\gamma^3, ^3\Gamma^3, M=-1, \gamma_3) = |\bar{\gamma}_1\gamma_3|$$

$$\Psi_2(\gamma^1\gamma^3, ^3\Gamma^3, M=0, \gamma_3) = \frac{\sqrt{2}|\bar{\gamma}_1\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_1\bar{\gamma}_3|}{2}$$

$$\Psi_3(\gamma^1\gamma^3, ^3\Gamma^3, M=1, \gamma_3) = |\gamma_1\gamma_3|$$

$$\gamma^2\gamma^8$$

$$\boxed{\Delta E = \langle \gamma_2\gamma_8 || \gamma_2\gamma_8 \rangle}$$

$$\Psi_4(\gamma^2\gamma^8, ^3\Gamma^3, M=-1, \gamma_3) = |\bar{\gamma}_2\gamma_8|$$

$$\Psi_5(\gamma^2\gamma^8, ^3\Gamma^3, M=0, \gamma_3) = \frac{\sqrt{2}|\bar{\gamma}_2\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_2\bar{\gamma}_8|}{2}$$

$$\Psi_6(\gamma^2\gamma^8, ^3\Gamma^3, M=1, \gamma_3) = |\gamma_2\gamma_8|$$

$$\gamma^4\gamma^6$$

$$\boxed{\Delta E = \langle \gamma_4\gamma_6 || \gamma_4\gamma_6 \rangle}$$

2.11.3 $^1\Gamma^2$

$$\gamma^1\gamma^2$$

$$\boxed{\Delta E = \langle \gamma_1\gamma_2 || \gamma_1\gamma_2 \rangle}$$

$$\Psi_7(\gamma^4\gamma^6, ^3\Gamma^3, M=-1, \gamma_3) = |\bar{\gamma}_4\gamma_6|$$

$$\Psi_8(\gamma^4\gamma^6, ^3\Gamma^3, M=0, \gamma_3) = \frac{\sqrt{2}|\bar{\gamma}_4\gamma_6|}{2} + \frac{\sqrt{2}|\gamma_4\bar{\gamma}_6|}{2}$$

$$\Psi_9(\gamma^4\gamma^6, ^3\Gamma^3, M=1, \gamma_3) = |\gamma_4\gamma_6|$$

$$\gamma^5\gamma^7$$

$$\boxed{\Delta E = \langle \gamma_5\gamma_7 || \gamma_5\gamma_7 \rangle}$$

$$\Psi_{10}(\gamma^5\gamma^7, ^3\Gamma^3, M=-1, \gamma_3) = |\bar{\gamma}_5\gamma_7|$$

$$\Psi_{11}(\gamma^5\gamma^7, ^3\Gamma^3, M=0, \gamma_3) = \frac{\sqrt{2}|\bar{\gamma}_5\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_5\bar{\gamma}_7|}{2}$$

$$\Psi_{12}(\gamma^5\gamma^7, ^3\Gamma^3, M=1, \gamma_3) = |\gamma_5\gamma_7|$$

$$\gamma^3\gamma^8$$

$$\boxed{\Delta E = \langle \gamma_3\gamma_8 || \gamma_3\gamma_8 \rangle}$$

$$\Psi_2(\gamma^3\gamma^8, ^1\Gamma^2, M=0, \gamma_2) = -\frac{\sqrt{2}|\bar{\gamma}_3\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_3\bar{\gamma}_8|}{2}$$

$$\gamma^4\gamma^7$$

$$\boxed{\Delta E = \langle \gamma_4\gamma_7 || \gamma_4\gamma_7 \rangle}$$

2.11.5 $^1\Gamma^3$

$$\gamma^1 \gamma^3$$

$$\boxed{\Delta E = \langle \gamma_1 \gamma_3 || \gamma_1 \gamma_3 \rangle}$$

$$\Psi_1(\gamma^1 \gamma^3, ^1\Gamma^3, M=0, \gamma_3) = -\frac{\sqrt{2}|\bar{\gamma}_1 \gamma_3|}{2} + \frac{\sqrt{2}|\gamma_1 \bar{\gamma}_3|}{2}$$

$$\gamma^2 \gamma^8$$

$$\boxed{\Delta E = \langle \gamma_2 \gamma_8 || \gamma_2 \gamma_8 \rangle}$$

$$\Psi_2(\gamma^2 \gamma^8, ^1\Gamma^3, M=0, \gamma_3) = -\frac{\sqrt{2}|\bar{\gamma}_2 \gamma_8|}{2} + \frac{\sqrt{2}|\gamma_2 \bar{\gamma}_8|}{2}$$

$$\gamma^4 \gamma^6$$

$$\boxed{\Delta E = \langle \gamma_4 \gamma_6 || \gamma_4 \gamma_6 \rangle}$$

$$\Psi_3(\gamma^4 \gamma^6, ^1\Gamma^3, M=0, \gamma_3) = -\frac{\sqrt{2}|\bar{\gamma}_4 \gamma_6|}{2} + \frac{\sqrt{2}|\gamma_4 \bar{\gamma}_6|}{2}$$

$$\gamma^5 \gamma^7$$

$$\boxed{\Delta E = \langle \gamma_5 \gamma_7 || \gamma_5 \gamma_7 \rangle}$$

$$\Psi_4(\gamma^5 \gamma^7, ^1\Gamma^3, M=0, \gamma_3) = -\frac{\sqrt{2}|\bar{\gamma}_5 \gamma_7|}{2} + \frac{\sqrt{2}|\gamma_5 \bar{\gamma}_7|}{2}$$

2.11.6 $^3\Gamma^4$

$$\gamma^1 \gamma^4$$

$$\boxed{\Delta E = -\langle \gamma_1 \gamma_1 || \gamma_4 \gamma_4 \rangle + \langle \gamma_1 \gamma_4 || \gamma_1 \gamma_4 \rangle}$$

$$\Psi_1(\gamma^1 \gamma^4, ^3\Gamma^4, M=-1, \gamma_4) = |\bar{\gamma}_1 \gamma_4|$$

$$\Psi_2(\gamma^1 \gamma^4, ^3\Gamma^4, M=0, \gamma_4) = \frac{\sqrt{2}|\bar{\gamma}_1 \gamma_4|}{2} + \frac{\sqrt{2}|\gamma_1 \bar{\gamma}_4|}{2}$$

$$\Psi_3(\gamma^1 \gamma^4, ^3\Gamma^4, M=1, \gamma_4) = |\gamma_1 \gamma_4|$$

$$\gamma^2 \gamma^6$$

$$\boxed{\Delta E = -\langle \gamma_2 \gamma_2 || \gamma_6 \gamma_6 \rangle + \langle \gamma_2 \gamma_6 || \gamma_2 \gamma_6 \rangle}$$

$$\Psi_4(\gamma^2 \gamma^6, ^3\Gamma^4, M=-1, \gamma_4) = |\bar{\gamma}_2 \gamma_6|$$

$$\Psi_5(\gamma^2 \gamma^6, ^3\Gamma^4, M=0, \gamma_4) = \frac{\sqrt{2}|\bar{\gamma}_2 \gamma_6|}{2} + \frac{\sqrt{2}|\gamma_2 \bar{\gamma}_6|}{2}$$

$$\Psi_6(\gamma^2 \gamma^6, ^3\Gamma^4, M=1, \gamma_4) = |\gamma_2 \gamma_6|$$

$$\gamma^3 \gamma^7$$

$$\boxed{\Delta E = -\langle \gamma_3 \gamma_3 || \gamma_7 \gamma_7 \rangle + \langle \gamma_3 \gamma_7 || \gamma_3 \gamma_7 \rangle}$$

$$\Psi_7(\gamma^3 \gamma^7, ^3\Gamma^4, M=-1, \gamma_4) = |\bar{\gamma}_3 \gamma_7|$$

$$\Psi_8(\gamma^3 \gamma^7, ^3\Gamma^4, M=0, \gamma_4) = \frac{\sqrt{2}|\bar{\gamma}_3 \gamma_7|}{2} + \frac{\sqrt{2}|\gamma_3 \bar{\gamma}_7|}{2}$$

$$\Psi_9(\gamma^3 \gamma^7, ^3\Gamma^4, M=1, \gamma_4) = |\gamma_3 \gamma_7|$$

$$\gamma^5 \gamma^8$$

$$\boxed{\Delta E = -\langle \gamma_5 \gamma_5 || \gamma_8 \gamma_8 \rangle + \langle \gamma_5 \gamma_8 || \gamma_5 \gamma_8 \rangle}$$

$$\Psi_{10}(\gamma^5 \gamma^8, ^3\Gamma^4, M=-1, \gamma_4) = |\bar{\gamma}_5 \gamma_8|$$

$$\Psi_{11}(\gamma^5 \gamma^8, ^3\Gamma^4, M=0, \gamma_4) = \frac{\sqrt{2}|\bar{\gamma}_5 \gamma_8|}{2} + \frac{\sqrt{2}|\gamma_5 \bar{\gamma}_8|}{2}$$

$$\Psi_{12}(\gamma^5 \gamma^8, ^3\Gamma^4, M=1, \gamma_4) = |\gamma_5 \gamma_8|$$

2.11.7 $^1\Gamma^4$

$$\gamma^1 \gamma^4$$

$$\boxed{\Delta E = \langle \gamma_1 \gamma_1 || \gamma_4 \gamma_4 \rangle + \langle \gamma_1 \gamma_4 || \gamma_1 \gamma_4 \rangle}$$

$$\Psi_1(\gamma^1 \gamma^4, ^1\Gamma^4, M=0, \gamma_4) = -\frac{\sqrt{2}|\bar{\gamma}_1 \gamma_4|}{2} + \frac{\sqrt{2}|\gamma_1 \bar{\gamma}_4|}{2}$$

$$\gamma^2 \gamma^6$$

$$\boxed{\Delta E = \langle \gamma_2 \gamma_2 || \gamma_6 \gamma_6 \rangle + \langle \gamma_2 \gamma_6 || \gamma_2 \gamma_6 \rangle}$$

$$\Psi_2(\gamma^2 \gamma^6, ^1\Gamma^4, M=0, \gamma_4) = -\frac{\sqrt{2}|\bar{\gamma}_2 \gamma_6|}{2} + \frac{\sqrt{2}|\gamma_2 \bar{\gamma}_6|}{2}$$

$$\gamma^3 \gamma^7$$

$$\boxed{\Delta E = \langle \gamma_3 \gamma_3 || \gamma_7 \gamma_7 \rangle + \langle \gamma_3 \gamma_7 || \gamma_3 \gamma_7 \rangle}$$

$$\Psi_3(\gamma^3 \gamma^7, ^1\Gamma^4, M=0, \gamma_4) = -\frac{\sqrt{2}|\bar{\gamma}_3 \gamma_7|}{2} + \frac{\sqrt{2}|\gamma_3 \bar{\gamma}_7|}{2}$$

$$\gamma^5 \gamma^8$$

$$\boxed{\Delta E = \langle \gamma_5 \gamma_5 || \gamma_8 \gamma_8 \rangle + \langle \gamma_5 \gamma_8 || \gamma_5 \gamma_8 \rangle}$$

$$\Psi_4(\gamma^5 \gamma^8, ^1\Gamma^4, M=0, \gamma_4) = -\frac{\sqrt{2}|\bar{\gamma}_5 \gamma_8|}{2} + \frac{\sqrt{2}|\gamma_5 \bar{\gamma}_8|}{2}$$

2.11.8 $^3\Gamma^5$

$$\gamma^1 \gamma^5$$

$$\boxed{\Delta E = -\langle \gamma_1 \gamma_1 || \gamma_5 \gamma_5 \rangle + \langle \gamma_1 \gamma_5 || \gamma_1 \gamma_5 \rangle}$$

$$\Psi_1(\gamma^1 \gamma^5, ^3\Gamma^5, M=-1, \gamma_5) = |\bar{\gamma}_1 \gamma_5|$$

$$\Psi_2(\gamma^1 \gamma^5, ^3\Gamma^5, M=0, \gamma_5) = \frac{\sqrt{2}|\bar{\gamma}_1 \gamma_5|}{2} + \frac{\sqrt{2}|\gamma_1 \bar{\gamma}_5|}{2}$$

$$\Psi_3(\gamma^1 \gamma^5, ^3\Gamma^5, M=1, \gamma_5) = |\gamma_1 \gamma_5|$$

$$\gamma^2 \gamma^7$$

$$\boxed{\Delta E = -\langle \gamma_2 \gamma_2 || \gamma_7 \gamma_7 \rangle + \langle \gamma_2 \gamma_7 || \gamma_2 \gamma_7 \rangle}$$

$$\Psi_4(\gamma^2 \gamma^7, ^3\Gamma^5, M=-1, \gamma_5) = |\bar{\gamma}_2 \gamma_7|$$

$$\Psi_5(\gamma^2 \gamma^7, ^3\Gamma^5, M=0, \gamma_5) = \frac{\sqrt{2}|\bar{\gamma}_2 \gamma_7|}{2} + \frac{\sqrt{2}|\gamma_2 \bar{\gamma}_7|}{2}$$

$$\Psi_6(\gamma^2 \gamma^7, ^3\Gamma^5, M=1, \gamma_5) = |\gamma_2 \gamma_7|$$

$\gamma^3\gamma^6$

$$\Delta E = -\langle \gamma_3 \gamma_3 || \gamma_6 \gamma_6 \rangle + \langle \gamma_3 \gamma_6 || \gamma_3 \gamma_6 \rangle$$

$$\Psi_7(\gamma^3\gamma^6, {}^3\Gamma^5, M=-1, \gamma_5) = |\overline{\gamma_3}\gamma_6|$$

$$\Psi_8(\gamma^3\gamma^6, {}^3\Gamma^5, M=0, \gamma_5) = \frac{\sqrt{2}|\overline{\gamma_3}\gamma_6|}{2} + \frac{\sqrt{2}|\gamma_3\overline{\gamma_6}|}{2}$$

$$\Psi_9(\gamma^3\gamma^6, {}^3\Gamma^5, M=1, \gamma_5) = |\gamma_3\gamma_6|$$

 $\gamma^4\gamma^8$

$$\Delta E = -\langle \gamma_4 \gamma_4 || \gamma_8 \gamma_8 \rangle + \langle \gamma_4 \gamma_8 || \gamma_4 \gamma_8 \rangle$$

$$\Psi_{10}(\gamma^4\gamma^8, {}^3\Gamma^5, M=-1, \gamma_5) = |\overline{\gamma_4}\gamma_8|$$

$$\Psi_{11}(\gamma^4\gamma^8, {}^3\Gamma^5, M=0, \gamma_5) = \frac{\sqrt{2}|\overline{\gamma_4}\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_4\overline{\gamma_8}|}{2}$$

$$\Psi_{12}(\gamma^4\gamma^8, {}^3\Gamma^5, M=1, \gamma_5) = |\gamma_4\gamma_8|$$

2.11.9 ${}^1\Gamma^5$ $\gamma^1\gamma^5$

$$\Delta E = \langle \gamma_1 \gamma_1 || \gamma_5 \gamma_5 \rangle + \langle \gamma_1 \gamma_5 || \gamma_1 \gamma_5 \rangle$$

$$\Psi_1(\gamma^1\gamma^5, {}^1\Gamma^5, M=0, \gamma_5) = -\frac{\sqrt{2}|\overline{\gamma_1}\gamma_5|}{2} + \frac{\sqrt{2}|\gamma_1\overline{\gamma_5}|}{2}$$

 $\gamma^2\gamma^7$

$$\Delta E = \langle \gamma_2 \gamma_2 || \gamma_7 \gamma_7 \rangle + \langle \gamma_2 \gamma_7 || \gamma_2 \gamma_7 \rangle$$

$$\Psi_2(\gamma^2\gamma^7, {}^1\Gamma^5, M=0, \gamma_5) = -\frac{\sqrt{2}|\overline{\gamma_2}\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_2\overline{\gamma_7}|}{2}$$

 $\gamma^3\gamma^6$

$$\Delta E = \langle \gamma_3 \gamma_3 || \gamma_6 \gamma_6 \rangle + \langle \gamma_3 \gamma_6 || \gamma_3 \gamma_6 \rangle$$

$$\Psi_3(\gamma^3\gamma^6, {}^1\Gamma^5, M=0, \gamma_5) = -\frac{\sqrt{2}|\overline{\gamma_3}\gamma_6|}{2} + \frac{\sqrt{2}|\gamma_3\overline{\gamma_6}|}{2}$$

 $\gamma^4\gamma^8$

$$\Delta E = \langle \gamma_4 \gamma_4 || \gamma_8 \gamma_8 \rangle + \langle \gamma_4 \gamma_8 || \gamma_4 \gamma_8 \rangle$$

$$\Psi_4(\gamma^4\gamma^8, {}^1\Gamma^5, M=0, \gamma_5) = -\frac{\sqrt{2}|\overline{\gamma_4}\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_4\overline{\gamma_8}|}{2}$$

2.11.10 ${}^3\Gamma^6$ $\gamma^1\gamma^6$

$$\Delta E = \langle \gamma_1 \gamma_6 || \gamma_1 \gamma_6 \rangle$$

$$\Psi_1(\gamma^1\gamma^6, {}^3\Gamma^6, M=-1, \gamma_6) = |\overline{\gamma_1}\gamma_6|$$

$$\Psi_2(\gamma^1\gamma^6, {}^3\Gamma^6, M=0, \gamma_6) = \frac{\sqrt{2}|\overline{\gamma_1}\gamma_6|}{2} + \frac{\sqrt{2}|\gamma_1\overline{\gamma_6}|}{2}$$

$$\Psi_3(\gamma^1\gamma^6, {}^3\Gamma^6, M=1, \gamma_6) = |\gamma_1\gamma_6|$$

 $\gamma^2\gamma^5$

$$\Delta E = \langle \gamma_2 \gamma_5 || \gamma_2 \gamma_5 \rangle$$

$$\Psi_4(\gamma^2\gamma^5, {}^3\Gamma^6, M=-1, \gamma_6) = |\overline{\gamma_2}\gamma_5|$$

$$\Psi_5(\gamma^2\gamma^5, {}^3\Gamma^6, M=0, \gamma_6) = \frac{\sqrt{2}|\overline{\gamma_2}\gamma_5|}{2} + \frac{\sqrt{2}|\gamma_2\overline{\gamma_5}|}{2}$$

$$\Psi_6(\gamma^2\gamma^5, {}^3\Gamma^6, M=1, \gamma_6) = |\gamma_2\gamma_5|$$

 $\gamma^3\gamma^4$

$$\Delta E = \langle \gamma_3 \gamma_4 || \gamma_3 \gamma_4 \rangle$$

$$\Psi_7(\gamma^3\gamma^4, {}^3\Gamma^6, M=-1, \gamma_6) = |\overline{\gamma_3}\gamma_4|$$

$$\Psi_8(\gamma^3\gamma^4, {}^3\Gamma^6, M=0, \gamma_6) = \frac{\sqrt{2}|\overline{\gamma_3}\gamma_4|}{2} + \frac{\sqrt{2}|\gamma_3\overline{\gamma_4}|}{2}$$

$$\Psi_9(\gamma^3\gamma^4, {}^3\Gamma^6, M=1, \gamma_6) = |\gamma_3\gamma_4|$$

 $\gamma^7\gamma^8$

$$\Delta E = \langle \gamma_7 \gamma_8 || \gamma_7 \gamma_8 \rangle$$

$$\Psi_{10}(\gamma^7\gamma^8, {}^3\Gamma^6, M=-1, \gamma_6) = |\overline{\gamma_7}\gamma_8|$$

$$\Psi_{11}(\gamma^7\gamma^8, {}^3\Gamma^6, M=0, \gamma_6) = \frac{\sqrt{2}|\overline{\gamma_7}\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_7\overline{\gamma_8}|}{2}$$

$$\Psi_{12}(\gamma^7\gamma^8, {}^3\Gamma^6, M=1, \gamma_6) = |\gamma_7\gamma_8|$$

2.11.11 ${}^1\Gamma^6$ $\gamma^1\gamma^6$

$$\Delta E = \langle \gamma_1 \gamma_6 || \gamma_1 \gamma_6 \rangle$$

$$\Psi_1(\gamma^1\gamma^6, {}^1\Gamma^6, M=0, \gamma_6) = -\frac{\sqrt{2}|\overline{\gamma_1}\gamma_6|}{2} + \frac{\sqrt{2}|\gamma_1\overline{\gamma_6}|}{2}$$

 $\gamma^2\gamma^5$

$$\Delta E = \langle \gamma_2 \gamma_5 || \gamma_2 \gamma_5 \rangle$$

$$\Psi_2(\gamma^2\gamma^5, {}^1\Gamma^6, M=0, \gamma_6) = -\frac{\sqrt{2}|\overline{\gamma_2}\gamma_5|}{2} + \frac{\sqrt{2}|\gamma_2\overline{\gamma_5}|}{2}$$

 $\gamma^3\gamma^4$

$$\Delta E = \langle \gamma_3 \gamma_4 || \gamma_3 \gamma_4 \rangle$$

$$\Psi_3(\gamma^3\gamma^4, {}^1\Gamma^6, M=0, \gamma_6) = -\frac{\sqrt{2}|\overline{\gamma_3}\gamma_4|}{2} + \frac{\sqrt{2}|\gamma_3\overline{\gamma_4}|}{2}$$

 $\gamma^7\gamma^8$

$$\Delta E = \langle \gamma_7 \gamma_8 || \gamma_7 \gamma_8 \rangle$$

$$\Psi_4(\gamma^7\gamma^8, {}^1\Gamma^6, M=0, \gamma_6) = -\frac{\sqrt{2}|\overline{\gamma_7}\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_7\overline{\gamma_8}|}{2}$$

2.11.12 ${}^3\Gamma^7$

$$\Psi_3(\gamma^3\gamma^5, {}^1\Gamma^7, M=0, \gamma_7) = -\frac{\sqrt{2}|\gamma_3\gamma_5|}{2} + \frac{\sqrt{2}|\gamma_3\gamma_5|}{2}$$

 $\gamma^1\gamma^7$

$$\boxed{\Delta E = \langle \gamma_1\gamma_7 || \gamma_1\gamma_7 \rangle}$$

 $\gamma^6\gamma^8$

$$\boxed{\Delta E = \langle \gamma_6\gamma_8 || \gamma_6\gamma_8 \rangle}$$

$$\Psi_1(\gamma^1\gamma^7, {}^3\Gamma^7, M=-1, \gamma_7) = |\gamma_1\gamma_7|$$

$$\Psi_2(\gamma^1\gamma^7, {}^3\Gamma^7, M=0, \gamma_7) = \frac{\sqrt{2}|\gamma_1\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_1\gamma_7|}{2}$$

$$\Psi_3(\gamma^1\gamma^7, {}^3\Gamma^7, M=1, \gamma_7) = |\gamma_1\gamma_7|$$

 $\gamma^2\gamma^4$

$$\boxed{\Delta E = \langle \gamma_2\gamma_4 || \gamma_2\gamma_4 \rangle}$$

$$\Psi_4(\gamma^2\gamma^4, {}^3\Gamma^7, M=-1, \gamma_7) = |\gamma_2\gamma_4|$$

$$\Psi_5(\gamma^2\gamma^4, {}^3\Gamma^7, M=0, \gamma_7) = \frac{\sqrt{2}|\gamma_2\gamma_4|}{2} + \frac{\sqrt{2}|\gamma_2\gamma_4|}{2}$$

$$\Psi_6(\gamma^2\gamma^4, {}^3\Gamma^7, M=1, \gamma_7) = |\gamma_2\gamma_4|$$

 $\gamma^3\gamma^5$

$$\boxed{\Delta E = \langle \gamma_3\gamma_5 || \gamma_3\gamma_5 \rangle}$$

$$\Psi_7(\gamma^3\gamma^5, {}^3\Gamma^7, M=-1, \gamma_7) = |\gamma_3\gamma_5|$$

$$\Psi_8(\gamma^3\gamma^5, {}^3\Gamma^7, M=0, \gamma_7) = \frac{\sqrt{2}|\gamma_3\gamma_5|}{2} + \frac{\sqrt{2}|\gamma_3\gamma_5|}{2}$$

$$\Psi_9(\gamma^3\gamma^5, {}^3\Gamma^7, M=1, \gamma_7) = |\gamma_3\gamma_5|$$

 $\gamma^6\gamma^8$

$$\boxed{\Delta E = \langle \gamma_6\gamma_8 || \gamma_6\gamma_8 \rangle}$$

$$\Psi_{10}(\gamma^6\gamma^8, {}^3\Gamma^7, M=-1, \gamma_7) = |\gamma_6\gamma_8|$$

$$\Psi_{11}(\gamma^6\gamma^8, {}^3\Gamma^7, M=0, \gamma_7) = \frac{\sqrt{2}|\gamma_6\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_6\gamma_8|}{2}$$

$$\Psi_{12}(\gamma^6\gamma^8, {}^3\Gamma^7, M=1, \gamma_7) = |\gamma_6\gamma_8|$$

2.11.13 ${}^1\Gamma^7$ $\gamma^1\gamma^7$

$$\boxed{\Delta E = \langle \gamma_1\gamma_7 || \gamma_1\gamma_7 \rangle}$$

$$\Psi_1(\gamma^1\gamma^7, {}^1\Gamma^7, M=0, \gamma_7) = -\frac{\sqrt{2}|\gamma_1\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_1\gamma_7|}{2}$$

 $\gamma^2\gamma^4$

$$\boxed{\Delta E = \langle \gamma_2\gamma_4 || \gamma_2\gamma_4 \rangle}$$

$$\Psi_2(\gamma^2\gamma^4, {}^1\Gamma^7, M=0, \gamma_7) = -\frac{\sqrt{2}|\gamma_2\gamma_4|}{2} + \frac{\sqrt{2}|\gamma_2\gamma_4|}{2}$$

 $\gamma^3\gamma^5$

$$\boxed{\Delta E = \langle \gamma_3\gamma_5 || \gamma_3\gamma_5 \rangle}$$

2.11.14 ${}^3\Gamma^8$ $\gamma^1\gamma^8$

$$\boxed{\Delta E = -\langle \gamma_1\gamma_1 || \gamma_8\gamma_8 \rangle + \langle \gamma_1\gamma_8 || \gamma_1\gamma_8 \rangle}$$

$$\Psi_1(\gamma^1\gamma^8, {}^3\Gamma^8, M=-1, \gamma_8) = |\gamma_1\gamma_8|$$

$$\Psi_2(\gamma^1\gamma^8, {}^3\Gamma^8, M=0, \gamma_8) = \frac{\sqrt{2}|\gamma_1\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_1\gamma_8|}{2}$$

$$\Psi_3(\gamma^1\gamma^8, {}^3\Gamma^8, M=1, \gamma_8) = |\gamma_1\gamma_8|$$

 $\gamma^4\gamma^5$

$$\boxed{\Delta E = -\langle \gamma_4\gamma_4 || \gamma_5\gamma_5 \rangle + \langle \gamma_4\gamma_5 || \gamma_4\gamma_5 \rangle}$$

$$\Psi_4(\gamma^4\gamma^5, {}^3\Gamma^8, M=-1, \gamma_8) = |\gamma_4\gamma_5|$$

$$\Psi_5(\gamma^4\gamma^5, {}^3\Gamma^8, M=0, \gamma_8) = \frac{\sqrt{2}|\gamma_4\gamma_5|}{2} + \frac{\sqrt{2}|\gamma_4\gamma_5|}{2}$$

$$\Psi_6(\gamma^4\gamma^5, {}^3\Gamma^8, M=1, \gamma_8) = |\gamma_4\gamma_5|$$

2.11.15 ${}^1\Gamma^8$ $\gamma^1\gamma^8$

$$\boxed{\Delta E = \langle \gamma_1\gamma_1 || \gamma_8\gamma_8 \rangle + \langle \gamma_1\gamma_8 || \gamma_1\gamma_8 \rangle}$$

$$\Psi_1(\gamma^1\gamma^8, {}^1\Gamma^8, M=0, \gamma_8) = -\frac{\sqrt{2}|\gamma_1\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_1\gamma_8|}{2}$$

 $(\gamma^2)^2$

$$\boxed{\Delta E = \langle \gamma_2\gamma_2 || \gamma_2\gamma_2 \rangle}$$

$$\Psi_2((\gamma^2)^2, {}^1\Gamma^8, M=0, \gamma_8) = -|\gamma_2\gamma_2|$$

 $(\gamma^3)^2$

$$\boxed{\Delta E = \langle \gamma_3\gamma_3 || \gamma_3\gamma_3 \rangle}$$

$$\Psi_3((\gamma^3)^2, {}^1\Gamma^8, M=0, \gamma_8) = -|\gamma_3\gamma_3|$$

 $\gamma^4\gamma^5$

$$\boxed{\Delta E = \langle \gamma_4\gamma_4 || \gamma_5\gamma_5 \rangle + \langle \gamma_4\gamma_5 || \gamma_4\gamma_5 \rangle}$$

$$\Psi_4(\gamma^4\gamma^5, {}^1\Gamma^8, M=0, \gamma_8) = -\frac{\sqrt{2}|\bar{\gamma}_4\gamma_5|}{2} + \frac{\sqrt{2}|\gamma_4\bar{\gamma}_5|}{2}$$

$$\boxed{\Delta E = \langle \gamma_6\gamma_6 || \gamma_6\gamma_6 \rangle}$$

$$\Psi_5((\gamma^6)^2, {}^1\Gamma^8, M=0, \gamma_8) = -|\bar{\gamma}_6\gamma_6|$$

$$\boxed{\Delta E = \langle \gamma_7\gamma_7 || \gamma_7\gamma_7 \rangle}$$

$$\Psi_6((\gamma^7)^2, {}^1\Gamma^8, M=0, \gamma_8) = -|\bar{\gamma}_7\gamma_7|$$

$$\boxed{\Delta E = -\langle \gamma_2\gamma_2 || \gamma_3\gamma_3 \rangle + \langle \gamma_2\gamma_3 || \gamma_2\gamma_3 \rangle}$$

$$\Psi_1(\gamma^2\gamma^3, {}^3\Gamma^1, M=-1, \gamma_1) = |\bar{\gamma}_2\gamma_3|$$

$$\Psi_2(\gamma^2\gamma^3, {}^3\Gamma^1, M=0, \gamma_1) = \frac{\sqrt{2}|\bar{\gamma}_2\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_2\bar{\gamma}_3|}{2}$$

$$\Psi_3(\gamma^2\gamma^3, {}^3\Gamma^1, M=1, \gamma_1) = |\gamma_2\gamma_3|$$

$$\gamma^6\gamma^7$$

$$\boxed{\Delta E = -\langle \gamma_6\gamma_6 || \gamma_7\gamma_7 \rangle + \langle \gamma_6\gamma_7 || \gamma_6\gamma_7 \rangle}$$

2.11.16 ${}^3\Gamma^1$

$$\gamma^2\gamma^3$$

$$\Psi_4(\gamma^6\gamma^7, {}^3\Gamma^1, M=-1, \gamma_1) = |\bar{\gamma}_6\gamma_7|$$

$$\Psi_5(\gamma^6\gamma^7, {}^3\Gamma^1, M=0, \gamma_1) = \frac{\sqrt{2}|\bar{\gamma}_6\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_6\bar{\gamma}_7|}{2}$$

$$\Psi_6(\gamma^6\gamma^7, {}^3\Gamma^1, M=1, \gamma_1) = |\gamma_6\gamma_7|$$

2.12 Group D_4

Component labels

$$A_1 : \{\alpha\} \longrightarrow A_2 : \{\beta\} \longrightarrow B_2 : \{\zeta\} \longrightarrow B_1 : \{\gamma\} \longrightarrow E : \{\eta, \mu\}$$

2.12.1 1A_1

$$a_1^2$$

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_1(a_1^2, {}^1A_1, M=0, \alpha) = -|\bar{\alpha}\alpha|$$

$$\boxed{\Delta E = \langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_5(e^2, {}^1A_1, M=0, \alpha) = -\frac{\sqrt{2}|\bar{\eta}\eta|}{2} - \frac{\sqrt{2}|\bar{\mu}\mu|}{2}$$

2.12.2 3A_2

$$a_1a_2$$

$$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_2(a_2^2, {}^1A_1, M=0, \alpha) = -|\bar{\beta}\beta|$$

$$\Psi_1(a_1a_2, {}^3A_2, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$b_2^2$$

$$\boxed{\Delta E = \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\Psi_3(b_2^2, {}^1A_1, M=0, \alpha) = -|\bar{\zeta}\zeta|$$

$$\Psi_2(a_1a_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(a_1a_2, {}^3A_2, M=1, \beta) = |\alpha\beta|$$

$$b_1b_2$$

$$\boxed{\Delta E = \langle \zeta\gamma || \zeta\gamma \rangle - \langle \zeta\zeta || \gamma\gamma \rangle}$$

$$\Psi_4(b_1b_2, {}^3A_2, M=-1, \beta) = |\bar{\zeta}\bar{\gamma}|$$

$$\Psi_5(b_1b_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

$$\Psi_6(b_1b_2, {}^3A_2, M=1, \beta) = |\zeta\gamma|$$

$$\boxed{\Delta E = \langle \gamma\gamma || \gamma\gamma \rangle}$$

$$e^2$$

$$e^2$$

2.12.5 1B_2

$$\Delta E = \langle \mu\eta || \mu\eta \rangle - \langle \mu\mu || \eta\eta \rangle$$

$$\Psi_7(e^2, ^3A_2, M=-1, \beta) = -|\overline{\eta}\mu|$$

$$\Psi_8(e^2, ^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\overline{\eta}\mu|}{2} + \frac{\sqrt{2}|\overline{\mu}\eta|}{2}$$

$$\Psi_9(e^2, ^3A_2, M=1, \beta) = -|\eta\mu|$$

a₁b₂

$$\boxed{\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1b_2, ^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\overline{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\overline{\zeta}|}{2}$$

a₂b₁

$$\boxed{\Delta E = \langle \beta\beta || \gamma\gamma \rangle + \langle \beta\gamma || \beta\gamma \rangle}$$

2.12.3 1A_2

a₁a₂

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a_1a_2, ^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\overline{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\overline{\beta}|}{2}$$

b₁b₂

$$\boxed{\Delta E = \langle \zeta\gamma || \zeta\gamma \rangle + \langle \zeta\zeta || \gamma\gamma \rangle}$$

$$\Psi_2(b_1b_2, ^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\overline{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\overline{\gamma}|}{2}$$

2.12.4 3B_2

a₁b₂

$$\boxed{\Delta E = -\langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1b_2, ^3B_2, M=-1, \zeta) = |\overline{\alpha}\overline{\zeta}|$$

$$\Psi_2(a_1b_2, ^3B_2, M=0, \zeta) = \frac{\sqrt{2}|\overline{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\overline{\zeta}|}{2}$$

$$\Psi_3(a_1b_2, ^3B_2, M=1, \zeta) = |\alpha\zeta|$$

a₂b₁

$$\boxed{\Delta E = -\langle \beta\beta || \gamma\gamma \rangle + \langle \beta\gamma || \beta\gamma \rangle}$$

$$\Psi_4(a_2b_1, ^3B_2, M=-1, \zeta) = |\overline{\beta}\overline{\gamma}|$$

$$\Psi_5(a_2b_1, ^3B_2, M=0, \zeta) = \frac{\sqrt{2}|\overline{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\overline{\gamma}|}{2}$$

$$\Psi_6(a_2b_1, ^3B_2, M=1, \zeta) = |\beta\gamma|$$

2.12.6 3B_1

a₁b₁

$$\boxed{\Delta E = -\langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(a_1b_1, ^3B_1, M=-1, \gamma) = |\overline{\alpha}\overline{\gamma}|$$

$$\Psi_2(a_1b_1, ^3B_1, M=0, \gamma) = \frac{\sqrt{2}|\overline{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\overline{\gamma}|}{2}$$

$$\Psi_3(a_1b_1, ^3B_1, M=1, \gamma) = |\alpha\gamma|$$

a₂b₂

$$\boxed{\Delta E = -\langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle}$$

$$\Psi_4(a_2b_2, ^3B_1, M=-1, \gamma) = |\overline{\beta}\overline{\zeta}|$$

$$\Psi_5(a_2b_2, ^3B_1, M=0, \gamma) = \frac{\sqrt{2}|\overline{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\overline{\zeta}|}{2}$$

$$\Psi_6(a_2b_2, ^3B_1, M=1, \gamma) = |\beta\zeta|$$

2.12.7 1B_1

a₁b₁

$$\boxed{\Delta E = \langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(a_1b_1, ^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\overline{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\overline{\gamma}|}{2}$$

a₂b₂

$$\boxed{\Delta E = \langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle}$$

$$\Psi_2(a_2 b_2, {}^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\beta\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

*e*²

$$\boxed{\Delta E = -\langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_3(e^2, {}^1B_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\eta}\eta|}{2} - \frac{\sqrt{2}|\bar{\mu}\mu|}{2}$$

2.12.8 3E

*a*₁*e*

$$\boxed{\Delta E = -\langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle}$$

$$\Psi_1(a_1 e, {}^3E, M=-1, \eta) = |\bar{\alpha}\eta|$$

$$\Psi_2(a_1 e, {}^3E, M=-1, \mu) = |\bar{\alpha}\mu|$$

$$\Psi_3(a_1 e, {}^3E, M=0, \eta) = \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_4(a_1 e, {}^3E, M=0, \mu) = \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_5(a_1 e, {}^3E, M=1, \eta) = |\alpha\eta|$$

$$\Psi_6(a_1 e, {}^3E, M=1, \mu) = |\alpha\mu|$$

*a*₂*e*

$$\boxed{\Delta E = -\langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle}$$

$$\Psi_7(a_2 e, {}^3E, M=-1, \mu) = -|\bar{\beta}\bar{\eta}|$$

$$\Psi_8(a_2 e, {}^3E, M=-1, \eta) = |\bar{\beta}\mu|$$

$$\Psi_9(a_2 e, {}^3E, M=0, \mu) = -\frac{\sqrt{2}|\bar{\beta}\eta|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_{10}(a_2 e, {}^3E, M=0, \eta) = \frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_{11}(a_2 e, {}^3E, M=1, \mu) = -|\beta\eta|$$

$$\Psi_{12}(a_2 e, {}^3E, M=1, \eta) = |\beta\mu|$$

*b*₂*e*

$$\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle - \langle \zeta\zeta || \mu\mu \rangle}$$

$$\Psi_{13}(b_2 e, {}^3E, M=-1, \mu) = |\bar{\zeta}\bar{\eta}|$$

$$\Psi_{14}(b_2 e, {}^3E, M=-1, \eta) = |\bar{\zeta}\mu|$$

$$\Psi_{15}(b_2 e, {}^3E, M=0, \mu) = \frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}$$

$$\Psi_{16}(b_2 e, {}^3E, M=0, \eta) = \frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$\Psi_{17}(b_2 e, {}^3E, M=1, \mu) = |\zeta\eta|$$

$$\Psi_{18}(b_2 e, {}^3E, M=1, \eta) = |\zeta\mu|$$

*b*₁*e*

$$\boxed{\Delta E = -\langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle}$$

$$\Psi_{19}(b_1 e, {}^3E, M=-1, \eta) = |\bar{\gamma}\eta|$$

$$\Psi_{20}(b_1 e, {}^3E, M=-1, \mu) = -|\bar{\gamma}\mu|$$

$$\Psi_{21}(b_1 e, {}^3E, M=0, \eta) = \frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

$$\Psi_{22}(b_1 e, {}^3E, M=0, \mu) = -\frac{\sqrt{2}|\bar{\gamma}\mu|}{2} - \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}$$

$$\Psi_{23}(b_1 e, {}^3E, M=1, \eta) = |\gamma\eta|$$

$$\Psi_{24}(b_1 e, {}^3E, M=1, \mu) = -|\gamma\mu|$$

2.12.9 1E

*a*₁*e*

$$\boxed{\Delta E = \langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle}$$

$$\Psi_1(a_1 e, {}^1E, M=0, \eta) = -\frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_2(a_1 e, {}^1E, M=0, \mu) = -\frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

*a*₂*e*

$$\boxed{\Delta E = \langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle}$$

$$\Psi_3(a_2 e, {}^1E, M=0, \mu) = \frac{\sqrt{2}|\bar{\beta}\eta|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_4(a_2 e, {}^1E, M=0, \eta) = -\frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

*b*₂*e*

$$\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle + \langle \zeta\zeta || \mu\mu \rangle}$$

$$\Psi_5(b_2 e, {}^1E, M=0, \mu) = -\frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}$$

$$\Psi_6(b_2 e, {}^1E, M=0, \eta) = -\frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

*b*₁*e*

$$\boxed{\Delta E = \langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle}$$

$$\Psi_7(b_1 e, {}^1E, M=0, \eta) = -\frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

$$\Psi_8(b_1 e, {}^1E, M=0, \mu) = \frac{\sqrt{2}|\bar{\gamma}\mu|}{2} - \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}$$

2.13 Group C_{4v}

Component labels

$$A_1 : \{\alpha\} \longrightarrow A_2 : \{\beta\} \longrightarrow B_2 : \{\zeta\} \longrightarrow B_1 : \{\gamma\} \longrightarrow E : \{\eta, \mu\}$$

e^2

2.13.1 1A_1

$$\boxed{\Delta E = \langle \mu\eta | \mu\eta \rangle - \langle \mu\mu | \eta\eta \rangle}$$

a_1^2

$$\boxed{\Delta E = \langle \alpha\alpha | \alpha\alpha \rangle}$$

$$\Psi_7(e^2, {}^3A_2, M=-1, \beta) = -|\bar{\eta}\mu|$$

$$\Psi_8(e^2, {}^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} + \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

$$\Psi_9(e^2, {}^3A_2, M=1, \beta) = -|\eta\mu|$$

$$\Psi_1(a_1^2, {}^1A_1, M=0, \alpha) = -|\bar{\alpha}\alpha|$$

a_2^2

$$\boxed{\Delta E = \langle \beta\beta | \beta\beta \rangle}$$

2.13.3 1A_2

a_1a_2

$$\boxed{\Delta E = \langle \alpha\alpha | \beta\beta \rangle + \langle \alpha\beta | \alpha\beta \rangle}$$

$$\Psi_2(a_2^2, {}^1A_1, M=0, \alpha) = -|\bar{\beta}\beta|$$

b_2^2

$$\boxed{\Delta E = \langle \zeta\zeta | \zeta\zeta \rangle}$$

$$\Psi_1(a_1a_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

b_1^2

$$\boxed{\Delta E = \langle \gamma\gamma | \gamma\gamma \rangle}$$

b_1b_2

$$\boxed{\Delta E = \langle \zeta\gamma | \zeta\gamma \rangle + \langle \zeta\zeta | \gamma\gamma \rangle}$$

$$\Psi_4(b_1^2, {}^1A_1, M=0, \alpha) = -|\bar{\gamma}\gamma|$$

e^2

$$\boxed{\Delta E = \langle \mu\mu | \eta\eta \rangle + \langle \mu\mu | \mu\mu \rangle}$$

$$\Psi_2(b_1b_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

$$\Psi_5(e^2, {}^1A_1, M=0, \alpha) = -\frac{\sqrt{2}|\bar{\eta}\eta|}{2} - \frac{\sqrt{2}|\bar{\mu}\mu|}{2}$$

2.13.4 3B_2

a_1b_2

$$\boxed{\Delta E = -\langle \alpha\alpha | \zeta\zeta \rangle + \langle \alpha\zeta | \alpha\zeta \rangle}$$

a_1a_2

$$\boxed{\Delta E = -\langle \alpha\alpha | \beta\beta \rangle + \langle \alpha\beta | \alpha\beta \rangle}$$

$$\Psi_1(a_1b_2, {}^3B_2, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}|$$

$$\Psi_1(a_1a_2, {}^3A_2, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$\Psi_2(a_1b_2, {}^3B_2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_3(a_1b_2, {}^3B_2, M=1, \zeta) = |\alpha\zeta|$$

a_2b_1

$$\boxed{\Delta E = -\langle \beta\beta | \gamma\gamma \rangle + \langle \beta\gamma | \beta\gamma \rangle}$$

$$\Psi_4(a_2b_1, {}^3B_2, M=-1, \zeta) = |\bar{\beta}\bar{\gamma}|$$

$$\Psi_2(a_1a_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(a_1a_2, {}^3A_2, M=1, \beta) = |\alpha\beta|$$

b_1b_2

$$\boxed{\Delta E = \langle \zeta\gamma | \zeta\gamma \rangle - \langle \zeta\zeta | \gamma\gamma \rangle}$$

a_2b_1

$$\Psi_4(b_1b_2, {}^3A_2, M=-1, \beta) = |\bar{\zeta}\bar{\gamma}|$$

$$\Psi_5(a_2b_1, {}^3B_2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_6(a_2b_1, {}^3B_2, M=1, \zeta) = |\beta\gamma|$$

2.13.5 1B_2

$$\Psi_2(a_2 b_2, ^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

 $a_1 b_2$

$$\boxed{\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1 b_2, ^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

 $a_2 b_1$

$$\boxed{\Delta E = \langle \beta\beta || \gamma\gamma \rangle + \langle \beta\gamma || \beta\gamma \rangle}$$

$$\Psi_2(a_2 b_1, ^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

 e^2

$$\boxed{\Delta E = \langle \mu\eta || \mu\eta \rangle + \langle \mu\mu || \eta\eta \rangle}$$

$$\Psi_3(e^2, ^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} - \frac{\sqrt{2}|\mu\bar{\eta}|}{2}$$

2.13.6 3B_1 $a_1 b_1$

$$\boxed{\Delta E = -\langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(a_1 b_1, ^3B_1, M=-1, \gamma) = |\bar{\alpha}\bar{\gamma}|$$

$$\Psi_2(a_1 b_1, ^3B_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(a_1 b_1, ^3B_1, M=1, \gamma) = |\alpha\gamma|$$

 $a_2 b_2$

$$\boxed{\Delta E = -\langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle}$$

$$\Psi_4(a_2 b_2, ^3B_1, M=-1, \gamma) = |\bar{\beta}\bar{\zeta}|$$

$$\Psi_5(a_2 b_2, ^3B_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

$$\Psi_6(a_2 b_2, ^3B_1, M=1, \gamma) = |\beta\zeta|$$

2.13.7 1B_1 $a_1 b_1$

$$\boxed{\Delta E = \langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(a_1 b_1, ^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

 $a_2 b_2$

$$\boxed{\Delta E = \langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle}$$

 e^2

$$\boxed{\Delta E = -\langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_3(e^2, ^1B_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\eta}\eta|}{2} - \frac{\sqrt{2}|\mu\bar{\mu}|}{2}$$

2.13.8 3E $a_1 e$

$$\boxed{\Delta E = -\langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle}$$

$$\Psi_1(a_1 e, ^3E, M=-1, \eta) = |\bar{\alpha}\bar{\eta}|$$

$$\Psi_2(a_1 e, ^3E, M=-1, \mu) = |\bar{\alpha}\bar{\mu}|$$

$$\Psi_3(a_1 e, ^3E, M=0, \eta) = \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_4(a_1 e, ^3E, M=0, \mu) = \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_5(a_1 e, ^3E, M=1, \eta) = |\alpha\eta|$$

$$\Psi_6(a_1 e, ^3E, M=1, \mu) = |\alpha\mu|$$

 $a_2 e$

$$\boxed{\Delta E = -\langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle}$$

$$\Psi_7(a_2 e, ^3E, M=-1, \mu) = -|\bar{\beta}\bar{\eta}|$$

$$\Psi_8(a_2 e, ^3E, M=-1, \eta) = |\bar{\beta}\bar{\mu}|$$

$$\Psi_9(a_2 e, ^3E, M=0, \mu) = -\frac{\sqrt{2}|\bar{\beta}\eta|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_{10}(a_2 e, ^3E, M=0, \eta) = \frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_{11}(a_2 e, ^3E, M=1, \mu) = -|\beta\eta|$$

$$\Psi_{12}(a_2 e, ^3E, M=1, \eta) = |\beta\mu|$$

 $b_2 e$

$$\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle - \langle \zeta\zeta || \mu\mu \rangle}$$

$$\Psi_{13}(b_2 e, ^3E, M=-1, \mu) = |\bar{\zeta}\bar{\eta}|$$

$$\Psi_{14}(b_2 e, ^3E, M=-1, \eta) = |\bar{\zeta}\bar{\mu}|$$

$$\Psi_{15}(b_2 e, ^3E, M=0, \mu) = \frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}$$

$$\Psi_{16}(b_2 e, ^3E, M=0, \eta) = \frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$\Psi_{17}(b_2 e, ^3E, M=1, \mu) = |\zeta\eta|$$

$$\Psi_{18}(b_2 e, ^3E, M=1, \eta) = |\zeta\mu|$$

 $b_1 e$

$$\boxed{\Delta E = -\langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle}$$

$$\Psi_{19}(b_1 e, ^3E, M=-1, \eta) = |\bar{\gamma}\bar{\eta}|$$

$$\begin{aligned}
\Psi_{20}(b_1e, {}^3E, M=-1, \mu) &= -|\bar{\gamma}\bar{\mu}| \\
\Psi_{21}(b_1e, {}^3E, M=0, \eta) &= \frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2} \\
\Psi_{22}(b_1e, {}^3E, M=0, \mu) &= -\frac{\sqrt{2}|\bar{\gamma}\mu|}{2} - \frac{\sqrt{2}|\gamma\bar{\mu}|}{2} \\
\Psi_{23}(b_1e, {}^3E, M=1, \eta) &= |\gamma\eta| \\
\Psi_{24}(b_1e, {}^3E, M=1, \mu) &= -|\gamma\mu|
\end{aligned}$$

$$\begin{aligned}
\Psi_3(a_2e, {}^1E, M=0, \mu) &= \frac{\sqrt{2}|\bar{\beta}\eta|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2} \\
\Psi_4(a_2e, {}^1E, M=0, \eta) &= -\frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2} \\
&\quad b_2e \\
\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle + \langle \zeta\zeta || \mu\mu \rangle}
\end{aligned}$$

$$\begin{aligned}
\mathbf{2.13.9} \quad {}^1E \\
a_1e \\
\boxed{\Delta E = \langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle} \\
\Psi_1(a_1e, {}^1E, M=0, \eta) &= -\frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2} \\
\Psi_2(a_1e, {}^1E, M=0, \mu) &= -\frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2} \\
&\quad a_2e \\
\boxed{\Delta E = \langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle} \\
\Psi_5(b_2e, {}^1E, M=0, \mu) &= -\frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2} \\
\Psi_6(b_2e, {}^1E, M=0, \eta) &= -\frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2} \\
&\quad b_1e \\
\boxed{\Delta E = \langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle} \\
\Psi_7(b_1e, {}^1E, M=0, \eta) &= -\frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2} \\
\Psi_8(b_1e, {}^1E, M=0, \mu) &= \frac{\sqrt{2}|\bar{\gamma}\mu|}{2} - \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}
\end{aligned}$$

2.14 Group D_{2d}

Component labels

$$A_1 : \{\alpha\} \longrightarrow B_1 : \{\gamma\} \longrightarrow A_2 : \{\beta\} \longrightarrow B_2 : \{\zeta\} \longrightarrow E : \{\eta, \mu\}$$

$$\begin{aligned}
\mathbf{2.14.1} \quad {}^1A_1 \\
a_1^2 \\
\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle} \\
\Psi_1(a_1^2, {}^1A_1, M=0, \alpha) &= -|\bar{\alpha}\alpha| \\
&\quad b_1^2 \\
&\quad \boxed{\Delta E = \langle \gamma\gamma || \gamma\gamma \rangle} \\
\Psi_2(b_1^2, {}^1A_1, M=0, \alpha) &= -|\bar{\gamma}\gamma| \\
&\quad a_2^2 \\
&\quad \boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle} \\
\Psi_3(a_2^2, {}^1A_1, M=0, \alpha) &= -|\bar{\beta}\beta| \\
&\quad b_2^2 \\
&\quad \boxed{\Delta E = \langle \zeta\zeta || \zeta\zeta \rangle} \\
\Psi_4(b_2^2, {}^1A_1, M=0, \alpha) &= -|\bar{\zeta}\zeta|
\end{aligned}$$

$$\begin{aligned}
&\quad e^2 \\
&\quad \boxed{\Delta E = \langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle} \\
\Psi_5(e^2, {}^1A_1, M=0, \alpha) &= -\frac{\sqrt{2}|\bar{\eta}\eta|}{2} - \frac{\sqrt{2}|\bar{\mu}\mu|}{2} \\
&\quad \mathbf{2.14.2} \quad {}^3B_1 \\
&\quad a_1b_1 \\
&\quad \boxed{\Delta E = -\langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle} \\
&\quad \Psi_1(a_1b_1, {}^3B_1, M=-1, \gamma) = |\bar{\alpha}\gamma| \\
&\quad \Psi_2(a_1b_1, {}^3B_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2} \\
&\quad \Psi_3(a_1b_1, {}^3B_1, M=1, \gamma) = |\alpha\gamma| \\
&\quad a_2b_2 \\
&\quad \boxed{\Delta E = -\langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle} \\
&\quad \Psi_4(a_2b_2, {}^3B_1, M=-1, \gamma) = |\bar{\beta}\zeta| \\
&\quad \Psi_5(a_2b_2, {}^3B_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2} \\
&\quad \Psi_6(a_2b_2, {}^3B_1, M=1, \gamma) = |\beta\zeta|
\end{aligned}$$

2.14.5 1A_2 **2.14.3** 1B_1 $a_1 b_1$

$$\boxed{\Delta E = \langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(a_1 b_1, ^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

 $a_2 b_2$

$$\boxed{\Delta E = \langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle}$$

$$\Psi_2(a_2 b_2, ^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

 e^2

$$\boxed{\Delta E = \langle \mu\eta || \mu\eta \rangle + \langle \mu\mu || \eta\eta \rangle}$$

$$\Psi_3(e^2, ^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} - \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

2.14.4 3A_2 $a_1 a_2$

$$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a_1 a_2, ^3A_2, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$\Psi_2(a_1 a_2, ^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(a_1 a_2, ^3A_2, M=1, \beta) = |\alpha\beta|$$

 $b_1 b_2$

$$\boxed{\Delta E = -\langle \gamma\gamma || \zeta\zeta \rangle + \langle \gamma\zeta || \gamma\zeta \rangle}$$

$$\Psi_4(b_1 b_2, ^3A_2, M=-1, \beta) = |\bar{\gamma}\bar{\zeta}|$$

$$\Psi_5(b_1 b_2, ^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\gamma\bar{\zeta}|}{2}$$

$$\Psi_6(b_1 b_2, ^3A_2, M=1, \beta) = |\gamma\zeta|$$

 e^2

$$\boxed{\Delta E = \langle \mu\eta || \mu\eta \rangle - \langle \mu\mu || \eta\eta \rangle}$$

$$\Psi_7(e^2, ^3A_2, M=-1, \beta) = -|\bar{\eta}\mu|$$

$$\Psi_8(e^2, ^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} + \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

$$\Psi_9(e^2, ^3A_2, M=1, \beta) = -|\eta\mu|$$

 $a_1 a_2$

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a_1 a_2, ^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

 $b_1 b_2$

$$\boxed{\Delta E = \langle \gamma\gamma || \zeta\zeta \rangle + \langle \gamma\zeta || \gamma\zeta \rangle}$$

$$\Psi_2(b_1 b_2, ^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\gamma\bar{\zeta}|}{2}$$

2.14.6 3B_2 $a_1 b_2$

$$\boxed{\Delta E = -\langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1 b_2, ^3B_2, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}|$$

$$\Psi_2(a_1 b_2, ^3B_2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_3(a_1 b_2, ^3B_2, M=1, \zeta) = |\alpha\zeta|$$

 $a_2 b_1$

$$\boxed{\Delta E = \langle \gamma\beta || \gamma\beta \rangle - \langle \gamma\gamma || \beta\beta \rangle}$$

$$\Psi_4(a_2 b_1, ^3B_2, M=-1, \zeta) = |\bar{\gamma}\bar{\beta}|$$

$$\Psi_5(a_2 b_1, ^3B_2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

$$\Psi_6(a_2 b_1, ^3B_2, M=1, \zeta) = |\gamma\beta|$$

2.14.7 1B_2 $a_1 b_2$

$$\boxed{\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1 b_2, ^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

 $a_2 b_1$

$$\boxed{\Delta E = \langle \gamma\beta || \gamma\beta \rangle + \langle \gamma\gamma || \beta\beta \rangle}$$

$$\Psi_2(a_2 b_1, ^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

 e^2

$$\boxed{\Delta E = -\langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_3(e^2, ^1B_2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\eta}\mu|}{2} - \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

2.14.8 3E *a₁e*

$$\boxed{\Delta E = -\langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle}$$

$$\Psi_1(a_1e, ^3E, M=-1, \eta) = |\overline{\alpha\eta}|$$

$$\Psi_2(a_1e, ^3E, M=-1, \mu) = |\overline{\alpha\mu}|$$

$$\Psi_3(a_1e, ^3E, M=0, \eta) = \frac{\sqrt{2}|\overline{\alpha\eta}|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_4(a_1e, ^3E, M=0, \mu) = \frac{\sqrt{2}|\overline{\alpha\mu}|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_5(a_1e, ^3E, M=1, \eta) = |\alpha\eta|$$

$$\Psi_6(a_1e, ^3E, M=1, \mu) = |\alpha\mu|$$

b₁e

$$\boxed{\Delta E = -\langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle}$$

$$\Psi_7(b_1e, ^3E, M=-1, \mu) = |\overline{\gamma\eta}|$$

$$\Psi_8(b_1e, ^3E, M=-1, \eta) = |\overline{\gamma\mu}|$$

$$\Psi_9(b_1e, ^3E, M=0, \mu) = \frac{\sqrt{2}|\overline{\gamma\eta}|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

$$\Psi_{10}(b_1e, ^3E, M=0, \eta) = \frac{\sqrt{2}|\overline{\gamma\mu}|}{2} + \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}$$

$$\Psi_{11}(b_1e, ^3E, M=1, \mu) = |\gamma\eta|$$

$$\Psi_{12}(b_1e, ^3E, M=1, \eta) = |\gamma\mu|$$

a₂e

$$\boxed{\Delta E = -\langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle}$$

$$\Psi_{13}(a_2e, ^3E, M=-1, \mu) = -|\overline{\beta\eta}|$$

$$\Psi_{14}(a_2e, ^3E, M=-1, \eta) = |\overline{\beta\mu}|$$

$$\Psi_{15}(a_2e, ^3E, M=0, \mu) = -\frac{\sqrt{2}|\overline{\beta\eta}|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_{16}(a_2e, ^3E, M=0, \eta) = \frac{\sqrt{2}|\overline{\beta\mu}|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_{17}(a_2e, ^3E, M=1, \mu) = -|\beta\eta|$$

$$\Psi_{18}(a_2e, ^3E, M=1, \eta) = |\beta\mu|$$

b₂e

$$\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle - \langle \zeta\zeta || \mu\mu \rangle}$$

$$\Psi_{19}(b_2e, ^3E, M=-1, \eta) = |\overline{\zeta\eta}|$$

$$\Psi_{20}(b_2e, ^3E, M=-1, \mu) = -|\overline{\zeta\mu}|$$

$$\Psi_{21}(b_2e, ^3E, M=0, \eta) = \frac{\sqrt{2}|\overline{\zeta\eta}|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}$$

$$\Psi_{22}(b_2e, ^3E, M=0, \mu) = -\frac{\sqrt{2}|\overline{\zeta\mu}|}{2} - \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$\Psi_{23}(b_2e, ^3E, M=1, \eta) = |\zeta\eta|$$

$$\Psi_{24}(b_2e, ^3E, M=1, \mu) = -|\zeta\mu|$$

2.14.9 1E *a₁e*

$$\boxed{\Delta E = \langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle}$$

$$\Psi_1(a_1e, ^1E, M=0, \eta) = -\frac{\sqrt{2}|\overline{\alpha\eta}|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_2(a_1e, ^1E, M=0, \mu) = -\frac{\sqrt{2}|\overline{\alpha\mu}|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

b₁e

$$\boxed{\Delta E = \langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle}$$

$$\Psi_3(b_1e, ^1E, M=0, \mu) = -\frac{\sqrt{2}|\overline{\gamma\eta}|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

$$\Psi_4(b_1e, ^1E, M=0, \eta) = -\frac{\sqrt{2}|\overline{\gamma\mu}|}{2} + \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}$$

a₂e

$$\boxed{\Delta E = \langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle}$$

$$\Psi_5(a_2e, ^1E, M=0, \mu) = \frac{\sqrt{2}|\overline{\beta\eta}|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_6(a_2e, ^1E, M=0, \eta) = -\frac{\sqrt{2}|\overline{\beta\mu}|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

b₂e

$$\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle + \langle \zeta\zeta || \mu\mu \rangle}$$

$$\Psi_7(b_2e, ^1E, M=0, \eta) = -\frac{\sqrt{2}|\overline{\zeta\eta}|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}$$

$$\Psi_8(b_2e, ^1E, M=0, \mu) = \frac{\sqrt{2}|\overline{\zeta\mu}|}{2} - \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

2.15 Group D_{4h} Component labels

$$A_{1g} : \{\alpha_g\} \longrightarrow A_{2g} : \{\beta_g\} \longrightarrow B_{2g} : \{\zeta_g\} \longrightarrow A_{2u} : \{\beta_u\} \longrightarrow B_{2u} : \{\zeta_u\} \longrightarrow B_{1u} : \{\gamma_u\} \longrightarrow \\ A_{1u} : \{\alpha_u\} \longrightarrow B_{1g} : \{\gamma_g\} \longrightarrow E_u : \{\eta_u, \mu_u\} \longrightarrow E_g : \{\eta_g, \mu_g\}$$

	2.15.2	$^3A_{2g}$
2.15.1	$^1A_{1g}$	
	a_{1g}^2	$\Delta E = -\langle \alpha_g \alpha_g \beta_g \beta_g \rangle + \langle \alpha_g \beta_g \alpha_g \beta_g \rangle$
$\Psi_1(a_{1g}^2, ^1A_{1g}, M=0, \alpha_g)$	$= - \overline{\alpha_g} \alpha_g $	$\Psi_1(a_{1g} a_{2g}, ^3A_{2g}, M=-1, \beta_g) = \overline{\alpha_g} \overline{\beta_g} $
	a_{2g}^2	$\Psi_2(a_{1g} a_{2g}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2} \overline{\alpha_g} \beta_g }{2} + \frac{\sqrt{2} \alpha_g \overline{\beta_g} }{2}$
$\Psi_2(a_{2g}^2, ^1A_{1g}, M=0, \alpha_g)$	$= - \overline{\beta_g} \beta_g $	$\Psi_3(a_{1g} a_{2g}, ^3A_{2g}, M=1, \beta_g) = \alpha_g \beta_g $
	b_{2g}^2	$b_{1g} b_{2g}$
$\Psi_3(b_{2g}^2, ^1A_{1g}, M=0, \alpha_g)$	$= - \overline{\zeta_g} \zeta_g $	$\Delta E = \langle \zeta_g \gamma_g \zeta_g \gamma_g \rangle - \langle \zeta_g \zeta_g \gamma_g \gamma_g \rangle$
	a_{2u}^2	$\Psi_4(b_{1g} b_{2g}, ^3A_{2g}, M=-1, \beta_g) = \overline{\zeta_g} \overline{\gamma_g} $
$\Psi_4(a_{2u}^2, ^1A_{1g}, M=0, \alpha_g)$	$= - \overline{\beta_u} \beta_u $	$\Psi_5(b_{1g} b_{2g}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2} \overline{\zeta_g} \gamma_g }{2} + \frac{\sqrt{2} \zeta_g \overline{\gamma_g} }{2}$
	b_{2u}^2	$\Psi_6(b_{1g} b_{2g}, ^3A_{2g}, M=1, \beta_g) = \zeta_g \gamma_g $
$\Psi_5(b_{2u}^2, ^1A_{1g}, M=0, \alpha_g)$	$= - \overline{\zeta_u} \zeta_u $	$a_{1u} a_{2u}$
	b_{1u}^2	$\Delta E = \langle \beta_u \alpha_u \beta_u \alpha_u \rangle - \langle \beta_u \beta_u \alpha_u \alpha_u \rangle$
$\Psi_6(b_{1u}^2, ^1A_{1g}, M=0, \alpha_g)$	$= - \overline{\gamma_u} \gamma_u $	$\Psi_7(a_{1u} a_{2u}, ^3A_{2g}, M=-1, \beta_g) = \overline{\beta_u} \overline{\alpha_u} $
	a_{1u}^2	$\Psi_8(a_{1u} a_{2u}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2} \overline{\beta_u} \alpha_u }{2} + \frac{\sqrt{2} \beta_u \overline{\alpha_u} }{2}$
$\Psi_7(a_{1u}^2, ^1A_{1g}, M=0, \alpha_g)$	$= - \overline{\alpha_u} \alpha_u $	$\Psi_9(a_{1u} a_{2u}, ^3A_{2g}, M=1, \beta_g) = \beta_u \alpha_u $
	b_{1g}^2	$b_{1u} b_{2u}$
$\Psi_8(b_{1g}^2, ^1A_{1g}, M=0, \alpha_g)$	$= - \overline{\gamma_g} \gamma_g $	$\Delta E = \langle \zeta_u \gamma_u \zeta_u \gamma_u \rangle - \langle \zeta_u \zeta_u \gamma_u \gamma_u \rangle$
	e_u^2	$\Psi_{10}(b_{1u} b_{2u}, ^3A_{2g}, M=-1, \beta_g) = \overline{\zeta_u} \overline{\gamma_u} $
$\Delta E = \langle \mu_u \alpha_u \alpha_u \alpha_u \rangle$		$\Psi_{11}(b_{1u} b_{2u}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2} \overline{\zeta_u} \gamma_u }{2} + \frac{\sqrt{2} \zeta_u \overline{\gamma_u} }{2}$
$\Psi_9(e_u^2, ^1A_{1g}, M=0, \alpha_g)$	$= - \overline{\alpha_u} \alpha_u $	$\Psi_{12}(b_{1u} b_{2u}, ^3A_{2g}, M=1, \beta_g) = \zeta_u \gamma_u $
	b_{1g}^2	e_u^2
$\Delta E = \langle \mu_u \eta_u \mu_u \eta_u \rangle + \langle \mu_u \mu_u \mu_u \mu_u \rangle$		$\Delta E = \langle \mu_u \eta_u \mu_u \eta_u \rangle - \langle \mu_u \mu_u \eta_u \eta_u \rangle$
$\Psi_{13}(e_u^2, ^3A_{2g}, M=-1, \beta_g)$	$= - \overline{\eta_u} \mu_u $	$\Psi_{13}(e_u^2, ^3A_{2g}, M=-1, \beta_g) = - \overline{\eta_u} \mu_u $
$\Psi_{14}(e_u^2, ^3A_{2g}, M=0, \beta_g)$	$= -\frac{\sqrt{2} \overline{\eta_u} \mu_u }{2} + \frac{\sqrt{2} \mu_u \eta_u }{2}$	$\Psi_{14}(e_u^2, ^3A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2} \overline{\eta_u} \mu_u }{2} + \frac{\sqrt{2} \mu_u \eta_u }{2}$
	e_u^2	$\Psi_{15}(e_u^2, ^3A_{2g}, M=1, \beta_g) = - \eta_u \mu_u $
$\Delta E = \langle \mu_g \eta_g \mu_g \eta_g \rangle + \langle \mu_g \mu_g \mu_g \mu_g \rangle$		e_g^2
$\Psi_{16}(e_g^2, ^3A_{2g}, M=-1, \beta_g)$	$= - \overline{\eta_g} \mu_g $	$\Delta E = \langle \mu_g \eta_g \mu_g \eta_g \rangle - \langle \mu_g \mu_g \eta_g \eta_g \rangle$
$\Psi_{17}(e_g^2, ^3A_{2g}, M=0, \beta_g)$	$= -\frac{\sqrt{2} \overline{\eta_g} \mu_g }{2} + \frac{\sqrt{2} \mu_g \eta_g }{2}$	$\Psi_{16}(e_g^2, ^3A_{2g}, M=-1, \beta_g) = - \overline{\eta_g} \mu_g $
$\Psi_{18}(e_g^2, ^3A_{2g}, M=1, \beta_g)$	$= - \eta_g \mu_g $	$\Psi_{17}(e_g^2, ^3A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2} \overline{\eta_g} \mu_g }{2} + \frac{\sqrt{2} \mu_g \eta_g }{2}$

2.15.3 $^1A_{2g}$ $a_{1g}a_{2g}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g | | \beta_g \beta_g \rangle + \langle \alpha_g \beta_g | | \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_{1g}a_{2g}, ^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\beta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\beta_g}|}{2}$$

$$b_{1g}b_{2g}$$

$$\boxed{\Delta E = \langle \zeta_g \gamma_g | | \zeta_g \gamma_g \rangle + \langle \zeta_g \zeta_g | | \gamma_g \gamma_g \rangle}$$

$$\Psi_2(b_{1g}b_{2g}, ^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\zeta_g}\gamma_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\gamma_g}|}{2}$$

$$a_{1u}a_{2u}$$

$$\boxed{\Delta E = \langle \beta_u \alpha_u | | \beta_u \alpha_u \rangle + \langle \beta_u \beta_u | | \alpha_u \alpha_u \rangle}$$

$$\Psi_3(a_{1u}a_{2u}, ^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\beta_u}\alpha_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\alpha_u}|}{2}$$

$$b_{1u}b_{2u}$$

$$\boxed{\Delta E = \langle \zeta_u \gamma_u | | \zeta_u \gamma_u \rangle + \langle \zeta_u \zeta_u | | \gamma_u \gamma_u \rangle}$$

$$\Psi_4(b_{1u}b_{2u}, ^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\zeta_u}\gamma_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\gamma_u}|}{2}$$

2.15.4 $^3B_{2g}$ $a_{1g}b_{2g}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g | | \zeta_g \zeta_g \rangle + \langle \alpha_g \zeta_g | | \alpha_g \zeta_g \rangle}$$

$$\Psi_1(a_{1g}b_{2g}, ^3B_{2g}, M=-1, \zeta_g) = |\overline{\alpha_g}\overline{\zeta_g}|$$

$$\Psi_2(a_{1g}b_{2g}, ^3B_{2g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\alpha_g}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\zeta_g}|}{2}$$

$$\Psi_3(a_{1g}b_{2g}, ^3B_{2g}, M=1, \zeta_g) = |\alpha_g\zeta_g|$$

$$a_{2g}b_{1g}$$

$$\boxed{\Delta E = -\langle \beta_g \beta_g | | \gamma_g \gamma_g \rangle + \langle \beta_g \gamma_g | | \beta_g \gamma_g \rangle}$$

$$\Psi_4(a_{2g}b_{1g}, ^3B_{2g}, M=-1, \zeta_g) = |\overline{\beta_g}\overline{\gamma_g}|$$

$$\Psi_5(a_{2g}b_{1g}, ^3B_{2g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_g}\gamma_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\gamma_g}|}{2}$$

$$\Psi_6(a_{2g}b_{1g}, ^3B_{2g}, M=1, \zeta_g) = |\beta_g\gamma_g|$$

 $a_{2u}b_{1u}$

$$\boxed{\Delta E = -\langle \beta_u \beta_u | | \gamma_u \gamma_u \rangle + \langle \beta_u \gamma_u | | \beta_u \gamma_u \rangle}$$

$$\Psi_7(a_{2u}b_{1u}, ^3B_{2g}, M=-1, \zeta_g) = |\overline{\beta_u}\overline{\gamma_u}|$$

$$\Psi_8(a_{2u}b_{1u}, ^3B_{2g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_u}\gamma_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\gamma_u}|}{2}$$

$$\Psi_9(a_{2u}b_{1u}, ^3B_{2g}, M=1, \zeta_g) = |\beta_u\gamma_u|$$

 $a_{1u}b_{2u}$

$$\boxed{\Delta E = \langle \zeta_u \alpha_u | | \zeta_u \alpha_u \rangle - \langle \zeta_u \zeta_u | | \alpha_u \alpha_u \rangle}$$

$$\Psi_{10}(a_{1u}b_{2u}, ^3B_{2g}, M=-1, \zeta_g) = |\overline{\zeta_u}\overline{\alpha_u}|$$

$$\Psi_{11}(a_{1u}b_{2u}, ^3B_{2g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\zeta_u}\alpha_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\alpha_u}|}{2}$$

$$\Psi_{12}(a_{1u}b_{2u}, ^3B_{2g}, M=1, \zeta_g) = |\zeta_u\alpha_u|$$

2.15.5 $^1B_{2g}$ $a_{1g}b_{2g}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g | | \zeta_g \zeta_g \rangle + \langle \alpha_g \zeta_g | | \alpha_g \zeta_g \rangle}$$

$$\Psi_1(a_{1g}b_{2g}, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\zeta_g}|}{2}$$

 $a_{2g}b_{1g}$

$$\boxed{\Delta E = \langle \beta_g \beta_g | | \gamma_g \gamma_g \rangle + \langle \beta_g \gamma_g | | \beta_g \gamma_g \rangle}$$

$$\Psi_2(a_{2g}b_{1g}, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\beta_g}\gamma_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\gamma_g}|}{2}$$

 $a_{2u}b_{1u}$

$$\boxed{\Delta E = \langle \beta_u \beta_u | | \gamma_u \gamma_u \rangle + \langle \beta_u \gamma_u | | \beta_u \gamma_u \rangle}$$

$$\Psi_3(a_{2u}b_{1u}, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\beta_u}\gamma_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\gamma_u}|}{2}$$

 $a_{1u}b_{2u}$

$$\boxed{\Delta E = \langle \zeta_u \alpha_u | | \zeta_u \alpha_u \rangle + \langle \zeta_u \zeta_u | | \alpha_u \alpha_u \rangle}$$

$$\Psi_4(a_{1u}b_{2u}, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\zeta_u}\alpha_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\alpha_u}|}{2}$$

 e_u^2

$$\boxed{\Delta E = \langle \mu_u \eta_u | | \mu_u \eta_u \rangle + \langle \mu_u \mu_u | | \eta_u \eta_u \rangle}$$

$$\Psi_5(e_u^2, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\eta_u}\mu_u|}{2} - \frac{\sqrt{2}|\mu_u\overline{\eta_u}|}{2}$$

 e_g^2

$$\boxed{\Delta E = \langle \mu_g \eta_g | | \mu_g \eta_g \rangle + \langle \mu_g \mu_g | | \eta_g \eta_g \rangle}$$

$$\Psi_6(e_g^2, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\eta_g}\mu_g|}{2} - \frac{\sqrt{2}|\mu_g\overline{\eta_g}|}{2}$$

2.15.6 $^3A_{2u}$ **2.15.7** $^1A_{2u}$ $a_{1g}a_{2u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \beta_u \beta_u \rangle + \langle \alpha_g \beta_u || \alpha_g \beta_u \rangle}$$

$$\Psi_1(a_{1g}a_{2u}, ^3A_{2u}, M=-1, \beta_u) = |\overline{\alpha_g} \overline{\beta_u}|$$

$$\Psi_2(a_{1g}a_{2u}, ^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\alpha_g} \beta_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_u}|}{2}$$

$$\Psi_3(a_{1g}a_{2u}, ^3A_{2u}, M=1, \beta_u) = |\alpha_g \beta_u|$$

 $a_{1u}a_{2g}$

$$\boxed{\Delta E = \langle \beta_g \alpha_u || \beta_g \alpha_u \rangle - \langle \beta_g \beta_g || \alpha_u \alpha_u \rangle}$$

$$\Psi_4(a_{1u}a_{2g}, ^3A_{2u}, M=-1, \beta_u) = |\overline{\beta_g} \overline{\alpha_u}|$$

$$\Psi_5(a_{1u}a_{2g}, ^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\beta_g} \alpha_u|}{2} + \frac{\sqrt{2}|\beta_g \overline{\alpha_u}|}{2}$$

$$\Psi_6(a_{1u}a_{2g}, ^3A_{2u}, M=1, \beta_u) = |\beta_g \alpha_u|$$

 $b_{1u}b_{2g}$

$$\boxed{\Delta E = \langle \zeta_g \gamma_u || \zeta_g \gamma_u \rangle - \langle \zeta_g \zeta_g || \gamma_u \gamma_u \rangle}$$

$$\Psi_7(b_{1u}b_{2g}, ^3A_{2u}, M=-1, \beta_u) = |\overline{\zeta_g} \overline{\gamma_u}|$$

$$\Psi_8(b_{1u}b_{2g}, ^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\zeta_g} \gamma_u|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\gamma_u}|}{2}$$

$$\Psi_9(b_{1u}b_{2g}, ^3A_{2u}, M=1, \beta_u) = |\zeta_g \gamma_u|$$

 $b_{1g}b_{2u}$

$$\boxed{\Delta E = \langle \zeta_u \gamma_g || \zeta_u \gamma_g \rangle - \langle \zeta_u \zeta_u || \gamma_g \gamma_g \rangle}$$

$$\Psi_{10}(b_{1g}b_{2u}, ^3A_{2u}, M=-1, \beta_u) = |\overline{\zeta_u} \overline{\gamma_g}|$$

$$\Psi_{11}(b_{1g}b_{2u}, ^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\zeta_u} \gamma_g|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\gamma_g}|}{2}$$

$$\Psi_{12}(b_{1g}b_{2u}, ^3A_{2u}, M=1, \beta_u) = |\zeta_u \gamma_g|$$

 $e_g e_u$

$$\boxed{\Delta E = \langle \mu_u \mu_g || \eta_u \eta_g \rangle + \langle \mu_u \mu_g || \mu_u \mu_g \rangle - \langle \mu_u \mu_u || \mu_g \mu_g \rangle - \langle \mu_u \eta_u || \eta_g \mu_g \rangle}$$

$$\Psi_{13}(e_g e_u, ^3A_{2u}, M=-1, \beta_u) = \frac{\sqrt{2}|\overline{\eta_u} \eta_g|}{2} + \frac{\sqrt{2}|\mu_u \mu_g|}{2}$$

$$\Psi_{14}(e_g e_u, ^3A_{2u}, M=0, \beta_u) = \frac{|\overline{\eta_u} \eta_g|}{2} + \frac{|\overline{\mu_u} \mu_g|}{2} + \frac{|\eta_u \overline{\eta_g}|}{2} + \frac{|\mu_u \overline{\mu_g}|}{2}$$

$$\Psi_{15}(e_g e_u, ^3A_{2u}, M=1, \beta_u) = \frac{\sqrt{2}|\eta_u \eta_g|}{2} + \frac{\sqrt{2}|\mu_u \mu_g|}{2}$$

 $a_{1g}a_{2u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_u \beta_u \rangle + \langle \alpha_g \beta_u || \alpha_g \beta_u \rangle}$$

$$\Psi_1(a_{1g}a_{2u}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\alpha_g} \beta_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_u}|}{2}$$

 $a_{1u}a_{2g}$

$$\boxed{\Delta E = \langle \beta_g \alpha_u || \beta_g \alpha_u \rangle + \langle \beta_g \beta_g || \alpha_u \alpha_u \rangle}$$

$$\Psi_2(a_{1u}a_{2g}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\beta_g} \alpha_u|}{2} + \frac{\sqrt{2}|\beta_g \overline{\alpha_u}|}{2}$$

 $b_{1u}b_{2g}$

$$\boxed{\Delta E = \langle \zeta_g \gamma_u || \zeta_g \gamma_u \rangle + \langle \zeta_g \zeta_g || \gamma_u \gamma_u \rangle}$$

$$\Psi_3(b_{1u}b_{2g}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\zeta_g} \gamma_u|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\gamma_u}|}{2}$$

 $b_{1g}b_{2u}$

$$\boxed{\Delta E = \langle \zeta_u \gamma_g || \zeta_u \gamma_g \rangle + \langle \zeta_u \zeta_u || \gamma_g \gamma_g \rangle}$$

$$\Psi_4(b_{1g}b_{2u}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\zeta_u} \gamma_g|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\gamma_g}|}{2}$$

 $e_g e_u$

$$\boxed{\Delta E = \langle \mu_u \mu_g || \eta_u \eta_g \rangle + \langle \mu_u \mu_g || \mu_u \mu_g \rangle + \langle \mu_u \mu_u || \mu_g \mu_g \rangle + \langle \mu_u \eta_u || \eta_g \mu_g \rangle}$$

$$\Psi_5(e_g e_u, ^1A_{2u}, M=0, \beta_u) = -\frac{|\overline{\eta_u} \eta_g|}{2} - \frac{|\overline{\mu_u} \mu_g|}{2} + \frac{|\eta_u \overline{\eta_g}|}{2} + \frac{|\mu_u \overline{\mu_g}|}{2}$$

2.15.8 $^3B_{2u}$ $a_{1g}b_{2u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u || \alpha_g \zeta_u \rangle}$$

$$\Psi_1(a_{1g}b_{2u}, ^3B_{2u}, M=-1, \zeta_u) = |\overline{\alpha_g} \overline{\zeta_u}|$$

$$\Psi_2(a_{1g}b_{2u}, ^3B_{2u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_g} \zeta_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\zeta_u}|}{2}$$

$$\Psi_3(a_{1g}b_{2u}, ^3B_{2u}, M=1, \zeta_u) = |\alpha_g \zeta_u|$$

 $a_{2g}b_{1u}$

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \gamma_u \gamma_u \rangle + \langle \beta_g \gamma_u || \beta_g \gamma_u \rangle}$$

$$\Psi_4(a_{2g}b_{1u}, ^3B_{2u}, M=-1, \zeta_u) = |\overline{\beta_g} \overline{\gamma_u}|$$

$$\Psi_5(a_{2g}b_{1u}, ^3B_{2u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\beta_g} \gamma_u|}{2} + \frac{\sqrt{2}|\beta_g \overline{\gamma_u}|}{2}$$

$$\Psi_6(a_{2g}b_{1u}, ^3B_{2u}, M=1, \zeta_u) = |\beta_g \gamma_u|$$

$a_{1u}b_{2g}$

$$\Delta E = \langle \zeta_g \alpha_u | \zeta_g \alpha_u \rangle - \langle \zeta_g \zeta_g | \alpha_u \alpha_u \rangle$$

$$\Psi_7(a_{1u}b_{2g}, {}^3B_{2u}, M=-1, \zeta_u) = |\overline{\zeta_g \alpha_u}|$$

$$\Psi_8(a_{1u}b_{2g}, {}^3B_{2u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\zeta_g \alpha_u}|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\alpha_u}|}{2}$$

$$\Psi_9(a_{1u}b_{2g}, {}^3B_{2u}, M=1, \zeta_u) = |\zeta_g \alpha_u|$$

 $a_{2u}b_{1g}$

$$\Delta E = -\langle \beta_u \beta_u | \gamma_g \gamma_g \rangle + \langle \beta_u \gamma_g | \beta_u \gamma_g \rangle$$

$$\Psi_{10}(a_{2u}b_{1g}, {}^3B_{2u}, M=-1, \zeta_u) = |\overline{\beta_u \gamma_g}|$$

$$\Psi_{11}(a_{2u}b_{1g}, {}^3B_{2u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\beta_u \gamma_g}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\gamma_g}|}{2}$$

$$\Psi_{12}(a_{2u}b_{1g}, {}^3B_{2u}, M=1, \zeta_u) = |\beta_u \gamma_g|$$

 $e_g e_u$

$$\Delta E = -\langle \mu_u \mu_g | \eta_u \eta_g \rangle + \langle \mu_u \mu_g | \mu_u \mu_g \rangle - \langle \mu_u \mu_u | \mu_g \mu_g \rangle \\ + \langle \mu_u \eta_u | \eta_g \mu_g \rangle$$

$$\Psi_{13}(e_g e_u, {}^3B_{2u}, M=-1, \zeta_u) = -\frac{\sqrt{2}|\overline{\eta_u \eta_g}|}{2} + \frac{\sqrt{2}|\overline{\mu_u \mu_g}|}{2}$$

$$\Psi_{14}(e_g e_u, {}^3B_{2u}, M=0, \zeta_u) = -\frac{|\overline{\eta_u \eta_g}|}{2} + \frac{|\overline{\mu_u \mu_g}|}{2} - \frac{|\eta_u \overline{\eta_g}|}{2} + \frac{|\mu_u \overline{\mu_g}|}{2}$$

$$\Psi_{15}(e_g e_u, {}^3B_{2u}, M=1, \zeta_u) = -\frac{\sqrt{2}|\eta_u \eta_g|}{2} + \frac{\sqrt{2}|\mu_u \mu_g|}{2}$$

2.15.9 ${}^1B_{2u}$ $a_{1g}b_{2u}$

$$\Delta E = \langle \alpha_g \alpha_g | \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u | \alpha_g \zeta_u \rangle$$

$$\Psi_1(a_{1g}b_{2u}, {}^1B_{2u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_g \zeta_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\zeta_u}|}{2}$$

 $a_{2g}b_{1u}$

$$\Delta E = \langle \beta_g \beta_g | \gamma_u \gamma_u \rangle + \langle \beta_g \gamma_u | \beta_g \gamma_u \rangle$$

$$\Psi_2(a_{2g}b_{1u}, {}^1B_{2u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\beta_g \gamma_u}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\gamma_u}|}{2}$$

 $a_{1u}b_{2g}$

$$\Delta E = \langle \zeta_g \alpha_u | \zeta_g \alpha_u \rangle + \langle \zeta_g \zeta_g | \alpha_u \alpha_u \rangle$$

$$\Psi_3(a_{1u}b_{2g}, {}^1B_{2u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\zeta_g \alpha_u}|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\alpha_u}|}{2}$$

 $a_{2u}b_{1g}$

$$\Delta E = \langle \beta_u \beta_u | \gamma_g \gamma_g \rangle + \langle \beta_u \gamma_g | \beta_u \gamma_g \rangle$$

$$\Psi_4(a_{2u}b_{1g}, {}^1B_{2u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\beta_u \gamma_g}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\gamma_g}|}{2}$$

 $e_g e_u$

$$\Delta E = -\langle \mu_u \mu_g | \eta_u \eta_g \rangle + \langle \mu_u \mu_g | \mu_u \mu_g \rangle + \langle \mu_u \mu_u | \mu_g \mu_g \rangle \\ - \langle \mu_u \eta_u | \eta_g \mu_g \rangle$$

$$\Psi_5(e_g e_u, {}^1B_{2u}, M=0, \zeta_u) = \frac{|\overline{\eta_u \eta_g}|}{2} - \frac{|\overline{\mu_u \mu_g}|}{2} - \frac{|\eta_u \overline{\eta_g}|}{2} + \frac{|\mu_u \overline{\mu_g}|}{2}$$

2.15.10 ${}^3B_{1u}$ $a_{1g}b_{1u}$

$$\Delta E = -\langle \alpha_g \alpha_g | \gamma_u \gamma_u \rangle + \langle \alpha_g \gamma_u | \alpha_g \gamma_u \rangle$$

$$\Psi_1(a_{1g}b_{1u}, {}^3B_{1u}, M=-1, \gamma_u) = |\overline{\alpha_g \gamma_u}|$$

$$\Psi_2(a_{1g}b_{1u}, {}^3B_{1u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_g \gamma_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\gamma_u}|}{2}$$

$$\Psi_3(a_{1g}b_{1u}, {}^3B_{1u}, M=1, \gamma_u) = |\alpha_g \gamma_u|$$

 $a_{2g}b_{2u}$

$$\Delta E = -\langle \beta_g \beta_g | \zeta_u \zeta_u \rangle + \langle \beta_g \zeta_u | \beta_g \zeta_u \rangle$$

$$\Psi_4(a_{2g}b_{2u}, {}^3B_{1u}, M=-1, \gamma_u) = |\overline{\beta_g \zeta_u}|$$

$$\Psi_5(a_{2g}b_{2u}, {}^3B_{1u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\beta_g \zeta_u}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\zeta_u}|}{2}$$

$$\Psi_6(a_{2g}b_{2u}, {}^3B_{1u}, M=1, \gamma_u) = |\beta_g \zeta_u|$$

 $a_{2u}b_{2g}$

$$\Delta E = \langle \zeta_g \beta_u | \zeta_g \beta_u \rangle - \langle \zeta_g \zeta_g | \beta_u \beta_u \rangle$$

$$\Psi_7(a_{2u}b_{2g}, {}^3B_{1u}, M=-1, \gamma_u) = |\overline{\zeta_g \beta_u}|$$

$$\Psi_8(a_{2u}b_{2g}, {}^3B_{1u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\zeta_g \beta_u}|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\beta_u}|}{2}$$

$$\Psi_9(a_{2u}b_{2g}, {}^3B_{1u}, M=1, \gamma_u) = |\zeta_g \beta_u|$$

 $a_{1u}b_{1g}$

$$\Delta E = -\langle \alpha_u \alpha_u | \gamma_g \gamma_g \rangle + \langle \alpha_u \gamma_g | \alpha_u \gamma_g \rangle$$

$$\Psi_{10}(a_{1u}b_{1g}, {}^3B_{1u}, M=-1, \gamma_u) = |\overline{\alpha_u \gamma_g}|$$

$$\Psi_{11}(a_{1u}b_{1g}, {}^3B_{1u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_u \gamma_g}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\gamma_g}|}{2}$$

$$\Psi_{12}(a_{1u}b_{1g}, {}^3B_{1u}, M=1, \gamma_u) = |\alpha_u \gamma_g|$$

 $e_g e_u$

$$\Delta E = \langle \mu_u \eta_g | \mu_u \eta_g \rangle + \langle \mu_u \mu_g | \eta_u \eta_g \rangle - \langle \mu_u \mu_u | \eta_g \eta_g \rangle \\ - \langle \mu_u \eta_u | \mu_g \eta_g \rangle$$

$$\Psi_{13}(e_g e_u, {}^3B_{1u}, M=-1, \gamma_u) = \frac{\sqrt{2}|\overline{\eta_u \mu_g}|}{2} + \frac{\sqrt{2}|\mu_u \overline{\eta_g}|}{2}$$

$$\begin{aligned}\Psi_{14}(e_g e_u, {}^3B_{1u}, M=0, \gamma_u) &= \\ \frac{|\eta_u \mu_g|}{2} + \frac{|\mu_u \eta_g|}{2} + \frac{|\eta_u \bar{\mu}_g|}{2} + \frac{|\mu_u \bar{\eta}_g|}{2} \\ \Psi_{15}(e_g e_u, {}^3B_{1u}, M=1, \gamma_u) &= \frac{\sqrt{2}|\eta_u \mu_g|}{2} + \frac{\sqrt{2}|\mu_u \eta_g|}{2}\end{aligned}$$

2.15.11 ${}^1B_{1u}$ *a_{1g}b_{1u}*

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \gamma_u \gamma_u \rangle + \langle \alpha_g \gamma_u || \alpha_g \gamma_u \rangle}$$

$$\Psi_1(a_{1g} b_{1u}, {}^1B_{1u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\bar{\alpha}_g \gamma_u|}{2} + \frac{\sqrt{2}|\alpha_g \bar{\gamma}_u|}{2}$$

a_{2g}b_{2u}

$$\boxed{\Delta E = \langle \beta_g \beta_g || \zeta_u \zeta_u \rangle + \langle \beta_g \zeta_u || \beta_g \zeta_u \rangle}$$

$$\Psi_2(a_{2g} b_{2u}, {}^1B_{1u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\bar{\beta}_g \zeta_u|}{2} + \frac{\sqrt{2}|\beta_g \bar{\zeta}_u|}{2}$$

a_{2u}b_{2g}

$$\boxed{\Delta E = \langle \zeta_g \beta_u || \zeta_g \beta_u \rangle + \langle \zeta_g \zeta_u || \beta_u \beta_u \rangle}$$

$$\Psi_3(a_{2u} b_{2g}, {}^1B_{1u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\bar{\zeta}_g \beta_u|}{2} + \frac{\sqrt{2}|\zeta_g \bar{\beta}_u|}{2}$$

a_{1u}b_{1g}

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \gamma_g \gamma_g \rangle + \langle \alpha_u \gamma_g || \alpha_u \gamma_g \rangle}$$

$$\Psi_4(a_{1u} b_{1g}, {}^1B_{1u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\bar{\alpha}_u \gamma_g|}{2} + \frac{\sqrt{2}|\alpha_u \bar{\gamma}_g|}{2}$$

e_ge_u

$$\boxed{\Delta E = \langle \mu_u \eta_g || \mu_u \eta_g \rangle + \langle \mu_u \mu_g || \eta_u \eta_g \rangle + \langle \mu_u \mu_u || \eta_g \eta_g \rangle + \langle \mu_u \eta_u || \mu_g \eta_g \rangle}$$

$$\Psi_5(e_g e_u, {}^1B_{1u}, M=0, \gamma_u) = \\ -\frac{|\eta_u \mu_g|}{2} - \frac{|\mu_u \eta_g|}{2} + \frac{|\eta_u \bar{\mu}_g|}{2} + \frac{|\mu_u \bar{\eta}_g|}{2}$$

2.15.12 ${}^3A_{1u}$ *a_{1g}a_{1u}*

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\begin{aligned}\Psi_1(a_{1g} a_{1u}, {}^3A_{1u}, M=-1, \alpha_u) &= |\bar{\alpha}_g \alpha_u| \\ \Psi_2(a_{1g} a_{1u}, {}^3A_{1u}, M=0, \alpha_u) &= \frac{\sqrt{2}|\bar{\alpha}_g \alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g \bar{\alpha}_u|}{2} \\ \Psi_3(a_{1g} a_{1u}, {}^3A_{1u}, M=1, \alpha_u) &= |\alpha_g \alpha_u|\end{aligned}$$

a_{2g}a_{2u}

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \beta_u \beta_u \rangle + \langle \beta_g \beta_u || \beta_g \beta_u \rangle}$$

$$\Psi_4(a_{2g} a_{2u}, {}^3A_{1u}, M=-1, \alpha_u) = |\bar{\beta}_g \beta_u|$$

$$\Psi_5(a_{2g} a_{2u}, {}^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\bar{\beta}_g \beta_u|}{2} + \frac{\sqrt{2}|\beta_g \bar{\beta}_u|}{2}$$

$$\Psi_6(a_{2g} a_{2u}, {}^3A_{1u}, M=1, \alpha_u) = |\beta_g \beta_u|$$

b_{2g}b_{2u}

$$\boxed{\Delta E = -\langle \zeta_g \zeta_g || \zeta_u \zeta_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle}$$

$$\Psi_7(b_{2g} b_{2u}, {}^3A_{1u}, M=-1, \alpha_u) = |\bar{\zeta}_g \zeta_u|$$

$$\Psi_8(b_{2g} b_{2u}, {}^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\bar{\zeta}_g \zeta_u|}{2} + \frac{\sqrt{2}|\zeta_g \bar{\zeta}_u|}{2}$$

$$\Psi_9(b_{2g} b_{2u}, {}^3A_{1u}, M=1, \alpha_u) = |\zeta_g \zeta_u|$$

b_{1g}b_{1u}

$$\boxed{\Delta E = \langle \gamma_u \gamma_g || \gamma_u \gamma_g \rangle - \langle \gamma_u \gamma_u || \gamma_g \gamma_g \rangle}$$

$$\Psi_{10}(b_{1g} b_{1u}, {}^3A_{1u}, M=-1, \alpha_u) = |\bar{\gamma}_u \gamma_g|$$

$$\Psi_{11}(b_{1g} b_{1u}, {}^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\bar{\gamma}_u \gamma_g|}{2} + \frac{\sqrt{2}|\gamma_u \bar{\gamma}_g|}{2}$$

$$\Psi_{12}(b_{1g} b_{1u}, {}^3A_{1u}, M=1, \alpha_u) = |\gamma_u \gamma_g|$$

e_ge_u

$$\boxed{\Delta E = \langle \mu_u \eta_g || \mu_u \eta_g \rangle - \langle \mu_u \mu_g || \eta_u \eta_g \rangle - \langle \mu_u \mu_u || \eta_g \eta_g \rangle + \langle \mu_u \eta_u || \mu_g \eta_g \rangle}$$

$$\Psi_{13}(e_g e_u, {}^3A_{1u}, M=-1, \alpha_u) = -\frac{\sqrt{2}|\bar{\eta}_u \mu_g|}{2} + \frac{\sqrt{2}|\mu_u \bar{\eta}_g|}{2}$$

$$\Psi_{14}(e_g e_u, {}^3A_{1u}, M=0, \alpha_u) = \\ -\frac{|\eta_u \mu_g|}{2} + \frac{|\mu_u \eta_g|}{2} - \frac{|\eta_u \bar{\mu}_g|}{2} + \frac{|\mu_u \bar{\eta}_g|}{2}$$

$$\Psi_{15}(e_g e_u, {}^3A_{1u}, M=1, \alpha_u) = -\frac{\sqrt{2}|\eta_u \mu_g|}{2} + \frac{\sqrt{2}|\mu_u \eta_g|}{2}$$

2.15.13 ${}^1A_{1u}$ *a_{1g}a_{1u}*

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_{1g} a_{1u}, {}^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\bar{\alpha}_g \alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g \bar{\alpha}_u|}{2}$$

a_{2g}a_{2u}

$$\boxed{\Delta E = \langle \beta_g \beta_g || \beta_u \beta_u \rangle + \langle \beta_g \beta_u || \beta_g \beta_u \rangle}$$

$$\Psi_2(a_{2g} a_{2u}, {}^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\bar{\beta}_g \beta_u|}{2} + \frac{\sqrt{2}|\beta_g \bar{\beta}_u|}{2}$$

b_{2g}b_{2u}

$$\boxed{\Delta E = \langle \zeta_g \zeta_g || \zeta_u \zeta_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle}$$

$$\Psi_3(b_{2g} b_{2u}, {}^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\bar{\zeta}_g \zeta_u|}{2} + \frac{\sqrt{2}|\zeta_g \bar{\zeta}_u|}{2}$$

$b_{1g}b_{1u}$

$$\boxed{\Delta E = \langle \gamma_u \gamma_g || \gamma_u \gamma_g \rangle + \langle \gamma_u \gamma_u || \gamma_g \gamma_g \rangle}$$

$$\Psi_4(b_{1g}b_{1u}, {}^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\bar{\gamma}_u \gamma_g|}{2} + \frac{\sqrt{2}|\gamma_u \bar{\gamma}_g|}{2}$$

 $e_g e_u$

$$\boxed{\Delta E = \langle \mu_u \eta_g || \mu_u \eta_g \rangle - \langle \mu_u \mu_g || \eta_u \eta_g \rangle + \langle \mu_u \mu_u || \eta_g \eta_g \rangle - \langle \mu_u \eta_u || \mu_g \eta_g \rangle}$$

$$\boxed{\Psi_5(e_g e_u, {}^1A_{1u}, M=0, \alpha_u) = \frac{|\eta_u \mu_g|}{2} - \frac{|\mu_u \eta_g|}{2} - \frac{|\eta_u \bar{\mu}_g|}{2} + \frac{|\mu_u \bar{\eta}_g|}{2}}$$

2.15.14 ${}^3B_{1g}$ $a_{1g}b_{1g}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \gamma_g \gamma_g \rangle + \langle \alpha_g \gamma_g || \alpha_g \gamma_g \rangle}$$

$$\Psi_1(a_{1g}b_{1g}, {}^3B_{1g}, M=-1, \gamma_g) = |\bar{\alpha}_g \gamma_g|$$

$$\Psi_2(a_{1g}b_{1g}, {}^3B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\bar{\alpha}_g \gamma_g|}{2} + \frac{\sqrt{2}|\alpha_g \bar{\gamma}_g|}{2}$$

$$\Psi_3(a_{1g}b_{1g}, {}^3B_{1g}, M=1, \gamma_g) = |\alpha_g \gamma_g|$$

 $a_{2g}b_{2g}$

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \zeta_g \zeta_g \rangle + \langle \beta_g \zeta_g || \beta_g \zeta_g \rangle}$$

$$\Psi_4(a_{2g}b_{2g}, {}^3B_{1g}, M=-1, \gamma_g) = |\bar{\beta}_g \zeta_g|$$

$$\Psi_5(a_{2g}b_{2g}, {}^3B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\bar{\beta}_g \zeta_g|}{2} + \frac{\sqrt{2}|\beta_g \bar{\zeta}_g|}{2}$$

$$\Psi_6(a_{2g}b_{2g}, {}^3B_{1g}, M=1, \gamma_g) = |\beta_g \zeta_g|$$

 $a_{2u}b_{2u}$

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \zeta_u \zeta_u \rangle + \langle \beta_u \zeta_u || \beta_u \zeta_u \rangle}$$

$$\Psi_7(a_{2u}b_{2u}, {}^3B_{1g}, M=-1, \gamma_g) = |\bar{\beta}_u \zeta_u|$$

$$\Psi_8(a_{2u}b_{2u}, {}^3B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\bar{\beta}_u \zeta_u|}{2} + \frac{\sqrt{2}|\beta_u \bar{\zeta}_u|}{2}$$

$$\Psi_9(a_{2u}b_{2u}, {}^3B_{1g}, M=1, \gamma_g) = |\beta_u \zeta_u|$$

 $a_{1u}b_{1u}$

$$\boxed{\Delta E = \langle \gamma_u \alpha_u || \gamma_u \alpha_u \rangle - \langle \gamma_u \gamma_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_{10}(a_{1u}b_{1u}, {}^3B_{1g}, M=-1, \gamma_g) = |\bar{\gamma}_u \alpha_u|$$

$$\Psi_{11}(a_{1u}b_{1u}, {}^3B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\bar{\gamma}_u \alpha_u|}{2} + \frac{\sqrt{2}|\gamma_u \bar{\alpha}_u|}{2}$$

$$\Psi_{12}(a_{1u}b_{1u}, {}^3B_{1g}, M=1, \gamma_g) = |\gamma_u \alpha_u|$$

2.15.15 ${}^1B_{1g}$ $a_{1g}b_{1g}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \gamma_g \gamma_g \rangle + \langle \alpha_g \gamma_g || \alpha_g \gamma_g \rangle}$$

$$\Psi_1(a_{1g}b_{1g}, {}^1B_{1g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\bar{\alpha}_g \gamma_g|}{2} + \frac{\sqrt{2}|\alpha_g \bar{\gamma}_g|}{2}$$

 $a_{2g}b_{2g}$

$$\boxed{\Delta E = \langle \beta_g \beta_g || \zeta_g \zeta_g \rangle + \langle \beta_g \zeta_g || \beta_g \zeta_g \rangle}$$

$$\Psi_2(a_{2g}b_{2g}, {}^1B_{1g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\bar{\beta}_g \zeta_g|}{2} + \frac{\sqrt{2}|\beta_g \bar{\zeta}_g|}{2}$$

 $a_{2u}b_{2u}$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \zeta_u \zeta_u \rangle + \langle \beta_u \zeta_u || \beta_u \zeta_u \rangle}$$

$$\Psi_3(a_{2u}b_{2u}, {}^1B_{1g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\bar{\beta}_u \zeta_u|}{2} + \frac{\sqrt{2}|\beta_u \bar{\zeta}_u|}{2}$$

 $a_{1u}b_{1u}$

$$\boxed{\Delta E = \langle \gamma_u \alpha_u || \gamma_u \alpha_u \rangle + \langle \gamma_u \gamma_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_4(a_{1u}b_{1u}, {}^1B_{1g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\bar{\gamma}_u \alpha_u|}{2} + \frac{\sqrt{2}|\gamma_u \bar{\alpha}_u|}{2}$$

 e_u^2

$$\boxed{\Delta E = -\langle \mu_u \mu_u || \eta_u \eta_u \rangle + \langle \mu_u \mu_u || \mu_u \mu_u \rangle}$$

$$\Psi_5(e_u^2, {}^1B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\bar{\eta}_u \eta_u|}{2} - \frac{\sqrt{2}|\mu_u \mu_u|}{2}$$

 e_g^2

$$\boxed{\Delta E = -\langle \mu_g \mu_g || \eta_g \eta_g \rangle + \langle \mu_g \mu_g || \mu_g \mu_g \rangle}$$

$$\Psi_6(e_g^2, {}^1B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\bar{\eta}_g \eta_g|}{2} - \frac{\sqrt{2}|\mu_g \mu_g|}{2}$$

2.15.16 3E_u $a_{1g}e_u$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \mu_u \mu_u \rangle + \langle \alpha_g \mu_u || \alpha_g \mu_u \rangle}$$

$$\Psi_1(a_{1g}e_u, {}^3E_u, M=-1, \eta_u) = |\bar{\alpha}_g \eta_u|$$

$$\Psi_2(a_{1g}e_u, {}^3E_u, M=-1, \mu_u) = |\bar{\alpha}_g \mu_u|$$

$$\Psi_3(a_{1g}e_u, {}^3E_u, M=0, \eta_u) = \frac{\sqrt{2}|\bar{\alpha}_g \eta_u|}{2} + \frac{\sqrt{2}|\alpha_g \bar{\eta}_u|}{2}$$

$$\Psi_4(a_{1g}e_u, {}^3E_u, M=0, \mu_u) = \frac{\sqrt{2}|\bar{\alpha}_g \mu_u|}{2} + \frac{\sqrt{2}|\alpha_g \bar{\mu}_u|}{2}$$

$$\Psi_5(a_{1g}e_u, {}^3E_u, M=1, \eta_u) = |\alpha_g \eta_u|$$

$$\Psi_6(a_{1g}e_u, {}^3E_u, M=1, \mu_u) = |\alpha_g \mu_u|$$

 $a_{2g}e_u$

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \mu_u \mu_u \rangle + \langle \beta_g \mu_u || \beta_g \mu_u \rangle}$$

$$\Psi_7(a_{2g}e_u, {}^3E_u, M=-1, \mu_u) = -|\overline{\beta_g}\eta_u|$$

$$\Psi_8(a_{2g}e_u, {}^3E_u, M=-1, \eta_u) = |\overline{\beta_g}\mu_u|$$

$$\Psi_9(a_{2g}e_u, {}^3E_u, M=0, \mu_u) = -\frac{\sqrt{2}|\overline{\beta_g}\eta_u|}{2} - \frac{\sqrt{2}|\beta_g\overline{\eta_u}|}{2}$$

$$\Psi_{10}(a_{2g}e_u, {}^3E_u, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\beta_g}\mu_u|}{2} + \frac{\sqrt{2}|\beta_g\overline{\mu_u}|}{2}$$

$$\Psi_{11}(a_{2g}e_u, {}^3E_u, M=1, \mu_u) = -|\beta_g\eta_u|$$

$$\Psi_{12}(a_{2g}e_u, {}^3E_u, M=1, \eta_u) = |\beta_g\mu_u|$$

b_{2g}e_u

$$\boxed{\Delta E = \langle \zeta_g\mu_u || \zeta_g\mu_u \rangle - \langle \zeta_g\zeta_g || \mu_u\mu_u \rangle}$$

$$\Psi_{13}(b_{2g}e_u, {}^3E_u, M=-1, \mu_u) = |\overline{\zeta_g}\eta_u|$$

$$\Psi_{14}(b_{2g}e_u, {}^3E_u, M=-1, \eta_u) = |\overline{\zeta_g}\mu_u|$$

$$\Psi_{15}(b_{2g}e_u, {}^3E_u, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\zeta_g}\eta_u|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\eta_u}|}{2}$$

$$\Psi_{16}(b_{2g}e_u, {}^3E_u, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\zeta_g}\mu_u|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\mu_u}|}{2}$$

$$\Psi_{17}(b_{2g}e_u, {}^3E_u, M=1, \mu_u) = |\zeta_g\eta_u|$$

$$\Psi_{18}(b_{2g}e_u, {}^3E_u, M=1, \eta_u) = |\zeta_g\mu_u|$$

a_{2u}e_g

$$\boxed{\Delta E = -\langle \beta_u\beta_u || \mu_g\mu_g \rangle + \langle \beta_u\mu_g || \beta_u\mu_g \rangle}$$

$$\Psi_{19}(a_{2u}e_g, {}^3E_u, M=-1, \eta_u) = |\overline{\beta_u}\eta_g|$$

$$\Psi_{20}(a_{2u}e_g, {}^3E_u, M=-1, \mu_u) = |\overline{\beta_u}\mu_g|$$

$$\Psi_{21}(a_{2u}e_g, {}^3E_u, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\beta_u}\eta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\eta_g}|}{2}$$

$$\Psi_{22}(a_{2u}e_g, {}^3E_u, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\beta_u}\mu_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\mu_g}|}{2}$$

$$\Psi_{23}(a_{2u}e_g, {}^3E_u, M=1, \eta_u) = |\beta_u\eta_g|$$

$$\Psi_{24}(a_{2u}e_g, {}^3E_u, M=1, \mu_u) = |\beta_u\mu_g|$$

b_{2u}e_g

$$\boxed{\Delta E = \langle \zeta_u\mu_g || \zeta_u\mu_g \rangle - \langle \zeta_u\zeta_u || \mu_g\mu_g \rangle}$$

$$\Psi_{25}(b_{2u}e_g, {}^3E_u, M=-1, \eta_u) = |\overline{\zeta_u}\eta_g|$$

$$\Psi_{26}(b_{2u}e_g, {}^3E_u, M=-1, \mu_u) = -|\overline{\zeta_u}\mu_g|$$

$$\Psi_{27}(b_{2u}e_g, {}^3E_u, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\zeta_u}\eta_g|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\eta_g}|}{2}$$

$$\Psi_{28}(b_{2u}e_g, {}^3E_u, M=0, \mu_u) = -\frac{\sqrt{2}|\overline{\zeta_u}\mu_g|}{2} - \frac{\sqrt{2}|\zeta_u\overline{\mu_g}|}{2}$$

$$\Psi_{29}(b_{2u}e_g, {}^3E_u, M=1, \eta_u) = |\zeta_u\eta_g|$$

$$\Psi_{30}(b_{2u}e_g, {}^3E_u, M=1, \mu_u) = -|\zeta_u\mu_g|$$

b_{1u}e_g

$$\boxed{\Delta E = -\langle \gamma_u\gamma_u || \mu_g\mu_g \rangle + \langle \gamma_u\mu_g || \gamma_u\mu_g \rangle}$$

$$\Psi_{31}(b_{1u}e_g, {}^3E_u, M=-1, \mu_u) = |\overline{\gamma_u}\eta_g|$$

$$\Psi_{32}(b_{1u}e_g, {}^3E_u, M=-1, \eta_u) = |\overline{\gamma_u}\mu_g|$$

$$\Psi_{33}(b_{1u}e_g, {}^3E_u, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\gamma_u}\eta_g|}{2} + \frac{\sqrt{2}|\gamma_u\overline{\eta_g}|}{2}$$

$$\Psi_{34}(b_{1u}e_g, {}^3E_u, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\gamma_u}\mu_g|}{2} + \frac{\sqrt{2}|\gamma_u\overline{\mu_g}|}{2}$$

$$\Psi_{35}(b_{1u}e_g, {}^3E_u, M=1, \mu_u) = |\gamma_u\eta_g|$$

$$\Psi_{36}(b_{1u}e_g, {}^3E_u, M=1, \eta_u) = |\gamma_u\mu_g|$$

a_{1u}e_g

$$\boxed{\Delta E = -\langle \alpha_u\alpha_u || \mu_g\mu_g \rangle + \langle \alpha_u\mu_g || \alpha_u\mu_g \rangle}$$

$$\Psi_{37}(a_{1u}e_g, {}^3E_u, M=-1, \mu_u) = -|\overline{\alpha_u}\eta_g|$$

$$\Psi_{38}(a_{1u}e_g, {}^3E_u, M=-1, \eta_u) = |\overline{\alpha_u}\mu_g|$$

$$\Psi_{39}(a_{1u}e_g, {}^3E_u, M=0, \mu_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\eta_g|}{2} - \frac{\sqrt{2}|\alpha_u\overline{\eta_g}|}{2}$$

$$\Psi_{40}(a_{1u}e_g, {}^3E_u, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\alpha_u}\mu_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\mu_g}|}{2}$$

$$\Psi_{41}(a_{1u}e_g, {}^3E_u, M=1, \mu_u) = -|\alpha_u\eta_g|$$

$$\Psi_{42}(a_{1u}e_g, {}^3E_u, M=1, \eta_u) = |\alpha_u\mu_g|$$

b_{1g}e_u

$$\boxed{\Delta E = -\langle \gamma_g\gamma_g || \mu_u\mu_u \rangle + \langle \gamma_g\mu_u || \gamma_g\mu_u \rangle}$$

$$\Psi_{43}(b_{1g}e_u, {}^3E_u, M=-1, \eta_u) = |\overline{\gamma_g}\eta_u|$$

$$\Psi_{44}(b_{1g}e_u, {}^3E_u, M=-1, \mu_u) = -|\overline{\gamma_g}\mu_u|$$

$$\Psi_{45}(b_{1g}e_u, {}^3E_u, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\gamma_g}\eta_u|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\eta_u}|}{2}$$

$$\Psi_{46}(b_{1g}e_u, {}^3E_u, M=0, \mu_u) = -\frac{\sqrt{2}|\overline{\gamma_g}\mu_u|}{2} - \frac{\sqrt{2}|\gamma_g\overline{\mu_u}|}{2}$$

$$\Psi_{47}(b_{1g}e_u, {}^3E_u, M=1, \eta_u) = |\gamma_g\eta_u|$$

$$\Psi_{48}(b_{1g}e_u, {}^3E_u, M=1, \mu_u) = -|\gamma_g\mu_u|$$

2.15.17 ¹E_u

a_{1g}e_u

$$\boxed{\Delta E = \langle \alpha_g\alpha_g || \mu_u\mu_u \rangle + \langle \alpha_g\mu_u || \alpha_g\mu_u \rangle}$$

$$\Psi_1(a_{1g}e_u, {}^1E_u, M=0, \eta_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\eta_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\eta_u}|}{2}$$

$$\Psi_2(a_{1g}e_u, {}^1E_u, M=0, \mu_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\mu_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\mu_u}|}{2}$$

a_{2g}e_g

$$\boxed{\Delta E = \langle \beta_g\beta_g || \mu_u\mu_u \rangle + \langle \beta_g\mu_u || \beta_g\mu_u \rangle}$$

$$\Psi_3(a_{2g}e_u, {}^1E_u, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\beta_g}\eta_u|}{2} - \frac{\sqrt{2}|\beta_g\overline{\eta_u}|}{2}$$

$$\Psi_4(a_{2g}e_u, {}^1E_u, M=0, \eta_u) = -\frac{\sqrt{2}|\overline{\beta_g}\mu_u|}{2} + \frac{\sqrt{2}|\beta_g\overline{\mu_u}|}{2}$$

b_{2g}e_u

$$\boxed{\Delta E = \langle \zeta_g\zeta_g || \mu_u\mu_u \rangle + \langle \zeta_g\mu_u || \zeta_g\mu_u \rangle}$$

$$\Psi_5(b_{2g}e_u, {}^1E_u, M=0, \mu_u) = -\frac{\sqrt{2}|\overline{\zeta_g}\eta_u|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\eta_u}|}{2}$$

$$\Psi_6(b_{2g}e_u, {}^1E_u, M=0, \eta_u) = -\frac{\sqrt{2}|\overline{\zeta_g}\mu_u|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\mu_u}|}{2}$$

$a_{2u}e_g$

$$\Delta E = \langle \beta_u \beta_u || \mu_g \mu_g \rangle + \langle \beta_u \mu_g || \beta_u \mu_g \rangle$$

$$\Psi_7(a_{2u}e_g, {}^1E_u, M=0, \eta_u) = -\frac{\sqrt{2}|\beta_u \eta_g|}{2} + \frac{\sqrt{2}|\beta_u \bar{\eta}_g|}{2}$$

$$\Psi_8(a_{2u}e_g, {}^1E_u, M=0, \mu_u) = -\frac{\sqrt{2}|\beta_u \mu_g|}{2} + \frac{\sqrt{2}|\beta_u \bar{\mu}_g|}{2}$$

 $b_{2u}e_g$

$$\Delta E = \langle \zeta_u \mu_g || \zeta_u \mu_g \rangle + \langle \zeta_u \zeta_u || \mu_g \mu_g \rangle$$

$$\Psi_9(b_{2u}e_g, {}^1E_u, M=0, \eta_u) = -\frac{\sqrt{2}|\zeta_u \eta_g|}{2} + \frac{\sqrt{2}|\zeta_u \bar{\eta}_g|}{2}$$

$$\Psi_{10}(b_{2u}e_g, {}^1E_u, M=0, \mu_u) = \frac{\sqrt{2}|\zeta_u \mu_g|}{2} - \frac{\sqrt{2}|\zeta_u \bar{\mu}_g|}{2}$$

 $b_{1u}e_g$

$$\Delta E = \langle \gamma_u \gamma_u || \mu_g \mu_g \rangle + \langle \gamma_u \mu_g || \gamma_u \mu_g \rangle$$

$$\Psi_{11}(b_{1u}e_g, {}^1E_u, M=0, \mu_u) = -\frac{\sqrt{2}|\gamma_u \eta_g|}{2} + \frac{\sqrt{2}|\gamma_u \bar{\eta}_g|}{2}$$

$$\Psi_{12}(b_{1u}e_g, {}^1E_u, M=0, \eta_u) = -\frac{\sqrt{2}|\gamma_u \mu_g|}{2} + \frac{\sqrt{2}|\gamma_u \bar{\mu}_g|}{2}$$

 $a_{1u}e_g$

$$\Delta E = \langle \alpha_u \alpha_u || \mu_g \mu_g \rangle + \langle \alpha_u \mu_g || \alpha_u \mu_g \rangle$$

$$\Psi_{13}(a_{1u}e_g, {}^1E_u, M=0, \mu_u) = \frac{\sqrt{2}|\alpha_u \eta_g|}{2} - \frac{\sqrt{2}|\alpha_u \bar{\eta}_g|}{2}$$

$$\Psi_{14}(a_{1u}e_g, {}^1E_u, M=0, \eta_u) = -\frac{\sqrt{2}|\alpha_u \mu_g|}{2} + \frac{\sqrt{2}|\alpha_u \bar{\mu}_g|}{2}$$

 $b_{1g}e_u$

$$\Delta E = \langle \gamma_g \gamma_g || \mu_u \mu_u \rangle + \langle \gamma_g \mu_u || \gamma_g \mu_u \rangle$$

$$\Psi_{15}(b_{1g}e_u, {}^1E_u, M=0, \eta_u) = -\frac{\sqrt{2}|\gamma_g \eta_u|}{2} + \frac{\sqrt{2}|\gamma_g \bar{\eta}_u|}{2}$$

$$\Psi_{16}(b_{1g}e_u, {}^1E_u, M=0, \mu_u) = \frac{\sqrt{2}|\gamma_g \mu_u|}{2} - \frac{\sqrt{2}|\gamma_g \bar{\mu}_u|}{2}$$

2.15.18 3E_g $a_{1g}e_g$

$$\Delta E = -\langle \alpha_g \alpha_g || \mu_g \mu_g \rangle + \langle \alpha_g \mu_g || \alpha_g \mu_g \rangle$$

$$\Psi_1(a_{1g}e_g, {}^3E_g, M=-1, \eta_g) = |\alpha_g \eta_g|$$

$$\Psi_2(a_{1g}e_g, {}^3E_g, M=-1, \mu_g) = |\alpha_g \mu_g|$$

$$\Psi_3(a_{1g}e_g, {}^3E_g, M=0, \eta_g) = \frac{\sqrt{2}|\alpha_g \eta_g|}{2} + \frac{\sqrt{2}|\alpha_g \bar{\eta}_g|}{2}$$

$$\Psi_4(a_{1g}e_g, {}^3E_g, M=0, \mu_g) = \frac{\sqrt{2}|\alpha_g \mu_g|}{2} + \frac{\sqrt{2}|\alpha_g \bar{\mu}_g|}{2}$$

$$\Psi_5(a_{1g}e_g, {}^3E_g, M=1, \eta_g) = |\alpha_g \eta_g|$$

$$\Psi_6(a_{1g}e_g, {}^3E_g, M=1, \mu_g) = |\alpha_g \mu_g|$$

 $a_{2g}e_g$

$$\Delta E = -\langle \beta_g \beta_g || \mu_g \mu_g \rangle + \langle \beta_g \mu_g || \beta_g \mu_g \rangle$$

$$\Psi_7(a_{2g}e_g, {}^3E_g, M=-1, \mu_g) = -|\beta_g \bar{\eta}_g|$$

$$\Psi_8(a_{2g}e_g, {}^3E_g, M=-1, \eta_g) = |\beta_g \bar{\mu}_g|$$

$$\Psi_9(a_{2g}e_g, {}^3E_g, M=0, \mu_g) = -\frac{\sqrt{2}|\beta_g \eta_g|}{2} - \frac{\sqrt{2}|\beta_g \bar{\eta}_g|}{2}$$

$$\Psi_{10}(a_{2g}e_g, {}^3E_g, M=0, \eta_g) = \frac{\sqrt{2}|\beta_g \mu_g|}{2} + \frac{\sqrt{2}|\beta_g \bar{\mu}_g|}{2}$$

$$\Psi_{11}(a_{2g}e_g, {}^3E_g, M=1, \mu_g) = -|\beta_g \eta_g|$$

$$\Psi_{12}(a_{2g}e_g, {}^3E_g, M=1, \eta_g) = |\beta_g \mu_g|$$

 $b_{2g}e_g$

$$\Delta E = \langle \zeta_g \mu_g || \zeta_g \mu_g \rangle - \langle \zeta_g \zeta_g || \mu_g \mu_g \rangle$$

$$\Psi_{13}(b_{2g}e_g, {}^3E_g, M=-1, \mu_g) = |\zeta_g \bar{\eta}_g|$$

$$\Psi_{14}(b_{2g}e_g, {}^3E_g, M=-1, \eta_g) = |\zeta_g \bar{\mu}_g|$$

$$\Psi_{15}(b_{2g}e_g, {}^3E_g, M=0, \mu_g) = \frac{\sqrt{2}|\zeta_g \eta_g|}{2} + \frac{\sqrt{2}|\zeta_g \bar{\eta}_g|}{2}$$

$$\Psi_{16}(b_{2g}e_g, {}^3E_g, M=0, \eta_g) = \frac{\sqrt{2}|\zeta_g \mu_g|}{2} + \frac{\sqrt{2}|\zeta_g \bar{\mu}_g|}{2}$$

$$\Psi_{17}(b_{2g}e_g, {}^3E_g, M=1, \mu_g) = |\zeta_g \eta_g|$$

$$\Psi_{18}(b_{2g}e_g, {}^3E_g, M=1, \eta_g) = |\zeta_g \mu_g|$$

 $a_{2u}e_u$

$$\Delta E = -\langle \beta_u \beta_u || \mu_u \mu_u \rangle + \langle \beta_u \mu_u || \beta_u \mu_u \rangle$$

$$\Psi_{19}(a_{2u}e_u, {}^3E_g, M=-1, \eta_g) = |\beta_u \bar{\eta}_u|$$

$$\Psi_{20}(a_{2u}e_u, {}^3E_g, M=-1, \mu_g) = |\beta_u \bar{\mu}_u|$$

$$\Psi_{21}(a_{2u}e_u, {}^3E_g, M=0, \eta_g) = \frac{\sqrt{2}|\beta_u \eta_u|}{2} + \frac{\sqrt{2}|\beta_u \bar{\eta}_u|}{2}$$

$$\Psi_{22}(a_{2u}e_u, {}^3E_g, M=0, \mu_g) = \frac{\sqrt{2}|\beta_u \mu_u|}{2} + \frac{\sqrt{2}|\beta_u \bar{\mu}_u|}{2}$$

$$\Psi_{23}(a_{2u}e_u, {}^3E_g, M=1, \eta_g) = |\beta_u \eta_u|$$

$$\Psi_{24}(a_{2u}e_u, {}^3E_g, M=1, \mu_g) = |\beta_u \mu_u|$$

 $b_{2u}e_u$

$$\Delta E = \langle \zeta_u \mu_u || \zeta_u \mu_u \rangle - \langle \zeta_u \zeta_u || \mu_u \mu_u \rangle$$

$$\Psi_{25}(b_{2u}e_u, {}^3E_g, M=-1, \eta_g) = |\zeta_u \bar{\eta}_u|$$

$$\Psi_{26}(b_{2u}e_u, {}^3E_g, M=-1, \mu_g) = -|\zeta_u \bar{\mu}_u|$$

$$\Psi_{27}(b_{2u}e_u, {}^3E_g, M=0, \eta_g) = \frac{\sqrt{2}|\zeta_u \eta_u|}{2} + \frac{\sqrt{2}|\zeta_u \bar{\eta}_u|}{2}$$

$$\Psi_{28}(b_{2u}e_u, {}^3E_g, M=0, \mu_g) = -\frac{\sqrt{2}|\zeta_u \mu_u|}{2} - \frac{\sqrt{2}|\zeta_u \bar{\mu}_u|}{2}$$

$$\Psi_{29}(b_{2u}e_u, {}^3E_g, M=1, \eta_g) = |\zeta_u \eta_u|$$

$$\Psi_{30}(b_{2u}e_u, {}^3E_g, M=1, \mu_g) = -|\zeta_u \mu_u|$$

 $b_{1u}e_u$

$$\Delta E = -\langle \gamma_u \gamma_u || \mu_u \mu_u \rangle + \langle \gamma_u \mu_u || \gamma_u \mu_u \rangle$$

$$\Psi_{31}(b_{1u}e_u, {}^3E_g, M=-1, \mu_g) = |\gamma_u \bar{\eta}_u|$$

$$\Psi_{32}(b_{1u}e_u, {}^3E_g, M=-1, \eta_g) = |\gamma_u \bar{\mu}_u|$$

$$\begin{aligned}\Psi_{33}(b_{1u}e_u, {}^3E_g, M=0, \mu_g) &= \frac{\sqrt{2}|\gamma_u\eta_u|}{2} + \frac{\sqrt{2}|\gamma_u\bar{\eta}_u|}{2} \\ \Psi_{34}(b_{1u}e_u, {}^3E_g, M=0, \eta_g) &= \frac{\sqrt{2}|\gamma_u\mu_u|}{2} + \frac{\sqrt{2}|\gamma_u\bar{\mu}_u|}{2} \\ \Psi_{35}(b_{1u}e_u, {}^3E_g, M=1, \mu_g) &= |\gamma_u\eta_u| \\ \Psi_{36}(b_{1u}e_u, {}^3E_g, M=1, \eta_g) &= |\gamma_u\mu_u|\end{aligned}$$

 $a_{1u}e_u$

$$\boxed{\Delta E = -\langle \alpha_u\alpha_u || \mu_u\mu_u \rangle + \langle \alpha_u\mu_u || \alpha_u\mu_u \rangle}$$

$$\Psi_{37}(a_{1u}e_u, {}^3E_g, M=-1, \mu_g) = -|\overline{\alpha_u\eta_u}|$$

$$\Psi_{38}(a_{1u}e_u, {}^3E_g, M=-1, \eta_g) = |\overline{\alpha_u\mu_u}|$$

$$\Psi_{39}(a_{1u}e_u, {}^3E_g, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\alpha_u\eta_u}|}{2} - \frac{\sqrt{2}|\alpha_u\bar{\eta}_u|}{2}$$

$$\Psi_{40}(a_{1u}e_u, {}^3E_g, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\alpha_u\mu_u}|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\mu}_u|}{2}$$

$$\Psi_{41}(a_{1u}e_u, {}^3E_g, M=1, \mu_g) = -|\alpha_u\eta_u|$$

$$\Psi_{42}(a_{1u}e_u, {}^3E_g, M=1, \eta_g) = |\alpha_u\mu_u|$$

 $b_{1g}e_g$

$$\boxed{\Delta E = -\langle \gamma_g\gamma_g || \mu_g\mu_g \rangle + \langle \gamma_g\mu_g || \gamma_g\mu_g \rangle}$$

$$\Psi_{43}(b_{1g}e_g, {}^3E_g, M=-1, \eta_g) = |\overline{\gamma_g\eta_g}|$$

$$\Psi_{44}(b_{1g}e_g, {}^3E_g, M=-1, \mu_g) = -|\overline{\gamma_g\mu_g}|$$

$$\Psi_{45}(b_{1g}e_g, {}^3E_g, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\gamma_g\eta_g}|}{2} + \frac{\sqrt{2}|\gamma_g\bar{\eta}_g|}{2}$$

$$\Psi_{46}(b_{1g}e_g, {}^3E_g, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\gamma_g\mu_g}|}{2} - \frac{\sqrt{2}|\gamma_g\bar{\mu}_g|}{2}$$

$$\Psi_{47}(b_{1g}e_g, {}^3E_g, M=1, \eta_g) = |\gamma_g\eta_g|$$

$$\Psi_{48}(b_{1g}e_g, {}^3E_g, M=1, \mu_g) = -|\gamma_g\mu_g|$$

2.15.19 1E_g $a_{1g}e_g$

$$\boxed{\Delta E = \langle \alpha_g\alpha_g || \mu_g\mu_g \rangle + \langle \alpha_g\mu_g || \alpha_g\mu_g \rangle}$$

$$\Psi_1(a_{1g}e_g, {}^1E_g, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\alpha_g\eta_g}|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\eta}_g|}{2}$$

$$\Psi_2(a_{1g}e_g, {}^1E_g, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\alpha_g\mu_g}|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\mu}_g|}{2}$$

 $a_{2g}e_g$

$$\boxed{\Delta E = \langle \beta_g\beta_g || \mu_g\mu_g \rangle + \langle \beta_g\mu_g || \beta_g\mu_g \rangle}$$

$$\Psi_3(a_{2g}e_g, {}^1E_g, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\beta_g\eta_g}|}{2} - \frac{\sqrt{2}|\beta_g\bar{\eta}_g|}{2}$$

$$\Psi_4(a_{2g}e_g, {}^1E_g, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\beta_g\mu_g}|}{2} + \frac{\sqrt{2}|\beta_g\bar{\mu}_g|}{2}$$

 $b_{2g}e_g$

$$\boxed{\Delta E = \langle \zeta_g\mu_g || \zeta_g\mu_g \rangle + \langle \zeta_g\zeta_g || \mu_g\mu_g \rangle}$$

$$\Psi_5(b_{2g}e_g, {}^1E_g, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\zeta_g\eta_g}|}{2} + \frac{\sqrt{2}|\zeta_g\bar{\eta}_g|}{2}$$

$$\Psi_6(b_{2g}e_g, {}^1E_g, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\zeta_g\mu_g}|}{2} + \frac{\sqrt{2}|\zeta_g\bar{\mu}_g|}{2}$$

 $a_{2u}e_u$

$$\boxed{\Delta E = \langle \beta_u\beta_u || \mu_u\mu_u \rangle + \langle \beta_u\mu_u || \beta_u\mu_u \rangle}$$

$$\Psi_7(a_{2u}e_u, {}^1E_g, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\beta_u\eta_u}|}{2} + \frac{\sqrt{2}|\beta_u\bar{\eta}_u|}{2}$$

$$\Psi_8(a_{2u}e_u, {}^1E_g, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\beta_u\mu_u}|}{2} + \frac{\sqrt{2}|\beta_u\bar{\mu}_u|}{2}$$

 $b_{2u}e_u$

$$\boxed{\Delta E = \langle \zeta_u\mu_u || \zeta_u\mu_u \rangle + \langle \zeta_u\zeta_u || \mu_u\mu_u \rangle}$$

$$\Psi_9(b_{2u}e_u, {}^1E_g, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\zeta_u\eta_u}|}{2} + \frac{\sqrt{2}|\zeta_u\bar{\eta}_u|}{2}$$

$$\Psi_{10}(b_{2u}e_u, {}^1E_g, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\zeta_u\mu_u}|}{2} - \frac{\sqrt{2}|\zeta_u\bar{\mu}_u|}{2}$$

 $b_{1u}e_u$

$$\boxed{\Delta E = \langle \gamma_u\gamma_u || \mu_u\mu_u \rangle + \langle \gamma_u\mu_u || \gamma_u\mu_u \rangle}$$

$$\Psi_{11}(b_{1u}e_u, {}^1E_g, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\gamma_u\eta_u}|}{2} + \frac{\sqrt{2}|\gamma_u\bar{\eta}_u|}{2}$$

$$\Psi_{12}(b_{1u}e_u, {}^1E_g, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\gamma_u\mu_u}|}{2} + \frac{\sqrt{2}|\gamma_u\bar{\mu}_u|}{2}$$

 $a_{1u}e_u$

$$\boxed{\Delta E = \langle \alpha_u\alpha_u || \mu_u\mu_u \rangle + \langle \alpha_u\mu_u || \alpha_u\mu_u \rangle}$$

$$\Psi_{13}(a_{1u}e_u, {}^1E_g, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\alpha_u\eta_u}|}{2} - \frac{\sqrt{2}|\alpha_u\bar{\eta}_u|}{2}$$

$$\Psi_{14}(a_{1u}e_u, {}^1E_g, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\alpha_u\mu_u}|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\mu}_u|}{2}$$

 $b_{1g}e_g$

$$\boxed{\Delta E = \langle \gamma_g\gamma_g || \mu_g\mu_g \rangle + \langle \gamma_g\mu_g || \gamma_g\mu_g \rangle}$$

$$\Psi_{15}(b_{1g}e_g, {}^1E_g, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\gamma_g\eta_g}|}{2} + \frac{\sqrt{2}|\gamma_g\bar{\eta}_g|}{2}$$

$$\Psi_{16}(b_{1g}e_g, {}^1E_g, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\gamma_g\mu_g}|}{2} - \frac{\sqrt{2}|\gamma_g\bar{\mu}_g|}{2}$$

2.16 Group C_3 Component labels

$$A : \{\alpha\} \longrightarrow E^1 : \{\beta\} \longrightarrow E^2 : \{\gamma\}$$

$$\Psi_2((e^2)^2, {}^1E^1, M=0, \beta) = -|\bar{\gamma}\gamma|$$

2.16.1 1A a^2

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_1(a^2, {}^1A, M=0, \alpha) = -|\bar{\alpha}\alpha|$$

 $e^1 e^2$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(e^1 e^2, {}^1A, M=0, \alpha) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

2.16.4 ${}^3E^2$ ae^2

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae^2, {}^3E^2, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

$$\Psi_2(ae^2, {}^3E^2, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(ae^2, {}^3E^2, M=1, \gamma) = |\alpha\gamma|$$

2.16.2 ${}^3E^1$ ae^1

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae^1, {}^3E^1, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$\Psi_2(ae^1, {}^3E^1, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(ae^1, {}^3E^1, M=1, \beta) = |\alpha\beta|$$

2.16.5 ${}^1E^2$ ae^2

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae^2, {}^1E^2, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

 $(e^1)^2$

$$\boxed{\Delta E = 0}$$

$$\Psi_2((e^1)^2, {}^1E^2, M=0, \gamma) = -|\bar{\beta}\beta|$$

2.16.3 ${}^1E^1$ ae^1

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae^1, {}^1E^1, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

 $(e^2)^2$

$$\boxed{\Delta E = 0}$$

2.16.6 3A $e^1 e^2$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(e^1 e^2, {}^3A, M=-1, \alpha) = |\bar{\beta}\bar{\gamma}|$$

$$\Psi_2(e^1 e^2, {}^3A, M=0, \alpha) = \frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_3(e^1 e^2, {}^3A, M=1, \alpha) = |\beta\gamma|$$

2.17 Group S_6 Component labels

$$A_g : \{\alpha_g\} \longrightarrow A_u : \{\alpha_u\} \longrightarrow E_u^1 : \{\beta_u\} \longrightarrow E_u^2 : \{\gamma_u\} \longrightarrow E_g^2 : \{\gamma_g\} \longrightarrow E_g^1 : \{\beta_g\}$$

2.17.1 1A_g

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \alpha_g \alpha_g \rangle}$$

 a_g^2

$$\Psi_1(a_g^2, {}^1A_g, M=0, \alpha_g) = -|\bar{\alpha}_g \alpha_g|$$

a_u^2	$e_g^1 e_u^1$
$\boxed{\Delta E = \langle \alpha_u \alpha_u \alpha_u \alpha_u \rangle}$	$\boxed{\Delta E = 0}$
$\Psi_2(a_u^2, {}^1A_g, M=0, \alpha_g) = - \overline{\alpha_u} \alpha_u $	$\Psi_2(e_g^1 e_u^1, {}^1A_u, M=0, \alpha_u) = -\frac{\sqrt{2} \overline{\beta_u} \beta_g }{2} + \frac{\sqrt{2} \beta_u \overline{\beta_g} }{2}$
$e_u^1 e_u^2$	$e_g^2 e_u^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_3(e_u^1 e_u^2, {}^1A_g, M=0, \alpha_g) = -\frac{\sqrt{2} \overline{\beta_u} \gamma_u }{2} + \frac{\sqrt{2} \beta_u \overline{\gamma_u} }{2}$	$\Psi_3(e_g^2 e_u^2, {}^1A_u, M=0, \alpha_u) = -\frac{\sqrt{2} \overline{\gamma_u} \gamma_g }{2} + \frac{\sqrt{2} \gamma_u \overline{\gamma_g} }{2}$
$e_g^1 e_g^2$	
$\boxed{\Delta E = 0}$	
$\Psi_4(e_g^1 e_g^2, {}^1A_g, M=0, \alpha_g) = -\frac{\sqrt{2} \overline{\gamma_g} \beta_g }{2} + \frac{\sqrt{2} \gamma_g \overline{\beta_g} }{2}$	
<hr/>	<hr/>
2.17.2	3A_u
$a_g a_u$	
$\boxed{\Delta E = -\langle \alpha_g \alpha_g \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u \alpha_g \alpha_u \rangle}$	
$\Psi_1(a_g a_u, {}^3A_u, M=-1, \alpha_u) = \overline{\alpha_g} \alpha_u $	$\Psi_1(a_g e_u^1, {}^3E_u^1, M=-1, \beta_u) = \overline{\alpha_g} \beta_u $
$\Psi_2(a_g a_u, {}^3A_u, M=0, \alpha_u) = \frac{\sqrt{2} \overline{\alpha_g} \alpha_u }{2} + \frac{\sqrt{2} \alpha_g \overline{\alpha_u} }{2}$	$\Psi_2(a_g e_u^1, {}^3E_u^1, M=0, \beta_u) = \frac{\sqrt{2} \overline{\alpha_g} \beta_u }{2} + \frac{\sqrt{2} \alpha_g \overline{\beta_u} }{2}$
$\Psi_3(a_g a_u, {}^3A_u, M=1, \alpha_u) = \alpha_g \alpha_u $	$\Psi_3(a_g e_u^1, {}^3E_u^1, M=1, \beta_u) = \alpha_g \beta_u $
$e_g^1 e_u^1$	$a_u e_g^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_4(e_g^1 e_u^1, {}^3A_u, M=-1, \alpha_u) = \overline{\beta_u} \beta_g $	$\Psi_4(a_u e_g^2, {}^3E_u^1, M=-1, \beta_u) = \overline{\alpha_u} \gamma_g $
$\Psi_5(e_g^1 e_u^1, {}^3A_u, M=0, \alpha_u) = \frac{\sqrt{2} \overline{\beta_u} \beta_g }{2} + \frac{\sqrt{2} \beta_u \overline{\beta_g} }{2}$	$\Psi_5(a_u e_g^2, {}^3E_u^1, M=0, \beta_u) = \frac{\sqrt{2} \overline{\alpha_u} \gamma_g }{2} + \frac{\sqrt{2} \alpha_u \overline{\gamma_g} }{2}$
$\Psi_6(e_g^1 e_u^1, {}^3A_u, M=1, \alpha_u) = \beta_u \beta_g $	$\Psi_6(a_u e_g^2, {}^3E_u^1, M=1, \beta_u) = \alpha_u \gamma_g $
$e_g^2 e_u^2$	$e_g^1 e_u^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_7(e_g^2 e_u^2, {}^3A_u, M=-1, \alpha_u) = \overline{\gamma_u} \gamma_g $	$\Psi_7(e_g^1 e_u^2, {}^3E_u^1, M=-1, \beta_u) = \overline{\gamma_u} \beta_g $
$\Psi_8(e_g^2 e_u^2, {}^3A_u, M=0, \alpha_u) = \frac{\sqrt{2} \overline{\gamma_u} \gamma_g }{2} + \frac{\sqrt{2} \gamma_u \overline{\gamma_g} }{2}$	$\Psi_8(e_g^1 e_u^2, {}^3E_u^1, M=0, \beta_u) = \frac{\sqrt{2} \overline{\gamma_u} \beta_g }{2} + \frac{\sqrt{2} \gamma_u \overline{\beta_g} }{2}$
$\Psi_9(e_g^2 e_u^2, {}^3A_u, M=1, \alpha_u) = \gamma_u \gamma_g $	$\Psi_9(e_g^1 e_u^2, {}^3E_u^1, M=1, \beta_u) = \gamma_u \beta_g $
<hr/>	<hr/>
2.17.3	1A_u
$a_g a_u$	
$\boxed{\Delta E = \langle \alpha_g \alpha_g \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u \alpha_g \alpha_u \rangle}$	$\boxed{\Delta E = 0}$
$\Psi_1(a_g a_u, {}^1A_u, M=0, \alpha_u) = -\frac{\sqrt{2} \overline{\alpha_g} \alpha_u }{2} + \frac{\sqrt{2} \alpha_g \overline{\alpha_u} }{2}$	$\Psi_1(a_g e_u^1, {}^1E_u^1, M=0, \beta_u) = -\frac{\sqrt{2} \overline{\alpha_g} \beta_u }{2} + \frac{\sqrt{2} \alpha_g \overline{\beta_u} }{2}$
$a_u e_g^2$	$a_u e_g^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_2(a_u e_g^2, {}^1E_u^1, M=0, \beta_u) = -\frac{\sqrt{2} \overline{\alpha_u} \gamma_g }{2} + \frac{\sqrt{2} \alpha_u \overline{\gamma_g} }{2}$	$\Psi_2(a_u e_g^2, {}^1E_u^1, M=0, \beta_u) = -\frac{\sqrt{2} \overline{\alpha_u} \gamma_g }{2} + \frac{\sqrt{2} \alpha_u \overline{\gamma_g} }{2}$

$e_g^1 e_u^2$	$\Delta E = 0$	—————
$\Psi_3(e_g^1 e_u^2, {}^1E_u^2, M=0, \gamma_u) = -\frac{\sqrt{2} \gamma_u \beta_g }{2} + \frac{\sqrt{2} \gamma_u \bar{\beta}_g }{2}$	$\mathbf{2.17.8} \quad {}^3E_g^2$	$a_g e_g^2$
$a_g e_u^2$	$\Delta E = 0$	—————
$\mathbf{2.17.6} \quad {}^3E_u^2$	$\Delta E = 0$	$\Psi_1(a_g e_g^2, {}^3E_g^2, M=-1, \gamma_g) = \alpha_g \gamma_g $
$a_g e_u^2$	$\Delta E = 0$	$\Psi_2(a_g e_g^2, {}^3E_g^2, M=0, \gamma_g) = \frac{\sqrt{2} \alpha_g \gamma_g }{2} + \frac{\sqrt{2} \alpha_g \bar{\gamma}_g }{2}$
$\Psi_1(a_g e_u^2, {}^3E_u^2, M=-1, \gamma_u) = \overline{\alpha_g} \gamma_u $	$\Delta E = 0$	$\Psi_3(a_g e_g^2, {}^3E_g^2, M=1, \gamma_g) = \alpha_g \gamma_g $
$a_u e_g^1$	$\Delta E = 0$	$a_u e_u^1$
$\Psi_4(a_u e_g^1, {}^3E_u^2, M=-1, \gamma_u) = \overline{\alpha_u} \beta_g $	$\Delta E = 0$	$\Psi_4(a_u e_u^1, {}^3E_g^2, M=-1, \gamma_g) = \overline{\alpha_u} \beta_u $
$\Psi_5(a_u e_g^1, {}^3E_u^2, M=0, \gamma_u) = \frac{\sqrt{2} \overline{\alpha_u} \beta_g }{2} + \frac{\sqrt{2} \alpha_u \beta_g }{2}$	$\Delta E = 0$	$\Psi_5(a_u e_g^1, {}^3E_g^2, M=0, \gamma_g) = \frac{\sqrt{2} \overline{\alpha_u} \beta_u }{2} + \frac{\sqrt{2} \alpha_u \bar{\beta}_u }{2}$
$\Psi_6(a_u e_g^1, {}^3E_u^2, M=1, \gamma_u) = \alpha_u \beta_g $	$\Delta E = 0$	$\Psi_6(a_u e_u^1, {}^3E_g^2, M=1, \gamma_g) = \alpha_u \beta_u $
$e_g^2 e_u^1$	$\Delta E = 0$	—————
$\Psi_7(e_g^2 e_u^1, {}^3E_u^2, M=-1, \gamma_u) = \overline{\beta_u} \gamma_g $	$\Delta E = 0$	$\mathbf{2.17.9} \quad {}^1E_g^2$
$\Psi_8(e_g^2 e_u^1, {}^3E_u^2, M=0, \gamma_u) = \frac{\sqrt{2} \overline{\beta_u} \gamma_g }{2} + \frac{\sqrt{2} \beta_u \overline{\gamma_g} }{2}$	$\Delta E = 0$	$a_g e_g^2$
$\Psi_9(e_g^2 e_u^1, {}^3E_u^2, M=1, \gamma_u) = \beta_u \gamma_g $	$\Delta E = 0$	$\Delta E = 0$
$\Psi_1(a_g e_g^2, {}^1E_g^2, M=0, \gamma_g) = -\frac{\sqrt{2} \overline{\alpha_g} \gamma_g }{2} + \frac{\sqrt{2} \alpha_g \overline{\gamma_g} }{2}$	$\Delta E = 0$	$a_u e_u^1$
$a_g e_u^2$	$\Delta E = 0$	$\Delta E = 0$
$\mathbf{2.17.7} \quad {}^1E_u^2$	$\Delta E = 0$	$\Psi_2(a_u e_u^1, {}^1E_g^2, M=0, \gamma_g) = -\frac{\sqrt{2} \overline{\alpha_u} \beta_u }{2} + \frac{\sqrt{2} \alpha_u \bar{\beta}_u }{2}$
$a_u e_g^1$	$\Delta E = 0$	$(e_u^2)^2$
$\Psi_1(a_g e_u^2, {}^1E_u^2, M=0, \gamma_u) = -\frac{\sqrt{2} \overline{\alpha_g} \gamma_u }{2} + \frac{\sqrt{2} \alpha_g \overline{\gamma_u} }{2}$	$\Delta E = 0$	$\Delta E = 0$
$a_u e_g^1$	$\Delta E = 0$	$\Psi_3((e_u^2)^2, {}^1E_g^2, M=0, \gamma_g) = - \overline{\gamma_u} \gamma_u $
$\Psi_2(a_u e_g^1, {}^1E_u^2, M=0, \gamma_u) = -\frac{\sqrt{2} \overline{\alpha_u} \beta_g }{2} + \frac{\sqrt{2} \alpha_u \bar{\beta}_g }{2}$	$\Delta E = 0$	$(e_g^1)^2$
$e_g^2 e_u^1$	$\Delta E = 0$	$\Delta E = 0$
$\Psi_3(e_g^2 e_u^1, {}^1E_u^2, M=0, \gamma_u) = -\frac{\sqrt{2} \overline{\beta_u} \gamma_g }{2} + \frac{\sqrt{2} \beta_u \overline{\gamma_g} }{2}$	$\Delta E = 0$	$\Psi_4((e_g^1)^2, {}^1E_g^2, M=0, \gamma_g) = - \overline{\beta_g} \beta_g $

2.17.10 $^3E_g^1$ $a_g e_g^1$ $\boxed{\Delta E = 0}$ $\Psi_1(a_g e_g^1, ^3E_g^1, M= -1, \beta_g) = \overline{\alpha_g} \beta_g $ $\Psi_2(a_g e_g^1, ^3E_g^1, M= 0, \beta_g) = \frac{\sqrt{2} \overline{\alpha_g} \beta_g }{2} + \frac{\sqrt{2} \alpha_g \overline{\beta_g} }{2}$ $\Psi_3(a_g e_g^1, ^3E_g^1, M= 1, \beta_g) = \alpha_g \beta_g $ $a_u e_u^2$ $\boxed{\Delta E = 0}$ $\Psi_4(a_u e_u^2, ^3E_g^1, M= -1, \beta_g) = \overline{\alpha_u} \gamma_u $ $\Psi_5(a_u e_u^2, ^3E_g^1, M= 0, \beta_g) = \frac{\sqrt{2} \overline{\alpha_u} \gamma_u }{2} + \frac{\sqrt{2} \alpha_u \overline{\gamma_u} }{2}$ $\Psi_6(a_u e_u^2, ^3E_g^1, M= 1, \beta_g) = \alpha_u \gamma_u $	$(e_u^1)^2$ $\boxed{\Delta E = 0}$ $\Psi_3((e_u^1)^2, ^1E_g^1, M= 0, \beta_g) = - \overline{\beta_u} \beta_u $ $(e_g^2)^2$ $\boxed{\Delta E = 0}$ $\Psi_4((e_g^2)^2, ^1E_g^1, M= 0, \beta_g) = - \overline{\gamma_g} \gamma_g $
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2.17.11 $^1E_g^1$ $a_g e_g^1$ $\boxed{\Delta E = 0}$ $\Psi_1(a_g e_g^1, ^1E_g^1, M= 0, \beta_g) = -\frac{\sqrt{2} \overline{\alpha_g} \beta_g }{2} + \frac{\sqrt{2} \alpha_g \overline{\beta_g} }{2}$ $a_u e_u^2$ $\boxed{\Delta E = 0}$ $\Psi_2(a_u e_u^2, ^1E_g^1, M= 0, \beta_g) = -\frac{\sqrt{2} \overline{\alpha_u} \gamma_u }{2} + \frac{\sqrt{2} \alpha_u \overline{\gamma_u} }{2}$	2.17.12 3A_g $e_u^1 e_u^2$ $\boxed{\Delta E = 0}$ $\Psi_1(e_u^1 e_u^2, ^3A_g, M= -1, \alpha_g) = \overline{\beta_u} \gamma_u $ $\Psi_2(e_u^1 e_u^2, ^3A_g, M= 0, \alpha_g) = \frac{\sqrt{2} \overline{\beta_u} \gamma_u }{2} + \frac{\sqrt{2} \beta_u \overline{\gamma_u} }{2}$ $\Psi_3(e_u^1 e_u^2, ^3A_g, M= 1, \alpha_g) = \beta_u \gamma_u $ $e_g^1 e_g^2$ $\boxed{\Delta E = 0}$ $\Psi_4(e_g^1 e_g^2, ^3A_g, M= -1, \alpha_g) = \overline{\gamma_g} \beta_g $ $\Psi_5(e_g^1 e_g^2, ^3A_g, M= 0, \alpha_g) = \frac{\sqrt{2} \overline{\gamma_g} \beta_g }{2} + \frac{\sqrt{2} \gamma_g \overline{\beta_g} }{2}$ $\Psi_6(e_g^1 e_g^2, ^3A_g, M= 1, \alpha_g) = \gamma_g \beta_g $
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2.18 Group D_3 <u>Component labels</u> $A_1 : \{\alpha\} \longrightarrow A_2 : \{\beta\} \longrightarrow E : \{\gamma, \zeta\}$	e^2 $\boxed{\Delta E = \langle \zeta \zeta \gamma \gamma \rangle + \langle \zeta \zeta \zeta \zeta \rangle}$ $\Psi_3(e^2, ^1A_1, M= 0, \alpha) = -\frac{\sqrt{2} \overline{\gamma} \gamma }{2} - \frac{\sqrt{2} \overline{\zeta} \zeta }{2}$
2.18.1 1A_1 a_1^2 $\boxed{\Delta E = \langle \alpha \alpha \alpha \alpha \rangle}$ $\Psi_1(a_1^2, ^1A_1, M= 0, \alpha) = - \overline{\alpha} \alpha $ a_2^2 $\boxed{\Delta E = \langle \beta \beta \beta \beta \rangle}$ $\Psi_2(a_2^2, ^1A_1, M= 0, \alpha) = - \overline{\beta} \beta $	2.18.2 3A_2 $a_1 a_2$ $\boxed{\Delta E = -\langle \alpha \alpha \beta \beta \rangle + \langle \alpha \beta \alpha \beta \rangle}$ $\Psi_1(a_1 a_2, ^3A_2, M= -1, \beta) = \overline{\alpha} \overline{\beta} $

$$\Psi_2(a_1a_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(a_1a_2, {}^3A_2, M=1, \beta) = |\alpha\beta|$$

a₂e

$$\boxed{\Delta E = -\langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle}$$

e²

$$\boxed{\Delta E = -3\langle \zeta\zeta || \gamma\gamma \rangle + \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\Psi_4(e^2, {}^3A_2, M=-1, \beta) = -|\bar{\gamma}\bar{\zeta}|$$

$$\Psi_5(e^2, {}^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\bar{\zeta}\gamma|}{2}$$

$$\Psi_6(e^2, {}^3A_2, M=1, \beta) = -|\gamma\zeta|$$

$$\Psi_7(a_2e, {}^3E, M=-1, \zeta) = -|\bar{\beta}\bar{\gamma}|$$

$$\Psi_8(a_2e, {}^3E, M=-1, \gamma) = |\bar{\beta}\zeta|$$

$$\Psi_9(a_2e, {}^3E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} - \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_{10}(a_2e, {}^3E, M=0, \gamma) = \frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

$$\Psi_{11}(a_2e, {}^3E, M=1, \zeta) = -|\beta\gamma|$$

$$\Psi_{12}(a_2e, {}^3E, M=1, \gamma) = |\beta\zeta|$$

2.18.3 ¹A₂*a₁a₂*

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a_1a_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

2.18.5 ¹E*a₁e*

$$\boxed{\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1e, {}^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_2(a_1e, {}^1E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

2.18.4 ³E*a₁e*

$$\boxed{\Delta E = -\langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1e, {}^3E, M=-1, \gamma) = |\bar{\alpha}\bar{\gamma}|$$

$$\Psi_2(a_1e, {}^3E, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}|$$

$$\Psi_3(a_1e, {}^3E, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_4(a_1e, {}^3E, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_5(a_1e, {}^3E, M=1, \gamma) = |\alpha\gamma|$$

$$\Psi_6(a_1e, {}^3E, M=1, \zeta) = |\alpha\zeta|$$

a₂e

$$\boxed{\Delta E = \langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle}$$

$$\Psi_3(a_2e, {}^1E, M=0, \zeta) = \frac{\sqrt{2}|\bar{\beta}\gamma|}{2} - \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_4(a_2e, {}^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

e²

$$\boxed{\Delta E = -\langle \zeta\zeta || \gamma\gamma \rangle + \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\Psi_5(e^2, {}^1E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\gamma|}{2} + \frac{\sqrt{2}|\gamma\bar{\gamma}|}{2}$$

$$\Psi_6(e^2, {}^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} - \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

2.19 Group C_{3v}Component labels

$$A_1 : \{\alpha\} \longrightarrow A_2 : \{\beta\} \longrightarrow E : \{\gamma, \zeta\}$$

$$\Psi_1(a_1^2, {}^1A_1, M=0, \alpha) = -|\bar{\alpha}\alpha|$$

2.19.1 ¹A₁*a₂²*

$$\boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle}$$

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_2(a_2^2, {}^1A_1, M=0, \alpha) = -|\bar{\beta}\beta|$$

e^2

$$\Delta E = \langle \zeta\zeta || \gamma\gamma \rangle + \langle \zeta\zeta || \zeta\zeta \rangle$$

$$\Psi_3(e^2, {}^1A_1, M=0, \alpha) = -\frac{\sqrt{2}|\bar{\gamma}\gamma|}{2} - \frac{\sqrt{2}|\bar{\zeta}\zeta|}{2}$$

$$\Psi_2(a_1e, {}^3E, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}|$$

$$\Psi_3(a_1e, {}^3E, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_4(a_1e, {}^3E, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_5(a_1e, {}^3E, M=1, \gamma) = |\alpha\gamma|$$

$$\Psi_6(a_1e, {}^3E, M=1, \zeta) = |\alpha\zeta|$$

2.19.2 3A_2 a_1a_2

$$\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle$$

$$\Psi_1(a_1a_2, {}^3A_2, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$\Psi_2(a_1a_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(a_1a_2, {}^3A_2, M=1, \beta) = |\alpha\beta|$$

 e^2

$$\Delta E = -3\langle \zeta\zeta || \gamma\gamma \rangle + \langle \zeta\zeta || \zeta\zeta \rangle$$

$$\Psi_4(e^2, {}^3A_2, M=-1, \beta) = -|\bar{\gamma}\bar{\zeta}|$$

$$\Psi_5(e^2, {}^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\bar{\zeta}\gamma|}{2}$$

$$\Psi_6(e^2, {}^3A_2, M=1, \beta) = -|\gamma\zeta|$$

2.19.3 1A_2 a_1a_2

$$\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle$$

$$\Psi_1(a_1a_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

2.19.4 3E a_1e

$$\Delta E = -\langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle$$

$$\Psi_1(a_1e, {}^3E, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

$$\Psi_2(a_1e, {}^3E, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}|$$

$$\Psi_3(a_1e, {}^3E, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_4(a_1e, {}^3E, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_5(a_1e, {}^3E, M=1, \gamma) = |\alpha\gamma|$$

$$\Psi_6(a_1e, {}^3E, M=1, \zeta) = |\alpha\zeta|$$

 a_2e

$$\Delta E = -\langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle$$

$$\Psi_7(a_2e, {}^3E, M=-1, \zeta) = -|\bar{\beta}\bar{\gamma}|$$

$$\Psi_8(a_2e, {}^3E, M=-1, \gamma) = |\bar{\beta}\gamma|$$

$$\Psi_9(a_2e, {}^3E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} - \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_{10}(a_2e, {}^3E, M=0, \gamma) = \frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

$$\Psi_{11}(a_2e, {}^3E, M=1, \zeta) = -|\beta\gamma|$$

$$\Psi_{12}(a_2e, {}^3E, M=1, \gamma) = |\beta\zeta|$$

2.19.5 1E a_1e

$$\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle$$

$$\Psi_1(a_1e, {}^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_2(a_1e, {}^1E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

 a_2e

$$\Delta E = \langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle$$

$$\Psi_3(a_2e, {}^1E, M=0, \zeta) = \frac{\sqrt{2}|\bar{\beta}\gamma|}{2} - \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_4(a_2e, {}^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

 e^2

$$\Delta E = -\langle \zeta\zeta || \gamma\gamma \rangle + \langle \zeta\zeta || \zeta\zeta \rangle$$

$$\Psi_5(e^2, {}^1E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\bar{\zeta}\gamma|}{2}$$

$$\Psi_6(e^2, {}^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\gamma}\gamma|}{2} - \frac{\sqrt{2}|\bar{\zeta}\zeta|}{2}$$

2.20 Group D_{3d} Component labels

$$A_{1g} : \{\alpha_g\} \longrightarrow A_{1u} : \{\alpha_u\} \longrightarrow A_{2u} : \{\beta_u\} \longrightarrow A_{2g} : \{\beta_g\} \longrightarrow E_g : \{\gamma_g, \zeta_g\} \longrightarrow E_u : \{\gamma_u, \zeta_u\}$$

2.20.1 $^1A_{1g}$ a_{1g}^2

$$\boxed{\Delta E = \langle \alpha_g \alpha_g | | \alpha_g \alpha_g \rangle}$$

$$\Psi_1(a_{1g}^2, ^1A_{1g}, M=0, \alpha_g) = -|\overline{\alpha_g} \alpha_g|$$

 a_{1u}^2

$$\boxed{\Delta E = \langle \alpha_u \alpha_u | | \alpha_u \alpha_u \rangle}$$

$$\Psi_2(a_{1u}^2, ^1A_{1g}, M=0, \alpha_g) = -|\overline{\alpha_u} \alpha_u|$$

 a_{2u}^2

$$\boxed{\Delta E = \langle \beta_u \beta_u | | \beta_u \beta_u \rangle}$$

$$\Psi_3(a_{2u}^2, ^1A_{1g}, M=0, \alpha_g) = -|\overline{\beta_u} \beta_u|$$

 a_{2g}^2

$$\boxed{\Delta E = \langle \beta_g \beta_g | | \beta_g \beta_g \rangle}$$

$$\Psi_4(a_{2g}^2, ^1A_{1g}, M=0, \alpha_g) = -|\overline{\beta_g} \beta_g|$$

 e_g^2

$$\boxed{\Delta E = \langle \zeta_g \zeta_g | | \gamma_g \gamma_g \rangle + \langle \zeta_g \zeta_g | | \zeta_g \zeta_g \rangle}$$

$$\Psi_5(e_g^2, ^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{2}|\overline{\gamma_g} \gamma_g|}{2} - \frac{\sqrt{2}|\overline{\zeta_g} \zeta_g|}{2}$$

 e_u^2

$$\boxed{\Delta E = \langle \zeta_u \zeta_u | | \gamma_u \gamma_u \rangle + \langle \zeta_u \zeta_u | | \zeta_u \zeta_u \rangle}$$

$$\Psi_6(e_u^2, ^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{2}|\overline{\gamma_u} \gamma_u|}{2} - \frac{\sqrt{2}|\overline{\zeta_u} \zeta_u|}{2}$$

2.20.2 $^3A_{1u}$
 $a_{1g} a_{1u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g | | \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u | | \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_{1g} a_{1u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\alpha_g} \alpha_u|$$

$$\Psi_2(a_{1g} a_{1u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\alpha_g} \alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\alpha_u}|}{2}$$

$$\Psi_3(a_{1g} a_{1u}, ^3A_{1u}, M=1, \alpha_u) = |\alpha_g \alpha_u|$$

 $a_{2g} a_{2u}$

$$\boxed{\Delta E = \langle \beta_u \beta_g | | \beta_u \beta_g \rangle - \langle \beta_u \beta_u | | \beta_g \beta_g \rangle}$$

$$\Psi_4(a_{2g} a_{2u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\beta_u} \beta_g|$$

$$\Psi_5(a_{2g} a_{2u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\beta_u} \beta_g|}{2} + \frac{\sqrt{2}|\beta_u \overline{\beta_g}|}{2}$$

$$\Psi_6(a_{2g} a_{2u}, ^3A_{1u}, M=1, \alpha_u) = |\beta_u \beta_g|$$

 $e_g e_u$

$$\boxed{\Delta E = -\langle \zeta_g \zeta_g | | \gamma_u \gamma_u \rangle - 3\langle \zeta_g \zeta_u | | \gamma_g \gamma_u \rangle + \langle \zeta_g \zeta_u | | \zeta_g \zeta_u \rangle + \langle \zeta_g \gamma_g | | \zeta_u \gamma_u \rangle}$$

$$\Psi_7(e_g e_u, ^3A_{1u}, M=-1, \alpha_u) = -\frac{\sqrt{2}|\overline{\gamma_g} \zeta_u|}{2} + \frac{\sqrt{2}|\overline{\zeta_g} \gamma_u|}{2}$$

$$\Psi_8(e_g e_u, ^3A_{1u}, M=0, \alpha_u) = -\frac{|\overline{\gamma_g} \zeta_u|}{2} + \frac{|\overline{\zeta_g} \gamma_u|}{2} - \frac{|\gamma_g \overline{\zeta_u}|}{2} + \frac{|\zeta_g \overline{\gamma_u}|}{2}$$

$$\Psi_9(e_g e_u, ^3A_{1u}, M=1, \alpha_u) = -\frac{\sqrt{2}|\gamma_g \zeta_u|}{2} + \frac{\sqrt{2}|\zeta_g \gamma_u|}{2}$$

2.20.3 $^1A_{1u}$
 $a_{1g} a_{1u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g | | \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u | | \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_{1g} a_{1u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\alpha_g} \alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\alpha_u}|}{2}$$

 $a_{2g} a_{2u}$

$$\boxed{\Delta E = \langle \beta_u \beta_g | | \beta_u \beta_g \rangle + \langle \beta_u \beta_u | | \beta_g \beta_g \rangle}$$

$$\Psi_2(a_{2g} a_{2u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\beta_u} \beta_g|}{2} + \frac{\sqrt{2}|\beta_u \overline{\beta_g}|}{2}$$

 $e_g e_u$

$$\boxed{\Delta E = \langle \zeta_g \zeta_g | | \gamma_u \gamma_u \rangle - 3\langle \zeta_g \zeta_u | | \gamma_g \gamma_u \rangle + \langle \zeta_g \zeta_u | | \zeta_g \zeta_u \rangle - \langle \zeta_g \gamma_g | | \zeta_u \gamma_u \rangle}$$

$$\Psi_3(e_g e_u, ^1A_{1u}, M=0, \alpha_u) = \frac{|\overline{\gamma_g} \zeta_u|}{2} - \frac{|\overline{\zeta_g} \gamma_u|}{2} - \frac{|\gamma_g \overline{\zeta_u}|}{2} + \frac{|\zeta_g \overline{\gamma_u}|}{2}$$

2.20.4 $^3A_{2u}$ *a_{1g}a_{2u}*

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \beta_u \beta_u \rangle + \langle \alpha_g \beta_u || \alpha_g \beta_u \rangle}$$

$$\Psi_1(a_{1g}a_{2u}, ^3A_{2u}, M=-1, \beta_u) = |\overline{\alpha_g} \overline{\beta_u}|$$

$$\Psi_2(a_{1g}a_{2u}, ^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\alpha_g} \beta_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_u}|}{2}$$

$$\Psi_3(a_{1g}a_{2u}, ^3A_{2u}, M=1, \beta_u) = |\alpha_g \beta_u|$$

a_{1u}a_{2g}

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \beta_g \beta_g \rangle + \langle \alpha_u \beta_g || \alpha_u \beta_g \rangle}$$

$$\Psi_4(a_{1u}a_{2g}, ^3A_{2u}, M=-1, \beta_u) = |\overline{\alpha_u} \overline{\beta_g}|$$

$$\Psi_5(a_{1u}a_{2g}, ^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\alpha_u} \beta_g|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\beta_g}|}{2}$$

$$\Psi_6(a_{1u}a_{2g}, ^3A_{2u}, M=1, \beta_u) = |\alpha_u \beta_g|$$

e_ge_u

$$\boxed{\Delta E = -2 \langle \zeta_g \zeta_g || \zeta_u \zeta_u \rangle + \langle \zeta_g \zeta_u || \gamma_g \gamma_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle \\ + \langle \zeta_g \gamma_g || \zeta_u \gamma_u \rangle + \langle \zeta_g \zeta_g || \gamma_u \gamma_u \rangle}$$

$$\Psi_7(e_g e_u, ^3A_{2u}, M=-1, \beta_u) = \frac{\sqrt{2}|\overline{\gamma_g} \overline{\gamma_u}|}{2} + \frac{\sqrt{2}|\zeta_g \zeta_u|}{2}$$

$$\Psi_8(e_g e_u, ^3A_{2u}, M=0, \beta_u) = \frac{|\overline{\gamma_g} \gamma_u|}{2} + \frac{|\zeta_g \zeta_u|}{2} + \frac{|\gamma_g \overline{\gamma_u}|}{2} + \frac{|\zeta_g \overline{\zeta_u}|}{2}$$

$$\Psi_9(e_g e_u, ^3A_{2u}, M=1, \beta_u) = \frac{\sqrt{2}|\gamma_g \gamma_u|}{2} + \frac{\sqrt{2}|\zeta_g \zeta_u|}{2}$$

2.20.5 $^1A_{2u}$ *a_{1g}a_{2u}*

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_u \beta_u \rangle + \langle \alpha_g \beta_u || \alpha_g \beta_u \rangle}$$

$$\Psi_1(a_{1g}a_{2u}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\alpha_g} \beta_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_u}|}{2}$$

a_{1u}a_{2g}

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \beta_g \beta_g \rangle + \langle \alpha_u \beta_g || \alpha_u \beta_g \rangle}$$

$$\Psi_2(a_{1u}a_{2g}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\alpha_u} \beta_g|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\beta_g}|}{2}$$

e_ge_u

$$\boxed{\Delta E = 2 \langle \zeta_g \zeta_g || \zeta_u \zeta_u \rangle + \langle \zeta_g \zeta_u || \gamma_g \gamma_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle \\ - \langle \zeta_g \gamma_g || \zeta_u \gamma_u \rangle - \langle \zeta_g \zeta_g || \gamma_u \gamma_u \rangle}$$

$$\Psi_3(e_g e_u, ^1A_{2u}, M=0, \beta_u) = -\frac{|\overline{\gamma_g} \gamma_u|}{2} - \frac{|\zeta_g \zeta_u|}{2} + \frac{|\gamma_g \overline{\gamma_u}|}{2} + \frac{|\zeta_g \overline{\zeta_u}|}{2}$$

2.20.6 $^3A_{2g}$ *a_{1g}a_{2g}*

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_{1g}a_{2g}, ^3A_{2g}, M=-1, \beta_g) = |\overline{\alpha_g} \overline{\beta_g}|$$

$$\Psi_2(a_{1g}a_{2g}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\alpha_g} \beta_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_g}|}{2}$$

$$\Psi_3(a_{1g}a_{2g}, ^3A_{2g}, M=1, \beta_g) = |\alpha_g \beta_g|$$

a_{1u}a_{2u}

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \beta_u \beta_u \rangle + \langle \alpha_u \beta_u || \alpha_u \beta_u \rangle}$$

$$\Psi_4(a_{1u}a_{2u}, ^3A_{2g}, M=-1, \beta_g) = |\overline{\alpha_u} \overline{\beta_u}|$$

$$\Psi_5(a_{1u}a_{2u}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\alpha_u} \beta_u|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\beta_u}|}{2}$$

$$\Psi_6(a_{1u}a_{2u}, ^3A_{2g}, M=1, \beta_g) = |\alpha_u \beta_u|$$

e_g²

$$\boxed{\Delta E = -3 \langle \zeta_g \zeta_g || \gamma_g \gamma_g \rangle + \langle \zeta_g \zeta_g || \zeta_g \zeta_g \rangle}$$

$$\Psi_7(e_g^2, ^3A_{2g}, M=-1, \beta_g) = -|\overline{\gamma_g} \overline{\zeta_g}|$$

$$\Psi_8(e_g^2, ^3A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\gamma_g} \zeta_g|}{2} + \frac{\sqrt{2}|\overline{\zeta_g} \gamma_g|}{2}$$

$$\Psi_9(e_g^2, ^3A_{2g}, M=1, \beta_g) = -|\gamma_g \zeta_g|$$

e_u²

$$\boxed{\Delta E = -3 \langle \zeta_u \zeta_u || \gamma_u \gamma_u \rangle + \langle \zeta_u \zeta_u || \zeta_u \zeta_u \rangle}$$

$$\Psi_{10}(e_u^2, ^3A_{2g}, M=-1, \beta_g) = -|\overline{\gamma_u} \overline{\zeta_u}|$$

$$\Psi_{11}(e_u^2, ^3A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\gamma_u} \zeta_u|}{2} + \frac{\sqrt{2}|\overline{\zeta_u} \gamma_u|}{2}$$

$$\Psi_{12}(e_u^2, ^3A_{2g}, M=1, \beta_g) = -|\gamma_u \zeta_u|$$

2.20.7 $^1A_{2g}$ *a_{1g}a_{2g}*

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_{1g}a_{2g}, ^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\alpha_g} \beta_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_g}|}{2}$$

a_{1u}a_{2u}

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \beta_u \beta_u \rangle + \langle \alpha_u \beta_u || \alpha_u \beta_u \rangle}$$

$$\Psi_2(a_{1u}a_{2g}, ^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\alpha_u} \beta_g|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\beta_g}|}{2}$$

2.20.8 3E_g **2.20.9** 1E_g $a_{1g}e_g$ $a_{1g}e_g$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \zeta_g \zeta_g \rangle + \langle \alpha_g \zeta_g || \alpha_g \zeta_g \rangle}$$

$$\Psi_1(a_{1g}e_g, ^3E_g, M=-1, \gamma_g) = |\overline{\alpha_g \gamma_g}|$$

$$\Psi_2(a_{1g}e_g, ^3E_g, M=-1, \zeta_g) = |\overline{\alpha_g \zeta_g}|$$

$$\Psi_3(a_{1g}e_g, ^3E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\alpha_g \gamma_g}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\gamma_g}|}{2}$$

$$\Psi_4(a_{1g}e_g, ^3E_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\alpha_g \zeta_g}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\zeta_g}|}{2}$$

$$\Psi_5(a_{1g}e_g, ^3E_g, M=1, \gamma_g) = |\alpha_g \gamma_g|$$

$$\Psi_6(a_{1g}e_g, ^3E_g, M=1, \zeta_g) = |\alpha_g \zeta_g|$$

 $a_{1u}e_u$ $a_{1u}e_u$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \zeta_u \zeta_u \rangle + \langle \alpha_u \zeta_u || \alpha_u \zeta_u \rangle}$$

$$\Psi_7(a_{1u}e_u, ^3E_g, M=-1, \zeta_g) = -|\overline{\alpha_u \gamma_u}|$$

$$\Psi_8(a_{1u}e_u, ^3E_g, M=-1, \gamma_g) = |\overline{\alpha_u \zeta_u}|$$

$$\Psi_9(a_{1u}e_u, ^3E_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\alpha_u \gamma_u}|}{2} - \frac{\sqrt{2}|\alpha_u \overline{\gamma_u}|}{2}$$

$$\Psi_{10}(a_{1u}e_u, ^3E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\alpha_u \zeta_u}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\zeta_u}|}{2}$$

$$\Psi_{11}(a_{1u}e_u, ^3E_g, M=1, \zeta_g) = -|\alpha_u \gamma_u|$$

$$\Psi_{12}(a_{1u}e_u, ^3E_g, M=1, \gamma_g) = |\alpha_u \zeta_u|$$

 $a_{2u}e_u$ $a_{2u}e_u$

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \zeta_u \zeta_u \rangle + \langle \beta_u \zeta_u || \beta_u \zeta_u \rangle}$$

$$\Psi_{13}(a_{2u}e_u, ^3E_g, M=-1, \gamma_g) = |\overline{\beta_u \gamma_u}|$$

$$\Psi_{14}(a_{2u}e_u, ^3E_g, M=-1, \zeta_g) = |\overline{\beta_u \zeta_u}|$$

$$\Psi_{15}(a_{2u}e_u, ^3E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\beta_u \gamma_u}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\gamma_u}|}{2}$$

$$\Psi_{16}(a_{2u}e_u, ^3E_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_u \zeta_u}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\zeta_u}|}{2}$$

$$\Psi_{17}(a_{2u}e_u, ^3E_g, M=1, \gamma_g) = |\beta_u \gamma_u|$$

$$\Psi_{18}(a_{2u}e_u, ^3E_g, M=1, \zeta_g) = |\beta_u \zeta_u|$$

 $a_{2g}e_g$ $a_{2g}e_g$

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \zeta_g \zeta_g \rangle + \langle \beta_g \zeta_g || \beta_g \zeta_g \rangle}$$

$$\Psi_{19}(a_{2g}e_g, ^3E_g, M=-1, \zeta_g) = -|\overline{\beta_g \gamma_g}|$$

$$\Psi_{20}(a_{2g}e_g, ^3E_g, M=-1, \gamma_g) = |\overline{\beta_g \zeta_g}|$$

$$\Psi_{21}(a_{2g}e_g, ^3E_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\beta_g \gamma_g}|}{2} - \frac{\sqrt{2}|\beta_g \overline{\gamma_g}|}{2}$$

$$\Psi_{22}(a_{2g}e_g, ^3E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\beta_g \zeta_g}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\zeta_g}|}{2}$$

$$\Psi_{23}(a_{2g}e_g, ^3E_g, M=1, \zeta_g) = -|\beta_g \gamma_g|$$

$$\Psi_{24}(a_{2g}e_g, ^3E_g, M=1, \gamma_g) = |\beta_g \zeta_g|$$

 $a_{2u}e_u$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \zeta_u \zeta_u \rangle + \langle \beta_u \zeta_u || \beta_u \zeta_u \rangle}$$

$$\Psi_5(a_{2u}e_u, ^1E_g, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\beta_u \gamma_u}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\gamma_u}|}{2}$$

$$\Psi_6(a_{2u}e_u, ^1E_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\beta_u \zeta_u}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\zeta_u}|}{2}$$

 $a_{2g}e_g$

$$\boxed{\Delta E = \langle \beta_g \beta_g || \zeta_g \zeta_g \rangle + \langle \beta_g \zeta_g || \beta_g \zeta_g \rangle}$$

$$\Psi_7(a_{2g}e_g, ^1E_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_g \gamma_g}|}{2} - \frac{\sqrt{2}|\beta_g \overline{\gamma_g}|}{2}$$

$$\Psi_8(a_{2g}e_g, ^1E_g, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\beta_g \zeta_g}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\zeta_g}|}{2}$$

 e_g^2

$$\boxed{\Delta E = -\langle \zeta_g \zeta_g || \gamma_g \gamma_g \rangle + \langle \zeta_g \zeta_g || \zeta_g \zeta_g \rangle}$$

$$\Psi_9(e_g^2, ^1E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\gamma_g \gamma_g}|}{2} - \frac{\sqrt{2}|\zeta_g \overline{\zeta_g}|}{2}$$

$$\Psi_{10}(e_g^2, ^1E_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\gamma_g \zeta_g}|}{2} - \frac{\sqrt{2}|\zeta_g \overline{\gamma_g}|}{2}$$

 e_u^2

$$\boxed{\Delta E = -\langle \zeta_u \zeta_u || \gamma_u \gamma_u \rangle + \langle \zeta_u \zeta_u || \zeta_u \zeta_u \rangle}$$

$$\Psi_{11}(e_u^2, ^1E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\gamma_u \gamma_u}|}{2} - \frac{\sqrt{2}|\zeta_u \overline{\zeta_u}|}{2}$$

$$\Psi_{12}(e_u^2, ^1E_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\gamma_u \zeta_u}|}{2} - \frac{\sqrt{2}|\zeta_u \overline{\gamma_u}|}{2}$$

2.20.10 3E_u $a_{1g}e_u$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u || \alpha_g \zeta_u \rangle}$$

$$\Psi_1(a_{1g}e_u, ^3E_u, M=-1, \gamma_u) = |\overline{\alpha_g \gamma_u}|$$

$$\Psi_2(a_{1g}e_u, ^3E_u, M=-1, \zeta_u) = |\overline{\alpha_g \zeta_u}|$$

$$\Psi_3(a_{1g}e_u, ^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_g \gamma_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\gamma_u}|}{2}$$

$$\Psi_4(a_{1g}e_u, ^3E_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_g \zeta_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\zeta_u}|}{2}$$

$$\Psi_5(a_{1g}e_u, ^3E_u, M=1, \gamma_u) = |\alpha_g \gamma_u|$$

$$\Psi_6(a_{1g}e_u, ^3E_u, M=1, \zeta_u) = |\alpha_g \zeta_u|$$

 $a_{1u}e_g$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \zeta_g \zeta_g \rangle + \langle \alpha_u \zeta_g || \alpha_u \zeta_g \rangle}$$

$$\Psi_7(a_{1u}e_g, ^3E_u, M=-1, \zeta_u) = -|\overline{\alpha_u \gamma_g}|$$

$$\Psi_8(a_{1u}e_g, ^3E_u, M=-1, \gamma_u) = |\overline{\alpha_u \zeta_g}|$$

$$\Psi_9(a_{1u}e_g, ^3E_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_u \gamma_g}|}{2} - \frac{\sqrt{2}|\alpha_u \overline{\gamma_g}|}{2}$$

$$\Psi_{10}(a_{1u}e_g, ^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_u \zeta_g}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\zeta_g}|}{2}$$

$$\Psi_{11}(a_{1u}e_g, ^3E_u, M=1, \zeta_u) = -|\alpha_u \gamma_g|$$

$$\Psi_{12}(a_{1u}e_g, ^3E_u, M=1, \gamma_u) = |\alpha_u \zeta_g|$$

 $a_{2u}e_g$

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \zeta_g \zeta_g \rangle + \langle \beta_u \zeta_g || \beta_u \zeta_g \rangle}$$

$$\Psi_{13}(a_{2u}e_g, ^3E_u, M=-1, \gamma_u) = |\overline{\beta_u \gamma_g}|$$

$$\Psi_{14}(a_{2u}e_g, ^3E_u, M=-1, \zeta_u) = |\overline{\beta_u \zeta_g}|$$

$$\Psi_{15}(a_{2u}e_g, ^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\beta_u \gamma_g}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\gamma_g}|}{2}$$

$$\Psi_{16}(a_{2u}e_g, ^3E_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\beta_u \zeta_g}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\zeta_g}|}{2}$$

$$\Psi_{17}(a_{2u}e_g, ^3E_u, M=1, \gamma_u) = |\beta_u \gamma_g|$$

$$\Psi_{18}(a_{2u}e_g, ^3E_u, M=1, \zeta_u) = |\beta_u \zeta_g|$$

 $a_{2g}e_u$

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \zeta_u \zeta_u \rangle + \langle \beta_g \zeta_u || \beta_g \zeta_u \rangle}$$

$$\Psi_{19}(a_{2g}e_u, ^3E_u, M=-1, \zeta_u) = -|\overline{\beta_g \gamma_u}|$$

$$\Psi_{20}(a_{2g}e_u, ^3E_u, M=-1, \gamma_u) = |\overline{\beta_g \zeta_u}|$$

$$\Psi_{21}(a_{2g}e_u, ^3E_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\beta_g \gamma_u}|}{2} - \frac{\sqrt{2}|\beta_g \overline{\gamma_u}|}{2}$$

$$\Psi_{22}(a_{2g}e_u, ^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\beta_g \zeta_u}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\zeta_u}|}{2}$$

$$\Psi_{23}(a_{2g}e_u, ^3E_u, M=1, \zeta_u) = -|\beta_g \gamma_u|$$

$$\Psi_{24}(a_{2g}e_u, ^3E_u, M=1, \gamma_u) = |\beta_g \zeta_u|$$

 $e_g e_u$

$$\boxed{\Delta E = -\langle \zeta_g \gamma_g || \zeta_u \gamma_u \rangle - \langle \zeta_g \zeta_u || \gamma_g \gamma_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle - \langle \zeta_g \zeta_g || \gamma_u \gamma_u \rangle}$$

$$\Psi_{25}(e_g e_u, ^3E_u, M=-1, \gamma_u) = -\frac{\sqrt{2}|\overline{\gamma_g \gamma_u}|}{2} + \frac{\sqrt{2}|\zeta_g \zeta_u|}{2}$$

$$\Psi_{26}(e_g e_u, ^3E_u, M=-1, \zeta_u) = \frac{\sqrt{2}|\overline{\gamma_g \zeta_u}|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\zeta_u}|}{2}$$

$$\Psi_{27}(e_g e_u, ^3E_u, M=0, \gamma_u) = -\frac{|\overline{\gamma_g \gamma_u}|}{2} + \frac{|\zeta_g \zeta_u|}{2} - \frac{|\gamma_g \overline{\gamma_u}|}{2} + \frac{|\zeta_g \overline{\zeta_u}|}{2}$$

$$\Psi_{28}(e_g e_u, ^3E_u, M=0, \zeta_u) = \frac{|\overline{\gamma_g \zeta_u}|}{2} + \frac{|\gamma_g \overline{\zeta_u}|}{2} + \frac{|\zeta_g \overline{\zeta_u}|}{2} + \frac{|\zeta_g \overline{\gamma_u}|}{2}$$

$$\Psi_{29}(e_g e_u, ^3E_u, M=1, \gamma_u) = -\frac{\sqrt{2}|\overline{\gamma_g \gamma_u}|}{2} + \frac{\sqrt{2}|\zeta_g \zeta_u|}{2}$$

$$\Psi_{30}(e_g e_u, ^3E_u, M=1, \zeta_u) = \frac{\sqrt{2}|\overline{\gamma_g \zeta_u}|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\zeta_u}|}{2}$$

2.20.11 1E_u $a_{1g}e_u$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u || \alpha_g \zeta_u \rangle}$$

$$\Psi_1(a_{1g}e_u, ^1E_u, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\alpha_g \gamma_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\gamma_u}|}{2}$$

$$\Psi_2(a_{1g}e_u, ^1E_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_g \zeta_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\zeta_u}|}{2}$$

 $a_{1u}e_g$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \zeta_g \zeta_g \rangle + \langle \alpha_u \zeta_g || \alpha_u \zeta_g \rangle}$$

$$\Psi_3(a_{1u}e_g, ^1E_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_u \gamma_g}|}{2} - \frac{\sqrt{2}|\alpha_u \overline{\gamma_g}|}{2}$$

$$\Psi_4(a_{1u}e_g, ^1E_u, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\alpha_u \zeta_g}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\zeta_g}|}{2}$$

 $a_{2u}e_g$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \zeta_g \zeta_g \rangle + \langle \beta_u \zeta_g || \beta_u \zeta_g \rangle}$$

$$\Psi_5(a_{2u}e_g, ^1E_u, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\beta_u \gamma_g}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\gamma_g}|}{2}$$

$$\Psi_6(a_{2u}e_g, ^1E_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\beta_u \zeta_g}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\zeta_g}|}{2}$$

 $a_{2g}e_u$

$$\boxed{\Delta E = \langle \beta_g \beta_g || \zeta_u \zeta_u \rangle + \langle \beta_g \zeta_u || \beta_g \zeta_u \rangle}$$

$$\Psi_7(a_{2g}e_u, ^1E_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\beta_g \gamma_u}|}{2} - \frac{\sqrt{2}|\beta_g \overline{\gamma_u}|}{2}$$

$$\Psi_8(a_{2g}e_u, ^1E_u, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\beta_g \zeta_u}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\zeta_u}|}{2}$$

 $e_g e_u$

$$\boxed{\Delta E = \langle \zeta_g \gamma_g || \zeta_u \gamma_u \rangle - \langle \zeta_g \zeta_u || \gamma_g \gamma_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle + \langle \zeta_g \zeta_g || \gamma_u \gamma_u \rangle}$$

$$\Psi_9(e_g e_u, ^1E_u, M=0, \gamma_u) = \frac{|\overline{\gamma_g \gamma_u}|}{2} - \frac{|\zeta_g \zeta_u|}{2} - \frac{|\gamma_g \overline{\gamma_u}|}{2} + \frac{|\zeta_g \overline{\zeta_u}|}{2}$$

$$\Psi_{10}(e_g e_u, ^1E_u, M=0, \zeta_u) = -\frac{|\overline{\gamma_g \zeta_u}|}{2} - \frac{|\zeta_g \gamma_u|}{2} + \frac{|\gamma_g \overline{\zeta_u}|}{2} + \frac{|\zeta_g \overline{\gamma_u}|}{2}$$

2.21 Group C_6

Component labels

$$A : \{\alpha\} \longrightarrow B : \{\beta\} \longrightarrow E'^1 : \{\eta\} \longrightarrow E'^2 : \{\mu\} \longrightarrow E''^2 : \{\zeta\} \longrightarrow E''^1 : \{\gamma\}$$

2.21.1 1A

a^2

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$e''^2 e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(e''^2 e'^2, {}^3B, M=-1, \beta) = |\bar{\mu}\bar{\zeta}|$$

$$\Psi_8(e''^2 e'^2, {}^3B, M=0, \beta) = \frac{\sqrt{2}|\bar{\mu}\bar{\zeta}|}{2} + \frac{\sqrt{2}|\mu\bar{\zeta}|}{2}$$

$$\Psi_9(e''^2 e'^2, {}^3B, M=1, \beta) = |\mu\bar{\zeta}|$$

$$\Psi_1(a^2, {}^1A, M=0, \alpha) = -|\bar{\alpha}\alpha|$$

b^2

$$\boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle}$$

2.21.3 1B

ab

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(ab, {}^1B, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$e''^1 e'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(e''^1 e'^1, {}^1B, M=0, \beta) = -\frac{\sqrt{2}|\bar{\eta}\gamma|}{2} + \frac{\sqrt{2}|\eta\bar{\gamma}|}{2}$$

$$e''^2 e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(e''^2 e'^2, {}^1B, M=0, \beta) = -\frac{\sqrt{2}|\bar{\mu}\bar{\zeta}|}{2} + \frac{\sqrt{2}|\mu\bar{\zeta}|}{2}$$

2.21.2 3B

ab

$$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

2.21.4 ${}^3E'^1$

$$ae'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae'^1, {}^3E'^1, M=-1, \eta) = |\bar{\alpha}\bar{\eta}|$$

$$\Psi_2(ae'^1, {}^3E'^1, M=0, \eta) = \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_3(ae'^1, {}^3E'^1, M=1, \eta) = |\alpha\eta|$$

$$be''^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(be''^2, {}^3E'^1, M=-1, \eta) = |\bar{\beta}\bar{\zeta}|$$

$$\begin{aligned} \Psi_1(e''^1 e'^1, {}^3B, M=-1, \beta) &= |\bar{\eta}\gamma| \\ \Psi_2(e''^1 e'^1, {}^3B, M=0, \beta) &= \frac{\sqrt{2}|\bar{\eta}\gamma|}{2} + \frac{\sqrt{2}|\eta\bar{\gamma}|}{2} \\ \Psi_3(e''^1 e'^1, {}^3B, M=1, \beta) &= |\eta\gamma| \end{aligned}$$

$$\Psi_5(be''^2, {}^3E'^1, M=0, \eta) = \frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

$$\Psi_6(be''^2, {}^3E'^1, M=1, \eta) = |\beta\zeta|$$

$$e''^1 e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(e''^2 e'^1, {}^3E'^2, M=-1, \mu) = |\bar{\eta}\bar{\zeta}|$$

$$\Psi_8(e''^2 e'^1, {}^3E'^2, M=0, \mu) = \frac{\sqrt{2}|\bar{\eta}\zeta|}{2} + \frac{\sqrt{2}|\eta\bar{\zeta}|}{2}$$

$$\Psi_9(e''^2 e'^1, {}^3E'^2, M=1, \mu) = |\eta\zeta|$$

2.21.7 ${}^1E'^2$

$$\boxed{ae'^2}$$

$$\boxed{\Delta E = 0}$$

$$2.21.5 \quad {}^1E'^1$$

$$ae'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae'^2, {}^1E'^2, M=0, \mu) = -\frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$be''^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(be''^1, {}^1E'^2, M=0, \mu) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$e''^2 e'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(e''^2 e'^1, {}^1E'^2, M=0, \mu) = -\frac{\sqrt{2}|\bar{\eta}\zeta|}{2} + \frac{\sqrt{2}|\eta\bar{\zeta}|}{2}$$

2.21.8 ${}^3E''^2$

$$\boxed{ae''^2}$$

$$\boxed{\Delta E = 0}$$

$$2.21.6 \quad {}^3E'^2$$

$$ae'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae'^2, {}^3E'^2, M=-1, \mu) = |\bar{\alpha}\mu|$$

$$\Psi_2(ae'^2, {}^3E'^2, M=0, \mu) = \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_3(ae'^2, {}^3E'^2, M=1, \mu) = |\alpha\mu|$$

$$be''^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(be''^1, {}^3E'^2, M=-1, \mu) = |\bar{\beta}\gamma|$$

$$\Psi_5(be''^1, {}^3E'^2, M=0, \mu) = \frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_6(be''^1, {}^3E'^2, M=1, \mu) = |\beta\gamma|$$

$$e''^2 e'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae''^2, {}^3E''^2, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}|$$

$$\Psi_2(ae''^2, {}^3E''^2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\bar{\zeta}|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_3(ae''^2, {}^3E''^2, M=1, \zeta) = |\alpha\zeta|$$

$$be'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(be'^1, {}^3E''^2, M=-1, \zeta) = |\bar{\beta}\bar{\eta}|$$

$$\Psi_5(be'^1, {}^3E''^2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\beta}\bar{\eta}|}{2} + \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_6(be'^1, {}^3E''^2, M=1, \zeta) = |\beta\eta|$$

2.21.9 ${}^1E''^2$

ae''^2	ae''^1
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_1(ae''^2, {}^1E''^2, M=0, \zeta) = -\frac{\sqrt{2} \bar{\alpha}\zeta }{2} + \frac{\sqrt{2} \alpha\bar{\zeta} }{2}$	$\Psi_1(ae''^1, {}^1E''^1, M=0, \gamma) = -\frac{\sqrt{2} \bar{\alpha}\gamma }{2} + \frac{\sqrt{2} \alpha\bar{\gamma} }{2}$
be'^1	be'^2
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_2(be'^1, {}^1E''^2, M=0, \zeta) = -\frac{\sqrt{2} \bar{\beta}\eta }{2} + \frac{\sqrt{2} \beta\bar{\eta} }{2}$	$\Psi_2(be'^2, {}^1E''^1, M=0, \gamma) = -\frac{\sqrt{2} \bar{\beta}\mu }{2} + \frac{\sqrt{2} \beta\bar{\mu} }{2}$
$(e'^2)^2$	$(e'^1)^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_3((e'^2)^2, {}^1E''^2, M=0, \zeta) = - \bar{\mu}\mu $	$\Psi_3((e'^1)^2, {}^1E''^1, M=0, \gamma) = - \bar{\eta}\eta $
$(e''^1)^2$	$(e''^2)^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_4((e''^1)^2, {}^1E''^2, M=0, \zeta) = - \bar{\gamma}\gamma $	$\Psi_4((e''^2)^2, {}^1E''^1, M=0, \gamma) = - \bar{\zeta}\zeta $

2.21.10 ${}^3E''^1$

ae''^1	$e'^1e'^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_1(ae''^1, {}^3E''^1, M=-1, \gamma) = \bar{\alpha}\gamma $	$\Psi_1(e'^1e'^2, {}^3A, M=-1, \alpha) = \bar{\eta}\mu $
$\Psi_2(ae''^1, {}^3E''^1, M=0, \gamma) = \frac{\sqrt{2} \bar{\alpha}\gamma }{2} + \frac{\sqrt{2} \alpha\bar{\gamma} }{2}$	$\Psi_2(e'^1e'^2, {}^3A, M=0, \alpha) = \frac{\sqrt{2} \bar{\eta}\mu }{2} + \frac{\sqrt{2} \eta\bar{\mu} }{2}$
$\Psi_3(ae''^1, {}^3E''^1, M=1, \gamma) = \alpha\gamma $	$\Psi_3(e'^1e'^2, {}^3A, M=1, \alpha) = \eta\mu $
be'^2	$e''^1e''^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_4(be'^2, {}^3E''^1, M=-1, \gamma) = \bar{\beta}\mu $	$\Psi_4(e''^1e''^2, {}^3A, M=-1, \alpha) = \bar{\zeta}\gamma $
$\Psi_5(be'^2, {}^3E''^1, M=0, \gamma) = \frac{\sqrt{2} \bar{\beta}\mu }{2} + \frac{\sqrt{2} \beta\bar{\mu} }{2}$	$\Psi_5(e''^1e''^2, {}^3A, M=0, \alpha) = \frac{\sqrt{2} \bar{\zeta}\gamma }{2} + \frac{\sqrt{2} \zeta\bar{\gamma} }{2}$
$\Psi_6(be'^2, {}^3E''^1, M=1, \gamma) = \beta\mu $	$\Psi_6(e''^1e''^2, {}^3A, M=1, \alpha) = \zeta\gamma $

2.21.12 3A

ae''^1	$e'^1e'^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_1(ae''^1, {}^3E''^1, M=-1, \gamma) = \bar{\alpha}\gamma $	$\Psi_1(e'^1e'^2, {}^3A, M=-1, \alpha) = \bar{\eta}\mu $
$\Psi_2(ae''^1, {}^3E''^1, M=0, \gamma) = \frac{\sqrt{2} \bar{\alpha}\gamma }{2} + \frac{\sqrt{2} \alpha\bar{\gamma} }{2}$	$\Psi_2(e'^1e'^2, {}^3A, M=0, \alpha) = \frac{\sqrt{2} \bar{\eta}\mu }{2} + \frac{\sqrt{2} \eta\bar{\mu} }{2}$
$\Psi_3(ae''^1, {}^3E''^1, M=1, \gamma) = \alpha\gamma $	$\Psi_3(e'^1e'^2, {}^3A, M=1, \alpha) = \eta\mu $
be'^2	$e''^1e''^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$
$\Psi_4(be'^2, {}^3E''^1, M=-1, \gamma) = \bar{\beta}\mu $	$\Psi_4(e''^1e''^2, {}^3A, M=-1, \alpha) = \bar{\zeta}\gamma $
$\Psi_5(be'^2, {}^3E''^1, M=0, \gamma) = \frac{\sqrt{2} \bar{\beta}\mu }{2} + \frac{\sqrt{2} \beta\bar{\mu} }{2}$	$\Psi_5(e''^1e''^2, {}^3A, M=0, \alpha) = \frac{\sqrt{2} \bar{\zeta}\gamma }{2} + \frac{\sqrt{2} \zeta\bar{\gamma} }{2}$
$\Psi_6(be'^2, {}^3E''^1, M=1, \gamma) = \beta\mu $	$\Psi_6(e''^1e''^2, {}^3A, M=1, \alpha) = \zeta\gamma $

2.22 Group C_{3h} Component labels

$A' : \{\alpha\} \longrightarrow A'' : \{\beta\} \longrightarrow E''^2 : \{\zeta\} \longrightarrow E''^1 : \{\gamma\} \longrightarrow E'^2 : \{\mu\} \longrightarrow E'^1 : \{\eta\}$

$$\Psi_8(e''^1 e'^1, {}^3A'', M=0, \beta) = \frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

$$\Psi_9(e''^1 e'^1, {}^3A'', M=1, \beta) = |\gamma\eta|$$

2.22.1 ${}^1A'$

$$\left(\begin{matrix} a' \\ a' \end{matrix}\right)^2$$

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_1(\left(\begin{matrix} a' \\ a' \end{matrix}\right)^2, {}^1A', M=0, \alpha) = -|\bar{\alpha}\alpha|$$

$$\left(\begin{matrix} a'' \\ a'' \end{matrix}\right)^2$$

$$\boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle}$$

$$\Psi_2(\left(\begin{matrix} a'' \\ a'' \end{matrix}\right)^2, {}^1A', M=0, \alpha) = -|\bar{\beta}\beta|$$

$$e''^1 e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(e''^1 e'^2, {}^1A', M=0, \alpha) = -\frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

$$e'^1 e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(e'^1 e'^2, {}^1A', M=0, \alpha) = -\frac{\sqrt{2}|\bar{\mu}\eta|}{2} + \frac{\sqrt{2}|\mu\bar{\eta}|}{2}$$

2.22.3 ${}^1A''$

$$a' a''$$

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a' a'', {}^1A'', M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$e''^2 e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(e''^2 e'^2, {}^1A'', M=0, \beta) = -\frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$e''^1 e'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(e''^1 e'^1, {}^1A'', M=0, \beta) = -\frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

2.22.2 ${}^3A''$

$$a' a''$$

$$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a' a'', {}^3A'', M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$\Psi_2(a' a'', {}^3A'', M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(a' a'', {}^3A'', M=1, \beta) = |\alpha\beta|$$

$$e''^2 e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(e''^2 e'^2, {}^3A'', M=-1, \beta) = |\bar{\zeta}\bar{\mu}|$$

$$\Psi_5(e''^2 e'^2, {}^3A'', M=0, \beta) = \frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$\Psi_6(e''^2 e'^2, {}^3A'', M=1, \beta) = |\zeta\mu|$$

$$e'^1 e'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(e''^1 e'^1, {}^3A'', M=-1, \beta) = |\bar{\gamma}\bar{\eta}|$$

$$a' e''^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(a' e''^2, {}^3E''^2, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}|$$

$$\Psi_2(a' e''^2, {}^3E''^2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_3(a' e''^2, {}^3E''^2, M=1, \zeta) = |\alpha\zeta|$$

$$a'' e'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(a'' e'^1, {}^3E''^2, M=-1, \zeta) = |\bar{\beta}\bar{\eta}|$$

$$\Psi_5(a'' e'^1, {}^3E''^2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\beta}\eta|}{2} + \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_6(a'' e'^1, {}^3E''^2, M=1, \zeta) = |\beta\eta|$$

$$e''^1 e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(e''^1 e'^2, {}^3E''^2, M=-1, \zeta) = |\bar{\gamma}\bar{\mu}|$$

$$\Psi_8(e''^1 e'^2, {}^3E''^2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\gamma}\mu|}{2} + \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}$$

$$\Psi_9(e''^1 e'^2, {}^3E''^2, M=1, \zeta) = |\gamma\mu|$$

2.22.5 ${}^1E''^2$

$$\Psi_1(a' e''^1, {}^1E''^1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$a' e''^2$	$a'' e'^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$

$$\Psi_2(a' e''^2, {}^1E''^2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$a'' e'^1$	$e''^2 e'^1$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$

$$\Psi_3(e''^1 e'^2, {}^1E''^2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

2.22.6 ${}^3E''^1$

$a' e''^1$	$a'' e'^2$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$

$$\Psi_1(a' e''^1, {}^3E''^1, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

$$\Psi_2(a' e''^1, {}^3E''^1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(a' e''^1, {}^3E''^1, M=1, \gamma) = |\alpha\gamma|$$

$a'' e'^2$	$a'' e''^1$
$\boxed{\Delta E = 0}$	$\boxed{\Delta E = 0}$

$$\Psi_4(a'' e'^2, {}^3E''^1, M=-1, \gamma) = |\bar{\beta}\mu|$$

$$\Psi_5(a'' e'^2, {}^3E''^1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_6(a'' e'^2, {}^3E''^1, M=1, \gamma) = |\beta\mu|$$

$$\Psi_1(a' e''^1, {}^1E''^1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$a'' e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(a'' e'^2, {}^1E''^1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$e''^2 e'^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(e''^2 e'^1, {}^1E''^1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}$$

2.22.8 ${}^3E'^2$

$$a' e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(a' e'^2, {}^3E'^2, M=-1, \mu) = |\bar{\alpha}\mu|$$

$$\Psi_2(a' e'^2, {}^3E'^2, M=0, \mu) = \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_3(a' e'^2, {}^3E'^2, M=1, \mu) = |\alpha\mu|$$

$$a'' e''^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(a'' e''^1, {}^3E'^2, M=-1, \mu) = |\bar{\beta}\gamma|$$

$$\Psi_5(a'' e''^1, {}^3E'^2, M=0, \mu) = \frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_6(a'' e''^1, {}^3E'^2, M=1, \mu) = |\beta\gamma|$$

2.22.9 ${}^1E'^2$

$$a' e'^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(a' e'^2, {}^1E'^2, M=0, \mu) = -\frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$a'' e''^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(a'' e''^1, {}^1E'^2, M=0, \mu) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

2.22.7 ${}^1E''^1$

$$a' e''^1$$

$$\boxed{\Delta E = 0}$$

$$\left(e''^2 \right)^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(\left(e''^2 \right)^2, {}^1E'^2, M=0, \mu) = -|\bar{\zeta}\zeta|$$

$$\begin{array}{|c|} \hline \left(e'^1\right)^2 \\ \hline \Delta E = 0 \\ \hline \end{array}$$

$$\begin{array}{|c|} \hline \boxed{\Delta E = 0} \\ \hline \Psi_2(a''e''^2, {}^1E'^1, M=0, \eta) = -\frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2} \\ \hline \end{array}$$

$$\Psi_4(\left(e'^1\right)^2, {}^1E'^2, M=0, \mu) = -|\bar{\eta}\eta|$$

$$\begin{array}{|c|} \hline \left(e''^1\right)^2 \\ \hline \Delta E = 0 \\ \hline \end{array}$$

2.22.10 ${}^3E'^1$

$$\Psi_3(\left(e''^1\right)^2, {}^1E'^1, M=0, \eta) = -|\bar{\gamma}\gamma|$$

$$\begin{array}{|c|} \hline a'e'^1 \\ \hline \boxed{\Delta E = 0} \\ \hline \end{array}$$

$$\begin{array}{|c|} \hline \left(e'^2\right)^2 \\ \hline \boxed{\Delta E = 0} \\ \hline \end{array}$$

$$\Psi_1(a'e'^1, {}^3E'^1, M=-1, \eta) = |\bar{\alpha}\eta|$$

$$\Psi_2(a'e'^1, {}^3E'^1, M=0, \eta) = \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_3(a'e'^1, {}^3E'^1, M=1, \eta) = |\alpha\eta|$$

$$\begin{array}{|c|} \hline a''e''^2 \\ \hline \boxed{\Delta E = 0} \\ \hline \end{array}$$

2.22.12 ${}^3A'$

$$\begin{array}{|c|} \hline e''^1e''^2 \\ \hline \boxed{\Delta E = 0} \\ \hline \end{array}$$

$$\Psi_1(e''^1e''^2, {}^3A', M=-1, \alpha) = |\bar{\zeta}\gamma|$$

$$\Psi_2(e''^1e''^2, {}^3A', M=0, \alpha) = \frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

$$\Psi_3(e''^1e''^2, {}^3A', M=1, \alpha) = |\zeta\gamma|$$

2.22.11 ${}^1E'^1$

$$\begin{array}{|c|} \hline a'e'^1 \\ \hline \boxed{\Delta E = 0} \\ \hline \end{array}$$

$$\Psi_1(a'e'^1, {}^1E'^1, M=0, \eta) = -\frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$a''e''^2$$

$$\begin{array}{|c|} \hline e'^1e'^2 \\ \hline \boxed{\Delta E = 0} \\ \hline \end{array}$$

$$\Psi_4(e'^1e'^2, {}^3A', M=-1, \alpha) = |\bar{\mu}\eta|$$

$$\Psi_5(e'^1e'^2, {}^3A', M=0, \alpha) = \frac{\sqrt{2}|\bar{\mu}\eta|}{2} + \frac{\sqrt{2}|\mu\bar{\eta}|}{2}$$

$$\Psi_6(e'^1e'^2, {}^3A', M=1, \alpha) = |\mu\eta|$$

2.23 Group C_{6h}

Component labels

$$\Gamma^1 : \{\gamma_4\} \longrightarrow \Gamma^2 : \{\gamma_5\} \longrightarrow \Gamma^3 : \{\gamma_6\} \longrightarrow \Gamma^4 : \{\gamma_7\} \longrightarrow \Gamma^5 : \{\gamma_8\} \longrightarrow \Gamma^6 : \{\gamma_9\} \longrightarrow \Gamma^7 : \{\gamma_{10}\} \longrightarrow \Gamma^8 : \{\gamma_{11}\} \longrightarrow \Gamma^9 : \{\gamma_{12}\} \longrightarrow \Gamma^{10} : \{\gamma_1\} \longrightarrow \Gamma^{11} : \{\gamma_2\} \longrightarrow \Gamma^{12} : \{\gamma_3\}$$

$$\Psi_1((\gamma^1)^2, {}^1\Gamma^1, M=0, \gamma_4) = -|\bar{\gamma}_4\gamma_4|$$

2.23.1 ${}^1\Gamma^1$

$$(\gamma^2)^2$$

$$(\gamma^1)^2$$

$$\boxed{\Delta E = \langle \gamma_5\gamma_5 || \gamma_5\gamma_5 \rangle}$$

$$\boxed{\Delta E = \langle \gamma_4\gamma_4 || \gamma_4\gamma_4 \rangle}$$

$$\Psi_2((\gamma^2)^2, {}^1\Gamma^1, M=0, \gamma_4) = -|\bar{\gamma}_5\gamma_5|$$

$$\begin{aligned} & \gamma^3 \gamma^4 \\ & \boxed{\Delta E = 0} \\ & \Psi_3(\gamma^3 \gamma^4, {}^1\Gamma^1, M=0, \gamma_4) = -\frac{\sqrt{2}|\gamma_6 \gamma_7|}{2} + \frac{\sqrt{2}|\gamma_6 \bar{\gamma}_7|}{2} \\ & (\gamma^5)^2 \\ & \boxed{\Delta E = \langle \gamma_8 \gamma_8 || \gamma_8 \gamma_8 \rangle} \\ & \Psi_4((\gamma^5)^2, {}^1\Gamma^1, M=0, \gamma_4) = -|\bar{\gamma}_8 \gamma_8| \\ & \gamma^6 \gamma^7 \\ & \boxed{\Delta E = 0} \\ & \Psi_5(\gamma^6 \gamma^7, {}^1\Gamma^1, M=0, \gamma_4) = -\frac{\sqrt{2}|\gamma_9 \gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_9 \bar{\gamma}_{10}|}{2} \\ & (\gamma^8)^2 \\ & \boxed{\Delta E = \langle \gamma_{11} \gamma_{11} || \gamma_{11} \gamma_{11} \rangle} \\ & \Psi_6((\gamma^8)^2, {}^1\Gamma^1, M=0, \gamma_4) = -|\bar{\gamma}_{11} \gamma_{11}| \\ & \gamma^9 \gamma^{10} \\ & \boxed{\Delta E = 0} \\ & \Psi_7(\gamma^9 \gamma^{10}, {}^1\Gamma^1, M=0, \gamma_4) = -\frac{\sqrt{2}|\gamma_{12} \gamma_1|}{2} + \frac{\sqrt{2}|\gamma_{12} \bar{\gamma}_1|}{2} \\ & \gamma^{11} \gamma^{12} \\ & \boxed{\Delta E = 0} \\ & \Psi_8(\gamma^{11} \gamma^{12}, {}^1\Gamma^1, M=0, \gamma_4) = -\frac{\sqrt{2}|\bar{\gamma}_2 \gamma_3|}{2} + \frac{\sqrt{2}|\gamma_2 \bar{\gamma}_3|}{2} \end{aligned}$$

2.23.2 ${}^3\Gamma^2$

$$\begin{aligned} & \gamma^1 \gamma^2 \\ & \boxed{\Delta E = -\langle \gamma_4 \gamma_4 || \gamma_5 \gamma_5 \rangle + \langle \gamma_4 \gamma_5 || \gamma_4 \gamma_5 \rangle} \\ & \Psi_1(\gamma^1 \gamma^2, {}^3\Gamma^2, M=-1, \gamma_5) = |\bar{\gamma}_4 \gamma_5| \\ & \Psi_2(\gamma^1 \gamma^2, {}^3\Gamma^2, M=0, \gamma_5) = \frac{\sqrt{2}|\bar{\gamma}_4 \gamma_5|}{2} + \frac{\sqrt{2}|\gamma_4 \bar{\gamma}_5|}{2} \\ & \Psi_3(\gamma^1 \gamma^2, {}^3\Gamma^2, M=1, \gamma_5) = |\gamma_4 \gamma_5| \\ & \gamma^3 \gamma^{12} \\ & \boxed{\Delta E = 0} \\ & \Psi_4(\gamma^3 \gamma^{12}, {}^3\Gamma^2, M=-1, \gamma_5) = |\bar{\gamma}_6 \gamma_3| \\ & \Psi_5(\gamma^3 \gamma^{12}, {}^3\Gamma^2, M=0, \gamma_5) = \frac{\sqrt{2}|\bar{\gamma}_6 \gamma_3|}{2} + \frac{\sqrt{2}|\gamma_6 \bar{\gamma}_3|}{2} \\ & \Psi_6(\gamma^3 \gamma^{12}, {}^3\Gamma^2, M=1, \gamma_5) = |\gamma_6 \gamma_3| \\ & \gamma^4 \gamma^{11} \end{aligned}$$

$$\begin{aligned} & \boxed{\Delta E = 0} \\ & \Psi_7(\gamma^4 \gamma^{11}, {}^3\Gamma^2, M=-1, \gamma_5) = |\bar{\gamma}_7 \gamma_2| \\ & \Psi_8(\gamma^4 \gamma^{11}, {}^3\Gamma^2, M=0, \gamma_5) = \frac{\sqrt{2}|\bar{\gamma}_7 \gamma_2|}{2} + \frac{\sqrt{2}|\gamma_7 \bar{\gamma}_2|}{2} \\ & \Psi_9(\gamma^4 \gamma^{11}, {}^3\Gamma^2, M=1, \gamma_5) = |\gamma_7 \gamma_2| \\ & \gamma^5 \gamma^8 \\ & \boxed{\Delta E = \langle \gamma_8 \gamma_{11} || \gamma_8 \gamma_{11} \rangle - \langle \gamma_8 \gamma_8 || \gamma_{11} \gamma_{11} \rangle} \\ & \Psi_{10}(\gamma^5 \gamma^8, {}^3\Gamma^2, M=-1, \gamma_5) = |\bar{\gamma}_8 \gamma_{11}| \\ & \Psi_{11}(\gamma^5 \gamma^8, {}^3\Gamma^2, M=0, \gamma_5) = \frac{\sqrt{2}|\bar{\gamma}_8 \gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_8 \bar{\gamma}_{11}|}{2} \\ & \Psi_{12}(\gamma^5 \gamma^8, {}^3\Gamma^2, M=1, \gamma_5) = |\gamma_8 \gamma_{11}| \\ & \gamma^6 \gamma^{10} \\ & \boxed{\Delta E = 0} \\ & \Psi_{13}(\gamma^6 \gamma^{10}, {}^3\Gamma^2, M=-1, \gamma_5) = |\bar{\gamma}_9 \gamma_1| \\ & \Psi_{14}(\gamma^6 \gamma^{10}, {}^3\Gamma^2, M=0, \gamma_5) = \frac{\sqrt{2}|\bar{\gamma}_9 \gamma_1|}{2} + \frac{\sqrt{2}|\gamma_9 \bar{\gamma}_1|}{2} \\ & \Psi_{15}(\gamma^6 \gamma^{10}, {}^3\Gamma^2, M=1, \gamma_5) = |\gamma_9 \gamma_1| \\ & \gamma^7 \gamma^9 \\ & \boxed{\Delta E = 0} \\ & \Psi_{16}(\gamma^7 \gamma^9, {}^3\Gamma^2, M=-1, \gamma_5) = |\bar{\gamma}_{10} \gamma_{12}| \\ & \Psi_{17}(\gamma^7 \gamma^9, {}^3\Gamma^2, M=0, \gamma_5) = \frac{\sqrt{2}|\bar{\gamma}_{10} \gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_{10} \bar{\gamma}_{12}|}{2} \\ & \Psi_{18}(\gamma^7 \gamma^9, {}^3\Gamma^2, M=1, \gamma_5) = |\gamma_{10} \gamma_{12}| \end{aligned}$$

2.23.3 ${}^1\Gamma^2$

$$\begin{aligned} & \gamma^1 \gamma^2 \\ & \boxed{\Delta E = \langle \gamma_4 \gamma_4 || \gamma_5 \gamma_5 \rangle + \langle \gamma_4 \gamma_5 || \gamma_4 \gamma_5 \rangle} \\ & \Psi_1(\gamma^1 \gamma^2, {}^1\Gamma^2, M=0, \gamma_5) = -\frac{\sqrt{2}|\bar{\gamma}_4 \gamma_5|}{2} + \frac{\sqrt{2}|\gamma_4 \bar{\gamma}_5|}{2} \\ & \gamma^3 \gamma^{12} \\ & \boxed{\Delta E = 0} \\ & \Psi_2(\gamma^3 \gamma^{12}, {}^1\Gamma^2, M=0, \gamma_5) = -\frac{\sqrt{2}|\bar{\gamma}_6 \gamma_3|}{2} + \frac{\sqrt{2}|\gamma_6 \bar{\gamma}_3|}{2} \\ & \gamma^4 \gamma^{11} \\ & \boxed{\Delta E = 0} \\ & \Psi_3(\gamma^4 \gamma^{11}, {}^1\Gamma^2, M=0, \gamma_5) = -\frac{\sqrt{2}|\bar{\gamma}_7 \gamma_2|}{2} + \frac{\sqrt{2}|\gamma_7 \bar{\gamma}_2|}{2} \\ & \gamma^5 \gamma^8 \\ & \boxed{\Delta E = \langle \gamma_8 \gamma_{11} || \gamma_8 \gamma_{11} \rangle + \langle \gamma_8 \gamma_8 || \gamma_{11} \gamma_{11} \rangle} \\ & \Psi_4(\gamma^5 \gamma^8, {}^1\Gamma^2, M=0, \gamma_5) = -\frac{\sqrt{2}|\bar{\gamma}_8 \gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_8 \bar{\gamma}_{11}|}{2} \end{aligned}$$

$$\begin{aligned} & \gamma^6\gamma^{10} \\ & \boxed{\Delta E = 0} \\ \Psi_5(\gamma^6\gamma^{10}, {}^1\Gamma^2, M=0, \gamma_5) &= -\frac{\sqrt{2}|\bar{\gamma}_9\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_9\bar{\gamma}_1|}{2} \\ & \gamma^7\gamma^9 \\ & \boxed{\Delta E = 0} \\ \Psi_6(\gamma^7\gamma^9, {}^1\Gamma^2, M=0, \gamma_5) &= -\frac{\sqrt{2}|\bar{\gamma}_{10}\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_{10}\bar{\gamma}_{12}|}{2} \end{aligned}$$

2.23.4 ${}^3\Gamma^3$

$$\begin{aligned} & \gamma^1\gamma^3 \\ & \boxed{\Delta E = 0} \\ \Psi_1(\gamma^1\gamma^3, {}^3\Gamma^3, M=-1, \gamma_6) &= |\bar{\gamma}_4\gamma_6| \\ \Psi_2(\gamma^1\gamma^3, {}^3\Gamma^3, M=0, \gamma_6) &= \frac{\sqrt{2}|\bar{\gamma}_4\gamma_6|}{2} + \frac{\sqrt{2}|\gamma_4\bar{\gamma}_6|}{2} \\ \Psi_3(\gamma^1\gamma^3, {}^3\Gamma^3, M=1, \gamma_6) &= |\gamma_4\gamma_6| \\ & \gamma^2\gamma^{11} \\ & \boxed{\Delta E = 0} \\ \Psi_4(\gamma^2\gamma^{11}, {}^3\Gamma^3, M=-1, \gamma_6) &= |\bar{\gamma}_5\gamma_2| \\ \Psi_5(\gamma^2\gamma^{11}, {}^3\Gamma^3, M=0, \gamma_6) &= \frac{\sqrt{2}|\bar{\gamma}_5\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_5\bar{\gamma}_2|}{2} \\ \Psi_6(\gamma^2\gamma^{11}, {}^3\Gamma^3, M=1, \gamma_6) &= |\gamma_5\gamma_2| \end{aligned}$$

$$\begin{aligned} & \gamma^4\gamma^{12} \\ & \boxed{\Delta E = 0} \\ \Psi_7(\gamma^4\gamma^{12}, {}^3\Gamma^3, M=-1, \gamma_6) &= |\bar{\gamma}_7\gamma_3| \\ \Psi_8(\gamma^4\gamma^{12}, {}^3\Gamma^3, M=0, \gamma_6) &= \frac{\sqrt{2}|\bar{\gamma}_7\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_7\bar{\gamma}_3|}{2} \\ \Psi_9(\gamma^4\gamma^{12}, {}^3\Gamma^3, M=1, \gamma_6) &= |\gamma_7\gamma_3| \end{aligned}$$

$$\begin{aligned} & \gamma^5\gamma^{10} \\ & \boxed{\Delta E = 0} \\ \Psi_{10}(\gamma^5\gamma^{10}, {}^3\Gamma^3, M=-1, \gamma_6) &= |\bar{\gamma}_8\gamma_1| \\ \Psi_{11}(\gamma^5\gamma^{10}, {}^3\Gamma^3, M=0, \gamma_6) &= \frac{\sqrt{2}|\bar{\gamma}_8\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_8\bar{\gamma}_1|}{2} \\ \Psi_{12}(\gamma^5\gamma^{10}, {}^3\Gamma^3, M=1, \gamma_6) &= |\gamma_8\gamma_1| \end{aligned}$$

$$\begin{aligned} & \gamma^6\gamma^9 \\ & \boxed{\Delta E = 0} \\ \Psi_{13}(\gamma^6\gamma^9, {}^3\Gamma^3, M=-1, \gamma_6) &= |\bar{\gamma}_9\gamma_{12}| \\ \Psi_{14}(\gamma^6\gamma^9, {}^3\Gamma^3, M=0, \gamma_6) &= \frac{\sqrt{2}|\bar{\gamma}_9\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_9\bar{\gamma}_{12}|}{2} \\ \Psi_{15}(\gamma^6\gamma^9, {}^3\Gamma^3, M=1, \gamma_6) &= |\gamma_9\gamma_{12}| \\ & \gamma^7\gamma^8 \end{aligned}$$

$$\begin{aligned} & \boxed{\Delta E = 0} \\ \Psi_{16}(\gamma^7\gamma^8, {}^3\Gamma^3, M=-1, \gamma_6) &= |\bar{\gamma}_{10}\gamma_{11}| \\ \Psi_{17}(\gamma^7\gamma^8, {}^3\Gamma^3, M=0, \gamma_6) &= \frac{\sqrt{2}|\bar{\gamma}_{10}\gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_{10}\bar{\gamma}_{11}|}{2} \\ \Psi_{18}(\gamma^7\gamma^8, {}^3\Gamma^3, M=1, \gamma_6) &= |\gamma_{10}\gamma_{11}| \end{aligned}$$

2.23.5 ${}^1\Gamma^3$

$$\begin{aligned} & \gamma^1\gamma^3 \\ & \boxed{\Delta E = 0} \\ \Psi_1(\gamma^1\gamma^3, {}^1\Gamma^3, M=0, \gamma_6) &= -\frac{\sqrt{2}|\bar{\gamma}_4\gamma_6|}{2} + \frac{\sqrt{2}|\gamma_4\bar{\gamma}_6|}{2} \\ & \gamma^2\gamma^{11} \\ & \boxed{\Delta E = 0} \\ \Psi_2(\gamma^2\gamma^{11}, {}^1\Gamma^3, M=0, \gamma_6) &= -\frac{\sqrt{2}|\bar{\gamma}_5\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_5\bar{\gamma}_2|}{2} \\ & \gamma^4\gamma^{12} \\ & \boxed{\Delta E = 0} \\ \Psi_3(\gamma^4\gamma^{12}, {}^1\Gamma^3, M=0, \gamma_6) &= -\frac{\sqrt{2}|\bar{\gamma}_7\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_7\bar{\gamma}_3|}{2} \\ & \gamma^5\gamma^{10} \\ & \boxed{\Delta E = 0} \\ \Psi_4(\gamma^5\gamma^{10}, {}^1\Gamma^3, M=0, \gamma_6) &= -\frac{\sqrt{2}|\bar{\gamma}_8\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_8\bar{\gamma}_1|}{2} \\ & \gamma^6\gamma^9 \\ & \boxed{\Delta E = 0} \\ \Psi_5(\gamma^6\gamma^9, {}^1\Gamma^3, M=0, \gamma_6) &= -\frac{\sqrt{2}|\bar{\gamma}_9\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_9\bar{\gamma}_{12}|}{2} \\ & \gamma^7\gamma^8 \\ & \boxed{\Delta E = 0} \\ \Psi_6(\gamma^7\gamma^8, {}^1\Gamma^3, M=0, \gamma_6) &= -\frac{\sqrt{2}|\bar{\gamma}_{10}\gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_{10}\bar{\gamma}_{11}|}{2} \end{aligned}$$

2.23.6 ${}^3\Gamma^4$

$$\begin{aligned} & \gamma^1\gamma^4 \\ & \boxed{\Delta E = 0} \\ \Psi_1(\gamma^1\gamma^4, {}^3\Gamma^4, M=-1, \gamma_7) &= |\bar{\gamma}_4\gamma_7| \\ \Psi_2(\gamma^1\gamma^4, {}^3\Gamma^4, M=0, \gamma_7) &= \frac{\sqrt{2}|\bar{\gamma}_4\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_4\bar{\gamma}_7|}{2} \\ \Psi_3(\gamma^1\gamma^4, {}^3\Gamma^4, M=1, \gamma_7) &= |\gamma_4\gamma_7| \end{aligned}$$

$\gamma^2\gamma^{12}$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^2\gamma^{12}, {}^3\Gamma^4, M=-1, \gamma_7) = |\overline{\gamma_5}\gamma_3|$$

$$\Psi_5(\gamma^2\gamma^{12}, {}^3\Gamma^4, M=0, \gamma_7) = \frac{\sqrt{2}|\overline{\gamma_5}\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_5\overline{\gamma_3}|}{2}$$

$$\Psi_6(\gamma^2\gamma^{12}, {}^3\Gamma^4, M=1, \gamma_7) = |\gamma_5\gamma_3|$$

 $\gamma^3\gamma^{11}$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(\gamma^3\gamma^{11}, {}^3\Gamma^4, M=-1, \gamma_7) = |\overline{\gamma_6}\gamma_2|$$

$$\Psi_8(\gamma^3\gamma^{11}, {}^3\Gamma^4, M=0, \gamma_7) = \frac{\sqrt{2}|\overline{\gamma_6}\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_6\overline{\gamma_2}|}{2}$$

$$\Psi_9(\gamma^3\gamma^{11}, {}^3\Gamma^4, M=1, \gamma_7) = |\gamma_6\gamma_2|$$

 $\gamma^5\gamma^9$

$$\boxed{\Delta E = 0}$$

$$\Psi_{10}(\gamma^5\gamma^9, {}^3\Gamma^4, M=-1, \gamma_7) = |\overline{\gamma_8}\gamma_{12}|$$

$$\Psi_{11}(\gamma^5\gamma^9, {}^3\Gamma^4, M=0, \gamma_7) = \frac{\sqrt{2}|\overline{\gamma_8}\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_8\overline{\gamma_{12}}|}{2}$$

$$\Psi_{12}(\gamma^5\gamma^9, {}^3\Gamma^4, M=1, \gamma_7) = |\gamma_8\gamma_{12}|$$

 $\gamma^6\gamma^8$

$$\boxed{\Delta E = 0}$$

$$\Psi_{13}(\gamma^6\gamma^8, {}^3\Gamma^4, M=-1, \gamma_7) = |\overline{\gamma_9}\gamma_{11}|$$

$$\Psi_{14}(\gamma^6\gamma^8, {}^3\Gamma^4, M=0, \gamma_7) = \frac{\sqrt{2}|\overline{\gamma_9}\gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_9\overline{\gamma_{11}}|}{2}$$

$$\Psi_{15}(\gamma^6\gamma^8, {}^3\Gamma^4, M=1, \gamma_7) = |\gamma_9\gamma_{11}|$$

 $\gamma^7\gamma^{10}$

$$\boxed{\Delta E = 0}$$

$$\Psi_{16}(\gamma^7\gamma^{10}, {}^3\Gamma^4, M=-1, \gamma_7) = |\overline{\gamma_{10}}\gamma_1|$$

$$\Psi_{17}(\gamma^7\gamma^{10}, {}^3\Gamma^4, M=0, \gamma_7) = \frac{\sqrt{2}|\overline{\gamma_{10}}\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_{10}\overline{\gamma_1}|}{2}$$

$$\Psi_{18}(\gamma^7\gamma^{10}, {}^3\Gamma^4, M=1, \gamma_7) = |\gamma_{10}\gamma_1|$$

2.23.7 ${}^1\Gamma^4$

 $\gamma^1\gamma^4$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(\gamma^1\gamma^4, {}^1\Gamma^4, M=0, \gamma_7) = -\frac{\sqrt{2}|\overline{\gamma_4}\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_4\overline{\gamma_7}|}{2}$$

 $\gamma^2\gamma^{12}$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(\gamma^2\gamma^{12}, {}^1\Gamma^4, M=0, \gamma_7) = -\frac{\sqrt{2}|\overline{\gamma_5}\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_5\overline{\gamma_3}|}{2}$$

 $\gamma^3\gamma^{11}$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(\gamma^3\gamma^{11}, {}^1\Gamma^4, M=0, \gamma_7) = -\frac{\sqrt{2}|\overline{\gamma_6}\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_6\overline{\gamma_2}|}{2}$$

 $\gamma^5\gamma^9$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^5\gamma^9, {}^1\Gamma^4, M=0, \gamma_7) = -\frac{\sqrt{2}|\overline{\gamma_8}\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_8\overline{\gamma_{12}}|}{2}$$

 $\gamma^6\gamma^8$

$$\boxed{\Delta E = 0}$$

$$\Psi_5(\gamma^6\gamma^8, {}^1\Gamma^4, M=0, \gamma_7) = -\frac{\sqrt{2}|\overline{\gamma_9}\gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_9\overline{\gamma_{11}}|}{2}$$

 $\gamma^7\gamma^{10}$

$$\boxed{\Delta E = 0}$$

$$\Psi_6(\gamma^7\gamma^{10}, {}^1\Gamma^4, M=0, \gamma_7) = -\frac{\sqrt{2}|\overline{\gamma_{10}}\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_{10}\overline{\gamma_1}|}{2}$$

2.23.8 ${}^3\Gamma^5$

 $\gamma^1\gamma^5$

$$\boxed{\Delta E = -\langle \gamma_4\gamma_4 || \gamma_8\gamma_8 \rangle + \langle \gamma_4\gamma_8 || \gamma_4\gamma_8 \rangle}$$

$$\Psi_1(\gamma^1\gamma^5, {}^3\Gamma^5, M=-1, \gamma_8) = |\overline{\gamma_4}\gamma_8|$$

$$\Psi_2(\gamma^1\gamma^5, {}^3\Gamma^5, M=0, \gamma_8) = \frac{\sqrt{2}|\overline{\gamma_4}\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_4\overline{\gamma_8}|}{2}$$

$$\Psi_3(\gamma^1\gamma^5, {}^3\Gamma^5, M=1, \gamma_8) = |\gamma_4\gamma_8|$$

 $\gamma^2\gamma^8$

$$\boxed{\Delta E = \langle \gamma_5\gamma_{11} || \gamma_5\gamma_{11} \rangle - \langle \gamma_5\gamma_5 || \gamma_{11}\gamma_{11} \rangle}$$

$$\Psi_4(\gamma^2\gamma^8, {}^3\Gamma^5, M=-1, \gamma_8) = |\overline{\gamma_5}\gamma_{11}|$$

$$\Psi_5(\gamma^2\gamma^8, {}^3\Gamma^5, M=0, \gamma_8) = \frac{\sqrt{2}|\overline{\gamma_5}\gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_5\overline{\gamma_{11}}|}{2}$$

$$\Psi_6(\gamma^2\gamma^8, {}^3\Gamma^5, M=1, \gamma_8) = |\gamma_5\gamma_{11}|$$

 $\gamma^3\gamma^9$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(\gamma^3\gamma^9, {}^3\Gamma^5, M=-1, \gamma_8) = |\overline{\gamma_6}\gamma_{12}|$$

$$\Psi_8(\gamma^3\gamma^9, {}^3\Gamma^5, M=0, \gamma_8) = \frac{\sqrt{2}|\overline{\gamma_6}\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_6\overline{\gamma_{12}}|}{2}$$

$$\Psi_9(\gamma^3\gamma^9, {}^3\Gamma^5, M=1, \gamma_8) = |\gamma_6\gamma_{12}|$$

 $\gamma^4\gamma^{10}$

$$\boxed{\Delta E = 0}$$

$$\Psi_{10}(\gamma^4\gamma^{10}, {}^3\Gamma^5, M=-1, \gamma_8) = |\overline{\gamma_7}\gamma_1|$$

$$\Psi_{11}(\gamma^4\gamma^{10}, {}^3\Gamma^5, M=0, \gamma_8) = \frac{\sqrt{2}|\overline{\gamma_7}\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_7\overline{\gamma_1}|}{2}$$

$$\Psi_{12}(\gamma^4\gamma^{10}, {}^3\Gamma^5, M=1, \gamma_8) = |\gamma_7\gamma_1|$$

 $\gamma^6\gamma^{11}$

$$\boxed{\Delta E = 0}$$

$$\Psi_{13}(\gamma^6\gamma^{11}, {}^3\Gamma^5, M=-1, \gamma_8) = |\overline{\gamma_9}\gamma_2|$$

$$\Psi_{14}(\gamma^6\gamma^{11}, {}^3\Gamma^5, M=0, \gamma_8) = \frac{\sqrt{2}|\overline{\gamma_9}\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_9\overline{\gamma_2}|}{2}$$

$$\Psi_{15}(\gamma^6\gamma^{11}, {}^3\Gamma^5, M=1, \gamma_8) = |\gamma_9\gamma_2|$$

$$\gamma^7\gamma^{12}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{16}(\gamma^7\gamma^{12}, {}^3\Gamma^5, M=-1, \gamma_8) = |\overline{\gamma_{10}}\gamma_3|$$

$$\Psi_{17}(\gamma^7\gamma^{12}, {}^3\Gamma^5, M=0, \gamma_8) = \frac{\sqrt{2}|\overline{\gamma_{10}}\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_{10}\overline{\gamma_3}|}{2}$$

$$\Psi_{18}(\gamma^7\gamma^{12}, {}^3\Gamma^5, M=1, \gamma_8) = |\gamma_{10}\gamma_3|$$

$$\boxed{\mathbf{2.23.10} \quad {}^3\Gamma^6}$$

$$\gamma^1\gamma^6$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(\gamma^1\gamma^6, {}^3\Gamma^6, M=-1, \gamma_9) = |\overline{\gamma_4}\gamma_9|$$

$$\Psi_2(\gamma^1\gamma^6, {}^3\Gamma^6, M=0, \gamma_9) = \frac{\sqrt{2}|\overline{\gamma_4}\gamma_9|}{2} + \frac{\sqrt{2}|\gamma_4\overline{\gamma_9}|}{2}$$

$$\Psi_3(\gamma^1\gamma^6, {}^3\Gamma^6, M=1, \gamma_9) = |\gamma_4\gamma_9|$$

$$\gamma^2\gamma^9$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^2\gamma^9, {}^3\Gamma^6, M=-1, \gamma_9) = |\overline{\gamma_5}\gamma_{12}|$$

$$\Psi_5(\gamma^2\gamma^9, {}^3\Gamma^6, M=0, \gamma_9) = \frac{\sqrt{2}|\overline{\gamma_5}\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_5\overline{\gamma_{12}}|}{2}$$

$$\Psi_6(\gamma^2\gamma^9, {}^3\Gamma^6, M=1, \gamma_9) = |\gamma_5\gamma_{12}|$$

$$\gamma^3\gamma^{10}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(\gamma^3\gamma^{10}, {}^3\Gamma^6, M=-1, \gamma_9) = |\overline{\gamma_6}\gamma_1|$$

$$\Psi_8(\gamma^3\gamma^{10}, {}^3\Gamma^6, M=0, \gamma_9) = \frac{\sqrt{2}|\overline{\gamma_6}\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_6\overline{\gamma_1}|}{2}$$

$$\Psi_9(\gamma^3\gamma^{10}, {}^3\Gamma^6, M=1, \gamma_9) = |\gamma_6\gamma_1|$$

$$\gamma^4\gamma^8$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{10}(\gamma^4\gamma^8, {}^3\Gamma^6, M=-1, \gamma_9) = |\overline{\gamma_7}\gamma_{11}|$$

$$\Psi_{11}(\gamma^4\gamma^8, {}^3\Gamma^6, M=0, \gamma_9) = \frac{\sqrt{2}|\overline{\gamma_7}\gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_7\overline{\gamma_{11}}|}{2}$$

$$\Psi_{12}(\gamma^4\gamma^8, {}^3\Gamma^6, M=1, \gamma_9) = |\gamma_7\gamma_{11}|$$

$$\gamma^5\gamma^{12}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{13}(\gamma^5\gamma^{12}, {}^3\Gamma^6, M=-1, \gamma_9) = |\overline{\gamma_8}\gamma_3|$$

$$\Psi_{14}(\gamma^5\gamma^{12}, {}^3\Gamma^6, M=0, \gamma_9) = \frac{\sqrt{2}|\overline{\gamma_8}\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_8\overline{\gamma_3}|}{2}$$

$$\Psi_{15}(\gamma^5\gamma^{12}, {}^3\Gamma^6, M=1, \gamma_9) = |\gamma_8\gamma_3|$$

$$\gamma^7\gamma^{11}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{16}(\gamma^7\gamma^{11}, {}^3\Gamma^6, M=-1, \gamma_9) = |\overline{\gamma_{10}}\gamma_2|$$

$$\Psi_{17}(\gamma^7\gamma^{11}, {}^3\Gamma^6, M=0, \gamma_9) = \frac{\sqrt{2}|\overline{\gamma_{10}}\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_{10}\overline{\gamma_2}|}{2}$$

$$\Psi_{18}(\gamma^7\gamma^{11}, {}^3\Gamma^6, M=1, \gamma_9) = |\gamma_{10}\gamma_2|$$

$$\boxed{\mathbf{2.23.9} \quad {}^1\Gamma^5}$$

$$\gamma^1\gamma^5$$

$$\boxed{\Delta E = \langle \gamma_4\gamma_4 || \gamma_8\gamma_8 \rangle + \langle \gamma_4\gamma_8 || \gamma_4\gamma_8 \rangle}$$

$$\Psi_1(\gamma^1\gamma^5, {}^1\Gamma^5, M=0, \gamma_8) = -\frac{\sqrt{2}|\overline{\gamma_4}\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_4\overline{\gamma_8}|}{2}$$

$$\gamma^2\gamma^8$$

$$\boxed{\Delta E = \langle \gamma_5\gamma_{11} || \gamma_5\gamma_{11} \rangle + \langle \gamma_5\gamma_5 || \gamma_{11}\gamma_{11} \rangle}$$

$$\Psi_2(\gamma^2\gamma^8, {}^1\Gamma^5, M=0, \gamma_8) = -\frac{\sqrt{2}|\overline{\gamma_5}\gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_5\overline{\gamma_{11}}|}{2}$$

$$\gamma^3\gamma^9$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(\gamma^3\gamma^9, {}^1\Gamma^5, M=0, \gamma_8) = -\frac{\sqrt{2}|\overline{\gamma_6}\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_6\overline{\gamma_{12}}|}{2}$$

$$\gamma^4\gamma^{10}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^4\gamma^{10}, {}^1\Gamma^5, M=0, \gamma_8) = -\frac{\sqrt{2}|\overline{\gamma_7}\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_7\overline{\gamma_1}|}{2}$$

$$\gamma^6\gamma^{11}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_5(\gamma^6\gamma^{11}, {}^1\Gamma^5, M=0, \gamma_8) = -\frac{\sqrt{2}|\overline{\gamma_9}\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_9\overline{\gamma_2}|}{2}$$

$$\gamma^7\gamma^{12}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_6(\gamma^7\gamma^{12}, {}^1\Gamma^5, M=0, \gamma_8) = -\frac{\sqrt{2}|\overline{\gamma_{10}}\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_{10}\overline{\gamma_3}|}{2}$$

2.23.11 $^1\Gamma^6$

$\gamma^1 \gamma^6$

 $\boxed{\Delta E = 0}$

$\Psi_1(\gamma^1 \gamma^6, ^1\Gamma^6, M=0, \gamma_9) = -\frac{\sqrt{2}|\gamma_4 \gamma_9|}{2} + \frac{\sqrt{2}|\gamma_4 \bar{\gamma}_9|}{2}$

$\gamma^2 \gamma^9$

 $\boxed{\Delta E = 0}$

$\Psi_2(\gamma^2 \gamma^9, ^1\Gamma^6, M=0, \gamma_9) = -\frac{\sqrt{2}|\gamma_5 \gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_5 \bar{\gamma}_{12}|}{2}$

$\gamma^3 \gamma^{10}$

 $\boxed{\Delta E = 0}$

$\Psi_3(\gamma^3 \gamma^{10}, ^1\Gamma^6, M=0, \gamma_9) = -\frac{\sqrt{2}|\gamma_6 \gamma_1|}{2} + \frac{\sqrt{2}|\gamma_6 \bar{\gamma}_1|}{2}$

$\gamma^4 \gamma^8$

 $\boxed{\Delta E = 0}$

$\Psi_4(\gamma^4 \gamma^8, ^1\Gamma^6, M=0, \gamma_9) = -\frac{\sqrt{2}|\gamma_7 \gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_7 \bar{\gamma}_{11}|}{2}$

$\gamma^5 \gamma^{12}$

 $\boxed{\Delta E = 0}$

$\Psi_5(\gamma^5 \gamma^{12}, ^1\Gamma^6, M=0, \gamma_9) = -\frac{\sqrt{2}|\gamma_8 \gamma_3|}{2} + \frac{\sqrt{2}|\gamma_8 \bar{\gamma}_3|}{2}$

$\gamma^7 \gamma^{11}$

 $\boxed{\Delta E = 0}$

$\Psi_6(\gamma^7 \gamma^{11}, ^1\Gamma^6, M=0, \gamma_9) = -\frac{\sqrt{2}|\gamma_{10} \gamma_2|}{2} + \frac{\sqrt{2}|\gamma_{10} \bar{\gamma}_2|}{2}$

2.23.12 $^3\Gamma^7$

$\gamma^1 \gamma^7$

 $\boxed{\Delta E = 0}$

$\Psi_1(\gamma^1 \gamma^7, ^3\Gamma^7, M=-1, \gamma_{10}) = |\gamma_4 \gamma_{10}|$

$\Psi_2(\gamma^1 \gamma^7, ^3\Gamma^7, M=0, \gamma_{10}) = \frac{\sqrt{2}|\gamma_4 \gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_4 \bar{\gamma}_{10}|}{2}$

$\Psi_3(\gamma^1 \gamma^7, ^3\Gamma^7, M=1, \gamma_{10}) = |\gamma_4 \gamma_{10}|$

$\gamma^2 \gamma^{10}$

 $\boxed{\Delta E = 0}$

$\Psi_4(\gamma^2 \gamma^{10}, ^3\Gamma^7, M=-1, \gamma_{10}) = |\gamma_5 \gamma_1|$

$\Psi_5(\gamma^2 \gamma^{10}, ^3\Gamma^7, M=0, \gamma_{10}) = \frac{\sqrt{2}|\gamma_5 \gamma_1|}{2} + \frac{\sqrt{2}|\gamma_5 \bar{\gamma}_1|}{2}$

$\Psi_6(\gamma^2 \gamma^{10}, ^3\Gamma^7, M=1, \gamma_{10}) = |\gamma_5 \gamma_1|$

$\gamma^3 \gamma^8$

 $\boxed{\Delta E = 0}$

$\Psi_7(\gamma^3 \gamma^8, ^3\Gamma^7, M=-1, \gamma_{10}) = |\gamma_6 \gamma_{11}|$

$\Psi_8(\gamma^3 \gamma^8, ^3\Gamma^7, M=0, \gamma_{10}) = \frac{\sqrt{2}|\gamma_6 \gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_6 \bar{\gamma}_{11}|}{2}$

$\Psi_9(\gamma^3 \gamma^8, ^3\Gamma^7, M=1, \gamma_{10}) = |\gamma_6 \gamma_{11}|$

$\gamma^4 \gamma^9$

 $\boxed{\Delta E = 0}$

$\Psi_{10}(\gamma^4 \gamma^9, ^3\Gamma^7, M=-1, \gamma_{10}) = |\gamma_7 \bar{\gamma}_{12}|$

$\Psi_{11}(\gamma^4 \gamma^9, ^3\Gamma^7, M=0, \gamma_{10}) = \frac{\sqrt{2}|\gamma_7 \gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_7 \bar{\gamma}_{12}|}{2}$

$\Psi_{12}(\gamma^4 \gamma^9, ^3\Gamma^7, M=1, \gamma_{10}) = |\gamma_7 \gamma_{12}|$

$\gamma^5 \gamma^{11}$

 $\boxed{\Delta E = 0}$

$\Psi_{13}(\gamma^5 \gamma^{11}, ^3\Gamma^7, M=-1, \gamma_{10}) = |\gamma_8 \bar{\gamma}_2|$

$\Psi_{14}(\gamma^5 \gamma^{11}, ^3\Gamma^7, M=0, \gamma_{10}) = \frac{\sqrt{2}|\gamma_8 \gamma_2|}{2} + \frac{\sqrt{2}|\gamma_8 \bar{\gamma}_2|}{2}$

$\Psi_{15}(\gamma^5 \gamma^{11}, ^3\Gamma^7, M=1, \gamma_{10}) = |\gamma_8 \gamma_2|$

$\gamma^6 \gamma^{12}$

 $\boxed{\Delta E = 0}$

$\Psi_{16}(\gamma^6 \gamma^{12}, ^3\Gamma^7, M=-1, \gamma_{10}) = |\gamma_9 \bar{\gamma}_3|$

$\Psi_{17}(\gamma^6 \gamma^{12}, ^3\Gamma^7, M=0, \gamma_{10}) = \frac{\sqrt{2}|\gamma_9 \gamma_3|}{2} + \frac{\sqrt{2}|\gamma_9 \bar{\gamma}_3|}{2}$

$\Psi_{18}(\gamma^6 \gamma^{12}, ^3\Gamma^7, M=1, \gamma_{10}) = |\gamma_9 \gamma_3|$

2.23.13 $^1\Gamma^7$

$\gamma^1 \gamma^7$

 $\boxed{\Delta E = 0}$

$\Psi_1(\gamma^1 \gamma^7, ^1\Gamma^7, M=0, \gamma_{10}) = -\frac{\sqrt{2}|\gamma_4 \gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_4 \bar{\gamma}_{10}|}{2}$

$\gamma^2 \gamma^{10}$

 $\boxed{\Delta E = 0}$

$\Psi_2(\gamma^2 \gamma^{10}, ^1\Gamma^7, M=0, \gamma_{10}) = -\frac{\sqrt{2}|\gamma_5 \gamma_1|}{2} + \frac{\sqrt{2}|\gamma_5 \bar{\gamma}_1|}{2}$

$\gamma^3 \gamma^8$

 $\boxed{\Delta E = 0}$

$\Psi_3(\gamma^3 \gamma^8, ^1\Gamma^7, M=0, \gamma_{10}) = -\frac{\sqrt{2}|\gamma_6 \gamma_{11}|}{2} + \frac{\sqrt{2}|\gamma_6 \bar{\gamma}_{11}|}{2}$

$\gamma^4 \gamma^9$

 $\boxed{\Delta E = 0}$

$\Psi_4(\gamma^4 \gamma^9, ^1\Gamma^7, M=0, \gamma_{10}) = -\frac{\sqrt{2}|\gamma_7 \gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_7 \bar{\gamma}_{12}|}{2}$

$\gamma^5\gamma^{11}$ <div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = 0$</div>	$\gamma^{10}\gamma^{12}$ <div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = 0$</div>
$\Psi_5(\gamma^5\gamma^{11}, {}^1\Gamma^7, M=0, \gamma_{10}) = -\frac{\sqrt{2} \bar{\gamma}_8\gamma_2 }{2} + \frac{\sqrt{2} \gamma_8\bar{\gamma}_2 }{2}$	
$\gamma^6\gamma^{12}$ <div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = 0$</div>	$\Psi_{16}(\gamma^{10}\gamma^{12}, {}^3\Gamma^8, M=-1, \gamma_{11}) = \bar{\gamma}_1\gamma_3 $
$\Psi_6(\gamma^6\gamma^{12}, {}^1\Gamma^7, M=0, \gamma_{10}) = -\frac{\sqrt{2} \bar{\gamma}_9\gamma_3 }{2} + \frac{\sqrt{2} \gamma_9\bar{\gamma}_3 }{2}$	
$\Psi_{17}(\gamma^{10}\gamma^{12}, {}^3\Gamma^8, M=0, \gamma_{11}) = \frac{\sqrt{2} \bar{\gamma}_1\gamma_3 }{2} + \frac{\sqrt{2} \gamma_1\bar{\gamma}_3 }{2}$	
$\Psi_{18}(\gamma^{10}\gamma^{12}, {}^3\Gamma^8, M=1, \gamma_{11}) = \gamma_1\gamma_3 $	

2.23.14 ${}^3\Gamma^8$	2.23.15 ${}^1\Gamma^8$
$\gamma^1\gamma^8$	
<div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = \langle \gamma_4\gamma_{11} \gamma_4\gamma_{11} \rangle - \langle \gamma_4\gamma_4 \gamma_{11}\gamma_{11} \rangle$</div>	
$\Psi_1(\gamma^1\gamma^8, {}^3\Gamma^8, M=-1, \gamma_{11}) = \bar{\gamma}_4\gamma_{11} $	
$\Psi_2(\gamma^1\gamma^8, {}^3\Gamma^8, M=0, \gamma_{11}) = \frac{\sqrt{2} \bar{\gamma}_4\gamma_{11} }{2} + \frac{\sqrt{2} \gamma_4\bar{\gamma}_{11} }{2}$	
$\Psi_3(\gamma^1\gamma^8, {}^3\Gamma^8, M=1, \gamma_{11}) = \gamma_4\gamma_{11} $	
$\gamma^2\gamma^5$	
<div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = -\langle \gamma_5\gamma_5 \gamma_8\gamma_8 \rangle + \langle \gamma_5\gamma_8 \gamma_5\gamma_8 \rangle$</div>	
$\Psi_4(\gamma^2\gamma^5, {}^3\Gamma^8, M=-1, \gamma_{11}) = \bar{\gamma}_5\gamma_8 $	
$\Psi_5(\gamma^2\gamma^5, {}^3\Gamma^8, M=0, \gamma_{11}) = \frac{\sqrt{2} \bar{\gamma}_5\gamma_8 }{2} + \frac{\sqrt{2} \gamma_5\bar{\gamma}_8 }{2}$	
$\Psi_6(\gamma^2\gamma^5, {}^3\Gamma^8, M=1, \gamma_{11}) = \gamma_5\gamma_8 $	
$\gamma^3\gamma^6$	
<div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = 0$</div>	
$\Psi_7(\gamma^3\gamma^6, {}^3\Gamma^8, M=-1, \gamma_{11}) = \bar{\gamma}_6\gamma_9 $	
$\Psi_8(\gamma^3\gamma^6, {}^3\Gamma^8, M=0, \gamma_{11}) = \frac{\sqrt{2} \bar{\gamma}_6\gamma_9 }{2} + \frac{\sqrt{2} \gamma_6\bar{\gamma}_9 }{2}$	
$\Psi_9(\gamma^3\gamma^6, {}^3\Gamma^8, M=1, \gamma_{11}) = \gamma_6\gamma_9 $	
$\gamma^4\gamma^7$	
<div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = 0$</div>	
$\Psi_{10}(\gamma^4\gamma^7, {}^3\Gamma^8, M=-1, \gamma_{11}) = \bar{\gamma}_7\gamma_{10} $	
$\Psi_{11}(\gamma^4\gamma^7, {}^3\Gamma^8, M=0, \gamma_{11}) = \frac{\sqrt{2} \bar{\gamma}_7\gamma_{10} }{2} + \frac{\sqrt{2} \gamma_7\bar{\gamma}_{10} }{2}$	
$\Psi_{12}(\gamma^4\gamma^7, {}^3\Gamma^8, M=1, \gamma_{11}) = \gamma_7\gamma_{10} $	
$\gamma^9\gamma^{11}$	
<div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = 0$</div>	
$\Psi_{13}(\gamma^9\gamma^{11}, {}^3\Gamma^8, M=-1, \gamma_{11}) = \bar{\gamma}_{12}\gamma_2 $	
$\Psi_{14}(\gamma^9\gamma^{11}, {}^3\Gamma^8, M=0, \gamma_{11}) = \frac{\sqrt{2} \bar{\gamma}_{12}\gamma_2 }{2} + \frac{\sqrt{2} \gamma_{12}\bar{\gamma}_2 }{2}$	
$\Psi_{15}(\gamma^9\gamma^{11}, {}^3\Gamma^8, M=1, \gamma_{11}) = \gamma_{12}\gamma_2 $	
$\Psi_3(\gamma^3\gamma^6, {}^1\Gamma^8, M=0, \gamma_{11}) = -\frac{\sqrt{2} \bar{\gamma}_6\gamma_9 }{2} + \frac{\sqrt{2} \gamma_6\bar{\gamma}_9 }{2}$	
$\gamma^3\gamma^6$	
<div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = 0$</div>	
$\Psi_4(\gamma^4\gamma^7, {}^1\Gamma^8, M=0, \gamma_{11}) = -\frac{\sqrt{2} \bar{\gamma}_7\gamma_{10} }{2} + \frac{\sqrt{2} \gamma_7\bar{\gamma}_{10} }{2}$	
$\gamma^4\gamma^7$	
<div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = 0$</div>	
$\Psi_5(\gamma^9\gamma^{11}, {}^1\Gamma^8, M=0, \gamma_{11}) = -\frac{\sqrt{2} \bar{\gamma}_{12}\gamma_2 }{2} + \frac{\sqrt{2} \gamma_{12}\bar{\gamma}_2 }{2}$	
$\gamma^9\gamma^{11}$	
<div style="border: 1px solid black; padding: 2px; display: inline-block;">$\Delta E = 0$</div>	
$\Psi_6(\gamma^{10}\gamma^{12}, {}^1\Gamma^8, M=0, \gamma_{11}) = -\frac{\sqrt{2} \bar{\gamma}_1\gamma_3 }{2} + \frac{\sqrt{2} \gamma_1\bar{\gamma}_3 }{2}$	

2.23.16 ${}^3\Gamma^9$

$\gamma^1 \gamma^9$

$\boxed{\Delta E = 0}$

$\Psi_1(\gamma^1 \gamma^9, {}^3\Gamma^9, M=0, \gamma_{12}) = |\overline{\gamma_4} \gamma_{12}|$

$\Psi_2(\gamma^1 \gamma^9, {}^3\Gamma^9, M=0, \gamma_{12}) = \frac{\sqrt{2}|\overline{\gamma_4} \gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_4 \overline{\gamma_{12}}|}{2}$

$\Psi_3(\gamma^1 \gamma^9, {}^3\Gamma^9, M=1, \gamma_{12}) = |\gamma_4 \gamma_{12}|$

$\gamma^2 \gamma^6$

$\boxed{\Delta E = 0}$

$\Psi_4(\gamma^2 \gamma^6, {}^3\Gamma^9, M=0, \gamma_{12}) = |\overline{\gamma_5} \gamma_9|$

$\Psi_5(\gamma^2 \gamma^6, {}^3\Gamma^9, M=0, \gamma_{12}) = \frac{\sqrt{2}|\overline{\gamma_5} \gamma_9|}{2} + \frac{\sqrt{2}|\gamma_5 \overline{\gamma_9}|}{2}$

$\Psi_6(\gamma^2 \gamma^6, {}^3\Gamma^9, M=1, \gamma_{12}) = |\gamma_5 \gamma_9|$

$\gamma^3 \gamma^7$

$\boxed{\Delta E = 0}$

$\Psi_7(\gamma^3 \gamma^7, {}^3\Gamma^9, M=0, \gamma_{12}) = |\overline{\gamma_6} \gamma_{10}|$

$\Psi_8(\gamma^3 \gamma^7, {}^3\Gamma^9, M=0, \gamma_{12}) = \frac{\sqrt{2}|\overline{\gamma_6} \gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_6 \overline{\gamma_{10}}|}{2}$

$\Psi_9(\gamma^3 \gamma^7, {}^3\Gamma^9, M=1, \gamma_{12}) = |\gamma_6 \gamma_{10}|$

$\gamma^4 \gamma^5$

$\boxed{\Delta E = 0}$

$\Psi_{10}(\gamma^4 \gamma^5, {}^3\Gamma^9, M=0, \gamma_{12}) = |\overline{\gamma_7} \gamma_8|$

$\Psi_{11}(\gamma^4 \gamma^5, {}^3\Gamma^9, M=0, \gamma_{12}) = \frac{\sqrt{2}|\overline{\gamma_7} \gamma_8|}{2} + \frac{\sqrt{2}|\gamma_7 \overline{\gamma_8}|}{2}$

$\Psi_{12}(\gamma^4 \gamma^5, {}^3\Gamma^9, M=1, \gamma_{12}) = |\gamma_7 \gamma_8|$

$\gamma^8 \gamma^{12}$

$\boxed{\Delta E = 0}$

$\Psi_{13}(\gamma^8 \gamma^{12}, {}^3\Gamma^9, M=0, \gamma_{12}) = |\overline{\gamma_{11}} \gamma_3|$

$\Psi_{14}(\gamma^8 \gamma^{12}, {}^3\Gamma^9, M=0, \gamma_{12}) = \frac{\sqrt{2}|\overline{\gamma_{11}} \gamma_3|}{2} + \frac{\sqrt{2}|\gamma_{11} \overline{\gamma_3}|}{2}$

$\Psi_{15}(\gamma^8 \gamma^{12}, {}^3\Gamma^9, M=1, \gamma_{12}) = |\gamma_{11} \gamma_3|$

$\gamma^{10} \gamma^{11}$

$\boxed{\Delta E = 0}$

$\Psi_{16}(\gamma^{10} \gamma^{11}, {}^3\Gamma^9, M=0, \gamma_{12}) = |\overline{\gamma_1} \gamma_2|$

$\Psi_{17}(\gamma^{10} \gamma^{11}, {}^3\Gamma^9, M=0, \gamma_{12}) = \frac{\sqrt{2}|\overline{\gamma_1} \gamma_2|}{2} + \frac{\sqrt{2}|\gamma_1 \overline{\gamma_2}|}{2}$

$\Psi_{18}(\gamma^{10} \gamma^{11}, {}^3\Gamma^9, M=1, \gamma_{12}) = |\gamma_1 \gamma_2|$

$\boxed{\Delta E = 0}$

$\Psi_1(\gamma^1 \gamma^9, {}^1\Gamma^9, M=0, \gamma_{12}) = -\frac{\sqrt{2}|\overline{\gamma_4} \gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_4 \overline{\gamma_{12}}|}{2}$

$\gamma^2 \gamma^6$

$\boxed{\Delta E = 0}$

$\Psi_2(\gamma^2 \gamma^6, {}^1\Gamma^9, M=0, \gamma_{12}) = -\frac{\sqrt{2}|\overline{\gamma_5} \gamma_9|}{2} + \frac{\sqrt{2}|\gamma_5 \overline{\gamma_9}|}{2}$

$\gamma^3 \gamma^7$

$\boxed{\Delta E = 0}$

$\Psi_3(\gamma^3 \gamma^7, {}^1\Gamma^9, M=0, \gamma_{12}) = -\frac{\sqrt{2}|\overline{\gamma_6} \gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_6 \overline{\gamma_{10}}|}{2}$

$\gamma^4 \gamma^5$

$\boxed{\Delta E = 0}$

$\Psi_4(\gamma^4 \gamma^5, {}^1\Gamma^9, M=0, \gamma_{12}) = -\frac{\sqrt{2}|\overline{\gamma_7} \gamma_8|}{2} + \frac{\sqrt{2}|\gamma_7 \overline{\gamma_8}|}{2}$

$\gamma^8 \gamma^{12}$

$\boxed{\Delta E = 0}$

$\Psi_5(\gamma^8 \gamma^{12}, {}^1\Gamma^9, M=0, \gamma_{12}) = -\frac{\sqrt{2}|\overline{\gamma_{11}} \gamma_3|}{2} + \frac{\sqrt{2}|\gamma_{11} \overline{\gamma_3}|}{2}$

$\gamma^{10} \gamma^{11}$

$\boxed{\Delta E = 0}$

$\Psi_6(\gamma^{10} \gamma^{11}, {}^1\Gamma^9, M=0, \gamma_{12}) = -\frac{\sqrt{2}|\overline{\gamma_1} \gamma_2|}{2} + \frac{\sqrt{2}|\gamma_1 \overline{\gamma_2}|}{2}$

2.23.17 ${}^1\Gamma^9$

$\gamma^1 \gamma^9$

2.23.18 ${}^3\Gamma^{10}$

$\gamma^1 \gamma^{10}$

$\boxed{\Delta E = 0}$

$\Psi_1(\gamma^1 \gamma^{10}, {}^3\Gamma^{10}, M=0, \gamma_1) = |\overline{\gamma_4} \gamma_1|$

$\Psi_2(\gamma^1 \gamma^{10}, {}^3\Gamma^{10}, M=0, \gamma_1) = \frac{\sqrt{2}|\overline{\gamma_4} \gamma_1|}{2} + \frac{\sqrt{2}|\gamma_4 \overline{\gamma_1}|}{2}$

$\Psi_3(\gamma^1 \gamma^{10}, {}^3\Gamma^{10}, M=1, \gamma_1) = |\gamma_4 \gamma_1|$

$\gamma^2 \gamma^7$

$\boxed{\Delta E = 0}$

$\Psi_4(\gamma^2 \gamma^7, {}^3\Gamma^{10}, M=0, \gamma_1) = |\overline{\gamma_5} \gamma_{10}|$

$\Psi_5(\gamma^2 \gamma^7, {}^3\Gamma^{10}, M=0, \gamma_1) = \frac{\sqrt{2}|\overline{\gamma_5} \gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_5 \overline{\gamma_{10}}|}{2}$

$\Psi_6(\gamma^2 \gamma^7, {}^3\Gamma^{10}, M=1, \gamma_1) = |\gamma_5 \gamma_{10}|$

$\gamma^3 \gamma^5$

$\boxed{\Delta E = 0}$

$\Psi_7(\gamma^3 \gamma^5, {}^3\Gamma^{10}, M=0, \gamma_1) = |\overline{\gamma_6} \gamma_8|$

$$\Psi_8(\gamma^3\gamma^5, {}^3\Gamma^{10}, M=0, \gamma_1) = \frac{\sqrt{2}|\gamma_6\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_6\bar{\gamma}_8|}{2}$$

$$\Psi_9(\gamma^3\gamma^5, {}^3\Gamma^{10}, M=1, \gamma_1) = |\gamma_6\gamma_8|$$

$$\gamma^4\gamma^6$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{10}(\gamma^4\gamma^6, {}^3\Gamma^{10}, M=-1, \gamma_1) = |\gamma_7\bar{\gamma}_9|$$

$$\Psi_{11}(\gamma^4\gamma^6, {}^3\Gamma^{10}, M=0, \gamma_1) = \frac{\sqrt{2}|\gamma_7\gamma_9|}{2} + \frac{\sqrt{2}|\gamma_7\bar{\gamma}_9|}{2}$$

$$\Psi_{12}(\gamma^4\gamma^6, {}^3\Gamma^{10}, M=1, \gamma_1) = |\gamma_7\gamma_9|$$

$$\gamma^8\gamma^{11}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{13}(\gamma^8\gamma^{11}, {}^3\Gamma^{10}, M=-1, \gamma_1) = |\gamma_{11}\bar{\gamma}_2|$$

$$\Psi_{14}(\gamma^8\gamma^{11}, {}^3\Gamma^{10}, M=0, \gamma_1) = \frac{\sqrt{2}|\gamma_{11}\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_{11}\bar{\gamma}_2|}{2}$$

$$\Psi_{15}(\gamma^8\gamma^{11}, {}^3\Gamma^{10}, M=1, \gamma_1) = |\gamma_{11}\gamma_2|$$

$$\gamma^9\gamma^{12}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{16}(\gamma^9\gamma^{12}, {}^3\Gamma^{10}, M=-1, \gamma_1) = |\gamma_{12}\bar{\gamma}_3|$$

$$\Psi_{17}(\gamma^9\gamma^{12}, {}^3\Gamma^{10}, M=0, \gamma_1) = \frac{\sqrt{2}|\gamma_{12}\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_{12}\bar{\gamma}_3|}{2}$$

$$\Psi_{18}(\gamma^9\gamma^{12}, {}^3\Gamma^{10}, M=1, \gamma_1) = |\gamma_{12}\gamma_3|$$

2.23.19 ${}^1\Gamma^{10}$

$$\gamma^1\gamma^{10}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(\gamma^1\gamma^{10}, {}^1\Gamma^{10}, M=0, \gamma_1) = -\frac{\sqrt{2}|\gamma_4\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_4\bar{\gamma}_1|}{2}$$

$$\gamma^2\gamma^7$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(\gamma^2\gamma^7, {}^1\Gamma^{10}, M=0, \gamma_1) = -\frac{\sqrt{2}|\gamma_5\gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_5\bar{\gamma}_{10}|}{2}$$

$$\gamma^3\gamma^5$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(\gamma^3\gamma^5, {}^1\Gamma^{10}, M=0, \gamma_1) = -\frac{\sqrt{2}|\gamma_6\gamma_8|}{2} + \frac{\sqrt{2}|\gamma_6\bar{\gamma}_8|}{2}$$

$$\gamma^4\gamma^6$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^4\gamma^6, {}^1\Gamma^{10}, M=0, \gamma_1) = -\frac{\sqrt{2}|\gamma_7\gamma_9|}{2} + \frac{\sqrt{2}|\gamma_7\bar{\gamma}_9|}{2}$$

$$\gamma^8\gamma^{11}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_5(\gamma^8\gamma^{11}, {}^1\Gamma^{10}, M=0, \gamma_1) = -\frac{\sqrt{2}|\gamma_{11}\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_{11}\bar{\gamma}_2|}{2}$$

$$\gamma^9\gamma^{12}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_6(\gamma^9\gamma^{12}, {}^1\Gamma^{10}, M=0, \gamma_1) = -\frac{\sqrt{2}|\gamma_{12}\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_{12}\bar{\gamma}_3|}{2}$$

2.23.20 ${}^3\Gamma^{11}$

$$\gamma^1\gamma^{11}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(\gamma^1\gamma^{11}, {}^3\Gamma^{11}, M=-1, \gamma_2) = |\gamma_4\bar{\gamma}_2|$$

$$\Psi_2(\gamma^1\gamma^{11}, {}^3\Gamma^{11}, M=0, \gamma_2) = \frac{\sqrt{2}|\gamma_4\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_4\bar{\gamma}_2|}{2}$$

$$\Psi_3(\gamma^1\gamma^{11}, {}^3\Gamma^{11}, M=1, \gamma_2) = |\gamma_4\gamma_2|$$

$$\gamma^2\gamma^3$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^2\gamma^3, {}^3\Gamma^{11}, M=-1, \gamma_2) = |\gamma_5\bar{\gamma}_6|$$

$$\Psi_5(\gamma^2\gamma^3, {}^3\Gamma^{11}, M=0, \gamma_2) = \frac{\sqrt{2}|\gamma_5\gamma_6|}{2} + \frac{\sqrt{2}|\gamma_5\bar{\gamma}_6|}{2}$$

$$\Psi_6(\gamma^2\gamma^3, {}^3\Gamma^{11}, M=1, \gamma_2) = |\gamma_5\gamma_6|$$

$$\gamma^5\gamma^7$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(\gamma^5\gamma^7, {}^3\Gamma^{11}, M=-1, \gamma_2) = |\gamma_8\bar{\gamma}_{10}|$$

$$\Psi_8(\gamma^5\gamma^7, {}^3\Gamma^{11}, M=0, \gamma_2) = \frac{\sqrt{2}|\gamma_8\gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_8\bar{\gamma}_{10}|}{2}$$

$$\Psi_9(\gamma^5\gamma^7, {}^3\Gamma^{11}, M=1, \gamma_2) = |\gamma_8\gamma_{10}|$$

$$\gamma^8\gamma^{10}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{10}(\gamma^8\gamma^{10}, {}^3\Gamma^{11}, M=-1, \gamma_2) = |\gamma_{11}\bar{\gamma}_1|$$

$$\Psi_{11}(\gamma^8\gamma^{10}, {}^3\Gamma^{11}, M=0, \gamma_2) = \frac{\sqrt{2}|\gamma_{11}\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_{11}\bar{\gamma}_1|}{2}$$

$$\Psi_{12}(\gamma^8\gamma^{10}, {}^3\Gamma^{11}, M=1, \gamma_2) = |\gamma_{11}\gamma_1|$$

2.23.21 ${}^1\Gamma^{11}$

$$\gamma^1\gamma^{11}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(\gamma^1\gamma^{11}, {}^1\Gamma^{11}, M=0, \gamma_2) = -\frac{\sqrt{2}|\gamma_4\gamma_2|}{2} + \frac{\sqrt{2}|\gamma_4\bar{\gamma}_2|}{2}$$

$$\gamma^2\gamma^3$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(\gamma^2\gamma^3, {}^1\Gamma^{11}, M=0, \gamma_2) = -\frac{\sqrt{2}|\gamma_5\gamma_6|}{2} + \frac{\sqrt{2}|\gamma_5\gamma_6|}{2}$$

$$(\gamma^4)^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3((\gamma^4)^2, {}^1\Gamma^{11}, M=0, \gamma_2) = -|\gamma_7\gamma_7|$$

$$\gamma^5\gamma^7$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^5\gamma^7, {}^1\Gamma^{11}, M=0, \gamma_2) = -\frac{\sqrt{2}|\gamma_8\gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_8\gamma_{10}|}{2}$$

$$(\gamma^6)^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_5((\gamma^6)^2, {}^1\Gamma^{11}, M=0, \gamma_2) = -|\gamma_9\gamma_9|$$

$$\gamma^8\gamma^{10}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_6(\gamma^8\gamma^{10}, {}^1\Gamma^{11}, M=0, \gamma_2) = -\frac{\sqrt{2}|\gamma_{11}\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_{11}\gamma_1|}{2}$$

$$(\gamma^9)^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7((\gamma^9)^2, {}^1\Gamma^{11}, M=0, \gamma_2) = -|\gamma_{12}\gamma_{12}|$$

$$(\gamma^{12})^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_8((\gamma^{12})^2, {}^1\Gamma^{11}, M=0, \gamma_2) = -|\gamma_3\gamma_3|$$

2.23.22 ${}^3\Gamma^{12}$

$$\gamma^1\gamma^{12}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(\gamma^1\gamma^{12}, {}^3\Gamma^{12}, M=-1, \gamma_3) = |\gamma_4\gamma_3|$$

$$\Psi_2(\gamma^1\gamma^{12}, {}^3\Gamma^{12}, M=0, \gamma_3) = \frac{\sqrt{2}|\gamma_4\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_4\gamma_3|}{2}$$

$$\Psi_3(\gamma^1\gamma^{12}, {}^3\Gamma^{12}, M=1, \gamma_3) = |\gamma_4\gamma_3|$$

$$\gamma^2\gamma^4$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^2\gamma^4, {}^3\Gamma^{12}, M=-1, \gamma_3) = |\gamma_5\gamma_7|$$

$$\Psi_5(\gamma^2\gamma^4, {}^3\Gamma^{12}, M=0, \gamma_3) = \frac{\sqrt{2}|\gamma_5\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_5\gamma_7|}{2}$$

$$\Psi_6(\gamma^2\gamma^4, {}^3\Gamma^{12}, M=1, \gamma_3) = |\gamma_5\gamma_7|$$

$$\gamma^5\gamma^6$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(\gamma^5\gamma^6, {}^3\Gamma^{12}, M=-1, \gamma_3) = |\gamma_8\gamma_9|$$

$$\Psi_8(\gamma^5\gamma^6, {}^3\Gamma^{12}, M=0, \gamma_3) = \frac{\sqrt{2}|\gamma_8\gamma_9|}{2} + \frac{\sqrt{2}|\gamma_8\gamma_9|}{2}$$

$$\Psi_9(\gamma^5\gamma^6, {}^3\Gamma^{12}, M=1, \gamma_3) = |\gamma_8\gamma_9|$$

$$\gamma^8\gamma^9$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{10}(\gamma^8\gamma^9, {}^3\Gamma^{12}, M=-1, \gamma_3) = |\gamma_{11}\gamma_{12}|$$

$$\Psi_{11}(\gamma^8\gamma^9, {}^3\Gamma^{12}, M=0, \gamma_3) = \frac{\sqrt{2}|\gamma_{11}\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_{11}\gamma_{12}|}{2}$$

$$\Psi_{12}(\gamma^8\gamma^9, {}^3\Gamma^{12}, M=1, \gamma_3) = |\gamma_{11}\gamma_{12}|$$

2.23.23 ${}^1\Gamma^{12}$

$$\gamma^1\gamma^{12}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(\gamma^1\gamma^{12}, {}^1\Gamma^{12}, M=0, \gamma_3) = -\frac{\sqrt{2}|\gamma_4\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_4\gamma_3|}{2}$$

$$\gamma^2\gamma^4$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(\gamma^2\gamma^4, {}^1\Gamma^{12}, M=0, \gamma_3) = -\frac{\sqrt{2}|\gamma_5\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_5\gamma_7|}{2}$$

$$(\gamma^3)^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3((\gamma^3)^2, {}^1\Gamma^{12}, M=0, \gamma_3) = -|\gamma_6\gamma_6|$$

$$\gamma^5\gamma^6$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^5\gamma^6, {}^1\Gamma^{12}, M=0, \gamma_3) = -\frac{\sqrt{2}|\gamma_8\gamma_9|}{2} + \frac{\sqrt{2}|\gamma_8\gamma_9|}{2}$$

$$(\gamma^7)^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_5((\gamma^7)^2, {}^1\Gamma^{12}, M=0, \gamma_3) = -|\gamma_{10}\gamma_{10}|$$

$$\gamma^8\gamma^9$$

$$\boxed{\Delta E = 0}$$

$$\Psi_6(\gamma^8\gamma^9, {}^1\Gamma^{12}, M=0, \gamma_3) = -\frac{\sqrt{2}|\gamma_{11}\gamma_{12}|}{2} + \frac{\sqrt{2}|\gamma_{11}\gamma_{12}|}{2}$$

$$(\gamma^{10})^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7((\gamma^{10})^2, {}^1\Gamma^{12}, M=0, \gamma_3) = -|\bar{\gamma}_1\gamma_1|$$

$$(\gamma^{11})^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_8((\gamma^{11})^2, {}^1\Gamma^{12}, M=0, \gamma_3) = -|\bar{\gamma}_2\gamma_2|$$

2.23.24 ${}^3\Gamma^1$

$$\gamma^3\gamma^4$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(\gamma^3\gamma^4, {}^3\Gamma^1, M=-1, \gamma_4) = |\bar{\gamma}_6\gamma_7|$$

$$\Psi_2(\gamma^3\gamma^4, {}^3\Gamma^1, M=0, \gamma_4) = \frac{\sqrt{2}|\bar{\gamma}_6\gamma_7|}{2} + \frac{\sqrt{2}|\gamma_6\bar{\gamma}_7|}{2}$$

$$\Psi_3(\gamma^3\gamma^4, {}^3\Gamma^1, M=1, \gamma_4) = |\gamma_6\bar{\gamma}_7|$$

$$\gamma^6\gamma^7$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\gamma^6\gamma^7, {}^3\Gamma^1, M=-1, \gamma_4) = |\bar{\gamma}_9\gamma_{10}|$$

$$\Psi_5(\gamma^6\gamma^7, {}^3\Gamma^1, M=0, \gamma_4) = \frac{\sqrt{2}|\bar{\gamma}_9\gamma_{10}|}{2} + \frac{\sqrt{2}|\gamma_9\bar{\gamma}_{10}|}{2}$$

$$\Psi_6(\gamma^6\gamma^7, {}^3\Gamma^1, M=1, \gamma_4) = |\gamma_9\bar{\gamma}_{10}|$$

$$\gamma^9\gamma^{10}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(\gamma^9\gamma^{10}, {}^3\Gamma^1, M=-1, \gamma_4) = |\bar{\gamma}_{12}\gamma_1|$$

$$\Psi_8(\gamma^9\gamma^{10}, {}^3\Gamma^1, M=0, \gamma_4) = \frac{\sqrt{2}|\bar{\gamma}_{12}\gamma_1|}{2} + \frac{\sqrt{2}|\gamma_{12}\bar{\gamma}_1|}{2}$$

$$\Psi_9(\gamma^9\gamma^{10}, {}^3\Gamma^1, M=1, \gamma_4) = |\gamma_{12}\bar{\gamma}_1|$$

$$\gamma^{11}\gamma^{12}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{10}(\gamma^{11}\gamma^{12}, {}^3\Gamma^1, M=-1, \gamma_4) = |\bar{\gamma}_2\gamma_3|$$

$$\Psi_{11}(\gamma^{11}\gamma^{12}, {}^3\Gamma^1, M=0, \gamma_4) = \frac{\sqrt{2}|\bar{\gamma}_2\gamma_3|}{2} + \frac{\sqrt{2}|\gamma_2\bar{\gamma}_3|}{2}$$

$$\Psi_{12}(\gamma^{11}\gamma^{12}, {}^3\Gamma^1, M=1, \gamma_4) = |\gamma_2\bar{\gamma}_3|$$

2.24 Group D_6

Component labels

$$A_1 : \{\alpha\} \longrightarrow B_1 : \{\gamma\} \longrightarrow B_2 : \{\zeta\} \longrightarrow A_2 : \{\beta\} \longrightarrow E_2 : \{\nu, \xi\} \longrightarrow E_1 : \{\eta, \mu\}$$

2.24.1 1A_1

$$a_1^2$$

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_1(a_1^2, {}^1A_1, M=0, \alpha) = -|\bar{\alpha}\alpha|$$

$$b_1^2$$

$$\boxed{\Delta E = \langle \gamma\gamma || \gamma\gamma \rangle}$$

$$\Psi_2(b_1^2, {}^1A_1, M=0, \alpha) = -|\bar{\gamma}\gamma|$$

$$b_2^2$$

$$\boxed{\Delta E = \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\Psi_3(b_2^2, {}^1A_1, M=0, \alpha) = -|\bar{\zeta}\zeta|$$

$$a_2^2$$

$$\boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle}$$

$$\Psi_4(a_2^2, {}^1A_1, M=0, \alpha) = -|\bar{\beta}\beta|$$

$$e_2^2$$

$$\boxed{\Delta E = \langle \xi\xi || \nu\nu \rangle + \langle \xi\xi || \xi\xi \rangle}$$

$$\Psi_5(e_2^2, {}^1A_1, M=0, \alpha) = -\frac{\sqrt{2}|\bar{\nu}\nu|}{2} - \frac{\sqrt{2}|\bar{\xi}\xi|}{2}$$

$$e_1^2$$

$$\boxed{\Delta E = \langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_6(e_1^2, {}^1A_1, M=0, \alpha) = -\frac{\sqrt{2}|\bar{\eta}\eta|}{2} - \frac{\sqrt{2}|\bar{\mu}\mu|}{2}$$

2.24.2 3B_1

$$a_1 b_1$$

$$\boxed{\Delta E = -\langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(a_1 b_1, {}^3B_1, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

$$\Psi_2(a_1 b_1, {}^3B_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(a_1 b_1, {}^3B_1, M=1, \gamma) = |\alpha\gamma|$$

$$a_2 b_2$$

$$\boxed{\Delta E = \langle \zeta\beta || \zeta\beta \rangle - \langle \zeta\zeta || \beta\beta \rangle}$$

$$\begin{aligned}\Psi_4(a_2b_2, {}^3B_1, M=-1, \gamma) &= |\zeta\beta| \\ \Psi_5(a_2b_2, {}^3B_1, M=0, \gamma) &= \frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2} \\ \Psi_6(a_2b_2, {}^3B_1, M=1, \gamma) &= |\zeta\beta|\end{aligned}$$

$$\begin{aligned}e_1e_2 \\ \Delta E = -\langle\xi\mu||\nu\eta\rangle + \langle\xi\mu||\xi\mu\rangle - 2\langle\xi\xi||\mu\mu\rangle \\ -\langle\xi\nu||\mu\eta\rangle + \langle\xi\xi||\eta\eta\rangle\end{aligned}$$

$$\begin{aligned}\Psi_7(e_1e_2, {}^3B_1, M=-1, \gamma) &= -\frac{\sqrt{2}|\bar{\nu}\eta|}{2} + \frac{\sqrt{2}|\bar{\xi}\mu|}{2} \\ \Psi_8(e_1e_2, {}^3B_1, M=0, \gamma) &= -\frac{|\bar{\nu}\eta|}{2} + \frac{|\bar{\xi}\mu|}{2} - \frac{|\nu\bar{\eta}|}{2} + \frac{|\xi\bar{\mu}|}{2} \\ \Psi_9(e_1e_2, {}^3B_1, M=1, \gamma) &= -\frac{\sqrt{2}|\nu\eta|}{2} + \frac{\sqrt{2}|\xi\mu|}{2}\end{aligned}$$

2.24.3 1B_1

$$\begin{aligned}a_1b_1 \\ \Delta E = \langle\alpha\alpha||\gamma\gamma\rangle + \langle\alpha\gamma||\alpha\gamma\rangle \\ \Psi_1(a_1b_1, {}^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2} \\ a_2b_2 \\ \Delta E = \langle\zeta\beta||\zeta\beta\rangle + \langle\zeta\zeta||\beta\beta\rangle \\ \Psi_2(a_2b_2, {}^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2} \\ e_1e_2 \\ \Delta E = -\langle\xi\mu||\nu\eta\rangle + \langle\xi\mu||\xi\mu\rangle + 2\langle\xi\xi||\mu\mu\rangle \\ +\langle\xi\nu||\mu\eta\rangle - \langle\xi\xi||\eta\eta\rangle \\ \Psi_3(e_1e_2, {}^1B_1, M=0, \gamma) = \frac{|\bar{\nu}\eta|}{2} - \frac{|\bar{\xi}\mu|}{2} - \frac{|\nu\bar{\eta}|}{2} + \frac{|\xi\bar{\mu}|}{2}\end{aligned}$$

2.24.4 3B_2

$$\begin{aligned}a_1b_2 \\ \Delta E = -\langle\alpha\alpha||\zeta\zeta\rangle + \langle\alpha\zeta||\alpha\zeta\rangle \\ \Psi_1(a_1b_2, {}^3B_2, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}| \\ \Psi_2(a_1b_2, {}^3B_2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2} \\ \Psi_3(a_1b_2, {}^3B_2, M=1, \zeta) = |\alpha\zeta| \\ a_2b_1 \\ \Delta E = \langle\gamma\beta||\gamma\beta\rangle - \langle\gamma\gamma||\beta\beta\rangle\end{aligned}$$

$$\begin{aligned}\Psi_4(a_2b_1, {}^3B_2, M=-1, \zeta) &= |\bar{\gamma}\bar{\beta}| \\ \Psi_5(a_2b_1, {}^3B_2, M=0, \zeta) &= \frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2} \\ \Psi_6(a_2b_1, {}^3B_2, M=1, \zeta) &= |\gamma\beta|\end{aligned}$$

$$\begin{aligned}e_1e_2 \\ \Delta E = 3\langle\xi\mu||\nu\eta\rangle + \langle\xi\mu||\xi\mu\rangle - \langle\xi\xi||\eta\eta\rangle \\ -\langle\xi\nu||\mu\eta\rangle\end{aligned}$$

$$\begin{aligned}\Psi_7(e_1e_2, {}^3B_2, M=-1, \zeta) &= \frac{\sqrt{2}|\bar{\nu}\mu|}{2} + \frac{\sqrt{2}|\bar{\xi}\eta|}{2} \\ \Psi_8(e_1e_2, {}^3B_2, M=0, \zeta) &= \frac{|\bar{\nu}\mu|}{2} + \frac{|\bar{\xi}\eta|}{2} + \frac{|\nu\bar{\mu}|}{2} + \frac{|\xi\bar{\eta}|}{2} \\ \Psi_9(e_1e_2, {}^3B_2, M=1, \zeta) &= \frac{\sqrt{2}|\nu\mu|}{2} + \frac{\sqrt{2}|\xi\eta|}{2}\end{aligned}$$

2.24.5 1B_2

$$\begin{aligned}a_1b_2 \\ \Delta E = \langle\alpha\alpha||\zeta\zeta\rangle + \langle\alpha\zeta||\alpha\zeta\rangle \\ \Psi_1(a_1b_2, {}^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2} \\ a_2b_1 \\ \Delta E = \langle\gamma\beta||\gamma\beta\rangle + \langle\gamma\gamma||\beta\beta\rangle \\ \Psi_2(a_2b_1, {}^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2} \\ e_1e_2 \\ \Delta E = 3\langle\xi\mu||\nu\eta\rangle + \langle\xi\mu||\xi\mu\rangle + \langle\xi\xi||\eta\eta\rangle \\ +\langle\xi\nu||\mu\eta\rangle \\ \Psi_3(e_1e_2, {}^1B_2, M=0, \zeta) = -\frac{|\bar{\nu}\mu|}{2} - \frac{|\bar{\xi}\eta|}{2} + \frac{|\nu\bar{\mu}|}{2} + \frac{|\xi\bar{\eta}|}{2}\end{aligned}$$

2.24.6 3A_2

$$\begin{aligned}a_1a_2 \\ \Delta E = -\langle\alpha\alpha||\beta\beta\rangle + \langle\alpha\beta||\alpha\beta\rangle \\ \Psi_1(a_1a_2, {}^3A_2, M=-1, \beta) = |\bar{\alpha}\bar{\beta}| \\ \Psi_2(a_1a_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2} \\ \Psi_3(a_1a_2, {}^3A_2, M=1, \beta) = |\alpha\beta| \\ b_1b_2 \\ \Delta E = -\langle\gamma\gamma||\zeta\zeta\rangle + \langle\gamma\zeta||\gamma\zeta\rangle \\ \Psi_4(b_1b_2, {}^3A_2, M=-1, \beta) = |\bar{\gamma}\bar{\zeta}|\end{aligned}$$

$$\Psi_5(b_1 b_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\gamma\bar{\zeta}|}{2}$$

$$\Psi_6(b_1 b_2, {}^3A_2, M=1, \beta) = |\gamma\zeta|$$

$$e_2^2$$

$$\boxed{\Delta E = -3 \langle \xi\xi || \nu\nu \rangle + \langle \xi\xi || \xi\xi \rangle}$$

$$\Psi_7(e_2^2, {}^3A_2, M=-1, \beta) = -|\bar{\nu}\bar{\xi}|$$

$$\Psi_8(e_2^2, {}^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\nu}\xi|}{2} + \frac{\sqrt{2}|\bar{\xi}\nu|}{2}$$

$$\Psi_9(e_2^2, {}^3A_2, M=1, \beta) = -|\nu\xi|$$

$$e_1^2$$

$$\boxed{\Delta E = -3 \langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_{10}(e_1^2, {}^3A_2, M=-1, \beta) = -|\bar{\eta}\mu|$$

$$\Psi_{11}(e_1^2, {}^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} + \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

$$\Psi_{12}(e_1^2, {}^3A_2, M=1, \beta) = -|\eta\mu|$$

2.24.7 1A_2

$$a_1 a_2$$

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a_1 a_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$b_1 b_2$$

$$\boxed{\Delta E = \langle \gamma\gamma || \zeta\zeta \rangle + \langle \gamma\zeta || \gamma\zeta \rangle}$$

$$\Psi_2(b_1 b_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\gamma\bar{\zeta}|}{2}$$

2.24.8 3E_2

$$a_1 e_2$$

$$\boxed{\Delta E = -\langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle}$$

$$\Psi_1(a_1 e_2, {}^3E_2, M=-1, \nu) = |\bar{\alpha}\bar{\nu}|$$

$$\Psi_2(a_1 e_2, {}^3E_2, M=-1, \xi) = |\bar{\alpha}\bar{\xi}|$$

$$\Psi_3(a_1 e_2, {}^3E_2, M=0, \nu) = \frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2}$$

$$\Psi_4(a_1 e_2, {}^3E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\alpha}\xi|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2}$$

$$\Psi_5(a_1 e_2, {}^3E_2, M=1, \nu) = |\alpha\nu|$$

$$\Psi_6(a_1 e_2, {}^3E_2, M=1, \xi) = |\alpha\xi|$$

$$b_1 e_1$$

$$\boxed{\Delta E = -\langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle}$$

$$\Psi_7(b_1 e_1, {}^3E_2, M=-1, \nu) = |\bar{\gamma}\bar{\eta}|$$

$$\Psi_8(b_1 e_1, {}^3E_2, M=-1, \xi) = -|\bar{\gamma}\bar{\mu}|$$

$$\Psi_9(b_1 e_1, {}^3E_2, M=0, \nu) = \frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

$$\Psi_{10}(b_1 e_1, {}^3E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\gamma}\mu|}{2} - \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}$$

$$\Psi_{11}(b_1 e_1, {}^3E_2, M=1, \nu) = |\gamma\eta|$$

$$\Psi_{12}(b_1 e_1, {}^3E_2, M=1, \xi) = -|\gamma\mu|$$

$$b_2 e_1$$

$$\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle - \langle \zeta\zeta || \mu\mu \rangle}$$

$$\Psi_{13}(b_2 e_1, {}^3E_2, M=-1, \xi) = |\bar{\zeta}\bar{\eta}|$$

$$\Psi_{14}(b_2 e_1, {}^3E_2, M=-1, \nu) = |\bar{\zeta}\bar{\mu}|$$

$$\Psi_{15}(b_2 e_1, {}^3E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}$$

$$\Psi_{16}(b_2 e_1, {}^3E_2, M=0, \nu) = \frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$\Psi_{17}(b_2 e_1, {}^3E_2, M=1, \xi) = |\zeta\eta|$$

$$\Psi_{18}(b_2 e_1, {}^3E_2, M=1, \nu) = |\zeta\mu|$$

$$a_2 e_2$$

$$\boxed{\Delta E = -\langle \beta\beta || \xi\xi \rangle + \langle \beta\xi || \beta\xi \rangle}$$

$$\Psi_{19}(a_2 e_2, {}^3E_2, M=-1, \xi) = -|\bar{\beta}\bar{\nu}|$$

$$\Psi_{20}(a_2 e_2, {}^3E_2, M=-1, \nu) = |\bar{\beta}\bar{\xi}|$$

$$\Psi_{21}(a_2 e_2, {}^3E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\beta}\nu|}{2} - \frac{\sqrt{2}|\beta\bar{\nu}|}{2}$$

$$\Psi_{22}(a_2 e_2, {}^3E_2, M=0, \nu) = \frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2}$$

$$\Psi_{23}(a_2 e_2, {}^3E_2, M=1, \xi) = -|\beta\nu|$$

$$\Psi_{24}(a_2 e_2, {}^3E_2, M=1, \nu) = |\beta\xi|$$

2.24.9 1E_2

$$a_1 e_2$$

$$\boxed{\Delta E = \langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle}$$

$$\Psi_1(a_1 e_2, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2}$$

$$\Psi_2(a_1 e_2, {}^1E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\alpha}\xi|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2}$$

$$b_1 e_1$$

$$\boxed{\Delta E = \langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle}$$

$$\Psi_3(b_1 e_1, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

$$\Psi_4(b_1 e_1, {}^1E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\gamma}\mu|}{2} - \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}$$

$$b_2 e_1$$

$$\Psi_{10}(b_1e_2, {}^3E_1, M=0, \mu) = -\frac{\sqrt{2}|\bar{\gamma}\xi|}{2} - \frac{\sqrt{2}|\gamma\bar{\xi}|}{2}$$

$$\Delta E = \langle \zeta\mu || \zeta\mu \rangle + \langle \zeta\xi || \mu\mu \rangle$$

$$\Psi_5(b_2e_1, {}^1E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}$$

$$\Psi_6(b_2e_1, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$a_2e_2$$

$$\Delta E = \langle \beta\beta || \xi\xi \rangle + \langle \beta\xi || \beta\xi \rangle$$

$$\Psi_7(a_2e_2, {}^1E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\beta}\nu|}{2} - \frac{\sqrt{2}|\beta\bar{\nu}|}{2}$$

$$\Psi_8(a_2e_2, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2}$$

$$e_2^2$$

$$\Delta E = -\langle \xi\xi || \nu\nu \rangle + \langle \xi\xi || \xi\xi \rangle$$

$$\Psi_9(e_2^2, {}^1E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\nu}\nu|}{2} + \frac{\sqrt{2}|\bar{\xi}\xi|}{2}$$

$$\Psi_{10}(e_2^2, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\nu}\xi|}{2} - \frac{\sqrt{2}|\xi\bar{\nu}|}{2}$$

$$e_1^2$$

$$\Delta E = -\langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle$$

$$\Psi_{11}(e_1^2, {}^1E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\eta}\eta|}{2} - \frac{\sqrt{2}|\bar{\mu}\mu|}{2}$$

$$\Psi_{12}(e_1^2, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} - \frac{\sqrt{2}|\mu\bar{\eta}|}{2}$$

2.24.10 3E_1 a_1e_1

$$\boxed{\Delta E = -\langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle}$$

$$\Psi_1(a_1e_1, {}^3E_1, M=-1, \eta) = |\bar{\alpha}\eta|$$

$$\Psi_2(a_1e_1, {}^3E_1, M=-1, \mu) = |\bar{\alpha}\mu|$$

$$\Psi_3(a_1e_1, {}^3E_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_4(a_1e_1, {}^3E_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_5(a_1e_1, {}^3E_1, M=1, \eta) = |\alpha\eta|$$

$$\Psi_6(a_1e_1, {}^3E_1, M=1, \mu) = |\alpha\mu|$$

 b_1e_2

$$\boxed{\Delta E = -\langle \gamma\gamma || \xi\xi \rangle + \langle \gamma\xi || \gamma\xi \rangle}$$

$$\Psi_7(b_1e_2, {}^3E_1, M=-1, \eta) = |\bar{\gamma}\nu|$$

$$\Psi_8(b_1e_2, {}^3E_1, M=-1, \mu) = -|\bar{\gamma}\bar{\xi}|$$

$$\Psi_9(b_1e_2, {}^3E_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\gamma}\nu|}{2} + \frac{\sqrt{2}|\gamma\bar{\nu}|}{2}$$

$$\Psi_{10}(b_1e_2, {}^3E_1, M=0, \mu) = -\frac{\sqrt{2}|\bar{\gamma}\xi|}{2} - \frac{\sqrt{2}|\gamma\bar{\xi}|}{2}$$

$$\Psi_{11}(b_1e_2, {}^3E_1, M=1, \eta) = |\gamma\nu|$$

$$\Psi_{12}(b_1e_2, {}^3E_1, M=1, \mu) = -|\gamma\xi|$$

 b_2e_2

$$\boxed{\Delta E = \langle \zeta\xi || \zeta\xi \rangle - \langle \zeta\xi || \xi\xi \rangle}$$

$$\Psi_{13}(b_2e_2, {}^3E_1, M=-1, \mu) = |\bar{\zeta}\nu|$$

$$\Psi_{14}(b_2e_2, {}^3E_1, M=-1, \eta) = |\bar{\zeta}\xi|$$

$$\Psi_{15}(b_2e_2, {}^3E_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\zeta}\nu|}{2} + \frac{\sqrt{2}|\zeta\bar{\nu}|}{2}$$

$$\Psi_{16}(b_2e_2, {}^3E_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\zeta}\xi|}{2} + \frac{\sqrt{2}|\zeta\bar{\xi}|}{2}$$

$$\Psi_{17}(b_2e_2, {}^3E_1, M=1, \mu) = |\zeta\nu|$$

$$\Psi_{18}(b_2e_2, {}^3E_1, M=1, \eta) = |\zeta\xi|$$

 a_2e_1

$$\boxed{\Delta E = -\langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle}$$

$$\Psi_{19}(a_2e_1, {}^3E_1, M=-1, \mu) = -|\bar{\beta}\eta|$$

$$\Psi_{20}(a_2e_1, {}^3E_1, M=-1, \eta) = |\bar{\beta}\mu|$$

$$\Psi_{21}(a_2e_1, {}^3E_1, M=0, \mu) = -\frac{\sqrt{2}|\bar{\beta}\eta|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_{22}(a_2e_1, {}^3E_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_{23}(a_2e_1, {}^3E_1, M=1, \mu) = -|\beta\eta|$$

$$\Psi_{24}(a_2e_1, {}^3E_1, M=1, \eta) = |\beta\mu|$$

 e_1e_2

$$\boxed{\Delta E = \langle \xi\mu || \nu\eta \rangle + \langle \xi\mu || \xi\mu \rangle - \langle \xi\xi || \eta\eta \rangle + \langle \xi\nu || \mu\eta \rangle}$$

$$\Psi_{25}(e_1e_2, {}^3E_1, M=-1, \mu) = -\frac{\sqrt{2}|\bar{\nu}\eta|}{2} - \frac{\sqrt{2}|\bar{\xi}\mu|}{2}$$

$$\Psi_{26}(e_1e_2, {}^3E_1, M=-1, \eta) = -\frac{\sqrt{2}|\bar{\nu}\mu|}{2} + \frac{\sqrt{2}|\bar{\xi}\bar{\eta}|}{2}$$

$$\Psi_{27}(e_1e_2, {}^3E_1, M=0, \mu) = -\frac{|\bar{\nu}\eta|}{2} - \frac{|\bar{\xi}\mu|}{2} - \frac{|\nu\bar{\eta}|}{2} - \frac{|\xi\bar{\mu}|}{2}$$

$$\Psi_{28}(e_1e_2, {}^3E_1, M=0, \eta) = -\frac{|\bar{\nu}\mu|}{2} + \frac{|\bar{\xi}\eta|}{2} - \frac{|\nu\bar{\mu}|}{2} + \frac{|\xi\bar{\eta}|}{2}$$

$$\Psi_{29}(e_1e_2, {}^3E_1, M=1, \mu) = -\frac{\sqrt{2}|\bar{\nu}\eta|}{2} - \frac{\sqrt{2}|\xi\mu|}{2}$$

$$\Psi_{30}(e_1e_2, {}^3E_1, M=1, \eta) = -\frac{\sqrt{2}|\bar{\nu}\mu|}{2} + \frac{\sqrt{2}|\xi\eta|}{2}$$

<p>2.24.11 1E_1</p> <p>$a_1 e_1$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \alpha\alpha \mu\mu \rangle + \langle \alpha\mu \alpha\mu \rangle$ </div> <p>$\Psi_1(a_1 e_1, ^1E_1, M=0, \eta) = -\frac{\sqrt{2} \bar{\alpha}\eta }{2} + \frac{\sqrt{2} \alpha\bar{\eta} }{2}$</p> <p>$\Psi_2(a_1 e_1, ^1E_1, M=0, \mu) = -\frac{\sqrt{2} \bar{\alpha}\mu }{2} + \frac{\sqrt{2} \alpha\bar{\mu} }{2}$</p> <p>$b_1 e_2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma\gamma \xi\xi \rangle + \langle \gamma\xi \gamma\xi \rangle$ </div> <p>$\Psi_3(b_1 e_2, ^1E_1, M=0, \eta) = -\frac{\sqrt{2} \bar{\gamma}\eta }{2} + \frac{\sqrt{2} \gamma\bar{\eta} }{2}$</p> <p>$\Psi_4(b_1 e_2, ^1E_1, M=0, \mu) = \frac{\sqrt{2} \bar{\gamma}\mu }{2} - \frac{\sqrt{2} \gamma\bar{\mu} }{2}$</p> <p>$b_2 e_2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \zeta\xi \zeta\xi \rangle + \langle \zeta\zeta \xi\xi \rangle$ </div>	<p>$a_2 e_1$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Psi_5(b_2 e_2, ^1E_1, M=0, \mu) = -\frac{\sqrt{2} \bar{\zeta}\nu }{2} + \frac{\sqrt{2} \zeta\bar{\nu} }{2}$ </div> <p>$\Psi_6(b_2 e_2, ^1E_1, M=0, \eta) = -\frac{\sqrt{2} \bar{\zeta}\xi }{2} + \frac{\sqrt{2} \zeta\bar{\xi} }{2}$</p> <p>$a_2 e_1$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \beta\beta \mu\mu \rangle + \langle \beta\mu \beta\mu \rangle$ </div> <p>$\Psi_7(a_2 e_1, ^1E_1, M=0, \mu) = \frac{\sqrt{2} \bar{\beta}\eta }{2} - \frac{\sqrt{2} \beta\bar{\eta} }{2}$</p> <p>$\Psi_8(a_2 e_1, ^1E_1, M=0, \eta) = -\frac{\sqrt{2} \bar{\beta}\mu }{2} + \frac{\sqrt{2} \beta\bar{\mu} }{2}$</p> <p>$e_1 e_2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \xi\mu \nu\eta \rangle + \langle \xi\mu \xi\mu \rangle + \langle \xi\xi \eta\eta \rangle - \langle \xi\nu \mu\eta \rangle$ </div> <p>$\Psi_9(e_1 e_2, ^1E_1, M=0, \mu) = \frac{ \bar{\nu}\eta }{2} + \frac{ \bar{\xi}\mu }{2} - \frac{ \nu\bar{\eta} }{2} - \frac{ \xi\bar{\mu} }{2}$</p> <p>$\Psi_{10}(e_1 e_2, ^1E_1, M=0, \eta) = \frac{ \bar{\nu}\mu }{2} - \frac{ \bar{\xi}\eta }{2} - \frac{ \nu\bar{\mu} }{2} + \frac{ \xi\bar{\eta} }{2}$</p>
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<p>2.25 Group C_{6v}</p> <p><u>Component labels</u></p> <p>$A_1 : \{\alpha\} \longrightarrow B_2 : \{\zeta\} \longrightarrow B_1 : \{\gamma\} \longrightarrow A_2 : \{\beta\} \longrightarrow E_2 : \{\nu, \xi\} \longrightarrow E_1 : \{\eta, \mu\}$</p> <hr style="border-top: 1px solid black; margin-top: 10px;"/> <p>2.25.1 1A_1</p> <p>a_1^2</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \alpha\alpha \alpha\alpha \rangle$ </div> <p>$\Psi_1(a_1^2, ^1A_1, M=0, \alpha) = - \bar{\alpha}\alpha$</p> <p>$b_2^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \zeta\zeta \zeta\zeta \rangle$ </div> <p>$\Psi_2(b_2^2, ^1A_1, M=0, \alpha) = - \bar{\zeta}\zeta$</p> <p>$b_1^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma\gamma \gamma\gamma \rangle$ </div> <p>$\Psi_3(b_1^2, ^1A_1, M=0, \alpha) = - \bar{\gamma}\gamma$</p> <p>$a_2^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \beta\beta \beta\beta \rangle$ </div> <p>$\Psi_4(a_2^2, ^1A_1, M=0, \alpha) = - \bar{\beta}\beta$</p>	<p>e_2^2</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \xi\xi \nu\nu \rangle + \langle \xi\xi \xi\xi \rangle$ </div> <p>$\Psi_5(e_2^2, ^1A_1, M=0, \alpha) = -\frac{\sqrt{2} \bar{\nu}\nu }{2} - \frac{\sqrt{2} \bar{\xi}\xi }{2}$</p> <p>$e_1^2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \mu\mu \eta\eta \rangle + \langle \mu\mu \mu\mu \rangle$ </div> <p>$\Psi_6(e_1^2, ^1A_1, M=0, \alpha) = -\frac{\sqrt{2} \bar{\eta}\eta }{2} - \frac{\sqrt{2} \bar{\mu}\mu }{2}$</p> <hr style="border-top: 1px solid black; margin-top: 20px;"/> <p>2.25.2 3B_2</p> <p>$a_1 b_2$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = -\langle \alpha\alpha \zeta\zeta \rangle + \langle \alpha\zeta \alpha\zeta \rangle$ </div> <p>$\Psi_1(a_1 b_2, ^3B_2, M=-1, \zeta) = \bar{\alpha}\zeta$</p> <p>$\Psi_2(a_1 b_2, ^3B_2, M=0, \zeta) = \frac{\sqrt{2} \bar{\alpha}\zeta }{2} + \frac{\sqrt{2} \alpha\bar{\zeta} }{2}$</p> <p>$\Psi_3(a_1 b_2, ^3B_2, M=1, \zeta) = \alpha\zeta$</p> <p>$a_2 b_1$</p> <div style="border: 1px solid black; padding: 5px; width: 100%;"> $\Delta E = \langle \gamma\beta \gamma\beta \rangle - \langle \gamma\gamma \beta\beta \rangle$ </div>
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$$\begin{aligned}\Psi_4(a_2b_1, {}^3B_2, M=-1, \zeta) &= |\bar{\gamma}\beta| \\ \Psi_5(a_2b_1, {}^3B_2, M=0, \zeta) &= \frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\beta|}{2} \\ \Psi_6(a_2b_1, {}^3B_2, M=1, \zeta) &= |\gamma\beta|\end{aligned}$$

e₁e₂

$$\Delta E = -\langle \xi\mu || \nu\eta \rangle + \langle \xi\mu || \xi\mu \rangle - 2\langle \xi\xi || \mu\mu \rangle - \langle \xi\nu || \mu\eta \rangle + \langle \xi\xi || \eta\eta \rangle$$

$$\begin{aligned}\Psi_7(e_1e_2, {}^3B_2, M=-1, \zeta) &= -\frac{\sqrt{2}|\bar{\nu}\eta|}{2} + \frac{\sqrt{2}|\bar{\xi}\mu|}{2} \\ \Psi_8(e_1e_2, {}^3B_2, M=0, \zeta) &= -\frac{|\bar{\nu}\eta|}{2} + \frac{|\bar{\xi}\mu|}{2} - \frac{|\nu\bar{\eta}|}{2} + \frac{|\xi\bar{\mu}|}{2} \\ \Psi_9(e_1e_2, {}^3B_2, M=1, \zeta) &= -\frac{\sqrt{2}|\nu\eta|}{2} + \frac{\sqrt{2}|\xi\mu|}{2}\end{aligned}$$

2.25.3 1B_2

a₁b₂

$$\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle$$

$$\Psi_1(a_1b_2, {}^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

a₂b₁

$$\Delta E = \langle \gamma\beta || \gamma\beta \rangle + \langle \gamma\gamma || \beta\beta \rangle$$

$$\Psi_2(a_2b_1, {}^1B_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

e₁e₂

$$\Delta E = -\langle \xi\mu || \nu\eta \rangle + \langle \xi\mu || \xi\mu \rangle + 2\langle \xi\xi || \mu\mu \rangle + \langle \xi\nu || \mu\eta \rangle - \langle \xi\xi || \eta\eta \rangle$$

$$\Psi_3(e_1e_2, {}^1B_2, M=0, \zeta) = \frac{|\bar{\nu}\eta|}{2} - \frac{|\bar{\xi}\mu|}{2} - \frac{|\nu\bar{\eta}|}{2} + \frac{|\xi\bar{\mu}|}{2}$$

2.25.4 3B_1

a₁b₁

$$\Delta E = -\langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle$$

$$\Psi_1(a_1b_1, {}^3B_1, M=-1, \gamma) = |\bar{\alpha}\bar{\gamma}|$$

$$\Psi_2(a_1b_1, {}^3B_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\bar{\gamma}|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(a_1b_1, {}^3B_1, M=1, \gamma) = |\alpha\gamma|$$

a₂b₂

$$\Delta E = \langle \zeta\beta || \zeta\beta \rangle - \langle \zeta\zeta || \beta\beta \rangle$$

$$\begin{aligned}\Psi_4(a_2b_2, {}^3B_1, M=-1, \gamma) &= |\bar{\zeta}\beta| \\ \Psi_5(a_2b_2, {}^3B_1, M=0, \gamma) &= \frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2} \\ \Psi_6(a_2b_2, {}^3B_1, M=1, \gamma) &= |\zeta\beta|\end{aligned}$$

e₁e₂

$$\Delta E = 3\langle \xi\mu || \nu\eta \rangle + \langle \xi\mu || \xi\mu \rangle - \langle \xi\xi || \eta\eta \rangle - \langle \xi\nu || \mu\eta \rangle$$

$$\begin{aligned}\Psi_7(e_1e_2, {}^3B_1, M=-1, \gamma) &= \frac{\sqrt{2}|\bar{\nu}\mu|}{2} + \frac{\sqrt{2}|\bar{\xi}\eta|}{2} \\ \Psi_8(e_1e_2, {}^3B_1, M=0, \gamma) &= \frac{|\bar{\nu}\mu|}{2} + \frac{|\bar{\xi}\eta|}{2} + \frac{|\nu\bar{\mu}|}{2} + \frac{|\xi\bar{\eta}|}{2} \\ \Psi_9(e_1e_2, {}^3B_1, M=1, \gamma) &= \frac{\sqrt{2}|\nu\mu|}{2} + \frac{\sqrt{2}|\xi\eta|}{2}\end{aligned}$$

2.25.5 1B_1

a₁b₁

$$\Delta E = \langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle$$

$$\Psi_1(a_1b_1, {}^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

a₂b₂

$$\Delta E = \langle \zeta\beta || \zeta\beta \rangle + \langle \zeta\zeta || \beta\beta \rangle$$

$$\Psi_2(a_2b_2, {}^1B_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2}$$

e₁e₂

$$\Delta E = 3\langle \xi\mu || \nu\eta \rangle + \langle \xi\mu || \xi\mu \rangle + \langle \xi\xi || \eta\eta \rangle + \langle \xi\nu || \mu\eta \rangle$$

$$\Psi_3(e_1e_2, {}^1B_1, M=0, \gamma) = -\frac{|\bar{\nu}\mu|}{2} - \frac{|\bar{\xi}\eta|}{2} + \frac{|\nu\bar{\mu}|}{2} + \frac{|\xi\bar{\eta}|}{2}$$

2.25.6 3A_2

a₁a₂

$$\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle$$

$$\Psi_1(a_1a_2, {}^3A_2, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$\Psi_2(a_1a_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\bar{\beta}|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(a_1a_2, {}^3A_2, M=1, \beta) = |\alpha\beta|$$

b₁b₂

$$\Delta E = \langle \zeta\gamma || \zeta\gamma \rangle - \langle \zeta\zeta || \gamma\gamma \rangle$$

$$\Psi_4(b_1b_2, {}^3A_2, M=-1, \beta) = |\bar{\zeta}\bar{\gamma}|$$

$$\Psi_5(b_1 b_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

$$\Psi_6(b_1 b_2, {}^3A_2, M=1, \beta) = |\zeta\gamma|$$

 e_2^2

$$\boxed{\Delta E = -3 \langle \xi\xi || \nu\nu \rangle + \langle \xi\xi || \xi\xi \rangle}$$

$$\Psi_7(e_2^2, {}^3A_2, M=-1, \beta) = -|\bar{\nu}\bar{\xi}|$$

$$\Psi_8(e_2^2, {}^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\nu}\xi|}{2} + \frac{\sqrt{2}|\bar{\xi}\nu|}{2}$$

$$\Psi_9(e_2^2, {}^3A_2, M=1, \beta) = -|\nu\xi|$$

 e_1^2

$$\boxed{\Delta E = -3 \langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_{10}(e_1^2, {}^3A_2, M=-1, \beta) = -|\bar{\eta}\mu|$$

$$\Psi_{11}(e_1^2, {}^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} + \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

$$\Psi_{12}(e_1^2, {}^3A_2, M=1, \beta) = -|\eta\mu|$$

2.25.7 1A_2 $a_1 a_2$

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a_1 a_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

 $b_1 b_2$

$$\boxed{\Delta E = \langle \zeta\gamma || \zeta\gamma \rangle + \langle \zeta\xi || \gamma\gamma \rangle}$$

$$\Psi_2(b_1 b_2, {}^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

2.25.8 3E_2 $a_1 e_2$

$$\boxed{\Delta E = -\langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle}$$

$$\Psi_1(a_1 e_2, {}^3E_2, M=-1, \nu) = |\bar{\alpha}\nu|$$

$$\Psi_2(a_1 e_2, {}^3E_2, M=-1, \xi) = |\bar{\alpha}\bar{\xi}|$$

$$\Psi_3(a_1 e_2, {}^3E_2, M=0, \nu) = \frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2}$$

$$\Psi_4(a_1 e_2, {}^3E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\alpha}\xi|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2}$$

$$\Psi_5(a_1 e_2, {}^3E_2, M=1, \nu) = |\alpha\nu|$$

$$\Psi_6(a_1 e_2, {}^3E_2, M=1, \xi) = |\alpha\xi|$$

 $b_2 e_1$

$$\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle - \langle \zeta\xi || \mu\mu \rangle}$$

$$\Psi_7(b_2 e_1, {}^3E_2, M=-1, \nu) = |\bar{\zeta}\bar{\eta}|$$

$$\Psi_8(b_2 e_1, {}^3E_2, M=-1, \xi) = -|\bar{\zeta}\bar{\mu}|$$

$$\Psi_9(b_2 e_1, {}^3E_2, M=0, \nu) = \frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}$$

$$\Psi_{10}(b_2 e_1, {}^3E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\zeta}\mu|}{2} - \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$\Psi_{11}(b_2 e_1, {}^3E_2, M=1, \nu) = |\zeta\eta|$$

$$\Psi_{12}(b_2 e_1, {}^3E_2, M=1, \xi) = -|\zeta\mu|$$

 $b_1 e_1$

$$\boxed{\Delta E = -\langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle}$$

$$\Psi_{13}(b_1 e_1, {}^3E_2, M=-1, \xi) = |\bar{\gamma}\bar{\eta}|$$

$$\Psi_{14}(b_1 e_1, {}^3E_2, M=-1, \nu) = |\bar{\gamma}\bar{\mu}|$$

$$\Psi_{15}(b_1 e_1, {}^3E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

$$\Psi_{16}(b_1 e_1, {}^3E_2, M=0, \nu) = \frac{\sqrt{2}|\bar{\gamma}\mu|}{2} + \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}$$

$$\Psi_{17}(b_1 e_1, {}^3E_2, M=1, \xi) = |\gamma\eta|$$

$$\Psi_{18}(b_1 e_1, {}^3E_2, M=1, \nu) = |\gamma\mu|$$

 $a_2 e_2$

$$\boxed{\Delta E = -\langle \beta\beta || \xi\xi \rangle + \langle \beta\xi || \beta\xi \rangle}$$

$$\Psi_{19}(a_2 e_2, {}^3E_2, M=-1, \xi) = -|\bar{\beta}\bar{\nu}|$$

$$\Psi_{20}(a_2 e_2, {}^3E_2, M=-1, \nu) = |\bar{\beta}\bar{\xi}|$$

$$\Psi_{21}(a_2 e_2, {}^3E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\beta}\nu|}{2} - \frac{\sqrt{2}|\beta\bar{\nu}|}{2}$$

$$\Psi_{22}(a_2 e_2, {}^3E_2, M=0, \nu) = \frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2}$$

$$\Psi_{23}(a_2 e_2, {}^3E_2, M=1, \xi) = -|\beta\nu|$$

$$\Psi_{24}(a_2 e_2, {}^3E_2, M=1, \nu) = |\beta\xi|$$

2.25.9 1E_2 $a_1 e_2$

$$\boxed{\Delta E = \langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle}$$

$$\Psi_1(a_1 e_2, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2}$$

$$\Psi_2(a_1 e_2, {}^1E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\alpha}\xi|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2}$$

 $b_2 e_1$

$$\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle + \langle \zeta\xi || \mu\mu \rangle}$$

$$\Psi_3(b_2 e_1, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\zeta}\bar{\eta}|}{2} + \frac{\sqrt{2}|\zeta\eta|}{2}$$

$$\Psi_4(b_2 e_1, {}^1E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\zeta}\mu|}{2} - \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$b_1 e_1$

$$\boxed{\Delta E = \langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle}$$

$$\Psi_5(b_1 e_1, {}^1E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{2}$$

$$\Psi_6(b_1 e_1, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\gamma}\mu|}{2} + \frac{\sqrt{2}|\gamma\bar{\mu}|}{2}$$

 $a_2 e_2$

$$\boxed{\Delta E = \langle \beta\beta || \xi\xi \rangle + \langle \beta\xi || \beta\xi \rangle}$$

$$\Psi_7(a_2 e_2, {}^1E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\beta}\nu|}{2} - \frac{\sqrt{2}|\beta\bar{\nu}|}{2}$$

$$\Psi_8(a_2 e_2, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2}$$

 e_2^2

$$\boxed{\Delta E = -\langle \xi\xi || \nu\nu \rangle + \langle \xi\xi || \xi\xi \rangle}$$

$$\Psi_9(e_2^2, {}^1E_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\nu}\nu|}{2} + \frac{\sqrt{2}|\bar{\xi}\xi|}{2}$$

$$\Psi_{10}(e_2^2, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\nu}\xi|}{2} - \frac{\sqrt{2}|\xi\nu|}{2}$$

 e_1^2

$$\boxed{\Delta E = -\langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_{11}(e_1^2, {}^1E_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\eta}\eta|}{2} - \frac{\sqrt{2}|\bar{\mu}\mu|}{2}$$

$$\Psi_{12}(e_1^2, {}^1E_2, M=0, \nu) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} - \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

2.25.10 3E_1 $a_1 e_1$

$$\boxed{\Delta E = -\langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle}$$

$$\Psi_1(a_1 e_1, {}^3E_1, M=-1, \eta) = |\bar{\alpha}\bar{\eta}|$$

$$\Psi_2(a_1 e_1, {}^3E_1, M=-1, \mu) = |\bar{\alpha}\bar{\mu}|$$

$$\Psi_3(a_1 e_1, {}^3E_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_4(a_1 e_1, {}^3E_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_5(a_1 e_1, {}^3E_1, M=1, \eta) = |\alpha\eta|$$

$$\Psi_6(a_1 e_1, {}^3E_1, M=1, \mu) = |\alpha\mu|$$

 $b_2 e_2$

$$\boxed{\Delta E = \langle \zeta\xi || \zeta\xi \rangle - \langle \zeta\zeta || \xi\xi \rangle}$$

$$\Psi_7(b_2 e_2, {}^3E_1, M=-1, \eta) = |\bar{\zeta}\bar{\nu}|$$

$$\Psi_8(b_2 e_2, {}^3E_1, M=-1, \mu) = -|\bar{\zeta}\bar{\xi}|$$

$$\Psi_9(b_2 e_2, {}^3E_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\zeta}\nu|}{2} + \frac{\sqrt{2}|\zeta\bar{\nu}|}{2}$$

$$\Psi_{10}(b_2 e_2, {}^3E_1, M=0, \mu) = -\frac{\sqrt{2}|\bar{\zeta}\xi|}{2} - \frac{\sqrt{2}|\zeta\bar{\xi}|}{2}$$

$$\Psi_{11}(b_2 e_2, {}^3E_1, M=1, \eta) = |\zeta\nu|$$

$$\Psi_{12}(b_2 e_2, {}^3E_1, M=1, \mu) = -|\zeta\xi|$$

 $b_1 e_2$

$$\boxed{\Delta E = -\langle \gamma\gamma || \xi\xi \rangle + \langle \gamma\xi || \gamma\xi \rangle}$$

$$\Psi_{13}(b_1 e_2, {}^3E_1, M=-1, \mu) = |\bar{\gamma}\bar{\nu}|$$

$$\Psi_{14}(b_1 e_2, {}^3E_1, M=-1, \eta) = |\bar{\gamma}\bar{\xi}|$$

$$\Psi_{15}(b_1 e_2, {}^3E_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\gamma}\nu|}{2} + \frac{\sqrt{2}|\gamma\bar{\nu}|}{2}$$

$$\Psi_{16}(b_1 e_2, {}^3E_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\gamma}\xi|}{2} + \frac{\sqrt{2}|\gamma\bar{\xi}|}{2}$$

$$\Psi_{17}(b_1 e_2, {}^3E_1, M=1, \mu) = |\gamma\nu|$$

$$\Psi_{18}(b_1 e_2, {}^3E_1, M=1, \eta) = |\gamma\xi|$$

 $a_2 e_1$

$$\boxed{\Delta E = -\langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle}$$

$$\Psi_{19}(a_2 e_1, {}^3E_1, M=-1, \mu) = -|\bar{\beta}\bar{\eta}|$$

$$\Psi_{20}(a_2 e_1, {}^3E_1, M=-1, \eta) = |\bar{\beta}\bar{\mu}|$$

$$\Psi_{21}(a_2 e_1, {}^3E_1, M=0, \mu) = -\frac{\sqrt{2}|\bar{\beta}\eta|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_{22}(a_2 e_1, {}^3E_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_{23}(a_2 e_1, {}^3E_1, M=1, \mu) = -|\beta\eta|$$

$$\Psi_{24}(a_2 e_1, {}^3E_1, M=1, \eta) = |\beta\mu|$$

 $e_1 e_2$

$$\boxed{\Delta E = \langle \xi\mu || \nu\eta \rangle + \langle \xi\mu || \xi\mu \rangle - \langle \xi\xi || \eta\eta \rangle + \langle \xi\nu || \mu\eta \rangle}$$

$$\Psi_{25}(e_1 e_2, {}^3E_1, M=-1, \mu) = -\frac{\sqrt{2}|\bar{\nu}\eta|}{2} - \frac{\sqrt{2}|\bar{\xi}\mu|}{2}$$

$$\Psi_{26}(e_1 e_2, {}^3E_1, M=-1, \eta) = -\frac{\sqrt{2}|\bar{\nu}\mu|}{2} + \frac{\sqrt{2}|\bar{\xi}\bar{\eta}|}{2}$$

$$\Psi_{27}(e_1 e_2, {}^3E_1, M=0, \mu) = -\frac{|\bar{\nu}\eta|}{2} - \frac{|\bar{\xi}\mu|}{2} - \frac{|\nu\bar{\eta}|}{2} - \frac{|\xi\bar{\mu}|}{2}$$

$$\Psi_{28}(e_1 e_2, {}^3E_1, M=0, \eta) = -\frac{|\bar{\nu}\mu|}{2} + \frac{|\bar{\xi}\eta|}{2} - \frac{|\nu\bar{\mu}|}{2} + \frac{|\xi\bar{\eta}|}{2}$$

$$\Psi_{29}(e_1 e_2, {}^3E_1, M=1, \mu) = -\frac{\sqrt{2}|\nu\eta|}{2} - \frac{\sqrt{2}|\xi\mu|}{2}$$

$$\Psi_{30}(e_1 e_2, {}^3E_1, M=1, \eta) = -\frac{\sqrt{2}|\nu\mu|}{2} + \frac{\sqrt{2}|\xi\eta|}{2}$$

2.25.11 1E_1 $a_1 e_1$

$$\boxed{\Delta E = \langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle}$$

$$\Psi_1(a_1 e_1, ^1E_1, M=0, \eta) = -\frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_2(a_1 e_1, ^1E_1, M=0, \mu) = -\frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

 $b_2 e_2$

$$\boxed{\Delta E = \langle \zeta\xi || \zeta\xi \rangle + \langle \zeta\zeta || \xi\xi \rangle}$$

$$\Psi_3(b_2 e_2, ^1E_1, M=0, \eta) = -\frac{\sqrt{2}|\bar{\zeta}\nu|}{2} + \frac{\sqrt{2}|\zeta\nu|}{2}$$

$$\Psi_4(b_2 e_2, ^1E_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\zeta}\xi|}{2} - \frac{\sqrt{2}|\zeta\xi|}{2}$$

 $b_1 e_2$

$$\boxed{\Delta E = \langle \gamma\gamma || \xi\xi \rangle + \langle \gamma\xi || \gamma\xi \rangle}$$

$$\Psi_5(b_1 e_2, ^1E_1, M=0, \mu) = -\frac{\sqrt{2}|\bar{\gamma}\nu|}{2} + \frac{\sqrt{2}|\gamma\nu|}{2}$$

$$\Psi_6(b_1 e_2, ^1E_1, M=0, \eta) = -\frac{\sqrt{2}|\bar{\gamma}\xi|}{2} + \frac{\sqrt{2}|\gamma\xi|}{2}$$

 $a_2 e_1$

$$\boxed{\Delta E = \langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle}$$

$$\Psi_7(a_2 e_1, ^1E_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\beta}\eta|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_8(a_2 e_1, ^1E_1, M=0, \eta) = -\frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

 $e_1 e_2$

$$\boxed{\Delta E = \langle \xi\mu || \nu\eta \rangle + \langle \xi\mu || \xi\mu \rangle + \langle \xi\xi || \eta\eta \rangle - \langle \xi\nu || \mu\eta \rangle}$$

$$\Psi_9(e_1 e_2, ^1E_1, M=0, \mu) = \frac{|\bar{\nu}\eta|}{2} + \frac{|\bar{\xi}\mu|}{2} - \frac{|\nu\bar{\eta}|}{2} - \frac{|\xi\bar{\mu}|}{2}$$

$$\Psi_{10}(e_1 e_2, ^1E_1, M=0, \eta) = \frac{|\bar{\nu}\mu|}{2} - \frac{|\bar{\xi}\eta|}{2} - \frac{|\nu\bar{\mu}|}{2} + \frac{|\xi\bar{\eta}|}{2}$$

2.26 Group D_{3h} Component labels

$$A'_1 : \{\alpha\} \longrightarrow A''_2 : \{\zeta\} \longrightarrow A''_1 : \{\gamma\} \longrightarrow A'_2 : \{\beta\} \longrightarrow E' : \{\eta, \mu\} \longrightarrow E'' : \{\nu, \xi\}$$

2.26.1 $^1A'_1$ $\left(\begin{smallmatrix} a'_1 \\ a_1 \end{smallmatrix}\right)^2$

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

$$\Psi_1\left(\left(\begin{smallmatrix} a'_1 \\ a_1 \end{smallmatrix}\right)^2, ^1A'_1, M=0, \alpha\right) = -|\bar{\alpha}\alpha|$$

 $\left(\begin{smallmatrix} a''_2 \\ a_2 \end{smallmatrix}\right)^2$

$$\boxed{\Delta E = \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\Psi_2\left(\left(\begin{smallmatrix} a''_2 \\ a_2 \end{smallmatrix}\right)^2, ^1A'_1, M=0, \alpha\right) = -|\bar{\zeta}\zeta|$$

 $\left(\begin{smallmatrix} a''_1 \\ a_1 \end{smallmatrix}\right)^2$

$$\boxed{\Delta E = \langle \gamma\gamma || \gamma\gamma \rangle}$$

$$\Psi_3\left(\left(\begin{smallmatrix} a''_1 \\ a_1 \end{smallmatrix}\right)^2, ^1A'_1, M=0, \alpha\right) = -|\bar{\gamma}\gamma|$$

 $\left(\begin{smallmatrix} a'_2 \\ a_2 \end{smallmatrix}\right)^2$

$$\boxed{\Delta E = \langle \beta\beta || \beta\beta \rangle}$$

$$\Psi_4\left(\left(\begin{smallmatrix} a'_2 \\ a_2 \end{smallmatrix}\right)^2, ^1A'_1, M=0, \alpha\right) = -|\bar{\beta}\beta|$$

 $\left(\begin{smallmatrix} e' \\ e \end{smallmatrix}\right)^2$

$$\boxed{\Delta E = \langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_5\left(\left(\begin{smallmatrix} e' \\ e \end{smallmatrix}\right)^2, ^1A'_1, M=0, \alpha\right) = -\frac{\sqrt{2}|\bar{\eta}\eta|}{2} - \frac{\sqrt{2}|\bar{\mu}\mu|}{2}$$

 $\left(\begin{smallmatrix} e'' \\ e \end{smallmatrix}\right)^2$

$$\boxed{\Delta E = \langle \xi\xi || \nu\nu \rangle + \langle \xi\xi || \xi\xi \rangle}$$

$$\Psi_6\left(\left(\begin{smallmatrix} e'' \\ e \end{smallmatrix}\right)^2, ^1A'_1, M=0, \alpha\right) = -\frac{\sqrt{2}|\bar{\nu}\nu|}{2} - \frac{\sqrt{2}|\bar{\xi}\xi|}{2}$$

2.26.2 $^3A''_2$ $\left(\begin{smallmatrix} a'_1 \\ a_1 \end{smallmatrix}\right)^2$

$$\boxed{\Delta E = -\langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a'_1 a''_2, ^3A''_2, M=-1, \zeta) = |\bar{\alpha}\bar{\zeta}|$$

$$\Psi_2(a'_1 a''_2, {}^3A''_2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_3(a'_1 a''_2, {}^3A''_2, M=1, \zeta) = |\alpha\zeta|$$

$$a''_1 a'_2$$

$$\boxed{\Delta E = \langle \gamma\beta || \gamma\beta \rangle - \langle \gamma\gamma || \beta\beta \rangle}$$

$$\Psi_4(a''_1 a'_2, {}^3A''_2, M=-1, \zeta) = |\bar{\gamma}\beta|$$

$$\Psi_5(a''_1 a'_2, {}^3A''_2, M=0, \zeta) = \frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

$$\Psi_6(a''_1 a'_2, {}^3A''_2, M=1, \zeta) = |\gamma\beta|$$

$$e' e''$$

$$\boxed{\Delta E = -2 \langle \mu\mu || \xi\xi \rangle + \langle \mu\xi || \eta\nu \rangle + \langle \mu\xi || \mu\xi \rangle + \langle \mu\eta || \xi\nu \rangle + \langle \mu\mu || \nu\nu \rangle}$$

$$\Psi_7(e' e'', {}^3A''_2, M=-1, \zeta) = \frac{\sqrt{2}|\bar{\eta}\bar{\nu}|}{2} + \frac{\sqrt{2}|\bar{\mu}\bar{\xi}|}{2}$$

$$\Psi_8(e' e'', {}^3A''_2, M=0, \zeta) = \frac{|\bar{\eta}\nu|}{2} + \frac{|\bar{\mu}\xi|}{2} + \frac{|\eta\bar{\nu}|}{2} + \frac{|\mu\bar{\xi}|}{2}$$

$$\Psi_9(e' e'', {}^3A''_2, M=1, \zeta) = \frac{\sqrt{2}|\eta\nu|}{2} + \frac{\sqrt{2}|\mu\xi|}{2}$$

2.26.3 ${}^1A''_2$

$$a'_1 a''_2$$

$$\boxed{\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a'_1 a''_2, {}^1A''_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$a''_1 a'_2$$

$$\boxed{\Delta E = \langle \gamma\beta || \gamma\beta \rangle + \langle \gamma\gamma || \beta\beta \rangle}$$

$$\Psi_2(a''_1 a'_2, {}^1A''_2, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\beta|}{2} + \frac{\sqrt{2}|\gamma\bar{\beta}|}{2}$$

$$e' e''$$

$$\boxed{\Delta E = 2 \langle \mu\mu || \xi\xi \rangle + \langle \mu\xi || \eta\nu \rangle + \langle \mu\xi || \mu\xi \rangle - \langle \mu\eta || \xi\nu \rangle - \langle \mu\mu || \nu\nu \rangle}$$

$$\Psi_3(e' e'', {}^1A''_2, M=0, \zeta) = -\frac{|\bar{\eta}\nu|}{2} - \frac{|\bar{\mu}\xi|}{2} + \frac{|\eta\bar{\nu}|}{2} + \frac{|\mu\bar{\xi}|}{2}$$

2.26.4 ${}^3A''_1$

$$a'_1 a''_1$$

$$\boxed{\Delta E = -\langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(a'_1 a''_1, {}^3A''_1, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

$$\Psi_2(a'_1 a''_1, {}^3A''_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(a'_1 a''_1, {}^3A''_1, M=1, \gamma) = |\alpha\gamma|$$

$$a'_2 a''_2$$

$$\boxed{\Delta E = \langle \zeta\beta || \zeta\beta \rangle - \langle \zeta\zeta || \beta\beta \rangle}$$

$$\Psi_4(a'_2 a''_2, {}^3A''_1, M=-1, \gamma) = |\bar{\zeta}\beta|$$

$$\Psi_5(a'_2 a''_2, {}^3A''_1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2}$$

$$\Psi_6(a'_2 a''_2, {}^3A''_1, M=1, \gamma) = |\zeta\beta|$$

$$e' e''$$

$$\boxed{\Delta E = -\langle \mu\mu || \nu\nu \rangle - 3 \langle \mu\xi || \eta\nu \rangle + \langle \mu\xi || \mu\xi \rangle + \langle \mu\eta || \xi\nu \rangle}$$

$$\Psi_7(e' e'', {}^3A''_1, M=-1, \gamma) = -\frac{\sqrt{2}|\bar{\eta}\bar{\xi}|}{2} + \frac{\sqrt{2}|\bar{\mu}\bar{\nu}|}{2}$$

$$\Psi_8(e' e'', {}^3A''_1, M=0, \gamma) = -\frac{|\bar{\eta}\xi|}{2} + \frac{|\bar{\mu}\nu|}{2} - \frac{|\eta\bar{\xi}|}{2} + \frac{|\mu\bar{\nu}|}{2}$$

$$\Psi_9(e' e'', {}^3A''_1, M=1, \gamma) = -\frac{\sqrt{2}|\eta\xi|}{2} + \frac{\sqrt{2}|\mu\nu|}{2}$$

2.26.5 ${}^1A''_1$

$$a'_1 a''_1$$

$$\boxed{\Delta E = \langle \alpha\alpha || \gamma\gamma \rangle + \langle \alpha\gamma || \alpha\gamma \rangle}$$

$$\Psi_1(a'_1 a''_1, {}^1A''_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$a'_2 a''_2$$

$$\boxed{\Delta E = \langle \zeta\beta || \zeta\beta \rangle + \langle \zeta\zeta || \beta\beta \rangle}$$

$$\Psi_2(a'_2 a''_2, {}^1A''_1, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\zeta}\beta|}{2} + \frac{\sqrt{2}|\zeta\bar{\beta}|}{2}$$

$$e' e''$$

$$\boxed{\Delta E = \langle \mu\mu || \nu\nu \rangle - 3 \langle \mu\xi || \eta\nu \rangle + \langle \mu\xi || \mu\xi \rangle - \langle \mu\eta || \xi\nu \rangle}$$

$$\Psi_3(e' e'', {}^1A''_1, M=0, \gamma) = \frac{|\bar{\eta}\xi|}{2} - \frac{|\bar{\mu}\nu|}{2} - \frac{|\eta\bar{\xi}|}{2} + \frac{|\mu\bar{\nu}|}{2}$$

2.26.6 $^3A'_2$ $a'_1 a'_2$

$$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a'_1 a'_2, ^3A'_2, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

$$\Psi_2(a'_1 a'_2, ^3A'_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_3(a'_1 a'_2, ^3A'_2, M=1, \beta) = |\alpha\beta|$$

 $a''_1 a''_2$

$$\boxed{\Delta E = \langle \zeta\gamma || \zeta\gamma \rangle - \langle \zeta\zeta || \gamma\gamma \rangle}$$

$$\Psi_4(a''_1 a''_2, ^3A'_2, M=-1, \beta) = |\bar{\zeta}\bar{\gamma}|$$

$$\Psi_5(a''_1 a''_2, ^3A'_2, M=0, \beta) = \frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

$$\Psi_6(a''_1 a''_2, ^3A'_2, M=1, \beta) = |\zeta\gamma|$$

 $(e')^2$

$$\boxed{\Delta E = -3 \langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle}$$

$$\Psi_7((e')^2, ^3A'_2, M=-1, \beta) = -|\bar{\eta}\bar{\mu}|$$

$$\Psi_8((e')^2, ^3A'_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} + \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

$$\Psi_9((e')^2, ^3A'_2, M=1, \beta) = -|\eta\mu|$$

 $(e'')^2$

$$\boxed{\Delta E = -3 \langle \xi\xi || \nu\nu \rangle + \langle \xi\xi || \xi\xi \rangle}$$

$$\Psi_{10}((e'')^2, ^3A'_2, M=-1, \beta) = -|\bar{\nu}\bar{\xi}|$$

$$\Psi_{11}((e'')^2, ^3A'_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\nu}\xi|}{2} + \frac{\sqrt{2}|\bar{\xi}\nu|}{2}$$

$$\Psi_{12}((e'')^2, ^3A'_2, M=1, \beta) = -|\nu\xi|$$

2.26.7 $^1A'_2$ $a'_1 a'_2$

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a'_1 a'_2, ^1A'_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

 $a''_1 a''_2$

$$\boxed{\Delta E = \langle \zeta\gamma || \zeta\gamma \rangle + \langle \zeta\zeta || \gamma\gamma \rangle}$$

$$\Psi_2(a''_1 a''_2, ^1A'_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} + \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

2.26.8 $^3E'$ $a'_1 e'$

$$\boxed{\Delta E = -\langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle}$$

$$\Psi_1(a'_1 e', ^3E', M=-1, \eta) = |\bar{\alpha}\bar{\eta}|$$

$$\Psi_2(a'_1 e', ^3E', M=-1, \mu) = |\bar{\alpha}\mu|$$

$$\Psi_3(a'_1 e', ^3E', M=0, \eta) = \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_4(a'_1 e', ^3E', M=0, \mu) = \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_5(a'_1 e', ^3E', M=1, \eta) = |\alpha\eta|$$

$$\Psi_6(a'_1 e', ^3E', M=1, \mu) = |\alpha\mu|$$

 $a''_2 e''$

$$\boxed{\Delta E = \langle \zeta\xi || \zeta\xi \rangle - \langle \zeta\zeta || \xi\xi \rangle}$$

$$\Psi_7(a''_2 e'', ^3E', M=-1, \eta) = |\bar{\zeta}\bar{\nu}|$$

$$\Psi_8(a''_2 e'', ^3E', M=-1, \mu) = |\bar{\zeta}\xi|$$

$$\Psi_9(a''_2 e'', ^3E', M=0, \eta) = \frac{\sqrt{2}|\bar{\zeta}\nu|}{2} + \frac{\sqrt{2}|\zeta\bar{\nu}|}{2}$$

$$\Psi_{10}(a''_2 e'', ^3E', M=0, \mu) = \frac{\sqrt{2}|\bar{\zeta}\xi|}{2} + \frac{\sqrt{2}|\zeta\bar{\xi}|}{2}$$

$$\Psi_{11}(a''_2 e'', ^3E', M=1, \eta) = |\zeta\nu|$$

$$\Psi_{12}(a''_2 e'', ^3E', M=1, \mu) = |\zeta\xi|$$

 $a''_1 e''$

$$\boxed{\Delta E = -\langle \gamma\gamma || \xi\xi \rangle + \langle \gamma\xi || \gamma\xi \rangle}$$

$$\Psi_{13}(a''_1 e'', ^3E', M=-1, \mu) = -|\bar{\gamma}\bar{\nu}|$$

$$\Psi_{14}(a''_1 e'', ^3E', M=-1, \eta) = |\bar{\gamma}\bar{\xi}|$$

$$\Psi_{15}(a''_1 e'', ^3E', M=0, \mu) = -\frac{\sqrt{2}|\bar{\gamma}\nu|}{2} - \frac{\sqrt{2}|\gamma\bar{\nu}|}{2}$$

$$\Psi_{16}(a''_1 e'', ^3E', M=0, \eta) = \frac{\sqrt{2}|\bar{\gamma}\xi|}{2} + \frac{\sqrt{2}|\gamma\bar{\xi}|}{2}$$

$$\Psi_{17}(a''_1 e'', ^3E', M=1, \mu) = -|\gamma\nu|$$

$$\Psi_{18}(a''_1 e'', ^3E', M=1, \eta) = |\gamma\xi|$$

 $a'_2 e'$

$$\boxed{\Delta E = -\langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle}$$

$$\Psi_{19}(a'_2 e', ^3E', M=-1, \mu) = -|\bar{\beta}\bar{\eta}|$$

$$\Psi_{20}(a'_2 e', ^3E', M=-1, \eta) = |\bar{\beta}\bar{\mu}|$$

$$\Psi_{21}(a'_2 e', ^3E', M=0, \mu) = -\frac{\sqrt{2}|\bar{\beta}\eta|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_{22}(a'_2 e', ^3E', M=0, \eta) = \frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_{23}(a'_2 e', ^3E', M=1, \mu) = -|\beta\eta|$$

$$\Psi_{24}(a'_2 e', ^3E', M=1, \eta) = |\beta\mu|$$

2.26.9 $^1E'$

$$\begin{aligned} & \textcolor{red}{a'_1 e'} \\ & \boxed{\Delta E = \langle \alpha\alpha || \mu\mu \rangle + \langle \alpha\mu || \alpha\mu \rangle} \\ & \Psi_1(a'_1 e', ^1E', M=0, \eta) = -\frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2} \\ & \Psi_2(a'_1 e', ^1E', M=0, \mu) = -\frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2} \\ & \textcolor{red}{a''_2 e''} \\ & \boxed{\Delta E = \langle \zeta\xi || \zeta\xi \rangle + \langle \zeta\zeta || \xi\xi \rangle} \\ & \Psi_3(a''_2 e'', ^1E', M=0, \eta) = -\frac{\sqrt{2}|\bar{\zeta}\nu|}{2} + \frac{\sqrt{2}|\zeta\bar{\nu}|}{2} \\ & \Psi_4(a''_2 e'', ^1E', M=0, \mu) = -\frac{\sqrt{2}|\bar{\zeta}\xi|}{2} + \frac{\sqrt{2}|\zeta\bar{\xi}|}{2} \\ & \textcolor{red}{a''_1 e''} \\ & \boxed{\Delta E = \langle \gamma\gamma || \xi\xi \rangle + \langle \gamma\xi || \gamma\xi \rangle} \\ & \Psi_5(a''_1 e'', ^1E', M=0, \mu) = \frac{\sqrt{2}|\bar{\gamma}\nu|}{2} - \frac{\sqrt{2}|\gamma\bar{\nu}|}{2} \\ & \Psi_6(a''_1 e'', ^1E', M=0, \eta) = -\frac{\sqrt{2}|\bar{\gamma}\xi|}{2} + \frac{\sqrt{2}|\gamma\bar{\xi}|}{2} \\ & \textcolor{red}{a'_2 e'} \\ & \boxed{\Delta E = \langle \beta\beta || \mu\mu \rangle + \langle \beta\mu || \beta\mu \rangle} \\ & \Psi_7(a'_2 e', ^1E', M=0, \mu) = \frac{\sqrt{2}|\bar{\beta}\eta|}{2} - \frac{\sqrt{2}|\beta\bar{\eta}|}{2} \\ & \Psi_8(a'_2 e', ^1E', M=0, \eta) = -\frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2} \\ & \textcolor{red}{(e')^2} \\ & \boxed{\Delta E = -\langle \mu\mu || \eta\eta \rangle + \langle \mu\mu || \mu\mu \rangle} \\ & \Psi_9((e')^2, ^1E', M=0, \mu) = -\frac{\sqrt{2}|\bar{\eta}\eta|}{2} + \frac{\sqrt{2}|\bar{\mu}\mu|}{2} \\ & \Psi_{10}((e')^2, ^1E', M=0, \eta) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} - \frac{\sqrt{2}|\bar{\mu}\eta|}{2} \\ & \textcolor{red}{(e'')^2} \\ & \boxed{\Delta E = -\langle \xi\xi || \nu\nu \rangle + \langle \xi\xi || \xi\xi \rangle} \\ & \Psi_{11}((e'')^2, ^1E', M=0, \mu) = -\frac{\sqrt{2}|\bar{\nu}\nu|}{2} + \frac{\sqrt{2}|\bar{\xi}\xi|}{2} \\ & \Psi_{12}((e'')^2, ^1E', M=0, \eta) = -\frac{\sqrt{2}|\bar{\nu}\xi|}{2} - \frac{\sqrt{2}|\bar{\xi}\nu|}{2} \end{aligned}$$

2.26.10 $^3E''$

$$\begin{aligned} & \textcolor{red}{a'_1 e''} \\ & \boxed{\Delta E = -\langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle} \\ & \Psi_1(a'_1 e'', ^3E'', M=-1, \nu) = |\bar{\alpha}\nu| \\ & \Psi_2(a'_1 e'', ^3E'', M=-1, \xi) = |\bar{\alpha}\bar{\xi}| \\ & \Psi_3(a'_1 e'', ^3E'', M=0, \nu) = \frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2} \\ & \Psi_4(a'_1 e'', ^3E'', M=0, \xi) = \frac{\sqrt{2}|\bar{\alpha}\xi|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2} \\ & \Psi_5(a'_1 e'', ^3E'', M=1, \nu) = |\alpha\nu| \\ & \Psi_6(a'_1 e'', ^3E'', M=1, \xi) = |\alpha\xi| \\ & \textcolor{red}{a''_2 e'} \\ & \boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle - \langle \zeta\xi || \mu\mu \rangle} \\ & \Psi_7(a''_2 e', ^3E'', M=-1, \nu) = |\bar{\zeta}\bar{\eta}| \\ & \Psi_8(a''_2 e', ^3E'', M=-1, \xi) = |\bar{\zeta}\bar{\mu}| \\ & \Psi_9(a''_2 e', ^3E'', M=0, \nu) = \frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2} \\ & \Psi_{10}(a''_2 e', ^3E'', M=0, \xi) = \frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2} \\ & \Psi_{11}(a''_2 e', ^3E'', M=1, \nu) = |\zeta\eta| \\ & \Psi_{12}(a''_2 e', ^3E'', M=1, \xi) = |\zeta\mu| \\ & \textcolor{red}{a''_1 e'} \\ & \boxed{\Delta E = -\langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle} \\ & \Psi_{13}(a''_1 e', ^3E'', M=-1, \xi) = -|\bar{\gamma}\bar{\eta}| \\ & \Psi_{14}(a''_1 e', ^3E'', M=-1, \nu) = |\bar{\gamma}\bar{\mu}| \\ & \Psi_{15}(a''_1 e', ^3E'', M=0, \xi) = -\frac{\sqrt{2}|\bar{\gamma}\eta|}{2} - \frac{\sqrt{2}|\gamma\bar{\eta}|}{2} \\ & \Psi_{16}(a''_1 e', ^3E'', M=0, \nu) = \frac{\sqrt{2}|\bar{\gamma}\mu|}{2} + \frac{\sqrt{2}|\gamma\bar{\mu}|}{2} \\ & \Psi_{17}(a''_1 e', ^3E'', M=1, \xi) = -|\gamma\eta| \\ & \Psi_{18}(a''_1 e', ^3E'', M=1, \nu) = |\gamma\mu| \\ & \textcolor{red}{a'_2 e''} \\ & \boxed{\Delta E = -\langle \beta\beta || \xi\xi \rangle + \langle \beta\xi || \beta\xi \rangle} \\ & \Psi_{19}(a'_2 e'', ^3E'', M=-1, \xi) = -|\bar{\beta}\bar{\nu}| \\ & \Psi_{20}(a'_2 e'', ^3E'', M=-1, \nu) = |\bar{\beta}\bar{\xi}| \\ & \Psi_{21}(a'_2 e'', ^3E'', M=0, \xi) = -\frac{\sqrt{2}|\bar{\beta}\nu|}{2} - \frac{\sqrt{2}|\beta\bar{\nu}|}{2} \\ & \Psi_{22}(a'_2 e'', ^3E'', M=0, \nu) = \frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2} \\ & \Psi_{23}(a'_2 e'', ^3E'', M=1, \xi) = -|\beta\nu| \\ & \Psi_{24}(a'_2 e'', ^3E'', M=1, \nu) = |\beta\xi| \\ & \textcolor{red}{e' e''} \\ & \boxed{\Delta E = -\langle \mu\mu || \nu\nu \rangle - \langle \mu\xi || \eta\nu \rangle + \langle \mu\xi || \mu\xi \rangle} \\ & \quad - \langle \mu\eta || \xi\nu \rangle \end{aligned}$$

$$\begin{aligned}\Psi_{25}(e' e'', {}^3E'', M=-1, \xi) &= \frac{\sqrt{2}|\bar{\eta}\nu|}{2} - \frac{\sqrt{2}|\bar{\mu}\bar{\xi}|}{2} \\ \Psi_{26}(e' e'', {}^3E'', M=-1, \nu) &= \frac{\sqrt{2}|\bar{\eta}\bar{\xi}|}{2} + \frac{\sqrt{2}|\bar{\mu}\nu|}{2} \\ \Psi_{27}(e' e'', {}^3E'', M=0, \xi) &= \frac{|\bar{\eta}\nu|}{2} - \frac{|\bar{\mu}\xi|}{2} + \frac{|\eta\bar{\nu}|}{2} - \frac{|\mu\bar{\xi}|}{2} \\ \Psi_{28}(e' e'', {}^3E'', M=0, \nu) &= \frac{|\bar{\eta}\xi|}{2} + \frac{|\bar{\mu}\nu|}{2} + \frac{|\eta\bar{\xi}|}{2} + \frac{|\mu\bar{\nu}|}{2} \\ \Psi_{29}(e' e'', {}^3E'', M=1, \xi) &= \frac{\sqrt{2}|\eta\nu|}{2} - \frac{\sqrt{2}|\mu\xi|}{2} \\ \Psi_{30}(e' e'', {}^3E'', M=1, \nu) &= \frac{\sqrt{2}|\eta\xi|}{2} + \frac{\sqrt{2}|\mu\nu|}{2}\end{aligned}$$

2.26.11 ${}^1E''$

$$\begin{aligned}a'_1 e'' \\ \Delta E = \langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle \\ \Psi_1(a'_1 e'', {}^1E'', M=0, \nu) = -\frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2} \\ \Psi_2(a'_1 e'', {}^1E'', M=0, \xi) = -\frac{\sqrt{2}|\bar{\alpha}\xi|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2} \\ a''_2 e' \\ \Delta E = \langle \zeta\mu || \zeta\mu \rangle + \langle \zeta\zeta || \mu\mu \rangle \\ \Psi_3(a''_2 e', {}^1E'', M=0, \nu) = -\frac{\sqrt{2}|\bar{\zeta}\eta|}{2} + \frac{\sqrt{2}|\zeta\bar{\eta}|}{2}\end{aligned}$$

$$\begin{aligned}\Psi_4(a''_2 e', {}^1E'', M=0, \xi) &= -\frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2} \\ a''_1 e' \\ \Delta E = \langle \gamma\gamma || \mu\mu \rangle + \langle \gamma\mu || \gamma\mu \rangle \\ \Psi_5(a''_1 e', {}^1E'', M=0, \xi) &= \frac{\sqrt{2}|\bar{\gamma}\eta|}{2} - \frac{\sqrt{2}|\gamma\bar{\eta}|}{2} \\ \Psi_6(a''_1 e', {}^1E'', M=0, \nu) &= -\frac{\sqrt{2}|\bar{\gamma}\mu|}{2} + \frac{\sqrt{2}|\gamma\bar{\mu}|}{2} \\ a'_2 e'' \\ \Delta E = \langle \beta\beta || \xi\xi \rangle + \langle \beta\xi || \beta\xi \rangle\end{aligned}$$

$$\begin{aligned}\Psi_7(a'_2 e'', {}^1E'', M=0, \xi) &= \frac{\sqrt{2}|\bar{\beta}\nu|}{2} - \frac{\sqrt{2}|\beta\bar{\nu}|}{2} \\ \Psi_8(a'_2 e'', {}^1E'', M=0, \nu) &= -\frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2} \\ e' e'' \\ \Delta E = \langle \mu\mu || \nu\nu \rangle - \langle \mu\xi || \eta\nu \rangle + \langle \mu\xi || \mu\xi \rangle \\ + \langle \mu\eta || \xi\nu \rangle \\ \Psi_9(e' e'', {}^1E'', M=0, \xi) &= -\frac{|\bar{\eta}\nu|}{2} + \frac{|\bar{\mu}\xi|}{2} + \frac{|\eta\bar{\nu}|}{2} - \frac{|\mu\bar{\xi}|}{2} \\ \Psi_{10}(e' e'', {}^1E'', M=0, \nu) &= -\frac{|\bar{\eta}\xi|}{2} - \frac{|\bar{\mu}\nu|}{2} + \frac{|\eta\bar{\xi}|}{2} + \frac{|\mu\bar{\nu}|}{2}\end{aligned}$$

2.27 Group D_{6h}

Component labels

$$\begin{aligned}A_{1g} : \{\alpha_g\} &\longrightarrow A_{2u} : \{\beta_u\} \longrightarrow A_{1u} : \{\alpha_u\} \longrightarrow B_{1g} : \{\gamma_g\} \longrightarrow B_{2g} : \{\zeta_g\} \longrightarrow B_{1u} : \{\gamma_u\} \longrightarrow \\ B_{2u} : \{\zeta_u\} &\longrightarrow A_{2g} : \{\beta_g\} \longrightarrow E_{2g} : \{\nu_g, \xi_g\} \longrightarrow E_{1u} : \{\eta_u, \mu_u\} \longrightarrow E_{1g} : \{\eta_g, \mu_g\} \longrightarrow E_{2u} : \{\nu_u, \xi_u\}\end{aligned}$$

$$\Psi_3(a_{1u}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\bar{\alpha}_u\alpha_u|$$

$$\begin{aligned}\mathbf{2.27.1} \quad {}^1A_{1g} \\ a_{1g}^2 \\ \Delta E = \langle \alpha_g \alpha_g || \alpha_g \alpha_g \rangle \\ \Psi_1(a_{1g}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\bar{\alpha}_g\alpha_g| \\ a_{2u}^2 \\ \Delta E = \langle \beta_u \beta_u || \beta_u \beta_u \rangle \\ \Psi_2(a_{2u}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\bar{\beta}_u\beta_u| \\ a_{1u}^2 \\ \Delta E = \langle \alpha_u \alpha_u || \alpha_u \alpha_u \rangle \\ b_{1g}^2 \\ \Delta E = \langle \gamma_g \gamma_g || \gamma_g \gamma_g \rangle \\ \Psi_4(b_{1g}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\bar{\gamma}_g\gamma_g| \\ b_{2g}^2 \\ \Delta E = \langle \zeta_g \zeta_g || \zeta_g \zeta_g \rangle \\ \Psi_5(b_{2g}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\bar{\zeta}_g\zeta_g| \\ b_{1u}^2 \\ \Delta E = \langle \gamma_u \gamma_u || \gamma_u \gamma_u \rangle \\ \Psi_6(b_{1u}^2, {}^1A_{1g}, M=0, \alpha_g) = -|\bar{\gamma}_u\gamma_u| \\ b_{2u}^2\end{aligned}$$

$\Psi_6(a_{1u}a_{2g}, {}^3A_{2u}, M=1, \beta_u) = \alpha_u\beta_g $	$b_{1g}b_{2u}$
$\Delta E = \langle \zeta_u \zeta_u \zeta_u \zeta_u \rangle$	
$\Psi_7(b_{2u}^2, {}^1A_{1g}, M=0, \alpha_g) = - \overline{\zeta_u} \zeta_u $	$ \overline{\gamma_g} \overline{\zeta_u} $
a_{2g}^2	$\Psi_8(b_{1g}b_{2u}, {}^3A_{2u}, M=-1, \beta_u) = \overline{\gamma_g} \overline{\zeta_u} $
$\Delta E = \langle \beta_g \beta_g \beta_g \beta_g \rangle$	$\Psi_8(b_{1g}b_{2u}, {}^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2} \overline{\gamma_g} \zeta_u }{2} + \frac{\sqrt{2} \gamma_g \overline{\zeta_u} }{2}$
$\Psi_8(a_{2g}^2, {}^1A_{1g}, M=0, \alpha_g) = - \overline{\beta_g} \beta_g $	$\Psi_9(b_{1g}b_{2u}, {}^3A_{2u}, M=1, \beta_u) = \gamma_g \zeta_u $
e_{2g}^2	$b_{1u}b_{2g}$
$\Delta E = \langle \xi_g \xi_g \nu_g \nu_g \rangle + \langle \xi_g \xi_g \xi_g \xi_g \rangle$	$\Delta E = \langle \zeta_g \gamma_u \zeta_g \gamma_u \rangle - \langle \zeta_g \zeta_g \gamma_u \gamma_u \rangle$
$\Psi_9(e_{2g}^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{2} \overline{\nu_g} \nu_g }{2} - \frac{\sqrt{2} \overline{\xi_g} \xi_g }{2}$	$\Psi_{10}(b_{1u}b_{2g}, {}^3A_{2u}, M=-1, \beta_u) = \overline{\zeta_g} \overline{\gamma_u} $
e_{1u}^2	$\Psi_{11}(b_{1u}b_{2g}, {}^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2} \overline{\zeta_g} \gamma_u }{2} + \frac{\sqrt{2} \zeta_g \overline{\gamma_u} }{2}$
$\Delta E = \langle \mu_u \mu_u \eta_u \eta_u \rangle + \langle \mu_u \mu_u \mu_u \mu_u \rangle$	$\Psi_{12}(b_{1u}b_{2g}, {}^3A_{2u}, M=1, \beta_u) = \zeta_g \gamma_u $
$\Psi_{10}(e_{1u}^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{2} \overline{\eta_u} \eta_u }{2} - \frac{\sqrt{2} \overline{\mu_u} \mu_u }{2}$	$e_{2g}e_{2u}$
e_{1g}^2	
$\Delta E = \langle \mu_g \mu_g \eta_g \eta_g \rangle + \langle \mu_g \mu_g \mu_g \mu_g \rangle$	$\Delta E = -2 \langle \xi_g \xi_g \xi_u \xi_u \rangle + \langle \xi_g \xi_u \nu_g \nu_u \rangle + \langle \xi_g \xi_u \xi_g \xi_u \rangle + \langle \xi_g \nu_g \xi_u \nu_u \rangle + \langle \xi_g \xi_g \nu_u \nu_u \rangle$
$\Psi_{11}(e_{1g}^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{2} \overline{\eta_g} \eta_g }{2} - \frac{\sqrt{2} \overline{\mu_g} \mu_g }{2}$	$\Psi_{13}(e_{2g}e_{2u}, {}^3A_{2u}, M=-1, \beta_u) = \frac{\sqrt{2} \overline{\nu_g} \nu_u }{2} + \frac{\sqrt{2} \overline{\xi_g} \xi_u }{2}$
e_{2u}^2	$\Psi_{14}(e_{2g}e_{2u}, {}^3A_{2u}, M=0, \beta_u) = \frac{ \overline{\nu_g} \nu_u }{2} + \frac{ \overline{\xi_g} \xi_u }{2} + \frac{ \nu_g \overline{\nu_u} }{2} + \frac{ \xi_g \overline{\xi_u} }{2}$
$\Delta E = \langle \xi_u \xi_u \nu_u \nu_u \rangle + \langle \xi_u \xi_u \xi_u \xi_u \rangle$	$\Psi_{15}(e_{2g}e_{2u}, {}^3A_{2u}, M=1, \beta_u) = \frac{\sqrt{2} \nu_g \nu_u }{2} + \frac{\sqrt{2} \xi_g \xi_u }{2}$
$\Psi_{12}(e_{2u}^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{2} \overline{\nu_u} \nu_u }{2} - \frac{\sqrt{2} \overline{\xi_u} \xi_u }{2}$	$e_{1g}e_{1u}$
<hr/>	
2.27.2	${}^3A_{2u}$
$a_{1g}a_{2u}$	
$\Delta E = -\langle \alpha_g \alpha_g \beta_u \beta_u \rangle + \langle \alpha_g \beta_u \alpha_g \beta_u \rangle$	$\Delta E = \langle \mu_u \mu_g \eta_u \eta_g \rangle + \langle \mu_u \mu_g \mu_u \mu_g \rangle - 2 \langle \mu_u \mu_u \mu_g \mu_g \rangle + \langle \mu_u \eta_u \mu_g \eta_g \rangle + \langle \mu_u \mu_u \eta_g \eta_g \rangle$
$\Psi_1(a_{1g}a_{2u}, {}^3A_{2u}, M=-1, \beta_u) = \overline{\alpha_g} \overline{\beta_u} $	$\Psi_{16}(e_{1g}e_{1u}, {}^3A_{2u}, M=-1, \beta_u) = \frac{\sqrt{2} \overline{\eta_u} \eta_g }{2} + \frac{\sqrt{2} \mu_u \mu_g }{2}$
$\Psi_2(a_{1g}a_{2u}, {}^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2} \overline{\alpha_g} \beta_u }{2} + \frac{\sqrt{2} \alpha_g \overline{\beta_u} }{2}$	$\Psi_{17}(e_{1g}e_{1u}, {}^3A_{2u}, M=0, \beta_u) = \frac{ \overline{\eta_u} \eta_g }{2} + \frac{ \overline{\mu_u} \mu_g }{2} + \frac{ \eta_u \overline{\eta_g} }{2} + \frac{ \mu_u \overline{\mu_g} }{2}$
$\Psi_3(a_{1g}a_{2u}, {}^3A_{2u}, M=1, \beta_u) = \alpha_g \beta_u $	$\Psi_{18}(e_{1g}e_{1u}, {}^3A_{2u}, M=1, \beta_u) = \frac{\sqrt{2} \eta_u \eta_g }{2} + \frac{\sqrt{2} \mu_u \mu_g }{2}$
$a_{1u}a_{2g}$	<hr/>
$\Delta E = -\langle \alpha_u \alpha_u \beta_g \beta_g \rangle + \langle \alpha_u \beta_g \alpha_u \beta_g \rangle$	
$\Psi_4(a_{1u}a_{2g}, {}^3A_{2u}, M=-1, \beta_u) = \overline{\alpha_u} \overline{\beta_g} $	
$\Psi_5(a_{1u}a_{2g}, {}^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2} \overline{\alpha_u} \beta_g }{2} + \frac{\sqrt{2} \alpha_u \overline{\beta_g} }{2}$	

2.27.3 $^1A_{2u}$ $a_{2g}a_{2u}$ $a_{1g}a_{2u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_u \beta_u \rangle + \langle \alpha_g \beta_u || \alpha_g \beta_u \rangle}$$

$$\Psi_1(a_{1g}a_{2u}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\beta_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\beta_u}|}{2}$$

$a_{1u}a_{2g}$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \beta_g \beta_g \rangle + \langle \alpha_u \beta_g || \alpha_u \beta_g \rangle}$$

$$\Psi_2(a_{1u}a_{2g}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\beta_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\beta_g}|}{2}$$

$b_{1g}b_{2u}$

$$\boxed{\Delta E = \langle \gamma_g \gamma_g || \zeta_u \zeta_u \rangle + \langle \gamma_g \zeta_u || \gamma_g \zeta_u \rangle}$$

$$\Psi_3(b_{1g}b_{2u}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\gamma_g}\zeta_u|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\zeta_u}|}{2}$$

 $b_{1u}b_{2g}$

$$\boxed{\Delta E = \langle \zeta_g \gamma_u || \zeta_g \gamma_u \rangle + \langle \zeta_g \zeta_u || \gamma_g \gamma_u \rangle}$$

$$\Psi_4(b_{1u}b_{2g}, ^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\overline{\zeta_g}\gamma_u|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\gamma_u}|}{2}$$

 $e_{2g}e_{2u}$

$$\boxed{\Delta E = 2 \langle \xi_g \xi_g || \xi_u \xi_u \rangle + \langle \xi_g \xi_u || \nu_g \nu_u \rangle + \langle \xi_g \xi_u || \xi_g \xi_u \rangle - \langle \xi_g \nu_g || \xi_u \nu_u \rangle - \langle \xi_g \xi_g || \nu_u \nu_u \rangle}$$

$$\Psi_5(e_{2g}e_{2u}, ^1A_{2u}, M=0, \beta_u) = -\frac{|\overline{\nu_g}\nu_u|}{2} - \frac{|\overline{\xi_g}\xi_u|}{2} + \frac{|\nu_g\overline{\nu_u}|}{2} + \frac{|\xi_g\overline{\xi_u}|}{2}$$

 $e_{1g}e_{1u}$

$$\boxed{\Delta E = \langle \mu_u \mu_g || \eta_u \eta_g \rangle + \langle \mu_u \mu_g || \mu_u \mu_g \rangle + 2 \langle \mu_u \mu_u || \mu_g \mu_g \rangle - \langle \mu_u \eta_u || \mu_g \eta_g \rangle - \langle \mu_u \mu_u || \eta_g \eta_g \rangle}$$

$$\Psi_6(e_{1g}e_{1u}, ^1A_{2u}, M=0, \beta_u) = -\frac{|\overline{\eta_u}\eta_g|}{2} - \frac{|\overline{\mu_u}\mu_g|}{2} + \frac{|\eta_u\overline{\eta_g}|}{2} + \frac{|\mu_u\overline{\mu_g}|}{2}$$

2.27.4 $^3A_{1u}$ $a_{1g}a_{1u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_{1g}a_{1u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\alpha_g}\alpha_u|$$

$$\Psi_2(a_{1g}a_{1u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\alpha_g}\alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\alpha_u}|}{2}$$

$\Psi_3(a_{1g}a_{1u}, ^3A_{1u}, M=1, \alpha_u) = |\alpha_g\alpha_u|$

 $a_{2g}a_{2u}$

$$\boxed{\Delta E = \langle \beta_u \beta_g || \beta_u \beta_g \rangle - \langle \beta_u \beta_u || \beta_g \beta_g \rangle}$$

$$\Psi_4(a_{2g}a_{2u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\beta_u}\beta_g|$$

$$\Psi_5(a_{2g}a_{2u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\beta_u}\beta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\beta_g}|}{2}$$

$$\Psi_6(a_{2g}a_{2u}, ^3A_{1u}, M=1, \alpha_u) = |\beta_u\beta_g|$$

 $b_{1g}b_{1u}$

$$\boxed{\Delta E = -\langle \gamma_g \gamma_g || \gamma_u \gamma_u \rangle + \langle \gamma_g \gamma_u || \gamma_g \gamma_u \rangle}$$

$$\Psi_7(b_{1g}b_{1u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\gamma_g}\gamma_u|$$

$$\Psi_8(b_{1g}b_{1u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\gamma_g}\gamma_u|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\gamma_u}|}{2}$$

$$\Psi_9(b_{1g}b_{1u}, ^3A_{1u}, M=1, \alpha_u) = |\gamma_g\gamma_u|$$

 $b_{2g}b_{2u}$

$$\boxed{\Delta E = -\langle \zeta_g \zeta_g || \zeta_u \zeta_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle}$$

$$\Psi_{10}(b_{2g}b_{2u}, ^3A_{1u}, M=-1, \alpha_u) = |\overline{\zeta_g}\zeta_u|$$

$$\Psi_{11}(b_{2g}b_{2u}, ^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\zeta_g}\zeta_u|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\zeta_u}|}{2}$$

$$\Psi_{12}(b_{2g}b_{2u}, ^3A_{1u}, M=1, \alpha_u) = |\zeta_g\zeta_u|$$

 $e_{2g}e_{2u}$

$$\boxed{\Delta E = -\langle \xi_g \xi_g || \nu_u \nu_u \rangle - 3 \langle \xi_g \xi_u || \nu_g \nu_u \rangle + \langle \xi_g \xi_u || \xi_g \xi_u \rangle + \langle \xi_g \nu_g || \xi_u \nu_u \rangle}$$

$$\Psi_{13}(e_{2g}e_{2u}, ^3A_{1u}, M=-1, \alpha_u) = -\frac{\sqrt{2}|\overline{\nu_g}\xi_u|}{2} + \frac{\sqrt{2}|\xi_g\overline{\nu_u}|}{2}$$

$$\Psi_{14}(e_{2g}e_{2u}, ^3A_{1u}, M=0, \alpha_u) = -\frac{|\overline{\nu_g}\xi_u|}{2} + \frac{|\overline{\xi_g}\nu_u|}{2} - \frac{|\nu_g\overline{\xi_u}|}{2} + \frac{|\xi_g\overline{\nu_u}|}{2}$$

$$\Psi_{15}(e_{2g}e_{2u}, ^3A_{1u}, M=1, \alpha_u) = -\frac{\sqrt{2}|\nu_g\xi_u|}{2} + \frac{\sqrt{2}|\xi_g\nu_u|}{2}$$

 $e_{1g}e_{1u}$

$$\boxed{\Delta E = -3 \langle \mu_u \mu_g || \eta_u \eta_g \rangle + \langle \mu_u \mu_g || \mu_u \mu_g \rangle - \langle \mu_u \mu_u || \eta_g \eta_g \rangle + \langle \mu_u \eta_u || \mu_g \eta_g \rangle}$$

$$\Psi_{16}(e_{1g}e_{1u}, ^3A_{1u}, M=-1, \alpha_u) = -\frac{\sqrt{2}|\overline{\eta_u}\mu_g|}{2} + \frac{\sqrt{2}|\mu_u\overline{\eta_g}|}{2}$$

$$\Psi_{17}(e_{1g}e_{1u}, ^3A_{1u}, M=0, \alpha_u) = -\frac{|\overline{\eta_u}\mu_g|}{2} + \frac{|\overline{\mu_u}\eta_g|}{2} - \frac{|\eta_u\overline{\mu_g}|}{2} + \frac{|\mu_u\overline{\eta_g}|}{2}$$

$$\Psi_{18}(e_{1g}e_{1u}, ^3A_{1u}, M=1, \alpha_u) = -\frac{\sqrt{2}|\eta_u\mu_g|}{2} + \frac{\sqrt{2}|\mu_u\eta_g|}{2}$$

2.27.5 $^1A_{1u}$ $a_{2u}b_{2u}$ $a_{1g}a_{1u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_{1g}a_{1u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\alpha_u}|}{2}$$

 $a_{2g}a_{2u}$

$$\boxed{\Delta E = \langle \beta_u \beta_g || \beta_u \beta_g \rangle + \langle \beta_u \beta_u || \beta_g \beta_g \rangle}$$

$$\Psi_2(a_{2g}a_{2u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\beta_u}\beta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\beta_g}|}{2}$$

 $b_{1g}b_{1u}$

$$\boxed{\Delta E = \langle \gamma_g \gamma_g || \gamma_u \gamma_u \rangle + \langle \gamma_g \gamma_u || \gamma_g \gamma_u \rangle}$$

$$\Psi_3(b_{1g}b_{1u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\gamma_g}\gamma_u|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\gamma_u}|}{2}$$

 $b_{2g}b_{2u}$

$$\boxed{\Delta E = \langle \zeta_g \zeta_g || \zeta_u \zeta_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle}$$

$$\Psi_4(b_{2g}b_{2u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\zeta_g}\zeta_u|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\zeta_u}|}{2}$$

 $e_{2g}e_{2u}$

$$\boxed{\Delta E = \langle \xi_g \xi_g || \nu_u \nu_u \rangle - 3 \langle \xi_g \xi_u || \nu_g \nu_u \rangle + \langle \xi_g \xi_u || \xi_g \xi_u \rangle - \langle \xi_g \nu_g || \xi_u \nu_u \rangle}$$

$$\Psi_5(e_{2g}e_{2u}, ^1A_{1u}, M=0, \alpha_u) = \frac{|\overline{\nu_g}\xi_u|}{2} - \frac{|\overline{\xi_g}\nu_u|}{2} - \frac{|\nu_g\overline{\xi_u}|}{2} + \frac{|\xi_g\overline{\nu_u}|}{2}$$

 $e_{1g}e_{1u}$

$$\boxed{\Delta E = -3 \langle \mu_u \mu_g || \eta_u \eta_g \rangle + \langle \mu_u \mu_g || \mu_u \mu_g \rangle + \langle \mu_u \mu_u || \eta_g \eta_g \rangle - \langle \mu_u \eta_u || \mu_g \eta_g \rangle}$$

$$\Psi_6(e_{1g}e_{1u}, ^1A_{1u}, M=0, \alpha_u) = \frac{|\overline{\eta_u}\mu_g|}{2} - \frac{|\overline{\mu_u}\eta_g|}{2} - \frac{|\eta_u\overline{\mu_g}|}{2} + \frac{|\mu_u\overline{\eta_g}|}{2}$$

2.27.6 $^3B_{1g}$ $a_{1g}b_{1g}$

$$\boxed{\Delta E = - \langle \alpha_g \alpha_g || \gamma_g \gamma_g \rangle + \langle \alpha_g \gamma_g || \alpha_g \gamma_g \rangle}$$

$$\Psi_1(a_{1g}b_{1g}, ^3B_{1g}, M=-1, \gamma_g) = |\overline{\alpha_g}\gamma_g|$$

$$\Psi_2(a_{1g}b_{1g}, ^3B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\alpha_g}\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\gamma_g}|}{2}$$

$$\Psi_3(a_{1g}b_{1g}, ^3B_{1g}, M=1, \gamma_g) = |\alpha_g\gamma_g|$$

 $a_{2u}b_{2u}$

$$\boxed{\Delta E = - \langle \beta_u \beta_u || \zeta_u \zeta_u \rangle + \langle \beta_u \zeta_u || \beta_u \zeta_u \rangle}$$

$$\Psi_4(a_{2u}b_{2u}, ^3B_{1g}, M=-1, \gamma_g) = |\overline{\beta_u}\zeta_u|$$

$$\Psi_5(a_{2u}b_{2u}, ^3B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\beta_u}\zeta_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\zeta_u}|}{2}$$

$$\Psi_6(a_{2u}b_{2u}, ^3B_{1g}, M=1, \gamma_g) = |\beta_u\zeta_u|$$

 $a_{1u}b_{1u}$

$$\boxed{\Delta E = - \langle \alpha_u \alpha_u || \gamma_u \gamma_u \rangle + \langle \alpha_u \gamma_u || \alpha_u \gamma_u \rangle}$$

$$\Psi_7(a_{1u}b_{1u}, ^3B_{1g}, M=-1, \gamma_g) = |\overline{\alpha_u}\gamma_u|$$

$$\Psi_8(a_{1u}b_{1u}, ^3B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\alpha_u}\gamma_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\gamma_u}|}{2}$$

$$\Psi_9(a_{1u}b_{1u}, ^3B_{1g}, M=1, \gamma_g) = |\alpha_u\gamma_u|$$

 $a_{2g}b_{2g}$

$$\boxed{\Delta E = \langle \zeta_g \beta_g || \zeta_g \beta_g \rangle - \langle \zeta_g \zeta_g || \beta_g \beta_g \rangle}$$

$$\Psi_{10}(a_{2g}b_{2g}, ^3B_{1g}, M=-1, \gamma_g) = |\overline{\zeta_g}\beta_g|$$

$$\Psi_{11}(a_{2g}b_{2g}, ^3B_{1g}, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\zeta_g}\beta_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\beta_g}|}{2}$$

$$\Psi_{12}(a_{2g}b_{2g}, ^3B_{1g}, M=1, \gamma_g) = |\zeta_g\beta_g|$$

 $e_{1g}e_{2g}$

$$\boxed{\Delta E = 3 \langle \xi_g \mu_g || \nu_g \eta_g \rangle + \langle \xi_g \mu_g || \xi_g \mu_g \rangle - \langle \xi_g \xi_g || \eta_g \eta_g \rangle - \langle \xi_g \nu_g || \mu_g \eta_g \rangle}$$

$$\Psi_{13}(e_{1g}e_{2g}, ^3B_{1g}, M=-1, \gamma_g) = \frac{\sqrt{2}|\overline{\nu_g}\mu_g|}{2} + \frac{\sqrt{2}|\overline{\xi_g}\eta_g|}{2}$$

$$\Psi_{14}(e_{1g}e_{2g}, ^3B_{1g}, M=0, \gamma_g) = \frac{|\overline{\nu_g}\mu_g|}{2} + \frac{|\overline{\xi_g}\eta_g|}{2} + \frac{|\nu_g\overline{\mu_g}|}{2} + \frac{|\xi_g\overline{\eta_g}|}{2}$$

$$\Psi_{15}(e_{1g}e_{2g}, ^3B_{1g}, M=1, \gamma_g) = \frac{\sqrt{2}|\nu_g\mu_g|}{2} + \frac{\sqrt{2}|\xi_g\eta_g|}{2}$$

 $e_{1u}e_{2u}$

$$\boxed{\Delta E = - \langle \mu_u \mu_u || \nu_u \nu_u \rangle + 3 \langle \mu_u \xi_u || \eta_u \nu_u \rangle + \langle \mu_u \xi_u || \mu_u \xi_u \rangle - \langle \mu_u \eta_u || \xi_u \nu_u \rangle}$$

$$\Psi_{16}(e_{1u}e_{2u}, ^3B_{1g}, M=-1, \gamma_g) = \frac{\sqrt{2}|\overline{\eta_u}\xi_u|}{2} + \frac{\sqrt{2}|\mu_u\overline{\nu_u}|}{2}$$

$$\Psi_{17}(e_{1u}e_{2u}, ^3B_{1g}, M=0, \gamma_g) = \frac{|\overline{\eta_u}\xi_u|}{2} + \frac{|\overline{\mu_u}\nu_u|}{2} + \frac{|\eta_u\overline{\xi_u}|}{2} + \frac{|\mu_u\overline{\nu_u}|}{2}$$

$$\Psi_{18}(e_{1u}e_{2u}, ^3B_{1g}, M=1, \gamma_g) = \frac{\sqrt{2}|\eta_u\xi_u|}{2} + \frac{\sqrt{2}|\mu_u\nu_u|}{2}$$

2.27.7 $^1B_{1g}$ $a_{2u}b_{1u}$ $a_{1g}b_{1g}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \gamma_g \gamma_g \rangle + \langle \alpha_g \gamma_g || \alpha_g \gamma_g \rangle}$$

$$\Psi_1(a_{1g}b_{1g}, ^1B_{1g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\gamma_g}|}{2}$$

 $a_{2u}b_{2u}$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \zeta_u \zeta_u \rangle + \langle \beta_u \zeta_u || \beta_u \zeta_u \rangle}$$

$$\Psi_2(a_{2u}b_{2u}, ^1B_{1g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\beta_u}\zeta_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\zeta_u}|}{2}$$

 $a_{1u}b_{1u}$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \gamma_u \gamma_u \rangle + \langle \alpha_u \gamma_u || \alpha_u \gamma_u \rangle}$$

$$\Psi_3(a_{1u}b_{1u}, ^1B_{1g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\alpha_u}\gamma_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\gamma_u}|}{2}$$

 $a_{2g}b_{2g}$

$$\boxed{\Delta E = \langle \zeta_g \beta_g || \zeta_g \beta_g \rangle + \langle \zeta_g \zeta_g || \beta_g \beta_g \rangle}$$

$$\Psi_4(a_{2g}b_{2g}, ^1B_{1g}, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\zeta_g}\beta_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\beta_g}|}{2}$$

 $e_{1g}e_{2g}$

$$\boxed{\Delta E = 3 \langle \xi_g \mu_g || \nu_g \eta_g \rangle + \langle \xi_g \mu_g || \xi_g \mu_g \rangle + \langle \xi_g \xi_g || \eta_g \eta_g \rangle + \langle \xi_g \nu_g || \mu_g \eta_g \rangle}$$

$$\Psi_5(e_{1g}e_{2g}, ^1B_{1g}, M=0, \gamma_g) = -\frac{|\overline{\nu_g}\mu_g|}{2} - \frac{|\overline{\xi_g}\eta_g|}{2} + \frac{|\nu_g\overline{\mu_g}|}{2} + \frac{|\xi_g\overline{\eta_g}|}{2}$$

 $e_{1u}e_{2u}$

$$\boxed{\Delta E = \langle \mu_u \mu_u || \nu_u \nu_u \rangle + 3 \langle \mu_u \xi_u || \eta_u \nu_u \rangle + \langle \mu_u \xi_u || \mu_u \xi_u \rangle + \langle \mu_u \eta_u || \xi_u \nu_u \rangle}$$

$$\Psi_6(e_{1u}e_{2u}, ^1B_{1g}, M=0, \gamma_g) = -\frac{|\overline{\eta_u}\xi_u|}{2} - \frac{|\overline{\mu_u}\nu_u|}{2} + \frac{|\eta_u\overline{\xi_u}|}{2} + \frac{|\mu_u\overline{\nu_u}|}{2}$$

2.27.8 $^3B_{2g}$ $a_{1g}b_{2g}$

$$\boxed{\Delta E = - \langle \alpha_g \alpha_g || \zeta_g \zeta_g \rangle + \langle \alpha_g \zeta_g || \alpha_g \zeta_g \rangle}$$

$$\Psi_1(a_{1g}b_{2g}, ^3B_{2g}, M=-1, \zeta_g) = |\overline{\alpha_g}\zeta_g|$$

$$\Psi_2(a_{1g}b_{2g}, ^3B_{2g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\alpha_g}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\zeta_g}|}{2}$$

$$\Psi_3(a_{1g}b_{2g}, ^3B_{2g}, M=1, \zeta_g) = |\alpha_g\zeta_g|$$

 $a_{2u}b_{1u}$

$$\boxed{\Delta E = - \langle \beta_u \beta_u || \gamma_u \gamma_u \rangle + \langle \beta_u \gamma_u || \beta_u \gamma_u \rangle}$$

$$\Psi_4(a_{2u}b_{1u}, ^3B_{2g}, M=-1, \zeta_g) = |\overline{\beta_u}\gamma_u|$$

$$\Psi_5(a_{2u}b_{1u}, ^3B_{2g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_u}\gamma_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\gamma_u}|}{2}$$

$$\Psi_6(a_{2u}b_{1u}, ^3B_{2g}, M=1, \zeta_g) = |\beta_u\gamma_u|$$

 $a_{1u}b_{2u}$

$$\boxed{\Delta E = - \langle \alpha_u \alpha_u || \zeta_u \zeta_u \rangle + \langle \alpha_u \zeta_u || \alpha_u \zeta_u \rangle}$$

$$\Psi_7(a_{1u}b_{2u}, ^3B_{2g}, M=-1, \zeta_g) = |\overline{\alpha_u}\zeta_u|$$

$$\Psi_8(a_{1u}b_{2u}, ^3B_{2g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\alpha_u}\zeta_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\zeta_u}|}{2}$$

$$\Psi_9(a_{1u}b_{2u}, ^3B_{2g}, M=1, \zeta_g) = |\alpha_u\zeta_u|$$

 $a_{2g}b_{1g}$

$$\boxed{\Delta E = \langle \gamma_g \beta_g || \gamma_g \beta_g \rangle - \langle \gamma_g \gamma_g || \beta_g \beta_g \rangle}$$

$$\Psi_{10}(a_{2g}b_{1g}, ^3B_{2g}, M=-1, \zeta_g) = |\overline{\gamma_g}\beta_g|$$

$$\Psi_{11}(a_{2g}b_{1g}, ^3B_{2g}, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\gamma_g}\beta_g|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\beta_g}|}{2}$$

$$\Psi_{12}(a_{2g}b_{1g}, ^3B_{2g}, M=1, \zeta_g) = |\gamma_g\beta_g|$$

 $e_{1g}e_{2g}$

$$\boxed{\Delta E = - \langle \xi_g \mu_g || \nu_g \eta_g \rangle + \langle \xi_g \mu_g || \xi_g \mu_g \rangle - 2 \langle \xi_g \xi_g || \mu_g \mu_g \rangle - \langle \xi_g \nu_g || \mu_g \eta_g \rangle + \langle \xi_g \xi_g || \eta_g \eta_g \rangle}$$

$$\Psi_{13}(e_{1g}e_{2g}, ^3B_{2g}, M=-1, \zeta_g) = -\frac{\sqrt{2}|\overline{\nu_g}\eta_g|}{2} + \frac{\sqrt{2}|\xi_g\overline{\mu_g}|}{2}$$

$$\Psi_{14}(e_{1g}e_{2g}, ^3B_{2g}, M=0, \zeta_g) = -\frac{|\overline{\nu_g}\eta_g|}{2} + \frac{|\xi_g\mu_g|}{2} - \frac{|\nu_g\overline{\eta_g}|}{2} + \frac{|\xi_g\overline{\mu_g}|}{2}$$

$$\Psi_{15}(e_{1g}e_{2g}, ^3B_{2g}, M=1, \zeta_g) = -\frac{\sqrt{2}|\nu_g\eta_g|}{2} + \frac{\sqrt{2}|\xi_g\mu_g|}{2}$$

 $e_{1u}e_{2u}$

$$\boxed{\Delta E = -2 \langle \mu_u \mu_u || \xi_u \xi_u \rangle - \langle \mu_u \xi_u || \eta_u \nu_u \rangle + \langle \mu_u \xi_u || \mu_u \xi_u \rangle - \langle \mu_u \eta_u || \xi_u \nu_u \rangle + \langle \mu_u \mu_u || \nu_u \nu_u \rangle}$$

$$\Psi_{16}(e_{1u}e_{2u}, ^3B_{2g}, M=-1, \zeta_g) = -\frac{\sqrt{2}|\overline{\eta_u}\nu_u|}{2} + \frac{\sqrt{2}|\mu_u\overline{\xi_u}|}{2}$$

$$\Psi_{17}(e_{1u}e_{2u}, ^3B_{2g}, M=0, \zeta_g) = -\frac{|\overline{\eta_u}\nu_u|}{2} + \frac{|\mu_u\xi_u|}{2} - \frac{|\eta_u\overline{\nu_u}|}{2} + \frac{|\mu_u\overline{\xi_u}|}{2}$$

$$\Psi_{18}(e_{1u}e_{2u}, ^3B_{2g}, M=1, \zeta_g) = -\frac{\sqrt{2}|\eta_u\nu_u|}{2} + \frac{\sqrt{2}|\mu_u\xi_u|}{2}$$

2.27.9 $^1B_{2g}$ $a_{2u}b_{2g}$ $a_{1g}b_{2g}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \zeta_g \zeta_g \rangle + \langle \alpha_g \zeta_g || \alpha_g \zeta_g \rangle}$$

$$\Psi_1(a_{1g}b_{2g}, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\zeta_g}|}{2}$$

$a_{2u}b_{1u}$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \gamma_u \gamma_u \rangle + \langle \beta_u \gamma_u || \beta_u \gamma_u \rangle}$$

$$\Psi_2(a_{2u}b_{1u}, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\beta_u}\gamma_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\gamma_u}|}{2}$$

$a_{1u}b_{2u}$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \zeta_u \zeta_u \rangle + \langle \alpha_u \zeta_u || \alpha_u \zeta_u \rangle}$$

$$\Psi_3(a_{1u}b_{2u}, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\alpha_u}\zeta_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\zeta_u}|}{2}$$

 $a_{2g}b_{1g}$

$$\boxed{\Delta E = \langle \gamma_g \beta_g || \gamma_g \beta_g \rangle + \langle \gamma_g \gamma_g || \beta_g \beta_g \rangle}$$

$$\Psi_4(a_{2g}b_{1g}, ^1B_{2g}, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\gamma_g}\beta_g|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\beta_g}|}{2}$$

$e_{1g}e_{2g}$

$$\boxed{\Delta E = -\langle \xi_g \mu_g || \nu_g \eta_g \rangle + \langle \xi_g \mu_g || \xi_g \mu_g \rangle + 2 \langle \xi_g \xi_g || \mu_g \mu_g \rangle + \langle \xi_g \nu_g || \mu_g \eta_g \rangle - \langle \xi_g \xi_g || \eta_g \eta_g \rangle}$$

$$\Psi_5(e_{1g}e_{2g}, ^1B_{2g}, M=0, \zeta_g) = \frac{|\overline{\xi_g}\mu_g|}{2} - \frac{|\overline{\xi_g}\mu_g|}{2} - \frac{|\nu_g\overline{\eta_g}|}{2} + \frac{|\xi_g\overline{\mu_g}|}{2}$$

 $e_{1u}e_{2u}$

$$\boxed{\Delta E = 2 \langle \mu_u \mu_u || \xi_u \xi_u \rangle - \langle \mu_u \xi_u || \eta_u \nu_u \rangle + \langle \mu_u \xi_u || \mu_u \xi_u \rangle + \langle \mu_u \eta_u || \xi_u \nu_u \rangle - \langle \mu_u \mu_u || \nu_u \nu_u \rangle}$$

$$\Psi_6(e_{1u}e_{2u}, ^1B_{2g}, M=0, \zeta_g) = \frac{|\overline{\eta_u}\nu_u|}{2} - \frac{|\overline{\mu_u}\xi_u|}{2} - \frac{|\eta_u\overline{\nu_u}|}{2} + \frac{|\mu_u\overline{\xi_u}|}{2}$$

2.27.10 $^3B_{1u}$ $a_{1g}b_{1u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \gamma_u \gamma_u \rangle + \langle \alpha_g \gamma_u || \alpha_g \gamma_u \rangle}$$

$$\Psi_1(a_{1g}b_{1u}, ^3B_{1u}, M=-1, \gamma_u) = |\overline{\alpha_g}\gamma_u|$$

$$\Psi_2(a_{1g}b_{1u}, ^3B_{1u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_g}\gamma_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\gamma_u}|}{2}$$

$$\Psi_3(a_{1g}b_{1u}, ^3B_{1u}, M=1, \gamma_u) = |\alpha_g\gamma_u|$$

 $a_{2u}b_{2g}$

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \zeta_g \zeta_g \rangle + \langle \beta_u \zeta_g || \beta_u \zeta_g \rangle}$$

$$\Psi_4(a_{2u}b_{2g}, ^3B_{1u}, M=-1, \gamma_u) = |\overline{\beta_u}\zeta_g|$$

$$\Psi_5(a_{2u}b_{2g}, ^3B_{1u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\beta_u}\zeta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\zeta_g}|}{2}$$

$$\Psi_6(a_{2u}b_{2g}, ^3B_{1u}, M=1, \gamma_u) = |\beta_u\zeta_g|$$

 $a_{1u}b_{1g}$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \gamma_g \gamma_g \rangle + \langle \alpha_u \gamma_g || \alpha_u \gamma_g \rangle}$$

$$\Psi_7(a_{1u}b_{1g}, ^3B_{1u}, M=-1, \gamma_u) = |\overline{\alpha_u}\gamma_g|$$

$$\Psi_8(a_{1u}b_{1g}, ^3B_{1u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_u}\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\gamma_g}|}{2}$$

$$\Psi_9(a_{1u}b_{1g}, ^3B_{1u}, M=1, \gamma_u) = |\alpha_u\gamma_g|$$

 $a_{2g}b_{2u}$

$$\boxed{\Delta E = \langle \zeta_u \beta_g || \zeta_u \beta_g \rangle - \langle \zeta_u \zeta_u || \beta_g \beta_g \rangle}$$

$$\Psi_{10}(a_{2g}b_{2u}, ^3B_{1u}, M=-1, \gamma_u) = |\overline{\zeta_u}\beta_g|$$

$$\Psi_{11}(a_{2g}b_{2u}, ^3B_{1u}, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\zeta_u}\beta_g|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\beta_g}|}{2}$$

$$\Psi_{12}(a_{2g}b_{2u}, ^3B_{1u}, M=1, \gamma_u) = |\zeta_u\beta_g|$$

 $e_{1u}e_{2g}$

$$\boxed{\Delta E = -\langle \xi_g \mu_u || \nu_g \eta_u \rangle + \langle \xi_g \mu_u || \xi_g \mu_u \rangle - 2 \langle \xi_g \xi_g || \mu_u \mu_u \rangle - \langle \xi_g \nu_g || \mu_u \eta_u \rangle + \langle \xi_g \xi_g || \eta_u \eta_u \rangle}$$

$$\Psi_{13}(e_{1u}e_{2g}, ^3B_{1u}, M=-1, \gamma_u) = -\frac{\sqrt{2}|\overline{\nu_g}\eta_u|}{2} + \frac{\sqrt{2}|\overline{\xi_g}\mu_u|}{2}$$

$$\Psi_{14}(e_{1u}e_{2g}, ^3B_{1u}, M=0, \gamma_u) = -\frac{|\overline{\nu_g}\eta_u|}{2} + \frac{|\overline{\xi_g}\mu_u|}{2} - \frac{|\nu_g\overline{\eta_u}|}{2} + \frac{|\xi_g\overline{\mu_u}|}{2}$$

$$\Psi_{15}(e_{1u}e_{2g}, ^3B_{1u}, M=1, \gamma_u) = -\frac{\sqrt{2}|\nu_g\eta_u|}{2} + \frac{\sqrt{2}|\xi_g\mu_u|}{2}$$

 $e_{1g}e_{2u}$

$$\boxed{\Delta E = -2 \langle \mu_g \mu_g || \xi_u \xi_u \rangle - \langle \mu_g \xi_u || \eta_g \nu_u \rangle + \langle \mu_g \xi_u || \mu_g \xi_u \rangle - \langle \mu_g \eta_g || \xi_u \nu_u \rangle + \langle \mu_g \mu_g || \nu_u \nu_u \rangle}$$

$$\Psi_{16}(e_{1g}e_{2u}, ^3B_{1u}, M=-1, \gamma_u) = -\frac{\sqrt{2}|\overline{\eta_g}\nu_u|}{2} + \frac{\sqrt{2}|\overline{\mu_g}\xi_u|}{2}$$

$$\Psi_{17}(e_{1g}e_{2u}, ^3B_{1u}, M=0, \gamma_u) = -\frac{|\overline{\eta_g}\nu_u|}{2} + \frac{|\overline{\mu_g}\xi_u|}{2} - \frac{|\eta_g\overline{\nu_u}|}{2} + \frac{|\mu_g\overline{\xi_u}|}{2}$$

$$\Psi_{18}(e_{1g}e_{2u}, ^3B_{1u}, M=1, \gamma_u) = -\frac{\sqrt{2}|\eta_g\nu_u|}{2} + \frac{\sqrt{2}|\mu_g\xi_u|}{2}$$

2.27.11 $^1B_{1u}$ $a_{2u}b_{1g}$

$a_{1g}b_{1u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \gamma_u \gamma_u \rangle + \langle \alpha_g \gamma_u || \alpha_g \gamma_u \rangle}$$

$$\Psi_1(a_{1g}b_{1u}, ^1B_{1u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\gamma_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\gamma_u}|}{2}$$

$a_{2u}b_{2g}$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \zeta_g \zeta_g \rangle + \langle \beta_u \zeta_g || \beta_u \zeta_g \rangle}$$

$$\Psi_2(a_{2u}b_{2g}, ^1B_{1u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\beta_u}\zeta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\zeta_g}|}{2}$$

$a_{1u}b_{1g}$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \gamma_g \gamma_g \rangle + \langle \alpha_u \gamma_g || \alpha_u \gamma_g \rangle}$$

$$\Psi_3(a_{1u}b_{1g}, ^1B_{1u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\gamma_g}|}{2}$$

$a_{2g}b_{2u}$

$$\boxed{\Delta E = \langle \zeta_u \beta_g || \zeta_u \beta_g \rangle + \langle \zeta_u \zeta_u || \beta_g \beta_g \rangle}$$

$$\Psi_4(a_{2g}b_{2u}, ^1B_{1u}, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\zeta_u}\beta_g|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\beta_g}|}{2}$$

$e_{1u}e_{2g}$

$$\boxed{\Delta E = -\langle \xi_g \mu_u || \nu_g \eta_u \rangle + \langle \xi_g \mu_u || \xi_g \mu_u \rangle + 2 \langle \xi_g \xi_g || \mu_u \mu_u \rangle + \langle \xi_g \nu_g || \mu_u \eta_u \rangle - \langle \xi_g \xi_g || \eta_u \eta_u \rangle}$$

$$\Psi_5(e_{1u}e_{2g}, ^1B_{1u}, M=0, \gamma_u) = \frac{|\overline{\nu_g}\eta_u|}{2} - \frac{|\overline{\xi_g}\mu_u|}{2} - \frac{|\nu_g\overline{\eta_u}|}{2} + \frac{|\xi_g\overline{\mu_u}|}{2}$$

$e_{1g}e_{2u}$

$$\boxed{\Delta E = 2 \langle \mu_g \mu_g || \xi_u \xi_u \rangle - \langle \mu_g \xi_u || \eta_g \nu_u \rangle + \langle \mu_g \xi_u || \mu_g \xi_u \rangle + \langle \mu_g \eta_g || \xi_u \nu_u \rangle - \langle \mu_g \mu_g || \nu_u \nu_u \rangle}$$

$$\Psi_6(e_{1g}e_{2u}, ^1B_{1u}, M=0, \gamma_u) = \frac{|\overline{\eta_g}\nu_u|}{2} - \frac{|\overline{\mu_g}\xi_u|}{2} - \frac{|\eta_g\overline{\nu_u}|}{2} + \frac{|\mu_g\overline{\xi_u}|}{2}$$

2.27.12 $^3B_{2u}$

$a_{1g}b_{2u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u || \alpha_g \zeta_u \rangle}$$

$$\Psi_1(a_{1g}b_{2u}, ^3B_{2u}, M=-1, \zeta_u) = |\overline{\alpha_g}\zeta_u|$$

$$\Psi_2(a_{1g}b_{2u}, ^3B_{2u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_g}\zeta_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\zeta_u}|}{2}$$

$$\Psi_3(a_{1g}b_{2u}, ^3B_{2u}, M=1, \zeta_u) = |\alpha_g\zeta_u|$$

 $a_{2u}b_{1g}$

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \gamma_g \gamma_g \rangle + \langle \beta_u \gamma_g || \beta_u \gamma_g \rangle}$$

$$\Psi_4(a_{2u}b_{1g}, ^3B_{2u}, M=-1, \zeta_u) = |\overline{\beta_u}\gamma_g|$$

$$\Psi_5(a_{2u}b_{1g}, ^3B_{2u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\beta_u}\gamma_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\gamma_g}|}{2}$$

$$\Psi_6(a_{2u}b_{1g}, ^3B_{2u}, M=1, \zeta_u) = |\beta_u\gamma_g|$$

 $a_{1u}b_{2g}$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \zeta_g \zeta_g \rangle + \langle \alpha_u \zeta_g || \alpha_u \zeta_g \rangle}$$

$$\Psi_7(a_{1u}b_{2g}, ^3B_{2u}, M=-1, \zeta_u) = |\overline{\alpha_u}\zeta_g|$$

$$\Psi_8(a_{1u}b_{2g}, ^3B_{2u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_u}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\zeta_g}|}{2}$$

$$\Psi_9(a_{1u}b_{2g}, ^3B_{2u}, M=1, \zeta_u) = |\alpha_u\zeta_g|$$

 $a_{2g}b_{1u}$

$$\boxed{\Delta E = \langle \gamma_u \beta_g || \gamma_u \beta_g \rangle - \langle \gamma_u \gamma_u || \beta_g \beta_g \rangle}$$

$$\Psi_{10}(a_{2g}b_{1u}, ^3B_{2u}, M=-1, \zeta_u) = |\overline{\gamma_u}\beta_g|$$

$$\Psi_{11}(a_{2g}b_{1u}, ^3B_{2u}, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\gamma_u}\beta_g|}{2} + \frac{\sqrt{2}|\gamma_u\overline{\beta_g}|}{2}$$

$$\Psi_{12}(a_{2g}b_{1u}, ^3B_{2u}, M=1, \zeta_u) = |\gamma_u\beta_g|$$

 $e_{1u}e_{2g}$

$$\boxed{\Delta E = 3 \langle \xi_g \mu_u || \nu_g \eta_u \rangle + \langle \xi_g \mu_u || \xi_g \mu_u \rangle - \langle \xi_g \xi_g || \eta_u \eta_u \rangle - \langle \xi_g \nu_g || \mu_u \eta_u \rangle}$$

$$\Psi_{13}(e_{1u}e_{2g}, ^3B_{2u}, M=-1, \zeta_u) = \frac{\sqrt{2}|\overline{\nu_g}\mu_u|}{2} + \frac{\sqrt{2}|\xi_g\overline{\eta_u}|}{2}$$

$$\Psi_{14}(e_{1u}e_{2g}, ^3B_{2u}, M=0, \zeta_u) = \frac{|\overline{\nu_g}\mu_u|}{2} + \frac{|\xi_g\overline{\eta_u}|}{2} + \frac{|\nu_g\overline{\mu_u}|}{2} + \frac{|\xi_g\overline{\eta_u}|}{2}$$

$$\Psi_{15}(e_{1u}e_{2g}, ^3B_{2u}, M=1, \zeta_u) = \frac{\sqrt{2}|\nu_g\mu_u|}{2} + \frac{\sqrt{2}|\xi_g\eta_u|}{2}$$

 $e_{1g}e_{2u}$

$$\boxed{\Delta E = -\langle \mu_g \mu_g || \nu_u \nu_u \rangle + 3 \langle \mu_g \xi_u || \eta_g \nu_u \rangle + \langle \mu_g \xi_u || \mu_g \xi_u \rangle - \langle \mu_g \eta_g || \xi_u \nu_u \rangle}$$

$$\Psi_{16}(e_{1g}e_{2u}, ^3B_{2u}, M=-1, \zeta_u) = \frac{\sqrt{2}|\overline{\eta_g}\xi_u|}{2} + \frac{\sqrt{2}|\mu_g\nu_u|}{2}$$

$$\Psi_{17}(e_{1g}e_{2u}, ^3B_{2u}, M=0, \zeta_u) = \frac{|\overline{\eta_g}\xi_u|}{2} + \frac{|\overline{\mu_g}\nu_u|}{2} + \frac{|\eta_g\overline{\xi_u}|}{2} + \frac{|\mu_g\overline{\nu_u}|}{2}$$

$$\Psi_{18}(e_{1g}e_{2u}, ^3B_{2u}, M=1, \zeta_u) = \frac{\sqrt{2}|\eta_g\xi_u|}{2} + \frac{\sqrt{2}|\mu_g\nu_u|}{2}$$

2.27.13 $^1B_{2u}$ $a_{1g}b_{2u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u || \alpha_g \zeta_u \rangle}$$

$$\Psi_1(a_{1g}b_{2u}, ^1B_{2u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\zeta_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\zeta_u}|}{2}$$

 $a_{2u}b_{1g}$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \gamma_g \gamma_g \rangle + \langle \beta_u \gamma_g || \beta_u \gamma_g \rangle}$$

$$\Psi_2(a_{2u}b_{1g}, ^1B_{2u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\beta_u}\gamma_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\gamma_g}|}{2}$$

 $a_{1u}b_{2g}$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \zeta_g \zeta_g \rangle + \langle \alpha_u \zeta_g || \alpha_u \zeta_g \rangle}$$

$$\Psi_3(a_{1u}b_{2g}, ^1B_{2u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\zeta_g}|}{2}$$

 $a_{2g}b_{1u}$

$$\boxed{\Delta E = \langle \gamma_u \beta_g || \gamma_u \beta_g \rangle + \langle \gamma_u \gamma_u || \beta_g \beta_g \rangle}$$

$$\Psi_4(a_{2g}b_{1u}, ^1B_{2u}, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\gamma_u}\beta_g|}{2} + \frac{\sqrt{2}|\gamma_u\overline{\beta_g}|}{2}$$

 $e_{1u}e_{2g}$

$$\boxed{\Delta E = 3 \langle \xi_g \mu_u || \nu_g \eta_u \rangle + \langle \xi_g \mu_u || \xi_g \mu_u \rangle + \langle \xi_g \xi_g || \eta_u \eta_u \rangle + \langle \xi_g \nu_g || \mu_u \eta_u \rangle}$$

$$\Psi_5(e_{1u}e_{2g}, ^1B_{2u}, M=0, \zeta_u) = -\frac{|\overline{\nu_g}\mu_u|}{2} - \frac{|\overline{\xi_g}\eta_u|}{2} + \frac{|\nu_g\overline{\mu_u}|}{2} + \frac{|\xi_g\overline{\eta_u}|}{2}$$

 $e_{1g}e_{2u}$

$$\boxed{\Delta E = \langle \mu_g \mu_g || \nu_u \nu_u \rangle + 3 \langle \mu_g \xi_u || \eta_g \nu_u \rangle + \langle \mu_g \xi_u || \mu_g \xi_u \rangle + \langle \mu_g \eta_g || \xi_u \nu_u \rangle}$$

$$\Psi_6(e_{1g}e_{2u}, ^1B_{2u}, M=0, \zeta_u) = -\frac{|\overline{\eta_g}\xi_u|}{2} - \frac{|\overline{\mu_g}\nu_u|}{2} + \frac{|\eta_g\overline{\xi_u}|}{2} + \frac{|\mu_g\overline{\nu_u}|}{2}$$

2.27.14 $^3A_{2g}$ $a_{1g}a_{2g}$

$$\boxed{\Delta E = - \langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_{1g}a_{2g}, ^3A_{2g}, M=-1, \beta_g) = |\overline{\alpha_g}\overline{\beta_g}|$$

$$\Psi_2(a_{1g}a_{2g}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\alpha_g}\beta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\beta_g}|}{2}$$

$$\Psi_3(a_{1g}a_{2g}, ^3A_{2g}, M=1, \beta_g) = |\alpha_g\beta_g|$$

 $a_{1u}a_{2u}$

$$\boxed{\Delta E = \langle \beta_u \alpha_u || \beta_u \alpha_u \rangle - \langle \beta_u \beta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_4(a_{1u}a_{2u}, ^3A_{2g}, M=-1, \beta_g) = |\overline{\beta_u}\overline{\alpha_u}|$$

$$\Psi_5(a_{1u}a_{2u}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\beta_u}\alpha_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\alpha_u}|}{2}$$

$$\Psi_6(a_{1u}a_{2u}, ^3A_{2g}, M=1, \beta_g) = |\beta_u\alpha_u|$$

 $b_{1g}b_{2g}$

$$\boxed{\Delta E = - \langle \gamma_g \gamma_g || \zeta_g \zeta_g \rangle + \langle \gamma_g \zeta_g || \gamma_g \zeta_g \rangle}$$

$$\Psi_7(b_{1g}b_{2g}, ^3A_{2g}, M=-1, \beta_g) = |\overline{\gamma_g}\overline{\zeta_g}|$$

$$\Psi_8(b_{1g}b_{2g}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\gamma_g}\zeta_g|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\zeta_g}|}{2}$$

$$\Psi_9(b_{1g}b_{2g}, ^3A_{2g}, M=1, \beta_g) = |\gamma_g\zeta_g|$$

 $b_{1u}b_{2u}$

$$\boxed{\Delta E = - \langle \gamma_u \gamma_u || \zeta_u \zeta_u \rangle + \langle \gamma_u \zeta_u || \gamma_u \zeta_u \rangle}$$

$$\Psi_{10}(b_{1u}b_{2u}, ^3A_{2g}, M=-1, \beta_g) = |\overline{\gamma_u}\overline{\zeta_u}|$$

$$\Psi_{11}(b_{1u}b_{2u}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\gamma_u}\zeta_u|}{2} + \frac{\sqrt{2}|\gamma_u\overline{\zeta_u}|}{2}$$

$$\Psi_{12}(b_{1u}b_{2u}, ^3A_{2g}, M=1, \beta_g) = |\gamma_u\zeta_u|$$

 e_{2g}^2

$$\boxed{\Delta E = -3 \langle \xi_g \xi_g || \nu_g \nu_g \rangle + \langle \xi_g \xi_g || \xi_g \xi_g \rangle}$$

$$\Psi_{13}(e_{2g}^2, ^3A_{2g}, M=-1, \beta_g) = -|\overline{\nu_g}\overline{\xi_g}|$$

$$\Psi_{14}(e_{2g}^2, ^3A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\nu_g}\xi_g|}{2} + \frac{\sqrt{2}|\xi_g\overline{\nu_g}|}{2}$$

$$\Psi_{15}(e_{2g}^2, ^3A_{2g}, M=1, \beta_g) = -|\nu_g\xi_g|$$

 e_{1u}^2

$$\boxed{\Delta E = -3 \langle \mu_u \mu_u || \eta_u \eta_u \rangle + \langle \mu_u \mu_u || \mu_u \mu_u \rangle}$$

$$\Psi_{16}(e_{1u}^2, ^3A_{2g}, M=-1, \beta_g) = -|\overline{\eta_u}\overline{\mu_u}|$$

$$\Psi_{17}(e_{1u}^2, ^3A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\eta_u}\mu_u|}{2} + \frac{\sqrt{2}|\mu_u\overline{\eta_u}|}{2}$$

$$\Psi_{18}(e_{1u}^2, ^3A_{2g}, M=1, \beta_g) = -|\eta_u\mu_u|$$

 e_{1g}^2

$$\boxed{\Delta E = -3 \langle \mu_g \mu_g || \eta_g \eta_g \rangle + \langle \mu_g \mu_g || \mu_g \mu_g \rangle}$$

$$\Psi_{19}(e_{1g}^2, ^3A_{2g}, M=-1, \beta_g) = -|\overline{\eta_g}\overline{\mu_g}|$$

$$\Psi_{20}(e_{1g}^2, ^3A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\eta_g}\mu_g|}{2} + \frac{\sqrt{2}|\mu_g\overline{\eta_g}|}{2}$$

$$\Psi_{21}(e_{1g}^2, ^3A_{2g}, M=1, \beta_g) = -|\eta_g\mu_g|$$

 e_{2u}^2

$$\boxed{\Delta E = -3 \langle \xi_u \xi_u || \nu_u \nu_u \rangle + \langle \xi_u \xi_u || \xi_u \xi_u \rangle}$$

$$\begin{aligned}\Psi_{22}(e_{2u}^2, {}^3A_{2g}, M=-1, \beta_g) &= -|\overline{\nu_u} \overline{\xi_u}| \\ \Psi_{23}(e_{2u}^2, {}^3A_{2g}, M=0, \beta_g) &= -\frac{\sqrt{2}|\overline{\nu_u} \xi_u|}{2} + \frac{\sqrt{2}|\overline{\xi_u} \nu_u|}{2} \\ \Psi_{24}(e_{2u}^2, {}^3A_{2g}, M=1, \beta_g) &= -|\nu_u \xi_u|\end{aligned}$$

2.27.15 ${}^1A_{2g}$ $a_{1g}a_{2g}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_{1g}a_{2g}, {}^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\alpha_g} \beta_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_g}|}{2}$$

 $a_{1u}a_{2u}$

$$\boxed{\Delta E = \langle \beta_u \alpha_u || \beta_u \alpha_u \rangle + \langle \beta_u \beta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_2(a_{1u}a_{2u}, {}^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\beta_u} \alpha_u|}{2} + \frac{\sqrt{2}|\beta_u \overline{\alpha_u}|}{2}$$

 $b_{1g}b_{2g}$

$$\boxed{\Delta E = \langle \gamma_g \gamma_g || \zeta_g \zeta_g \rangle + \langle \gamma_g \zeta_g || \gamma_g \zeta_g \rangle}$$

$$\Psi_3(b_{1g}b_{2g}, {}^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\gamma_g} \zeta_g|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\zeta_g}|}{2}$$

 $b_{1u}b_{2u}$

$$\boxed{\Delta E = \langle \gamma_u \gamma_u || \zeta_u \zeta_u \rangle + \langle \gamma_u \zeta_u || \gamma_u \zeta_u \rangle}$$

$$\Psi_4(b_{1u}b_{2u}, {}^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\gamma_u} \zeta_u|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\zeta_u}|}{2}$$

2.27.16 ${}^3E_{2g}$ $a_{1g}e_{2g}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \xi_g \xi_g \rangle + \langle \alpha_g \xi_g || \alpha_g \xi_g \rangle}$$

$$\Psi_1(a_{1g}e_{2g}, {}^3E_{2g}, M=-1, \nu_g) = |\overline{\alpha_g} \nu_g|$$

$$\Psi_2(a_{1g}e_{2g}, {}^3E_{2g}, M=-1, \xi_g) = |\overline{\alpha_g} \xi_g|$$

$$\Psi_3(a_{1g}e_{2g}, {}^3E_{2g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\alpha_g} \nu_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\nu_g}|}{2}$$

$$\Psi_4(a_{1g}e_{2g}, {}^3E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\alpha_g} \xi_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\xi_g}|}{2}$$

$$\Psi_5(a_{1g}e_{2g}, {}^3E_{2g}, M=1, \nu_g) = |\alpha_g \nu_g|$$

$$\Psi_6(a_{1g}e_{2g}, {}^3E_{2g}, M=1, \xi_g) = |\alpha_g \xi_g|$$

 $a_{2u}e_{2u}$

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \xi_u \xi_u \rangle + \langle \beta_u \xi_u || \beta_u \xi_u \rangle}$$

$$\Psi_7(a_{2u}e_{2u}, {}^3E_{2g}, M=-1, \nu_g) = |\overline{\beta_u} \nu_u|$$

$$\Psi_8(a_{2u}e_{2u}, {}^3E_{2g}, M=-1, \xi_g) = |\overline{\beta_u} \xi_u|$$

$$\Psi_9(a_{2u}e_{2u}, {}^3E_{2g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\beta_u} \nu_u|}{2} + \frac{\sqrt{2}|\beta_u \overline{\nu_u}|}{2}$$

$$\Psi_{10}(a_{2u}e_{2u}, {}^3E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\beta_u} \xi_u|}{2} + \frac{\sqrt{2}|\beta_u \overline{\xi_u}|}{2}$$

$$\Psi_{11}(a_{2u}e_{2u}, {}^3E_{2g}, M=1, \nu_g) = |\beta_u \nu_u|$$

$$\Psi_{12}(a_{2u}e_{2u}, {}^3E_{2g}, M=1, \xi_g) = |\beta_u \xi_u|$$

 $a_{1u}e_{2u}$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \xi_u \xi_u \rangle + \langle \alpha_u \xi_u || \alpha_u \xi_u \rangle}$$

$$\Psi_{13}(a_{1u}e_{2u}, {}^3E_{2g}, M=-1, \xi_g) = -|\overline{\alpha_u} \nu_u|$$

$$\Psi_{14}(a_{1u}e_{2u}, {}^3E_{2g}, M=-1, \nu_g) = |\overline{\alpha_u} \xi_u|$$

$$\Psi_{15}(a_{1u}e_{2u}, {}^3E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\alpha_u} \nu_u|}{2} - \frac{\sqrt{2}|\alpha_u \overline{\nu_u}|}{2}$$

$$\Psi_{16}(a_{1u}e_{2u}, {}^3E_{2g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\alpha_u} \xi_u|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\xi_u}|}{2}$$

$$\Psi_{17}(a_{1u}e_{2u}, {}^3E_{2g}, M=1, \xi_g) = -|\alpha_u \nu_u|$$

$$\Psi_{18}(a_{1u}e_{2u}, {}^3E_{2g}, M=1, \nu_g) = |\alpha_u \xi_u|$$

 $b_{1g}e_{1g}$

$$\boxed{\Delta E = -\langle \gamma_g \gamma_g || \mu_g \mu_g \rangle + \langle \gamma_g \mu_g || \gamma_g \mu_g \rangle}$$

$$\Psi_{19}(b_{1g}e_{1g}, {}^3E_{2g}, M=-1, \xi_g) = |\overline{\gamma_g} \eta_g|$$

$$\Psi_{20}(b_{1g}e_{1g}, {}^3E_{2g}, M=-1, \nu_g) = |\overline{\gamma_g} \mu_g|$$

$$\Psi_{21}(b_{1g}e_{1g}, {}^3E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\gamma_g} \eta_g|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\eta_g}|}{2}$$

$$\Psi_{22}(b_{1g}e_{1g}, {}^3E_{2g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\gamma_g} \mu_g|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\mu_g}|}{2}$$

$$\Psi_{23}(b_{1g}e_{1g}, {}^3E_{2g}, M=1, \xi_g) = |\gamma_g \eta_g|$$

$$\Psi_{24}(b_{1g}e_{1g}, {}^3E_{2g}, M=1, \nu_g) = |\gamma_g \mu_g|$$

 $b_{2g}e_{1g}$

$$\boxed{\Delta E = \langle \zeta_g \mu_g || \zeta_g \mu_g \rangle - \langle \zeta_g \zeta_g || \mu_g \mu_g \rangle}$$

$$\Psi_{25}(b_{2g}e_{1g}, {}^3E_{2g}, M=-1, \nu_g) = |\overline{\zeta_g} \eta_g|$$

$$\Psi_{26}(b_{2g}e_{1g}, {}^3E_{2g}, M=-1, \xi_g) = -|\overline{\zeta_g} \mu_g|$$

$$\Psi_{27}(b_{2g}e_{1g}, {}^3E_{2g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\zeta_g} \eta_g|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\eta_g}|}{2}$$

$$\Psi_{28}(b_{2g}e_{1g}, {}^3E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\zeta_g} \mu_g|}{2} - \frac{\sqrt{2}|\zeta_g \overline{\mu_g}|}{2}$$

$$\Psi_{29}(b_{2g}e_{1g}, {}^3E_{2g}, M=1, \nu_g) = |\zeta_g \eta_g|$$

$$\Psi_{30}(b_{2g}e_{1g}, {}^3E_{2g}, M=1, \xi_g) = -|\zeta_g \mu_g|$$

 $b_{1u}e_{1u}$

$$\boxed{\Delta E = -\langle \gamma_u \gamma_u || \mu_u \mu_u \rangle + \langle \gamma_u \mu_u || \gamma_u \mu_u \rangle}$$

$$\Psi_{31}(b_{1u}e_{1u}, {}^3E_{2g}, M=-1, \nu_g) = |\overline{\gamma_u} \eta_u|$$

$$\Psi_{32}(b_{1u}e_{1u}, {}^3E_{2g}, M=-1, \xi_g) = -|\overline{\gamma_u} \mu_u|$$

$$\Psi_{33}(b_{1u}e_{1u}, {}^3E_{2g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\gamma_u} \eta_u|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\eta_u}|}{2}$$

$$\Psi_{34}(b_{1u}e_{1u}, {}^3E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\gamma_u} \mu_u|}{2} - \frac{\sqrt{2}|\gamma_u \overline{\mu_u}|}{2}$$

$$\Psi_{35}(b_{1u}e_{1u}, {}^3E_{2g}, M=1, \nu_g) = |\gamma_u \eta_u|$$

$$\Psi_{36}(b_{1u}e_{1u}, {}^3E_{2g}, M=1, \xi_g) = -|\gamma_u\mu_u|$$

$$b_{2u}e_{1u}$$

$$\boxed{\Delta E = \langle \zeta_u\mu_u || \zeta_u\mu_u \rangle - \langle \zeta_u\zeta_u || \mu_u\mu_u \rangle}$$

$$\Psi_{37}(b_{2u}e_{1u}, {}^3E_{2g}, M=-1, \xi_g) = |\overline{\zeta_u}\overline{\eta_u}|$$

$$\Psi_{38}(b_{2u}e_{1u}, {}^3E_{2g}, M=-1, \nu_g) = |\overline{\zeta_u}\overline{\mu_u}|$$

$$\Psi_{39}(b_{2u}e_{1u}, {}^3E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\zeta_u}\eta_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\eta_u}|}{2}$$

$$\Psi_{40}(b_{2u}e_{1u}, {}^3E_{2g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\zeta_u}\mu_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\mu_u}|}{2}$$

$$\Psi_{41}(b_{2u}e_{1u}, {}^3E_{2g}, M=1, \xi_g) = |\zeta_u\eta_u|$$

$$\Psi_{42}(b_{2u}e_{1u}, {}^3E_{2g}, M=1, \nu_g) = |\zeta_u\mu_u|$$

$$a_{2g}e_{2g}$$

$$\boxed{\Delta E = -\langle \beta_g\beta_g || \xi_g\xi_g \rangle + \langle \beta_g\xi_g || \beta_g\xi_g \rangle}$$

$$\Psi_{43}(a_{2g}e_{2g}, {}^3E_{2g}, M=-1, \xi_g) = -|\overline{\beta_g}\overline{\nu_g}|$$

$$\Psi_{44}(a_{2g}e_{2g}, {}^3E_{2g}, M=-1, \nu_g) = |\overline{\beta_g}\overline{\xi_g}|$$

$$\Psi_{45}(a_{2g}e_{2g}, {}^3E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\beta_g}\nu_g|}{2} - \frac{\sqrt{2}|\beta_g\overline{\nu_g}|}{2}$$

$$\Psi_{46}(a_{2g}e_{2g}, {}^3E_{2g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\beta_g}\xi_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\xi_g}|}{2}$$

$$\Psi_{47}(a_{2g}e_{2g}, {}^3E_{2g}, M=1, \xi_g) = -|\beta_g\nu_g|$$

$$\Psi_{48}(a_{2g}e_{2g}, {}^3E_{2g}, M=1, \nu_g) = |\beta_g\xi_g|$$

2.27.17 ${}^1E_{2g}$

$$a_{1u}e_{2g}$$

$$\boxed{\Delta E = \langle \alpha_g\alpha_g || \xi_g\xi_g \rangle + \langle \alpha_g\xi_g || \alpha_g\xi_g \rangle}$$

$$\Psi_1(a_{1g}e_{2g}, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\nu_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\nu_g}|}{2}$$

$$\Psi_2(a_{1g}e_{2g}, {}^1E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\xi_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\xi_g}|}{2}$$

$$a_{2u}e_{2u}$$

$$\boxed{\Delta E = \langle \beta_u\beta_u || \xi_u\xi_u \rangle + \langle \beta_u\xi_u || \beta_u\xi_u \rangle}$$

$$\Psi_3(a_{2u}e_{2u}, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\beta_u}\nu_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\nu_u}|}{2}$$

$$\Psi_4(a_{2u}e_{2u}, {}^1E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\beta_u}\xi_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\xi_u}|}{2}$$

$$a_{1u}e_{2u}$$

$$\boxed{\Delta E = \langle \alpha_u\alpha_u || \xi_u\xi_u \rangle + \langle \alpha_u\xi_u || \alpha_u\xi_u \rangle}$$

$$\Psi_5(a_{1u}e_{2u}, {}^1E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\alpha_u}\nu_u|}{2} - \frac{\sqrt{2}|\alpha_u\overline{\nu_u}|}{2}$$

$$\Psi_6(a_{1u}e_{2u}, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\alpha_u}\xi_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\xi_u}|}{2}$$

$$b_{1g}e_{1g}$$

$$\boxed{\Delta E = \langle \gamma_g\gamma_g || \mu_g\mu_g \rangle + \langle \gamma_g\mu_g || \gamma_g\mu_g \rangle}$$

$$\Psi_7(b_{1g}e_{1g}, {}^1E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\gamma_g}\eta_g|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\eta_g}|}{2}$$

$$\Psi_8(b_{1g}e_{1g}, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\gamma_g}\mu_g|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\mu_g}|}{2}$$

$$b_{2g}e_{1g}$$

$$\boxed{\Delta E = \langle \zeta_g\mu_g || \zeta_g\mu_g \rangle + \langle \zeta_g\xi_g || \mu_g\mu_g \rangle}$$

$$\Psi_9(b_{2g}e_{1g}, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\zeta_g}\eta_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\eta_g}|}{2}$$

$$\Psi_{10}(b_{2g}e_{1g}, {}^1E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\zeta_g}\mu_g|}{2} - \frac{\sqrt{2}|\zeta_g\overline{\mu_g}|}{2}$$

$$b_{1u}e_{1u}$$

$$\boxed{\Delta E = \langle \gamma_u\gamma_u || \mu_u\mu_u \rangle + \langle \gamma_u\mu_u || \gamma_u\mu_u \rangle}$$

$$\Psi_{11}(b_{1u}e_{1u}, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\gamma_u}\eta_u|}{2} + \frac{\sqrt{2}|\gamma_u\overline{\eta_u}|}{2}$$

$$\Psi_{12}(b_{1u}e_{1u}, {}^1E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\gamma_u}\mu_u|}{2} - \frac{\sqrt{2}|\gamma_u\overline{\mu_u}|}{2}$$

$$b_{2u}e_{1u}$$

$$\boxed{\Delta E = \langle \zeta_u\mu_u || \zeta_u\mu_u \rangle + \langle \zeta_u\xi_u || \mu_u\mu_u \rangle}$$

$$\Psi_{13}(b_{2u}e_{1u}, {}^1E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\zeta_u}\eta_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\eta_u}|}{2}$$

$$\Psi_{14}(b_{2u}e_{1u}, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\zeta_u}\mu_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\mu_u}|}{2}$$

$$a_{2g}e_{2g}$$

$$\boxed{\Delta E = \langle \beta_g\beta_g || \xi_g\xi_g \rangle + \langle \beta_g\xi_g || \beta_g\xi_g \rangle}$$

$$\Psi_{15}(a_{2g}e_{2g}, {}^1E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\beta_g}\nu_g|}{2} - \frac{\sqrt{2}|\beta_g\overline{\nu_g}|}{2}$$

$$\Psi_{16}(a_{2g}e_{2g}, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\beta_g}\xi_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\xi_g}|}{2}$$

$$e_{2g}^2$$

$$\boxed{\Delta E = -\langle \xi_g\xi_g || \nu_g\nu_g \rangle + \langle \xi_g\xi_g || \xi_g\xi_g \rangle}$$

$$\Psi_{17}(e_{2g}^2, {}^1E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\nu_g}\nu_g|}{2} + \frac{\sqrt{2}|\xi_g\overline{\xi_g}|}{2}$$

$$\Psi_{18}(e_{2g}^2, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\nu_g}\xi_g|}{2} - \frac{\sqrt{2}|\xi_g\overline{\nu_g}|}{2}$$

$$e_{1u}^2$$

$$\boxed{\Delta E = -\langle \mu_u\mu_u || \eta_u\eta_u \rangle + \langle \mu_u\mu_u || \mu_u\mu_u \rangle}$$

$$\Psi_{19}(e_{1u}^2, {}^1E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\eta_u}\eta_u|}{2} - \frac{\sqrt{2}|\mu_u\overline{\mu_u}|}{2}$$

$$\Psi_{20}(e_{1u}^2, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\eta_u}\mu_u|}{2} - \frac{\sqrt{2}|\mu_u\overline{\eta_u}|}{2}$$

$$e_{1g}^2$$

$$\boxed{\Delta E = -\langle \mu_g\mu_g || \eta_g\eta_g \rangle + \langle \mu_g\mu_g || \mu_g\mu_g \rangle}$$

$$\Psi_{21}(e_{1g}^2, {}^1E_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\eta_g\eta_g|}{2} - \frac{\sqrt{2}|\mu_g\mu_g|}{2}$$

$$\Psi_{22}(e_{1g}^2, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\eta_g\mu_g|}{2} - \frac{\sqrt{2}|\mu_g\eta_g|}{2}$$

 e_{2u}^2

$$\boxed{\Delta E = -\langle \xi_u \xi_u || \nu_u \nu_u \rangle + \langle \xi_u \xi_u || \xi_u \xi_u \rangle}$$

$$\Psi_{23}(e_{2u}^2, {}^1E_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\nu_u\nu_u|}{2} + \frac{\sqrt{2}|\xi_u\xi_u|}{2}$$

$$\Psi_{24}(e_{2u}^2, {}^1E_{2g}, M=0, \nu_g) = -\frac{\sqrt{2}|\nu_u\xi_u|}{2} - \frac{\sqrt{2}|\xi_u\nu_u|}{2}$$

2.27.18 ${}^3E_{1u}$ $a_{1g}e_{1u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \mu_u \mu_u \rangle + \langle \alpha_g \mu_u || \alpha_g \mu_u \rangle}$$

$$\Psi_1(a_{1g}e_{1u}, {}^3E_{1u}, M=-1, \eta_u) = |\overline{\alpha_g}\eta_u|$$

$$\Psi_2(a_{1g}e_{1u}, {}^3E_{1u}, M=-1, \mu_u) = |\overline{\alpha_g}\mu_u|$$

$$\Psi_3(a_{1g}e_{1u}, {}^3E_{1u}, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\alpha_g}\eta_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\eta_u}|}{2}$$

$$\Psi_4(a_{1g}e_{1u}, {}^3E_{1u}, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\alpha_g}\mu_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\mu_u}|}{2}$$

$$\Psi_5(a_{1g}e_{1u}, {}^3E_{1u}, M=1, \eta_u) = |\alpha_g\eta_u|$$

$$\Psi_6(a_{1g}e_{1u}, {}^3E_{1u}, M=1, \mu_u) = |\alpha_g\mu_u|$$

 $a_{2u}e_{1g}$

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \mu_g \mu_g \rangle + \langle \beta_u \mu_g || \beta_u \mu_g \rangle}$$

$$\Psi_7(a_{2u}e_{1g}, {}^3E_{1u}, M=-1, \eta_u) = |\overline{\beta_u}\eta_g|$$

$$\Psi_8(a_{2u}e_{1g}, {}^3E_{1u}, M=-1, \mu_u) = |\overline{\beta_u}\mu_g|$$

$$\Psi_9(a_{2u}e_{1g}, {}^3E_{1u}, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\beta_u}\eta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\eta_g}|}{2}$$

$$\Psi_{10}(a_{2u}e_{1g}, {}^3E_{1u}, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\beta_u}\mu_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\mu_g}|}{2}$$

$$\Psi_{11}(a_{2u}e_{1g}, {}^3E_{1u}, M=1, \eta_u) = |\beta_u\eta_g|$$

$$\Psi_{12}(a_{2u}e_{1g}, {}^3E_{1u}, M=1, \mu_u) = |\beta_u\mu_g|$$

 $a_{1u}e_{1g}$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \mu_g \mu_g \rangle + \langle \alpha_u \mu_g || \alpha_u \mu_g \rangle}$$

$$\Psi_{13}(a_{1u}e_{1g}, {}^3E_{1u}, M=-1, \mu_u) = -|\overline{\alpha_u}\eta_g|$$

$$\Psi_{14}(a_{1u}e_{1g}, {}^3E_{1u}, M=-1, \eta_u) = |\overline{\alpha_u}\mu_g|$$

$$\Psi_{15}(a_{1u}e_{1g}, {}^3E_{1u}, M=0, \mu_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\eta_g|}{2} - \frac{\sqrt{2}|\alpha_u\overline{\eta_g}|}{2}$$

$$\Psi_{16}(a_{1u}e_{1g}, {}^3E_{1u}, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\alpha_u}\mu_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\mu_g}|}{2}$$

$$\Psi_{17}(a_{1u}e_{1g}, {}^3E_{1u}, M=1, \mu_u) = -|\alpha_u\eta_g|$$

$$\Psi_{18}(a_{1u}e_{1g}, {}^3E_{1u}, M=1, \eta_u) = |\alpha_u\mu_g|$$

 $b_{1g}e_{2u}$

$$\boxed{\Delta E = -\langle \gamma_g \gamma_g || \xi_u \xi_u \rangle + \langle \gamma_g \xi_u || \gamma_g \xi_u \rangle}$$

$$\Psi_{19}(b_{1g}e_{2u}, {}^3E_{1u}, M=-1, \mu_u) = |\overline{\gamma_g}\nu_u|$$

$$\Psi_{20}(b_{1g}e_{2u}, {}^3E_{1u}, M=-1, \eta_u) = |\overline{\gamma_g}\xi_u|$$

$$\Psi_{21}(b_{1g}e_{2u}, {}^3E_{1u}, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\gamma_g}\nu_u|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\nu_u}|}{2}$$

$$\Psi_{22}(b_{1g}e_{2u}, {}^3E_{1u}, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\gamma_g}\xi_u|}{2} + \frac{\sqrt{2}|\gamma_g\overline{\xi_u}|}{2}$$

$$\Psi_{23}(b_{1g}e_{2u}, {}^3E_{1u}, M=1, \mu_u) = |\gamma_g\nu_u|$$

$$\Psi_{24}(b_{1g}e_{2u}, {}^3E_{1u}, M=1, \eta_u) = |\gamma_g\xi_u|$$

 $b_{2g}e_{2u}$

$$\boxed{\Delta E = \langle \zeta_g \xi_u || \zeta_g \xi_u \rangle - \langle \zeta_g \zeta_g || \xi_u \xi_u \rangle}$$

$$\Psi_{25}(b_{2g}e_{2u}, {}^3E_{1u}, M=-1, \eta_u) = |\overline{\zeta_g}\nu_u|$$

$$\Psi_{26}(b_{2g}e_{2u}, {}^3E_{1u}, M=-1, \mu_u) = -|\overline{\zeta_g}\xi_u|$$

$$\Psi_{27}(b_{2g}e_{2u}, {}^3E_{1u}, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\zeta_g}\nu_u|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\nu_u}|}{2}$$

$$\Psi_{28}(b_{2g}e_{2u}, {}^3E_{1u}, M=0, \mu_u) = -\frac{\sqrt{2}|\overline{\zeta_g}\xi_u|}{2} - \frac{\sqrt{2}|\zeta_g\overline{\xi_u}|}{2}$$

$$\Psi_{29}(b_{2g}e_{2u}, {}^3E_{1u}, M=1, \eta_u) = |\zeta_g\nu_u|$$

$$\Psi_{30}(b_{2g}e_{2u}, {}^3E_{1u}, M=1, \mu_u) = -|\zeta_g\xi_u|$$

 $b_{1u}e_{2g}$

$$\boxed{\Delta E = -\langle \gamma_u \gamma_u || \xi_g \xi_g \rangle + \langle \gamma_u \xi_g || \gamma_u \xi_g \rangle}$$

$$\Psi_{31}(b_{1u}e_{2g}, {}^3E_{1u}, M=-1, \eta_u) = |\overline{\gamma_u}\nu_g|$$

$$\Psi_{32}(b_{1u}e_{2g}, {}^3E_{1u}, M=-1, \mu_u) = -|\overline{\gamma_u}\xi_g|$$

$$\Psi_{33}(b_{1u}e_{2g}, {}^3E_{1u}, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\gamma_u}\nu_g|}{2} + \frac{\sqrt{2}|\gamma_u\overline{\nu_g}|}{2}$$

$$\Psi_{34}(b_{1u}e_{2g}, {}^3E_{1u}, M=0, \mu_u) = -\frac{\sqrt{2}|\overline{\gamma_u}\xi_g|}{2} - \frac{\sqrt{2}|\gamma_u\overline{\xi_g}|}{2}$$

$$\Psi_{35}(b_{1u}e_{2g}, {}^3E_{1u}, M=1, \eta_u) = |\gamma_u\nu_g|$$

$$\Psi_{36}(b_{1u}e_{2g}, {}^3E_{1u}, M=1, \mu_u) = -|\gamma_u\xi_g|$$

 $b_{2u}e_{2g}$

$$\boxed{\Delta E = \langle \zeta_u \xi_g || \zeta_u \xi_g \rangle - \langle \zeta_u \zeta_u || \xi_g \xi_g \rangle}$$

$$\Psi_{37}(b_{2u}e_{2g}, {}^3E_{1u}, M=-1, \mu_u) = |\overline{\zeta_u}\nu_g|$$

$$\Psi_{38}(b_{2u}e_{2g}, {}^3E_{1u}, M=-1, \eta_u) = |\overline{\zeta_u}\xi_g|$$

$$\Psi_{39}(b_{2u}e_{2g}, {}^3E_{1u}, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\zeta_u}\nu_g|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\nu_g}|}{2}$$

$$\Psi_{40}(b_{2u}e_{2g}, {}^3E_{1u}, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\zeta_u}\xi_g|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\xi_g}|}{2}$$

$$\Psi_{41}(b_{2u}e_{2g}, {}^3E_{1u}, M=1, \mu_u) = |\zeta_u\nu_g|$$

$$\Psi_{42}(b_{2u}e_{2g}, {}^3E_{1u}, M=1, \eta_u) = |\zeta_u\xi_g|$$

 $a_{2g}e_{1u}$

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \mu_u \mu_u \rangle + \langle \beta_g \mu_u || \beta_g \mu_u \rangle}$$

$$\Psi_{43}(a_{2g}e_{1u}, {}^3E_{1u}, M=-1, \mu_u) = -|\overline{\beta_g}\eta_u|$$

$$\Psi_{44}(a_{2g}e_{1u}, {}^3E_{1u}, M=-1, \eta_u) = |\overline{\beta_g}\mu_u|$$

$$\Psi_{45}(a_{2g}e_{1u}, {}^3E_{1u}, M=0, \mu_u) = -\frac{\sqrt{2}|\beta_g\eta_u|}{2} - \frac{\sqrt{2}|\beta_g\bar{\eta}_u|}{2}$$

$$\Psi_{46}(a_{2g}e_{1u}, {}^3E_{1u}, M=0, \eta_u) = \frac{\sqrt{2}|\beta_g\mu_u|}{2} + \frac{\sqrt{2}|\beta_g\bar{\mu}_u|}{2}$$

$$\Psi_{47}(a_{2g}e_{1u}, {}^3E_{1u}, M=1, \mu_u) = -|\beta_g\eta_u|$$

$$\Psi_{48}(a_{2g}e_{1u}, {}^3E_{1u}, M=1, \eta_u) = |\beta_g\mu_u|$$

e_{1u}e_{2g}

$$\boxed{\Delta E = \langle \xi_g\mu_u || \nu_g\eta_u \rangle + \langle \xi_g\mu_u || \xi_g\mu_u \rangle - \langle \xi_g\xi_g || \eta_u\eta_u \rangle + \langle \xi_g\nu_g || \mu_u\eta_u \rangle}$$

$$\Psi_{49}(e_{1u}e_{2g}, {}^3E_{1u}, M=-1, \mu_u) = -\frac{\sqrt{2}|\nu_g\eta_u|}{2} - \frac{\sqrt{2}|\xi_g\bar{\mu}_u|}{2}$$

$$\Psi_{50}(e_{1u}e_{2g}, {}^3E_{1u}, M=-1, \eta_u) = -\frac{\sqrt{2}|\nu_g\mu_u|}{2} + \frac{\sqrt{2}|\xi_g\bar{\eta}_u|}{2}$$

$$\Psi_{51}(e_{1u}e_{2g}, {}^3E_{1u}, M=0, \mu_u) = -\frac{|\nu_g\eta_u|}{2} - \frac{|\xi_g\mu_u|}{2} - \frac{|\nu_g\bar{\eta}_u|}{2} - \frac{|\xi_g\bar{\mu}_u|}{2}$$

$$\Psi_{52}(e_{1u}e_{2g}, {}^3E_{1u}, M=0, \eta_u) = -\frac{|\nu_g\mu_u|}{2} + \frac{|\xi_g\eta_u|}{2} - \frac{|\nu_g\bar{\mu}_u|}{2} + \frac{|\xi_g\bar{\eta}_u|}{2}$$

$$\Psi_{53}(e_{1u}e_{2g}, {}^3E_{1u}, M=1, \mu_u) = -\frac{\sqrt{2}|\nu_g\eta_u|}{2} - \frac{\sqrt{2}|\xi_g\mu_u|}{2}$$

$$\Psi_{54}(e_{1u}e_{2g}, {}^3E_{1u}, M=1, \eta_u) = -\frac{\sqrt{2}|\nu_g\mu_u|}{2} + \frac{\sqrt{2}|\xi_g\eta_u|}{2}$$

e_{1g}e_{2u}

$$\boxed{\Delta E = -\langle \mu_g\mu_g || \nu_u\nu_u \rangle + \langle \mu_g\xi_u || \eta_g\nu_u \rangle + \langle \mu_g\xi_u || \mu_g\xi_u \rangle + \langle \mu_g\eta_g || \xi_u\nu_u \rangle}$$

$$\Psi_{55}(e_{1g}e_{2u}, {}^3E_{1u}, M=-1, \mu_u) = \frac{\sqrt{2}|\eta_g\nu_u|}{2} + \frac{\sqrt{2}|\mu_g\xi_u|}{2}$$

$$\Psi_{56}(e_{1g}e_{2u}, {}^3E_{1u}, M=-1, \eta_u) = -\frac{\sqrt{2}|\eta_g\xi_u|}{2} + \frac{\sqrt{2}|\mu_g\nu_u|}{2}$$

$$\Psi_{57}(e_{1g}e_{2u}, {}^3E_{1u}, M=0, \mu_u) = -\frac{|\eta_g\nu_u|}{2} + \frac{|\mu_g\xi_u|}{2} + \frac{|\eta_g\bar{\nu}_u|}{2} + \frac{|\mu_g\bar{\xi}_u|}{2}$$

$$\Psi_{58}(e_{1g}e_{2u}, {}^3E_{1u}, M=0, \eta_u) = -\frac{|\eta_g\xi_u|}{2} + \frac{|\mu_g\nu_u|}{2} - \frac{|\eta_g\bar{\xi}_u|}{2} + \frac{|\mu_g\bar{\nu}_u|}{2}$$

$$\Psi_{59}(e_{1g}e_{2u}, {}^3E_{1u}, M=1, \mu_u) = \frac{\sqrt{2}|\eta_g\nu_u|}{2} + \frac{\sqrt{2}|\mu_g\xi_u|}{2}$$

$$\Psi_{60}(e_{1g}e_{2u}, {}^3E_{1u}, M=1, \eta_u) = -\frac{\sqrt{2}|\eta_g\xi_u|}{2} + \frac{\sqrt{2}|\mu_g\nu_u|}{2}$$

2.27.19 ${}^1E_{1u}$

a_{1g}e_{1u}

$$\boxed{\Delta E = \langle \alpha_g\alpha_g || \mu_u\mu_u \rangle + \langle \alpha_g\mu_u || \alpha_g\mu_u \rangle}$$

$$\Psi_1(a_{1g}e_{1u}, {}^1E_{1u}, M=0, \eta_u) = -\frac{\sqrt{2}|\alpha_g\eta_u|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\eta}_u|}{2}$$

$$\Psi_2(a_{1g}e_{1u}, {}^1E_{1u}, M=0, \mu_u) = -\frac{\sqrt{2}|\alpha_g\mu_u|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\mu}_u|}{2}$$

a_{2u}e_{1g}

$$\boxed{\Delta E = \langle \beta_u\beta_u || \mu_g\mu_g \rangle + \langle \beta_u\mu_g || \beta_u\mu_g \rangle}$$

$$\Psi_3(a_{2u}e_{1g}, {}^1E_{1u}, M=0, \eta_u) = -\frac{\sqrt{2}|\beta_u\eta_g|}{2} + \frac{\sqrt{2}|\beta_u\bar{\eta}_g|}{2}$$

$$\Psi_4(a_{2u}e_{1g}, {}^1E_{1u}, M=0, \mu_u) = -\frac{\sqrt{2}|\beta_u\mu_g|}{2} + \frac{\sqrt{2}|\beta_u\bar{\mu}_g|}{2}$$

a_{1u}e_{1g}

$$\boxed{\Delta E = \langle \alpha_u\alpha_u || \mu_g\mu_g \rangle + \langle \alpha_u\mu_g || \alpha_u\mu_g \rangle}$$

$$\Psi_5(a_{1u}e_{1g}, {}^1E_{1u}, M=0, \mu_u) = \frac{\sqrt{2}|\alpha_u\eta_g|}{2} - \frac{\sqrt{2}|\alpha_u\bar{\eta}_g|}{2}$$

$$\Psi_6(a_{1u}e_{1g}, {}^1E_{1u}, M=0, \eta_u) = -\frac{\sqrt{2}|\alpha_u\mu_g|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\mu}_g|}{2}$$

b_{1g}e_{2u}

$$\boxed{\Delta E = \langle \gamma_g\gamma_g || \xi_u\xi_u \rangle + \langle \gamma_g\xi_u || \gamma_g\xi_u \rangle}$$

$$\Psi_7(b_{1g}e_{2u}, {}^1E_{1u}, M=0, \mu_u) = -\frac{\sqrt{2}|\gamma_g\nu_u|}{2} + \frac{\sqrt{2}|\gamma_g\bar{\nu}_u|}{2}$$

$$\Psi_8(b_{1g}e_{2u}, {}^1E_{1u}, M=0, \eta_u) = -\frac{\sqrt{2}|\gamma_g\xi_u|}{2} + \frac{\sqrt{2}|\gamma_g\bar{\xi}_u|}{2}$$

b_{2g}e_{2u}

$$\boxed{\Delta E = \langle \zeta_g\xi_u || \zeta_g\xi_u \rangle + \langle \zeta_g\zeta_g || \xi_u\xi_u \rangle}$$

$$\Psi_9(b_{2g}e_{2u}, {}^1E_{1u}, M=0, \eta_u) = -\frac{\sqrt{2}|\zeta_g\nu_u|}{2} + \frac{\sqrt{2}|\zeta_g\bar{\nu}_u|}{2}$$

$$\Psi_{10}(b_{2g}e_{2u}, {}^1E_{1u}, M=0, \mu_u) = \frac{\sqrt{2}|\zeta_g\xi_u|}{2} - \frac{\sqrt{2}|\zeta_g\bar{\xi}_u|}{2}$$

b_{1u}e_{2g}

$$\boxed{\Delta E = \langle \gamma_u\gamma_u || \xi_g\xi_g \rangle + \langle \gamma_u\xi_g || \gamma_u\xi_g \rangle}$$

$$\Psi_{11}(b_{1u}e_{2g}, {}^1E_{1u}, M=0, \eta_u) = -\frac{\sqrt{2}|\gamma_u\nu_g|}{2} + \frac{\sqrt{2}|\gamma_u\bar{\nu}_g|}{2}$$

$$\Psi_{12}(b_{1u}e_{2g}, {}^1E_{1u}, M=0, \mu_u) = \frac{\sqrt{2}|\gamma_u\xi_g|}{2} - \frac{\sqrt{2}|\gamma_u\bar{\xi}_g|}{2}$$

b_{2u}e_{2g}

$$\boxed{\Delta E = \langle \zeta_u\xi_g || \zeta_u\xi_g \rangle + \langle \zeta_u\zeta_u || \xi_g\xi_g \rangle}$$

$$\Psi_{13}(b_{2u}e_{2g}, {}^1E_{1u}, M=0, \mu_u) = -\frac{\sqrt{2}|\zeta_u\nu_g|}{2} + \frac{\sqrt{2}|\zeta_u\bar{\nu}_g|}{2}$$

$$\Psi_{14}(b_{2u}e_{2g}, {}^1E_{1u}, M=0, \eta_u) = -\frac{\sqrt{2}|\zeta_u\xi_g|}{2} + \frac{\sqrt{2}|\zeta_u\bar{\xi}_g|}{2}$$

a_{2g}e_{1u}

$$\boxed{\Delta E = \langle \beta_g\beta_g || \mu_u\mu_u \rangle + \langle \beta_g\mu_u || \beta_g\mu_u \rangle}$$

$$\Psi_{15}(a_{2g}e_{1u}, {}^1E_{1u}, M=0, \mu_u) = \frac{\sqrt{2}|\beta_g\eta_u|}{2} - \frac{\sqrt{2}|\beta_g\bar{\eta}_u|}{2}$$

$$\Psi_{16}(a_{2g}e_{1u}, {}^1E_{1u}, M=0, \eta_u) = -\frac{\sqrt{2}|\beta_g\mu_u|}{2} + \frac{\sqrt{2}|\beta_g\bar{\mu}_u|}{2}$$

e_{1u}e_{2g}

$$\boxed{\Delta E = \langle \xi_g\mu_u || \nu_g\eta_u \rangle + \langle \xi_g\mu_u || \xi_g\mu_u \rangle + \langle \xi_g\xi_g || \eta_u\eta_u \rangle - \langle \xi_g\nu_g || \mu_u\eta_u \rangle}$$

$$\Psi_{17}(e_{1u}e_{2g}, {}^1E_{1u}, M=0, \mu_u) = \frac{|\nu_g\eta_u|}{2} + \frac{|\xi_g\mu_u|}{2} - \frac{|\nu_g\eta_u|}{2} - \frac{|\xi_g\mu_u|}{2}$$

$$\Psi_{18}(e_{1u}e_{2g}, {}^1E_{1u}, M=0, \eta_u) = \frac{|\nu_g\mu_u|}{2} - \frac{|\xi_g\eta_u|}{2} - \frac{|\nu_g\mu_u|}{2} + \frac{|\xi_g\eta_u|}{2}$$

e_{1g}e_{2u}

$$\Delta E = \langle \mu_g\mu_g || \nu_u\nu_u \rangle + \langle \mu_g\xi_u || \eta_g\nu_u \rangle + \langle \mu_g\xi_u || \mu_g\xi_u \rangle - \langle \mu_g\eta_g || \xi_u\nu_u \rangle$$

$$\Psi_{19}(e_{1g}e_{2u}, {}^1E_{1u}, M=0, \mu_u) = -\frac{|\eta_g\nu_u|}{2} - \frac{|\mu_g\xi_u|}{2} + \frac{|\eta_g\nu_u|}{2} + \frac{|\mu_g\xi_u|}{2}$$

$$\Psi_{20}(e_{1g}e_{2u}, {}^1E_{1u}, M=0, \eta_u) = \frac{|\eta_g\xi_u|}{2} - \frac{|\mu_g\nu_u|}{2} - \frac{|\eta_g\xi_u|}{2} + \frac{|\mu_g\nu_u|}{2}$$

2.27.20 *{}^3E_{1g}*

a_{1g}e_{1g}

$$\Delta E = -\langle \alpha_g\alpha_g || \mu_g\mu_g \rangle + \langle \alpha_g\mu_g || \alpha_g\mu_g \rangle$$

$$\Psi_1(a_{1g}e_{1g}, {}^3E_{1g}, M=-1, \eta_g) = |\overline{\alpha_g}\eta_g|$$

$$\Psi_2(a_{1g}e_{1g}, {}^3E_{1g}, M=-1, \mu_g) = |\overline{\alpha_g}\mu_g|$$

$$\Psi_3(a_{1g}e_{1g}, {}^3E_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\alpha_g}\eta_g|}{2} + \frac{\sqrt{2}|\alpha_g\eta_g|}{2}$$

$$\Psi_4(a_{1g}e_{1g}, {}^3E_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\alpha_g}\mu_g|}{2} + \frac{\sqrt{2}|\alpha_g\mu_g|}{2}$$

$$\Psi_5(a_{1g}e_{1g}, {}^3E_{1g}, M=1, \eta_g) = |\alpha_g\eta_g|$$

$$\Psi_6(a_{1g}e_{1g}, {}^3E_{1g}, M=1, \mu_g) = |\alpha_g\mu_g|$$

a_{2u}e_{1u}

$$\Delta E = -\langle \beta_u\beta_u || \mu_u\mu_u \rangle + \langle \beta_u\mu_u || \beta_u\mu_u \rangle$$

$$\Psi_7(a_{2u}e_{1u}, {}^3E_{1g}, M=-1, \eta_g) = |\overline{\beta_u}\eta_u|$$

$$\Psi_8(a_{2u}e_{1u}, {}^3E_{1g}, M=-1, \mu_g) = |\overline{\beta_u}\mu_u|$$

$$\Psi_9(a_{2u}e_{1u}, {}^3E_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\beta_u}\eta_u|}{2} + \frac{\sqrt{2}|\beta_u\eta_u|}{2}$$

$$\Psi_{10}(a_{2u}e_{1u}, {}^3E_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\beta_u}\mu_u|}{2} + \frac{\sqrt{2}|\beta_u\mu_u|}{2}$$

$$\Psi_{11}(a_{2u}e_{1u}, {}^3E_{1g}, M=1, \eta_g) = |\beta_u\eta_u|$$

$$\Psi_{12}(a_{2u}e_{1u}, {}^3E_{1g}, M=1, \mu_g) = |\beta_u\mu_u|$$

a_{1u}e_{1u}

$$\Delta E = -\langle \alpha_u\alpha_u || \mu_u\mu_u \rangle + \langle \alpha_u\mu_u || \alpha_u\mu_u \rangle$$

$$\Psi_{13}(a_{1u}e_{1u}, {}^3E_{1g}, M=-1, \mu_g) = -|\overline{\alpha_u}\eta_u|$$

$$\Psi_{14}(a_{1u}e_{1u}, {}^3E_{1g}, M=-1, \eta_g) = |\overline{\alpha_u}\mu_u|$$

$$\Psi_{15}(a_{1u}e_{1u}, {}^3E_{1g}, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\alpha_u}\eta_u|}{2} - \frac{\sqrt{2}|\alpha_u\eta_u|}{2}$$

$$\Psi_{16}(a_{1u}e_{1u}, {}^3E_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\alpha_u}\mu_u|}{2} + \frac{\sqrt{2}|\alpha_u\mu_u|}{2}$$

$$\Psi_{17}(a_{1u}e_{1u}, {}^3E_{1g}, M=1, \mu_g) = -|\alpha_u\eta_u|$$

$$\Psi_{18}(a_{1u}e_{1u}, {}^3E_{1g}, M=1, \eta_g) = |\alpha_u\mu_u|$$

b_{1g}e_{2g}

$$\boxed{\Delta E = -\langle \gamma_g\gamma_g || \xi_g\xi_g \rangle + \langle \gamma_g\xi_g || \gamma_g\xi_g \rangle}$$

$$\Psi_{19}(b_{1g}e_{2g}, {}^3E_{1g}, M=-1, \mu_g) = |\overline{\gamma_g}\nu_g|$$

$$\Psi_{20}(b_{1g}e_{2g}, {}^3E_{1g}, M=-1, \eta_g) = |\overline{\gamma_g}\xi_g|$$

$$\Psi_{21}(b_{1g}e_{2g}, {}^3E_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\gamma_g}\nu_g|}{2} + \frac{\sqrt{2}|\gamma_g\nu_g|}{2}$$

$$\Psi_{22}(b_{1g}e_{2g}, {}^3E_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\gamma_g}\xi_g|}{2} + \frac{\sqrt{2}|\gamma_g\xi_g|}{2}$$

$$\Psi_{23}(b_{1g}e_{2g}, {}^3E_{1g}, M=1, \mu_g) = |\gamma_g\nu_g|$$

$$\Psi_{24}(b_{1g}e_{2g}, {}^3E_{1g}, M=1, \eta_g) = |\gamma_g\xi_g|$$

b_{2g}e_{2g}

$$\boxed{\Delta E = \langle \zeta_g\xi_g || \zeta_g\xi_g \rangle - \langle \zeta_g\zeta_g || \xi_g\xi_g \rangle}$$

$$\Psi_{25}(b_{2g}e_{2g}, {}^3E_{1g}, M=-1, \eta_g) = |\overline{\zeta_g}\nu_g|$$

$$\Psi_{26}(b_{2g}e_{2g}, {}^3E_{1g}, M=-1, \mu_g) = -|\overline{\zeta_g}\xi_g|$$

$$\Psi_{27}(b_{2g}e_{2g}, {}^3E_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\zeta_g}\nu_g|}{2} + \frac{\sqrt{2}|\zeta_g\nu_g|}{2}$$

$$\Psi_{28}(b_{2g}e_{2g}, {}^3E_{1g}, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\zeta_g}\xi_g|}{2} - \frac{\sqrt{2}|\zeta_g\xi_g|}{2}$$

$$\Psi_{29}(b_{2g}e_{2g}, {}^3E_{1g}, M=1, \eta_g) = |\zeta_g\nu_g|$$

$$\Psi_{30}(b_{2g}e_{2g}, {}^3E_{1g}, M=1, \mu_g) = -|\zeta_g\xi_g|$$

b_{1u}e_{2u}

$$\boxed{\Delta E = -\langle \gamma_u\gamma_u || \xi_u\xi_u \rangle + \langle \gamma_u\xi_u || \gamma_u\xi_u \rangle}$$

$$\Psi_{31}(b_{1u}e_{2u}, {}^3E_{1g}, M=-1, \eta_g) = |\overline{\gamma_u}\nu_u|$$

$$\Psi_{32}(b_{1u}e_{2u}, {}^3E_{1g}, M=-1, \mu_g) = -|\overline{\gamma_u}\xi_u|$$

$$\Psi_{33}(b_{1u}e_{2u}, {}^3E_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\gamma_u}\nu_u|}{2} + \frac{\sqrt{2}|\gamma_u\nu_u|}{2}$$

$$\Psi_{34}(b_{1u}e_{2u}, {}^3E_{1g}, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\gamma_u}\xi_u|}{2} - \frac{\sqrt{2}|\gamma_u\xi_u|}{2}$$

$$\Psi_{35}(b_{1u}e_{2u}, {}^3E_{1g}, M=1, \eta_g) = |\gamma_u\nu_u|$$

$$\Psi_{36}(b_{1u}e_{2u}, {}^3E_{1g}, M=1, \mu_g) = -|\gamma_u\xi_u|$$

b_{2u}e_{2u}

$$\boxed{\Delta E = \langle \zeta_u\xi_u || \zeta_u\xi_u \rangle - \langle \zeta_u\zeta_u || \xi_u\xi_u \rangle}$$

$$\Psi_{37}(b_{2u}e_{2u}, {}^3E_{1g}, M=-1, \mu_g) = |\overline{\zeta_u}\nu_u|$$

$$\Psi_{38}(b_{2u}e_{2u}, {}^3E_{1g}, M=-1, \eta_g) = |\overline{\zeta_u}\xi_u|$$

$$\Psi_{39}(b_{2u}e_{2u}, {}^3E_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\zeta_u}\nu_u|}{2} + \frac{\sqrt{2}|\zeta_u\nu_u|}{2}$$

$$\Psi_{40}(b_{2u}e_{2u}, {}^3E_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\zeta_u}\xi_u|}{2} + \frac{\sqrt{2}|\zeta_u\xi_u|}{2}$$

$$\Psi_{41}(b_{2u}e_{2u}, {}^3E_{1g}, M=1, \mu_g) = |\zeta_u\nu_u|$$

$$\Psi_{42}(b_{2u}e_{2u}, {}^3E_{1g}, M=1, \eta_g) = |\zeta_u\xi_u|$$

a_{2g}e_{1g}

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \mu_g \mu_g \rangle + \langle \beta_g \mu_g || \beta_g \mu_g \rangle}$$

$$\Psi_{43}(a_{2g}e_{1g}, {}^3E_{1g}, M=-1, \mu_g) = -|\overline{\beta_g \eta_g}|$$

$$\Psi_{44}(a_{2g}e_{1g}, {}^3E_{1g}, M=-1, \eta_g) = |\overline{\beta_g \mu_g}|$$

$$\Psi_{45}(a_{2g}e_{1g}, {}^3E_{1g}, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\beta_g \eta_g}|}{2} - \frac{\sqrt{2}|\beta_g \overline{\eta_g}|}{2}$$

$$\Psi_{46}(a_{2g}e_{1g}, {}^3E_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\beta_g \mu_g}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\mu_g}|}{2}$$

$$\Psi_{47}(a_{2g}e_{1g}, {}^3E_{1g}, M=1, \mu_g) = -|\beta_g \eta_g|$$

$$\Psi_{48}(a_{2g}e_{1g}, {}^3E_{1g}, M=1, \eta_g) = |\beta_g \mu_g|$$

e_{1g}e_{2g}

$$\boxed{\Delta E = \langle \xi_g \mu_g || \nu_g \eta_g \rangle + \langle \xi_g \mu_g || \xi_g \mu_g \rangle - \langle \xi_g \xi_g || \eta_g \eta_g \rangle + \langle \xi_g \nu_g || \mu_g \eta_g \rangle}$$

$$\Psi_{49}(e_{1g}e_{2g}, {}^3E_{1g}, M=-1, \mu_g) = -\frac{\sqrt{2}|\overline{\nu_g \eta_g}|}{2} - \frac{\sqrt{2}|\overline{\xi_g \mu_g}|}{2}$$

$$\Psi_{50}(e_{1g}e_{2g}, {}^3E_{1g}, M=-1, \eta_g) = -\frac{\sqrt{2}|\overline{\nu_g \mu_g}|}{2} + \frac{\sqrt{2}|\overline{\xi_g \eta_g}|}{2}$$

$$\Psi_{51}(e_{1g}e_{2g}, {}^3E_{1g}, M=0, \mu_g) = -\frac{|\overline{\nu_g \eta_g}|}{2} - \frac{|\overline{\xi_g \mu_g}|}{2} - \frac{|\nu_g \overline{\eta_g}|}{2} - \frac{|\xi_g \overline{\mu_g}|}{2}$$

$$\Psi_{52}(e_{1g}e_{2g}, {}^3E_{1g}, M=0, \eta_g) = -\frac{|\overline{\nu_g \mu_g}|}{2} + \frac{|\overline{\xi_g \eta_g}|}{2} - \frac{|\nu_g \overline{\mu_g}|}{2} + \frac{|\xi_g \overline{\eta_g}|}{2}$$

$$\Psi_{53}(e_{1g}e_{2g}, {}^3E_{1g}, M=1, \mu_g) = -\frac{\sqrt{2}|\nu_g \eta_g|}{2} - \frac{\sqrt{2}|\xi_g \mu_g|}{2}$$

$$\Psi_{54}(e_{1g}e_{2g}, {}^3E_{1g}, M=1, \eta_g) = -\frac{\sqrt{2}|\nu_g \mu_g|}{2} + \frac{\sqrt{2}|\xi_g \eta_g|}{2}$$

e_{1u}e_{2u}

$$\boxed{\Delta E = -\langle \mu_u \mu_u || \nu_u \nu_u \rangle + \langle \mu_u \xi_u || \eta_u \nu_u \rangle + \langle \mu_u \xi_u || \mu_u \xi_u \rangle + \langle \mu_u \eta_u || \xi_u \nu_u \rangle}$$

$$\Psi_{55}(e_{1u}e_{2u}, {}^3E_{1g}, M=-1, \mu_g) = \frac{\sqrt{2}|\overline{\eta_u \nu_u}|}{2} + \frac{\sqrt{2}|\overline{\mu_u \xi_u}|}{2}$$

$$\Psi_{56}(e_{1u}e_{2u}, {}^3E_{1g}, M=-1, \eta_g) = -\frac{\sqrt{2}|\overline{\eta_u \xi_u}|}{2} + \frac{\sqrt{2}|\overline{\mu_u \nu_u}|}{2}$$

$$\Psi_{57}(e_{1u}e_{2u}, {}^3E_{1g}, M=0, \mu_g) = -\frac{|\overline{\eta_u \nu_u}|}{2} + \frac{|\overline{\mu_u \xi_u}|}{2} + \frac{|\eta_u \overline{\nu_u}|}{2} + \frac{|\mu_u \overline{\xi_u}|}{2}$$

$$\Psi_{58}(e_{1u}e_{2u}, {}^3E_{1g}, M=0, \eta_g) = -\frac{|\overline{\eta_u \xi_u}|}{2} + \frac{|\overline{\mu_u \nu_u}|}{2} - \frac{|\eta_u \overline{\xi_u}|}{2} + \frac{|\mu_u \overline{\nu_u}|}{2}$$

$$\Psi_{59}(e_{1u}e_{2u}, {}^3E_{1g}, M=1, \mu_g) = \frac{\sqrt{2}|\eta_u \nu_u|}{2} + \frac{\sqrt{2}|\mu_u \xi_u|}{2}$$

$$\Psi_{60}(e_{1u}e_{2u}, {}^3E_{1g}, M=1, \eta_g) = -\frac{\sqrt{2}|\eta_u \xi_u|}{2} + \frac{\sqrt{2}|\mu_u \nu_u|}{2}$$

2.27.21 ${}^1E_{1g}$

a_{1g}e_{1g}

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \mu_g \mu_g \rangle + \langle \alpha_g \mu_g || \alpha_g \mu_g \rangle}$$

$$\Psi_1(a_{1g}e_{1g}, {}^1E_{1g}, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\alpha_g \eta_g}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\eta_g}|}{2}$$

$$\Psi_2(a_{1g}e_{1g}, {}^1E_{1g}, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\alpha_g \mu_g}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\mu_g}|}{2}$$

a_{2u}e_{1u}

$$\boxed{\Delta E = \langle \beta_u \beta_u || \mu_u \mu_u \rangle + \langle \beta_u \mu_u || \beta_u \mu_u \rangle}$$

$$\Psi_3(a_{2u}e_{1u}, {}^1E_{1g}, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\beta_u \eta_u}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\eta_u}|}{2}$$

$$\Psi_4(a_{2u}e_{1u}, {}^1E_{1g}, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\beta_u \mu_u}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\mu_u}|}{2}$$

a_{1u}e_{1u}

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \mu_u \mu_u \rangle + \langle \alpha_u \mu_u || \alpha_u \mu_u \rangle}$$

$$\Psi_5(a_{1u}e_{1u}, {}^1E_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\alpha_u \eta_u}|}{2} - \frac{\sqrt{2}|\alpha_u \overline{\eta_u}|}{2}$$

$$\Psi_6(a_{1u}e_{1u}, {}^1E_{1g}, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\alpha_u \mu_u}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\mu_u}|}{2}$$

b_{1g}e_{2g}

$$\boxed{\Delta E = \langle \gamma_g \gamma_g || \xi_g \xi_g \rangle + \langle \gamma_g \xi_g || \gamma_g \xi_g \rangle}$$

$$\Psi_7(b_{1g}e_{2g}, {}^1E_{1g}, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\gamma_g \nu_g}|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\nu_g}|}{2}$$

$$\Psi_8(b_{1g}e_{2g}, {}^1E_{1g}, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\gamma_g \xi_g}|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\xi_g}|}{2}$$

b_{2g}e_{2g}

$$\boxed{\Delta E = \langle \zeta_g \xi_g || \zeta_g \xi_g \rangle + \langle \zeta_g \zeta_g || \xi_g \xi_g \rangle}$$

$$\Psi_9(b_{2g}e_{2g}, {}^1E_{1g}, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\zeta_g \nu_g}|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\nu_g}|}{2}$$

$$\Psi_{10}(b_{2g}e_{2g}, {}^1E_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\zeta_g \xi_g}|}{2} - \frac{\sqrt{2}|\zeta_g \overline{\xi_g}|}{2}$$

b_{1u}e_{2u}

$$\boxed{\Delta E = \langle \gamma_u \gamma_u || \xi_u \xi_u \rangle + \langle \gamma_u \xi_u || \gamma_u \xi_u \rangle}$$

$$\Psi_{11}(b_{1u}e_{2u}, {}^1E_{1g}, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\gamma_u \nu_u}|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\nu_u}|}{2}$$

$$\Psi_{12}(b_{1u}e_{2u}, {}^1E_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\gamma_u \xi_u}|}{2} - \frac{\sqrt{2}|\gamma_u \overline{\xi_u}|}{2}$$

b_{2u}e_{2u}

$$\boxed{\Delta E = \langle \zeta_u \xi_u || \zeta_u \xi_u \rangle + \langle \zeta_u \zeta_u || \xi_u \xi_u \rangle}$$

$$\Psi_{13}(b_{2u}e_{2u}, {}^1E_{1g}, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\zeta_u \nu_u}|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\nu_u}|}{2}$$

$$\Psi_{14}(b_{2u}e_{2u}, {}^1E_{1g}, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\zeta_u \xi_u}|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\xi_u}|}{2}$$

a_{2g}e_{1g}

$$\boxed{\Delta E = \langle \beta_g \beta_g || \mu_g \mu_g \rangle + \langle \beta_g \mu_g || \beta_g \mu_g \rangle}$$

$$\Psi_{15}(a_{2g}e_{1g}, {}^1E_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\beta_g \eta_g}|}{2} - \frac{\sqrt{2}|\beta_g \overline{\eta_g}|}{2}$$

$$\Psi_{16}(a_{2g}e_{1g}, {}^1E_{1g}, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\beta_g \mu_g}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\mu_g}|}{2}$$

$e_{1g}e_{2g}$

$$\Delta E = \langle \xi_g \mu_g | \nu_g \eta_g \rangle + \langle \xi_g \mu_g | \xi_g \mu_g \rangle + \langle \xi_g \xi_g | \eta_g \eta_g \rangle - \langle \xi_g \nu_g | \mu_g \eta_g \rangle$$

$$\Psi_{17}(e_{1g}e_{2g}, {}^1E_{1g}, M=0, \mu_g) = \frac{|\nu_g \eta_g|}{2} + \frac{|\xi_g \mu_g|}{2} - \frac{|\nu_g \eta_g|}{2} - \frac{|\xi_g \mu_g|}{2}$$

$$\Psi_{18}(e_{1g}e_{2g}, {}^1E_{1g}, M=0, \eta_g) = \frac{|\nu_g \mu_g|}{2} - \frac{|\xi_g \eta_g|}{2} - \frac{|\nu_g \mu_g|}{2} + \frac{|\xi_g \eta_g|}{2}$$

 $e_{1u}e_{2u}$

$$\Delta E = \langle \mu_u \mu_u | \nu_u \nu_u \rangle + \langle \mu_u \xi_u | \eta_u \nu_u \rangle + \langle \mu_u \xi_u | \mu_u \xi_u \rangle - \langle \mu_u \eta_u | \xi_u \nu_u \rangle$$

$$\Psi_{19}(e_{1u}e_{2u}, {}^1E_{1g}, M=0, \mu_g) = -\frac{|\eta_u \nu_u|}{2} - \frac{|\mu_u \xi_u|}{2} + \frac{|\eta_u \nu_u|}{2} + \frac{|\mu_u \xi_u|}{2}$$

$$\Psi_{20}(e_{1u}e_{2u}, {}^1E_{1g}, M=0, \eta_g) = \frac{|\eta_u \xi_u|}{2} - \frac{|\mu_u \nu_u|}{2} - \frac{|\eta_u \xi_u|}{2} + \frac{|\mu_u \nu_u|}{2}$$

2.27.22 ${}^3E_{2u}$ $a_{1g}e_{2u}$

$$\Delta E = -\langle \alpha_g \alpha_g | \xi_u \xi_u \rangle + \langle \alpha_g \xi_u | \alpha_g \xi_u \rangle$$

$$\Psi_1(a_{1g}e_{2u}, {}^3E_{2u}, M=-1, \nu_u) = |\overline{\alpha_g \nu_u}|$$

$$\Psi_2(a_{1g}e_{2u}, {}^3E_{2u}, M=-1, \xi_u) = |\overline{\alpha_g \xi_u}|$$

$$\Psi_3(a_{1g}e_{2u}, {}^3E_{2u}, M=0, \nu_u) = \frac{\sqrt{2}|\overline{\alpha_g \nu_u}|}{2} + \frac{\sqrt{2}|\overline{\alpha_g \nu_u}|}{2}$$

$$\Psi_4(a_{1g}e_{2u}, {}^3E_{2u}, M=0, \xi_u) = \frac{\sqrt{2}|\overline{\alpha_g \xi_u}|}{2} + \frac{\sqrt{2}|\overline{\alpha_g \xi_u}|}{2}$$

$$\Psi_5(a_{1g}e_{2u}, {}^3E_{2u}, M=1, \nu_u) = |\alpha_g \nu_u|$$

$$\Psi_6(a_{1g}e_{2u}, {}^3E_{2u}, M=1, \xi_u) = |\alpha_g \xi_u|$$

 $a_{2u}e_{2g}$

$$\Delta E = -\langle \beta_u \beta_u | \xi_g \xi_g \rangle + \langle \beta_u \xi_g | \beta_u \xi_g \rangle$$

$$\Psi_7(a_{2u}e_{2g}, {}^3E_{2u}, M=-1, \nu_u) = |\overline{\beta_u \nu_g}|$$

$$\Psi_8(a_{2u}e_{2g}, {}^3E_{2u}, M=-1, \xi_u) = |\overline{\beta_u \xi_g}|$$

$$\Psi_9(a_{2u}e_{2g}, {}^3E_{2u}, M=0, \nu_u) = \frac{\sqrt{2}|\overline{\beta_u \nu_g}|}{2} + \frac{\sqrt{2}|\overline{\beta_u \nu_g}|}{2}$$

$$\Psi_{10}(a_{2u}e_{2g}, {}^3E_{2u}, M=0, \xi_u) = \frac{\sqrt{2}|\overline{\beta_u \xi_g}|}{2} + \frac{\sqrt{2}|\overline{\beta_u \xi_g}|}{2}$$

$$\Psi_{11}(a_{2u}e_{2g}, {}^3E_{2u}, M=1, \nu_u) = |\beta_u \nu_g|$$

$$\Psi_{12}(a_{2u}e_{2g}, {}^3E_{2u}, M=1, \xi_u) = |\beta_u \xi_g|$$

 $a_{1u}e_{2g}$

$$\Delta E = -\langle \alpha_u \alpha_u | \xi_g \xi_g \rangle + \langle \alpha_u \xi_g | \alpha_u \xi_g \rangle$$

$$\Psi_{13}(a_{1u}e_{2g}, {}^3E_{2u}, M=-1, \xi_u) = -|\overline{\alpha_u \nu_g}|$$

$$\Psi_{14}(a_{1u}e_{2g}, {}^3E_{2u}, M=-1, \nu_u) = |\overline{\alpha_u \xi_g}|$$

$$\Psi_{15}(a_{1u}e_{2g}, {}^3E_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\alpha_u \nu_g}|}{2} - \frac{\sqrt{2}|\overline{\alpha_u \nu_g}|}{2}$$

$$\Psi_{16}(a_{1u}e_{2g}, {}^3E_{2u}, M=0, \nu_u) = \frac{\sqrt{2}|\overline{\alpha_u \xi_g}|}{2} + \frac{\sqrt{2}|\overline{\alpha_u \xi_g}|}{2}$$

$$\Psi_{17}(a_{1u}e_{2g}, {}^3E_{2u}, M=1, \xi_u) = -|\alpha_u \nu_g|$$

$$\Psi_{18}(a_{1u}e_{2g}, {}^3E_{2u}, M=1, \nu_u) = |\alpha_u \xi_g|$$

 $b_{1g}e_{1u}$

$$\boxed{\Delta E = -\langle \gamma_g \gamma_g | \mu_u \mu_u \rangle + \langle \gamma_g \mu_u | \gamma_g \mu_u \rangle}$$

$$\Psi_{19}(b_{1g}e_{1u}, {}^3E_{2u}, M=-1, \xi_u) = |\overline{\gamma_g \eta_u}|$$

$$\Psi_{20}(b_{1g}e_{1u}, {}^3E_{2u}, M=-1, \nu_u) = |\overline{\gamma_g \mu_u}|$$

$$\Psi_{21}(b_{1g}e_{1u}, {}^3E_{2u}, M=0, \xi_u) = \frac{\sqrt{2}|\overline{\gamma_g \eta_u}|}{2} + \frac{\sqrt{2}|\overline{\gamma_g \eta_u}|}{2}$$

$$\Psi_{22}(b_{1g}e_{1u}, {}^3E_{2u}, M=0, \nu_u) = \frac{\sqrt{2}|\overline{\gamma_g \mu_u}|}{2} + \frac{\sqrt{2}|\overline{\gamma_g \mu_u}|}{2}$$

$$\Psi_{23}(b_{1g}e_{1u}, {}^3E_{2u}, M=1, \xi_u) = |\gamma_g \eta_u|$$

$$\Psi_{24}(b_{1g}e_{1u}, {}^3E_{2u}, M=1, \nu_u) = |\gamma_g \mu_u|$$

 $b_{2g}e_{1u}$

$$\boxed{\Delta E = \langle \zeta_g \mu_u | \zeta_g \mu_u \rangle - \langle \zeta_g \zeta_g | \mu_u \mu_u \rangle}$$

$$\Psi_{25}(b_{2g}e_{1u}, {}^3E_{2u}, M=-1, \nu_u) = |\overline{\zeta_g \eta_u}|$$

$$\Psi_{26}(b_{2g}e_{1u}, {}^3E_{2u}, M=-1, \xi_u) = -|\overline{\zeta_g \mu_u}|$$

$$\Psi_{27}(b_{2g}e_{1u}, {}^3E_{2u}, M=0, \nu_u) = \frac{\sqrt{2}|\overline{\zeta_g \eta_u}|}{2} + \frac{\sqrt{2}|\overline{\zeta_g \eta_u}|}{2}$$

$$\Psi_{28}(b_{2g}e_{1u}, {}^3E_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\zeta_g \mu_u}|}{2} - \frac{\sqrt{2}|\overline{\zeta_g \mu_u}|}{2}$$

$$\Psi_{29}(b_{2g}e_{1u}, {}^3E_{2u}, M=1, \nu_u) = |\zeta_g \eta_u|$$

$$\Psi_{30}(b_{2g}e_{1u}, {}^3E_{2u}, M=1, \xi_u) = -|\zeta_g \mu_u|$$

 $b_{1u}e_{1g}$

$$\boxed{\Delta E = -\langle \gamma_u \gamma_u | \mu_g \mu_g \rangle + \langle \gamma_u \mu_g | \gamma_u \mu_g \rangle}$$

$$\Psi_{31}(b_{1u}e_{1g}, {}^3E_{2u}, M=-1, \nu_u) = |\overline{\gamma_u \eta_g}|$$

$$\Psi_{32}(b_{1u}e_{1g}, {}^3E_{2u}, M=-1, \xi_u) = -|\overline{\gamma_u \mu_g}|$$

$$\Psi_{33}(b_{1u}e_{1g}, {}^3E_{2u}, M=0, \nu_u) = \frac{\sqrt{2}|\overline{\gamma_u \eta_g}|}{2} + \frac{\sqrt{2}|\overline{\gamma_u \eta_g}|}{2}$$

$$\Psi_{34}(b_{1u}e_{1g}, {}^3E_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\gamma_u \mu_g}|}{2} - \frac{\sqrt{2}|\overline{\gamma_u \mu_g}|}{2}$$

$$\Psi_{35}(b_{1u}e_{1g}, {}^3E_{2u}, M=1, \nu_u) = |\gamma_u \eta_g|$$

$$\Psi_{36}(b_{1u}e_{1g}, {}^3E_{2u}, M=1, \xi_u) = -|\gamma_u \mu_g|$$

 $b_{2u}e_{1g}$

$$\boxed{\Delta E = \langle \zeta_u \mu_g | \zeta_u \mu_g \rangle - \langle \zeta_u \zeta_u | \mu_g \mu_g \rangle}$$

$$\Psi_{37}(b_{2u}e_{1g}, {}^3E_{2u}, M=-1, \xi_u) = |\overline{\zeta_u \eta_g}|$$

$$\Psi_{38}(b_{2u}e_{1g}, {}^3E_{2u}, M=-1, \nu_u) = |\overline{\zeta_u \mu_g}|$$

$$\Psi_{39}(b_{2u}e_{1g}, {}^3E_{2u}, M=0, \xi_u) = \frac{\sqrt{2}|\overline{\zeta_u \eta_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \eta_g}|}{2}$$

$$\Psi_{40}(b_{2u}e_{1g}, {}^3E_{2u}, M=0, \nu_u) = \frac{\sqrt{2}|\overline{\zeta_u \mu_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \mu_g}|}{2}$$

$$\Psi_{41}(b_{2u}e_{1g}, {}^3E_{2u}, M=1, \xi_u) = |\zeta_u \eta_g|$$

$$\Psi_{42}(b_{2u}e_{1g}, {}^3E_{2u}, M=1, \nu_u) = |\zeta_u \mu_g|$$

a_{2g}e_{2u}

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \xi_u \xi_u \rangle + \langle \beta_g \xi_u || \beta_g \xi_u \rangle}$$

$$\Psi_{43}(a_{2g}e_{2u}, {}^3E_{2u}, M=-1, \xi_u) = -|\overline{\beta_g} \overline{\nu_u}|$$

$$\Psi_{44}(a_{2g}e_{2u}, {}^3E_{2u}, M=-1, \nu_u) = |\overline{\beta_g} \overline{\xi_u}|$$

$$\Psi_{45}(a_{2g}e_{2u}, {}^3E_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\beta_g} \nu_u|}{2} - \frac{\sqrt{2}|\beta_g \overline{\nu_u}|}{2}$$

$$\Psi_{46}(a_{2g}e_{2u}, {}^3E_{2u}, M=0, \nu_u) = \frac{\sqrt{2}|\overline{\beta_g} \xi_u|}{2} + \frac{\sqrt{2}|\beta_g \overline{\xi_u}|}{2}$$

$$\Psi_{47}(a_{2g}e_{2u}, {}^3E_{2u}, M=1, \xi_u) = -|\beta_g \nu_u|$$

$$\Psi_{48}(a_{2g}e_{2u}, {}^3E_{2u}, M=1, \nu_u) = |\beta_g \xi_u|$$

e_{2g}e_{2u}

$$\boxed{\Delta E = -\langle \xi_g \xi_g || \nu_u \nu_u \rangle - \langle \xi_g \xi_u || \nu_g \nu_u \rangle + \langle \xi_g \xi_u || \xi_g \xi_u \rangle - \langle \xi_g \nu_g || \xi_u \nu_u \rangle}$$

$$\Psi_{49}(e_{2g}e_{2u}, {}^3E_{2u}, M=-1, \xi_u) = \frac{\sqrt{2}|\overline{\nu_g} \overline{\nu_u}|}{2} - \frac{\sqrt{2}|\overline{\xi_g} \overline{\xi_u}|}{2}$$

$$\Psi_{50}(e_{2g}e_{2u}, {}^3E_{2u}, M=-1, \nu_u) = \frac{\sqrt{2}|\overline{\nu_g} \overline{\xi_u}|}{2} + \frac{\sqrt{2}|\overline{\xi_g} \overline{\nu_u}|}{2}$$

$$\Psi_{51}(e_{2g}e_{2u}, {}^3E_{2u}, M=0, \xi_u) = \frac{|\overline{\nu_g} \nu_u|}{2} - \frac{|\overline{\xi_g} \xi_u|}{2} + \frac{|\nu_g \overline{\nu_u}|}{2} - \frac{|\xi_g \overline{\xi_u}|}{2}$$

$$\Psi_{52}(e_{2g}e_{2u}, {}^3E_{2u}, M=0, \nu_u) = \frac{|\overline{\nu_g} \xi_u|}{2} + \frac{|\overline{\xi_g} \nu_u|}{2} + \frac{|\nu_g \overline{\xi_u}|}{2} + \frac{|\xi_g \overline{\nu_u}|}{2}$$

$$\Psi_{53}(e_{2g}e_{2u}, {}^3E_{2u}, M=1, \xi_u) = \frac{\sqrt{2}|\nu_g \nu_u|}{2} - \frac{\sqrt{2}|\xi_g \xi_u|}{2}$$

$$\Psi_{54}(e_{2g}e_{2u}, {}^3E_{2u}, M=1, \nu_u) = \frac{\sqrt{2}|\nu_g \xi_u|}{2} + \frac{\sqrt{2}|\xi_g \nu_u|}{2}$$

e_{1g}e_{1u}

$$\boxed{\Delta E = -\langle \mu_u \eta_u || \mu_g \eta_g \rangle - \langle \mu_u \mu_g || \eta_u \eta_g \rangle + \langle \mu_u \mu_g || \mu_u \mu_g \rangle - \langle \mu_u \mu_u || \eta_g \eta_g \rangle}$$

$$\Psi_{55}(e_{1g}e_{1u}, {}^3E_{2u}, M=-1, \xi_u) = -\frac{\sqrt{2}|\eta_u \eta_g|}{2} + \frac{\sqrt{2}|\mu_u \mu_g|}{2}$$

$$\Psi_{56}(e_{1g}e_{1u}, {}^3E_{2u}, M=-1, \nu_u) = \frac{\sqrt{2}|\eta_u \mu_g|}{2} + \frac{\sqrt{2}|\mu_u \eta_g|}{2}$$

$$\Psi_{57}(e_{1g}e_{1u}, {}^3E_{2u}, M=0, \xi_u) = -\frac{|\eta_u \eta_g|}{2} + \frac{|\mu_u \mu_g|}{2} - \frac{|\eta_u \overline{\eta_g}|}{2} + \frac{|\mu_u \overline{\mu_g}|}{2}$$

$$\Psi_{58}(e_{1g}e_{1u}, {}^3E_{2u}, M=0, \nu_u) = \frac{|\eta_u \mu_g|}{2} + \frac{|\mu_u \eta_g|}{2} + \frac{|\eta_u \overline{\mu_g}|}{2} + \frac{|\mu_u \overline{\eta_g}|}{2}$$

$$\Psi_{59}(e_{1g}e_{1u}, {}^3E_{2u}, M=1, \xi_u) = -\frac{\sqrt{2}|\eta_u \eta_g|}{2} + \frac{\sqrt{2}|\mu_u \mu_g|}{2}$$

$$\Psi_{60}(e_{1g}e_{1u}, {}^3E_{2u}, M=1, \nu_u) = \frac{\sqrt{2}|\eta_u \mu_g|}{2} + \frac{\sqrt{2}|\mu_u \eta_g|}{2}$$

2.27.23 ${}^1E_{2u}$ *a_{1g}e_{2u}*

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \xi_u \xi_u \rangle + \langle \alpha_g \xi_u || \alpha_g \xi_u \rangle}$$

$$\Psi_1(a_{1g}e_{2u}, {}^1E_{2u}, M=0, \nu_u) = -\frac{\sqrt{2}|\overline{\alpha_g} \nu_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\nu_u}|}{2}$$

$$\Psi_2(a_{1g}e_{2u}, {}^1E_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\alpha_g} \xi_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\xi_u}|}{2}$$

a_{2u}e_{2g}

$$\boxed{\Delta E = \langle \beta_u \beta_u || \xi_g \xi_g \rangle + \langle \beta_u \xi_g || \beta_u \xi_g \rangle}$$

$$\Psi_3(a_{2u}e_{2g}, {}^1E_{2u}, M=0, \nu_u) = -\frac{\sqrt{2}|\overline{\beta_u} \nu_g|}{2} + \frac{\sqrt{2}|\beta_u \overline{\nu_g}|}{2}$$

$$\Psi_4(a_{2u}e_{2g}, {}^1E_{2u}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\beta_u} \xi_g|}{2} + \frac{\sqrt{2}|\beta_u \overline{\xi_g}|}{2}$$

a_{1u}e_{2g}

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \xi_g \xi_g \rangle + \langle \alpha_u \xi_g || \alpha_u \xi_g \rangle}$$

$$\Psi_5(a_{1u}e_{2g}, {}^1E_{2u}, M=0, \xi_u) = \frac{\sqrt{2}|\overline{\alpha_u} \nu_g|}{2} - \frac{\sqrt{2}|\alpha_u \overline{\nu_g}|}{2}$$

$$\Psi_6(a_{1u}e_{2g}, {}^1E_{2u}, M=0, \nu_u) = -\frac{\sqrt{2}|\overline{\alpha_u} \xi_g|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\xi_g}|}{2}$$

b_{1g}e_{1u}

$$\boxed{\Delta E = \langle \gamma_g \gamma_g || \mu_u \mu_u \rangle + \langle \gamma_g \mu_u || \gamma_g \mu_u \rangle}$$

$$\Psi_7(b_{1g}e_{1u}, {}^1E_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\gamma_g} \eta_u|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\eta_u}|}{2}$$

$$\Psi_8(b_{1g}e_{1u}, {}^1E_{2u}, M=0, \nu_u) = -\frac{\sqrt{2}|\overline{\gamma_g} \mu_u|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\mu_u}|}{2}$$

b_{2g}e_{1u}

$$\boxed{\Delta E = \langle \zeta_g \mu_u || \zeta_g \mu_u \rangle + \langle \zeta_g \zeta_g || \mu_u \mu_u \rangle}$$

$$\Psi_9(b_{2g}e_{1u}, {}^1E_{2u}, M=0, \nu_u) = -\frac{\sqrt{2}|\overline{\zeta_g} \eta_u|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\eta_u}|}{2}$$

$$\Psi_{10}(b_{2g}e_{1u}, {}^1E_{2u}, M=0, \xi_u) = \frac{\sqrt{2}|\overline{\zeta_g} \mu_u|}{2} - \frac{\sqrt{2}|\zeta_g \overline{\mu_u}|}{2}$$

b_{1u}e_{1g}

$$\boxed{\Delta E = \langle \gamma_u \gamma_u || \mu_g \mu_g \rangle + \langle \gamma_u \mu_g || \gamma_u \mu_g \rangle}$$

$$\Psi_{11}(b_{1u}e_{1g}, {}^1E_{2u}, M=0, \nu_u) = -\frac{\sqrt{2}|\overline{\gamma_u} \eta_g|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\eta_g}|}{2}$$

$$\Psi_{12}(b_{1u}e_{1g}, {}^1E_{2u}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\gamma_u} \mu_g|}{2} - \frac{\sqrt{2}|\gamma_u \overline{\mu_g}|}{2}$$

b_{2u}e_{1g}

$$\boxed{\Delta E = \langle \zeta_u \mu_g || \zeta_u \mu_g \rangle + \langle \zeta_u \zeta_u || \mu_g \mu_g \rangle}$$

$$\Psi_{13}(b_{2u}e_{1g}, {}^1E_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\zeta_u} \eta_g|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\eta_g}|}{2}$$

$$\Psi_{14}(b_{2u}e_{1g}, {}^1E_{2u}, M=0, \nu_g) = -\frac{\sqrt{2}|\overline{\zeta_u} \mu_g|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\mu_g}|}{2}$$

a_{2g}e_{2u}

$$\boxed{\Delta E = \langle \beta_g \beta_g || \xi_u \xi_u \rangle + \langle \beta_g \xi_u || \beta_g \xi_u \rangle}$$

$$\Psi_{15}(a_{2g}e_{2u}, {}^1E_{2u}, M=0, \xi_u) = \frac{\sqrt{2}|\beta_g\nu_u|}{2} - \frac{\sqrt{2}|\beta_g\bar{\nu}_u|}{2} - \frac{|\bar{\nu}_g\xi_u|}{2} - \frac{|\xi_g\nu_u|}{2} + \frac{|\nu_g\bar{\xi}_u|}{2} + \frac{|\xi_g\bar{\nu}_u|}{2}$$

$$\Psi_{16}(a_{2g}e_{2u}, {}^1E_{2u}, M=0, \nu_u) = -\frac{\sqrt{2}|\beta_g\xi_u|}{2} + \frac{\sqrt{2}|\beta_g\bar{\xi}_u|}{2} \quad e_{1g}e_{1u}$$

$$e_{2g}e_{2u}$$

$$\boxed{\Delta E = \langle \xi_g\xi_g || \nu_u\nu_u \rangle - \langle \xi_g\xi_u || \nu_g\nu_u \rangle + \langle \xi_g\xi_u || \xi_g\xi_u \rangle + \langle \xi_g\nu_g || \xi_u\nu_u \rangle}$$

$$\Psi_{17}(e_{2g}e_{2u}, {}^1E_{2u}, M=0, \xi_u) = -\frac{|\bar{\nu}_g\nu_u|}{2} + \frac{|\bar{\xi}_g\xi_u|}{2} + \frac{|\nu_g\bar{\nu}_u|}{2} - \frac{|\xi_g\bar{\xi}_u|}{2}$$

$$\Psi_{18}(e_{2g}e_{2u}, {}^1E_{2u}, M=0, \nu_u) =$$

$$\boxed{\Delta E = \langle \mu_u\eta_u || \mu_g\eta_g \rangle - \langle \mu_u\mu_g || \eta_u\eta_g \rangle + \langle \mu_u\mu_g || \mu_u\mu_g \rangle + \langle \mu_u\mu_u || \eta_g\eta_g \rangle}$$

$$\Psi_{19}(e_{1g}e_{1u}, {}^1E_{2u}, M=0, \xi_u) = \frac{|\bar{\eta}_u\eta_g|}{2} - \frac{|\bar{\mu}_u\mu_g|}{2} - \frac{|\eta_u\bar{\eta}_g|}{2} + \frac{|\mu_u\bar{\mu}_g|}{2}$$

$$\Psi_{20}(e_{1g}e_{1u}, {}^1E_{2u}, M=0, \nu_u) = -\frac{|\bar{\eta}_u\mu_g|}{2} - \frac{|\bar{\mu}_u\eta_g|}{2} + \frac{|\eta_u\bar{\mu}_g|}{2} + \frac{|\mu_u\bar{\eta}_g|}{2}$$

2.28 Group T

Component labels

$$A : \{\alpha\} \longrightarrow E^1 : \{\beta\} \longrightarrow E^2 : \{\gamma\} \longrightarrow T : \{\zeta, \eta, \mu\}$$

2.28.3 ${}^1E^1$

2.28.1 1A

a^2

$$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$$

ae^1

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae^1, {}^1E^1, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$(e^2)^2$

$$\boxed{\Delta E = 0}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2((e^2)^2, {}^1E^1, M=0, \beta) = -|\bar{\gamma}\gamma|$$

t^2

t^2

$$\boxed{\Delta E = 3 \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(e^1e^2, {}^1A, M=0, \alpha) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_3(t^2, {}^1A, M=0, \alpha) = -\frac{\sqrt{3}|\bar{\eta}\eta|}{3} - \frac{\sqrt{3}|\bar{\mu}\mu|}{3} - \frac{\sqrt{3}|\bar{\zeta}\zeta|}{3}$$

$$\Psi_3(t^2, {}^1E^1, M=0, \beta) = \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\bar{\eta}\eta| - \frac{\sqrt{3}|\bar{\mu}\mu|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\zeta}\zeta|$$

2.28.2 ${}^3E^1$

ae^1

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae^1, {}^3E^1, M=-1, \beta) = |\bar{\alpha}\bar{\beta}|$$

ae^2

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae^2, {}^3E^1, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

$$\Psi_2(ae^1, {}^3E^1, M=0, \beta) = \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

$$\Psi_2(ae^2, {}^3E^1, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(ae^1, {}^3E^1, M=1, \beta) = |\alpha\beta|$$

$$\Psi_3(ae^2, {}^3E^1, M=1, \gamma) = |\alpha\gamma|$$

2.28.4 ${}^3E^2$

ae^2

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae^2, {}^3E^2, M=-1, \gamma) = |\bar{\alpha}\gamma|$$

$$\Psi_2(ae^2, {}^3E^2, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_3(ae^2, {}^3E^2, M=1, \gamma) = |\alpha\gamma|$$

2.28.5 $^1E^2$ ae^2

$$\boxed{\Delta E = 0}$$

$$\Psi_1(ae^2, ^1E^2, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

 $(e^1)^2$

$$\boxed{\Delta E = 0}$$

$$\Psi_2((e^1)^2, ^1E^2, M=0, \gamma) = -|\bar{\beta}\beta|$$

 t^2

$$\boxed{\Delta E = 0}$$

$$\begin{aligned} \Psi_3(t^2, ^1E^2, M=0, \gamma) &= \\ \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\bar{\eta}\eta| - \frac{\sqrt{3}|\bar{\mu}\mu|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\bar{\zeta}\zeta| \end{aligned}$$

2.28.6 3T *at*

$$\boxed{\Delta E = -\langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(at, ^3T, M=-1, \zeta) = |\bar{\alpha}\zeta|$$

$$\Psi_2(at, ^3T, M=-1, \eta) = |\bar{\alpha}\eta|$$

$$\Psi_3(at, ^3T, M=-1, \mu) = |\bar{\alpha}\mu|$$

$$\Psi_4(at, ^3T, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_5(at, ^3T, M=0, \eta) = \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_6(at, ^3T, M=0, \mu) = \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_7(at, ^3T, M=1, \zeta) = |\alpha\zeta|$$

$$\Psi_8(at, ^3T, M=1, \eta) = |\alpha\eta|$$

$$\Psi_9(at, ^3T, M=1, \mu) = |\alpha\mu|$$

 e^1t

$$\boxed{\Delta E = \langle \beta\zeta || \beta\zeta \rangle}$$

$$\Psi_{10}(e^1t, ^3T, M=-1, \zeta) = |\bar{\beta}\zeta|$$

$$\Psi_{11}(e^1t, ^3T, M=-1, \eta) = \frac{i(\sqrt{3}+i)|\bar{\beta}\eta|}{2}$$

$$\Psi_{12}(e^1t, ^3T, M=-1, \mu) = -\frac{i(\sqrt{3}-i)|\bar{\beta}\mu|}{2}$$

$$\Psi_{13}(e^1t, ^3T, M=0, \zeta) = \frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

$$\Psi_{14}(e^1t, ^3T, M=0, \eta) = \frac{\sqrt{2}i(\sqrt{3}+i)|\bar{\beta}\eta|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\beta\bar{\eta}|}{4}$$

$$\begin{aligned} \Psi_{15}(e^1t, ^3T, M=0, \mu) &= \\ -\frac{\sqrt{2}i(\sqrt{3}-i)|\bar{\beta}\mu|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\beta\bar{\mu}|}{4} \end{aligned}$$

$$\Psi_{16}(e^1t, ^3T, M=1, \zeta) = |\beta\zeta|$$

$$\Psi_{17}(e^1t, ^3T, M=1, \eta) = \frac{i(\sqrt{3}+i)|\beta\eta|}{2}$$

$$\Psi_{18}(e^1t, ^3T, M=1, \mu) = -\frac{i(\sqrt{3}-i)|\beta\mu|}{2}$$

 e^2t

$$\boxed{\Delta E = \langle \gamma\zeta || \gamma\zeta \rangle}$$

$$\Psi_{19}(e^2t, ^3T, M=-1, \zeta) = |\bar{\gamma}\zeta|$$

$$\Psi_{20}(e^2t, ^3T, M=-1, \eta) = -\frac{i(\sqrt{3}-i)|\bar{\gamma}\eta|}{2}$$

$$\Psi_{21}(e^2t, ^3T, M=-1, \mu) = \frac{i(\sqrt{3}+i)|\bar{\gamma}\mu|}{2}$$

$$\Psi_{22}(e^2t, ^3T, M=0, \zeta) = \frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\gamma\bar{\zeta}|}{2}$$

$$\begin{aligned} \Psi_{23}(e^2t, ^3T, M=0, \eta) &= \\ -\frac{\sqrt{2}i(\sqrt{3}-i)|\bar{\gamma}\eta|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\gamma\bar{\eta}|}{4} \end{aligned}$$

$$\Psi_{24}(e^2t, ^3T, M=0, \mu) = \frac{\sqrt{2}i(\sqrt{3}+i)|\bar{\gamma}\mu|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\gamma\bar{\mu}|}{4}$$

$$\Psi_{25}(e^2t, ^3T, M=1, \zeta) = |\gamma\zeta|$$

$$\Psi_{26}(e^2t, ^3T, M=1, \eta) = -\frac{i(\sqrt{3}-i)|\gamma\eta|}{2}$$

$$\Psi_{27}(e^2t, ^3T, M=1, \mu) = \frac{i(\sqrt{3}+i)|\gamma\mu|}{2}$$

 t^2

$$\boxed{\Delta E = \langle \zeta\mu || \zeta\mu \rangle - \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\Psi_{28}(t^2, ^3T, M=-1, \eta) = |\bar{\zeta}\mu|$$

$$\Psi_{29}(t^2, ^3T, M=-1, \mu) = |\bar{\eta}\zeta|$$

$$\Psi_{30}(t^2, ^3T, M=-1, \zeta) = |\bar{\mu}\eta|$$

$$\Psi_{31}(t^2, ^3T, M=0, \eta) = \frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$\Psi_{32}(t^2, ^3T, M=0, \mu) = \frac{\sqrt{2}|\bar{\eta}\zeta|}{2} + \frac{\sqrt{2}|\eta\bar{\zeta}|}{2}$$

$$\Psi_{33}(t^2, ^3T, M=0, \zeta) = \frac{\sqrt{2}|\bar{\mu}\eta|}{2} + \frac{\sqrt{2}|\mu\bar{\eta}|}{2}$$

$$\Psi_{34}(t^2, ^3T, M=1, \eta) = |\zeta\mu|$$

$$\Psi_{35}(t^2, ^3T, M=1, \mu) = |\eta\zeta|$$

$$\Psi_{36}(t^2, ^3T, M=1, \zeta) = |\mu\eta|$$

2.28.7 1T *at*

$$\boxed{\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(at, ^1T, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_2(at, ^1T, M=0, \eta) = -\frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_3(at, ^1T, M=0, \mu) = -\frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

 e^1t

$\Delta E = \langle \beta\zeta \beta\zeta \rangle$	t^2
$\Psi_4(e^1 t, {}^1 T, M=0, \zeta) = -\frac{\sqrt{2} \bar{\beta}\zeta }{2} + \frac{\sqrt{2} \beta\bar{\zeta} }{2}$	$\Delta E = \langle \zeta\mu \zeta\mu \rangle + \langle \zeta\zeta \zeta\zeta \rangle$
$\Psi_5(e^1 t, {}^1 T, M=0, \eta) = -\frac{\sqrt{2}i(\sqrt{3+i}) \bar{\beta}\eta }{4} + \frac{\sqrt{2}i(\sqrt{3+i}) \beta\bar{\eta} }{4}$	$\Psi_{10}(t^2, {}^1 T, M=0, \eta) = -\frac{\sqrt{2} \bar{\zeta}\mu }{2} + \frac{\sqrt{2} \zeta\bar{\mu} }{2}$
$\Psi_6(e^1 t, {}^1 T, M=0, \mu) = \frac{\sqrt{2}i(\sqrt{3-i}) \bar{\beta}\mu }{4} - \frac{\sqrt{2}i(\sqrt{3-i}) \beta\bar{\mu} }{4}$	$\Psi_{11}(t^2, {}^1 T, M=0, \mu) = -\frac{\sqrt{2} \bar{\eta}\zeta }{2} + \frac{\sqrt{2} \eta\bar{\zeta} }{2}$
$e^2 t$	$\Psi_{12}(t^2, {}^1 T, M=0, \zeta) = -\frac{\sqrt{2} \bar{\mu}\eta }{2} + \frac{\sqrt{2} \mu\bar{\eta} }{2}$
$\Delta E = \langle \gamma\zeta \gamma\zeta \rangle$	<hr/>
$\Psi_7(e^2 t, {}^1 T, M=0, \zeta) = -\frac{\sqrt{2} \bar{\gamma}\zeta }{2} + \frac{\sqrt{2} \gamma\bar{\zeta} }{2}$	$2.28.8 \quad {}^3 A$
$\Psi_8(e^2 t, {}^1 T, M=0, \eta) = \frac{\sqrt{2}i(\sqrt{3-i}) \bar{\gamma}\eta }{4} - \frac{\sqrt{2}i(\sqrt{3-i}) \gamma\bar{\eta} }{4}$	$e^1 e^2$
$\Psi_9(e^2 t, {}^1 T, M=0, \mu) = -\frac{\sqrt{2}i(\sqrt{3+i}) \bar{\gamma}\mu }{4} + \frac{\sqrt{2}i(\sqrt{3+i}) \gamma\bar{\mu} }{4}$	$\Delta E = 0$
<hr/>	$\Psi_1(e^1 e^2, {}^3 A, M=-1, \alpha) = \bar{\beta}\bar{\gamma} $
<hr/>	$\Psi_2(e^1 e^2, {}^3 A, M=0, \alpha) = \frac{\sqrt{2} \bar{\beta}\gamma }{2} + \frac{\sqrt{2} \beta\bar{\gamma} }{2}$
<hr/>	$\Psi_3(e^1 e^2, {}^3 A, M=1, \alpha) = \beta\gamma $

2.29 Group T_h Component labels

$$A_g : \{\alpha_g\} \longrightarrow A_u : \{\alpha_u\} \longrightarrow E_u^1 : \{\beta_u\} \longrightarrow E_u^2 : \{\gamma_u\} \longrightarrow E_g^2 : \{\gamma_g\} \longrightarrow E_g^1 : \{\beta_g\} \longrightarrow$$

$$T_g : \{\zeta_g, \eta_g, \mu_g\} \longrightarrow T_u : \{\zeta_u, \eta_u, \mu_u\}$$

$$\Psi_4(e_g^1 e_g^2, {}^1 A_g, M=0, \alpha_g) = -\frac{\sqrt{2}|\bar{\gamma}_g \beta_g|}{2} + \frac{\sqrt{2}|\gamma_g \bar{\beta}_g|}{2}$$

2.29.1 ${}^1 A_g$

$$a_g^2$$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \alpha_g \alpha_g \rangle}$$

$$\Psi_1(a_g^2, {}^1 A_g, M=0, \alpha_g) = -|\overline{\alpha_g} \alpha_g|$$

$$a_u^2$$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_2(a_u^2, {}^1 A_g, M=0, \alpha_g) = -|\overline{\alpha_u} \alpha_u|$$

$$e_u^1 e_u^2$$

$$\boxed{\Delta E = 0}$$

$$t_g^2$$

$$\boxed{\Delta E = 3 \langle \zeta_g \zeta_g || \zeta_g \zeta_g \rangle}$$

$$\Psi_5(t_g^2, {}^1 A_g, M=0, \alpha_g) = -\frac{\sqrt{3}|\bar{\eta}_g \eta_g|}{3} - \frac{\sqrt{3}|\bar{\mu}_g \mu_g|}{3} - \frac{\sqrt{3}|\bar{\zeta}_g \zeta_g|}{3}$$

$$t_u^2$$

$$\boxed{\Delta E = 3 \langle \zeta_u \zeta_u || \zeta_u \zeta_u \rangle}$$

$$\Psi_6(t_u^2, {}^1 A_g, M=0, \alpha_g) = -\frac{\sqrt{3}|\bar{\eta}_u \eta_u|}{3} - \frac{\sqrt{3}|\bar{\mu}_u \mu_u|}{3} - \frac{\sqrt{3}|\bar{\zeta}_u \zeta_u|}{3}$$

2.29.2 ${}^3 A_u$

$$a_g a_u$$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_g a_u, {}^3 A_u, M=-1, \alpha_u) = |\overline{\alpha_g} \alpha_u|$$

$$\Psi_2(a_g a_u, {}^3A_u, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\alpha}_g \alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\alpha}_u|}{2}$$

$$\Psi_3(a_g a_u, {}^3A_u, M=1, \alpha_u) = |\alpha_g \alpha_u|$$

$$e_g^2 e_u^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(e_g^2 e_u^1, {}^3A_u, M=-1, \alpha_u) = |\overline{\beta}_u \overline{\gamma}_g|$$

$$\Psi_5(e_g^2 e_u^1, {}^3A_u, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\beta}_u \gamma_g|}{2} + \frac{\sqrt{2}|\beta_u \overline{\gamma}_g|}{2}$$

$$\Psi_6(e_g^2 e_u^1, {}^3A_u, M=1, \alpha_u) = |\beta_u \gamma_g|$$

$$e_g^1 e_u^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(e_g^1 e_u^2, {}^3A_u, M=-1, \alpha_u) = |\overline{\gamma}_u \overline{\beta}_g|$$

$$\Psi_8(e_g^1 e_u^2, {}^3A_u, M=0, \alpha_u) = \frac{\sqrt{2}|\overline{\gamma}_u \beta_g|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\beta}_g|}{2}$$

$$\Psi_9(e_g^1 e_u^2, {}^3A_u, M=1, \alpha_u) = |\gamma_u \beta_g|$$

$$t_g t_u$$

$$\boxed{\Delta E = 3 \langle \zeta_g \eta_u | \zeta_g \eta_u \rangle - 3 \langle \zeta_g \zeta_g | \eta_u \eta_u \rangle}$$

$$\Psi_{10}(t_g t_u, {}^3A_u, M=-1, \alpha_u) = \frac{\sqrt{3}|\overline{\eta}_g \mu_u|}{3} + \frac{\sqrt{3}|\overline{\mu}_g \zeta_u|}{3} + \frac{\sqrt{3}|\zeta_g \overline{\eta}_u|}{3}$$

$$\Psi_{11}(t_g t_u, {}^3A_u, M=0, \alpha_u) = \frac{\sqrt{6}|\overline{\eta}_g \mu_u|}{6} + \frac{\sqrt{6}|\overline{\mu}_g \zeta_u|}{6} + \frac{\sqrt{6}|\zeta_g \eta_u|}{6} + \frac{\sqrt{6}|\eta_g \overline{\mu}_u|}{6} + \frac{\sqrt{6}|\mu_g \zeta_u|}{6} + \frac{\sqrt{6}|\zeta_g \overline{\eta}_u|}{6}$$

$$\Psi_{12}(t_g t_u, {}^3A_u, M=1, \alpha_u) = \frac{\sqrt{3}|\eta_g \mu_u|}{3} + \frac{\sqrt{3}|\mu_g \zeta_u|}{3} + \frac{\sqrt{3}|\zeta_g \eta_u|}{3}$$

2.29.3 1A_u

$$a_g a_u$$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g | \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u | \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_g a_u, {}^1A_u, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\alpha}_g \alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\alpha}_u|}{2}$$

$$e_g^2 e_u^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(e_g^2 e_u^1, {}^1A_u, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\beta}_u \gamma_g|}{2} + \frac{\sqrt{2}|\beta_u \overline{\gamma}_g|}{2}$$

$$e_g^1 e_u^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(e_g^1 e_u^2, {}^1A_u, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\gamma}_u \beta_g|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\beta}_g|}{2}$$

$$t_g t_u$$

$$\boxed{\Delta E = 3 \langle \zeta_g \eta_u | \zeta_g \eta_u \rangle + 3 \langle \zeta_g \zeta_g | \eta_u \eta_u \rangle}$$

$$\Psi_4(t_g t_u, {}^1A_u, M=0, \alpha_u) = -\frac{\sqrt{6}|\overline{\eta}_g \mu_u|}{6} - \frac{\sqrt{6}|\overline{\mu}_g \zeta_u|}{6} - \frac{\sqrt{6}|\zeta_g \eta_u|}{6} + \frac{\sqrt{6}|\eta_g \overline{\mu}_u|}{6} + \frac{\sqrt{6}|\mu_g \zeta_u|}{6} + \frac{\sqrt{6}|\zeta_g \overline{\eta}_u|}{6}$$

2.29.4 ${}^3E_u^1$

$$a_g e_u^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(a_g e_u^1, {}^3E_u^1, M=-1, \beta_u) = |\overline{\alpha}_g \overline{\beta}_u|$$

$$\Psi_2(a_g e_u^1, {}^3E_u^1, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\alpha}_g \beta_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta}_u|}{2}$$

$$\Psi_3(a_g e_u^1, {}^3E_u^1, M=1, \beta_u) = |\alpha_g \beta_u|$$

$$a_u e_g^1$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(a_u e_g^1, {}^3E_u^1, M=-1, \beta_u) = |\overline{\alpha}_u \overline{\beta}_g|$$

$$\Psi_5(a_u e_g^1, {}^3E_u^1, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\alpha}_u \beta_g|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\beta}_g|}{2}$$

$$\Psi_6(a_u e_g^1, {}^3E_u^1, M=1, \beta_u) = |\alpha_u \beta_g|$$

$$e_g^2 e_u^2$$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(e_g^2 e_u^2, {}^3E_u^1, M=-1, \beta_u) = |\overline{\gamma}_u \overline{\gamma}_g|$$

$$\Psi_8(e_g^2 e_u^2, {}^3E_u^1, M=0, \beta_u) = \frac{\sqrt{2}|\overline{\gamma}_u \gamma_g|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\gamma}_g|}{2}$$

$$\Psi_9(e_g^2 e_u^2, {}^3E_u^1, M=1, \beta_u) = |\gamma_u \gamma_g|$$

$$t_g t_u$$

$$\boxed{\Delta E = 0}$$

$$\Psi_{10}(t_g t_u, {}^3E_u^1, M=-1, \beta_u) = \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta}_g \mu_u| + \frac{\sqrt{3}|\overline{\mu}_g \zeta_u|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\zeta_g \overline{\eta}_u|$$

$$\Psi_{11}(t_g t_u, {}^3E_u^1, M=0, \beta_u) = \sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta}_g \mu_u| + \frac{\sqrt{6}|\overline{\mu}_g \zeta_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\zeta_g \overline{\eta}_u|}{2} + \sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\eta_g \overline{\mu}_u| + \frac{\sqrt{6}|\mu_g \zeta_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\zeta_g \overline{\eta}_u|}{2}$$

$$\Psi_{12}(t_g t_u, {}^3E_u^1, M=1, \beta_u) = \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\eta_g \mu_u| + \frac{\sqrt{3}|\mu_g \zeta_u|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\zeta_g \eta_u|$$

2.29.5 $^1E_u^1$

$a_g e_u^1$ $\boxed{\Delta E = 0}$ $\Psi_1(a_g e_u^1, ^1E_u^1, M=0, \beta_u) = -\frac{\sqrt{2} \overline{\alpha}_g \beta_u }{2} + \frac{\sqrt{2} \alpha_g \overline{\beta}_u }{2}$ $a_u e_g^1$ $\boxed{\Delta E = 0}$ $\Psi_2(a_u e_g^1, ^1E_u^1, M=0, \beta_u) = -\frac{\sqrt{2} \overline{\alpha}_u \beta_g }{2} + \frac{\sqrt{2} \alpha_u \overline{\beta}_g }{2}$ $e_g^2 e_u^2$ $\boxed{\Delta E = 0}$ $\Psi_3(e_g^2 e_u^2, ^1E_u^1, M=0, \beta_u) = -\frac{\sqrt{2} \overline{\gamma}_u \gamma_g }{2} + \frac{\sqrt{2} \gamma_u \overline{\gamma}_g }{2}$	$t_g t_u$ $\boxed{\Delta E = 0}$ $\Psi_{10}(t_g t_u, ^3E_u^2, M=-1, \gamma_u) = \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) \eta_g \mu_u + \frac{\sqrt{3} \overline{\mu}_g \zeta_u }{3} + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) \zeta_g \overline{\eta}_u $ $\Psi_{11}(t_g t_u, ^3E_u^2, M=0, \gamma_u) = \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) \overline{\eta}_g \mu_u }{2} + \frac{\sqrt{6} \overline{\mu}_g \zeta_u }{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) \zeta_g \eta_u }{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) \eta_g \overline{\mu}_u }{2} + \frac{\sqrt{6} \mu_g \overline{\zeta}_u }{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) \zeta_g \overline{\eta}_u }{2}$ $\Psi_{12}(t_g t_u, ^3E_u^2, M=1, \gamma_u) = \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) \eta_g \mu_u + \frac{\sqrt{3} \mu_g \zeta_u }{3} + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) \zeta_g \eta_u $
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2.29.6 $^3E_u^2$

$a_g e_u^2$ $\boxed{\Delta E = 0}$ $\Psi_1(a_g e_u^2, ^3E_u^2, M=-1, \gamma_u) = \overline{\alpha}_g \gamma_u $ $\Psi_2(a_g e_u^2, ^3E_u^2, M=0, \gamma_u) = \frac{\sqrt{2} \overline{\alpha}_g \gamma_u }{2} + \frac{\sqrt{2} \alpha_g \overline{\gamma}_u }{2}$ $\Psi_3(a_g e_u^2, ^3E_u^2, M=1, \gamma_u) = \alpha_g \gamma_u $ $a_u e_g^2$ $\boxed{\Delta E = 0}$ $\Psi_4(a_u e_g^2, ^3E_u^2, M=-1, \gamma_u) = \overline{\alpha}_u \gamma_g $ $\Psi_5(a_u e_g^2, ^3E_u^2, M=0, \gamma_u) = \frac{\sqrt{2} \overline{\alpha}_u \gamma_g }{2} + \frac{\sqrt{2} \alpha_u \overline{\gamma}_g }{2}$ $\Psi_6(a_u e_g^2, ^3E_u^2, M=1, \gamma_u) = \alpha_u \gamma_g $	$t_g t_u$ $\boxed{\Delta E = 0}$ $\Psi_3(e_g^1 e_u^1, ^1E_u^2, M=0, \gamma_u) = -\frac{\sqrt{2} \overline{\beta}_u \beta_g }{2} + \frac{\sqrt{2} \beta_u \overline{\beta}_g }{2}$ $e_g^1 e_u^1$ $\boxed{\Delta E = 0}$ $\Psi_4(t_g t_u, ^1E_u^2, M=0, \gamma_u) = \frac{\sqrt{2}(\overline{\eta}_g \mu_u - \frac{\sqrt{6} \overline{\mu}_g \zeta_u }{6})}{2} + \frac{\sqrt{2}(\zeta_g \overline{\eta}_u - \frac{\sqrt{6} \eta_g \overline{\mu}_u }{6})}{2} + \frac{\sqrt{2}(\zeta_g \overline{\eta}_u - \frac{\sqrt{6} \mu_g \overline{\zeta}_u }{6})}{2}$
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2.29.8 $^3E_g^2$

$e_g^1 e_u^1$ $\boxed{\Delta E = 0}$ $\Psi_7(e_g^1 e_u^1, ^3E_g^2, M=-1, \gamma_u) = \overline{\beta}_u \beta_g $ $\Psi_8(e_g^1 e_u^1, ^3E_g^2, M=0, \gamma_u) = \frac{\sqrt{2} \overline{\beta}_u \beta_g }{2} + \frac{\sqrt{2} \beta_u \overline{\beta}_g }{2}$ $\Psi_9(e_g^1 e_u^1, ^3E_g^2, M=1, \gamma_u) = \beta_u \beta_g $	$a_g e_g^2$ $\boxed{\Delta E = 0}$ $\Psi_1(a_g e_g^2, ^3E_g^2, M=-1, \gamma_g) = \overline{\alpha}_g \gamma_g $ $\Psi_2(a_g e_g^2, ^3E_g^2, M=0, \gamma_g) = \frac{\sqrt{2} \overline{\alpha}_g \gamma_g }{2} + \frac{\sqrt{2} \alpha_g \overline{\gamma}_g }{2}$ $\Psi_3(a_g e_g^2, ^3E_g^2, M=1, \gamma_g) = \alpha_g \gamma_g $
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$$\Psi_4(a_u e_u^2, {}^3E_g^2, M=-1, \gamma_g) = |\overline{\alpha_u \gamma_u}|$$

$$\Psi_5(a_u e_u^2, {}^3E_g^2, M=0, \gamma_g) = \frac{\sqrt{2}|\overline{\alpha_u \gamma_u}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\gamma_u}|}{2}$$

$$\Psi_6(a_u e_u^2, {}^3E_g^2, M=1, \gamma_g) = |\alpha_u \gamma_u|$$

$$\Psi_1(a_g e_g^1, {}^3E_g^1, M=-1, \beta_g) = |\overline{\alpha_g} \overline{\beta_g}|$$

$$\Psi_2(a_g e_g^1, {}^3E_g^1, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\alpha_g} \beta_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\beta_g}|}{2}$$

$$\Psi_3(a_g e_g^1, {}^3E_g^1, M=1, \beta_g) = |\alpha_g \beta_g|$$

2.29.9 $^1E_g^2$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(a_g e_g^2, {}^1E_g^2, M=0, \gamma_g) = -\frac{\sqrt{2}|\alpha_g\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_g\gamma_g|}{2}$$

$$a_u e_u^2$$

$$\Psi_2(a_u e_u^2, {}^1E_g^2, M=0, \gamma_g) = -\frac{\sqrt{2}[\overline{\alpha}_u \gamma_u]}{2} + \frac{\sqrt{2}[\alpha_u \overline{\gamma}_u]}{2}$$

$$\left(e_u^1\right)^2$$

$$\Psi_3(\left(e_u^1\right)^2, {}^1E_g^2, M=0, \gamma_g) = -|\overline{\beta_u}\beta_u|$$

$$\Delta E \equiv 0$$

$$\Psi_4(\left(e_q^1\right)^2, {}^1E_q^2, M=0, \gamma_q) = -|\overline{\beta}_q \beta_q|$$

$$t_g^2$$

$$\Psi_5(t_g^2, {}^1E_g^2, M=0, \gamma_g) =$$

$$\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta}_g \eta_g| - \frac{\sqrt{3}|\overline{\mu}_g \mu_g|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\zeta}_g \zeta_g|$$

$$t_u^2$$

$$\Psi_6(t_u^2, \overline{E_g^2}, M=0, \gamma_g) = \\ \left(\frac{\sqrt{3}}{6} - \frac{i}{2} \right) |\overline{\eta_u} \eta_u| - \frac{\sqrt{3} |\mu_u \mu_u|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2} \right) |\overline{\zeta_u} \zeta_u|$$

$$\begin{aligned}\Psi_4(a_u e_u^1, {}^3E_g^1, M=-1, \beta_g) &= |\overline{\alpha_u} \overline{\beta_u}| \\ \Psi_5(a_u e_u^1, {}^3E_g^1, M=0, \beta_g) &= \frac{\sqrt{2}|\overline{\alpha_u} \beta_u|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\beta_u}|}{2} \\ \Psi_6(a_u e_u^1, {}^3E_g^1, M=1, \beta_g) &= |\alpha_u \beta_u|\end{aligned}$$

$$a_g e_g^1$$

$$\Psi_1(a_g e_g^1, {}^1E_g^1, M=0, \beta_g) = -\frac{\sqrt{2}|\alpha_g \beta_g|}{2} + \frac{\sqrt{2}|\alpha_g \beta_g|}{2}$$

$$(e_u^2)^2$$

$$\Psi_3((e_u^2)^2, {}^1E_g^1, M=0, \beta_g) = -|\overline{\gamma_u}\gamma_u|$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(\left(e_a^2\right)^2, {}^1E_a^1, M=0, \beta_q) = -|\overline{\gamma}_q \gamma_q|$$

$$t_g^2$$

$$\Psi_5(t_g^2, {}^1E_g^1, M=0, \beta_g) =$$

$$\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\eta_g} \eta_g| - \frac{\sqrt{3}|\mu_g \mu_g|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\zeta_g} \zeta_g|$$

$$t_u^2$$

$$\Psi_6(t_u^2, \overline{E_g^1}, M=0, \beta_g) =$$

$$\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\eta_u} \eta_u| - \frac{\sqrt{3}|\mu_u \mu_u|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\zeta_u} \zeta_u|$$

$$\boxed{2.29.10} \quad {}^3E_g^1$$

2.29.12 3T_g $a_g t_g$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \zeta_g \zeta_g \rangle + \langle \alpha_g \zeta_g || \alpha_g \zeta_g \rangle}$$

$$\Psi_1(a_g t_g, ^3T_g, M=-1, \zeta_g) = |\overline{\alpha_g \zeta_g}|$$

$$\Psi_2(a_g t_g, ^3T_g, M=-1, \eta_g) = |\overline{\alpha_g \eta_g}|$$

$$\Psi_3(a_g t_g, ^3T_g, M=-1, \mu_g) = |\overline{\alpha_g \mu_g}|$$

$$\Psi_4(a_g t_g, ^3T_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\alpha_g \zeta_g}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\zeta_g}|}{2}$$

$$\Psi_5(a_g t_g, ^3T_g, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\alpha_g \eta_g}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\eta_g}|}{2}$$

$$\Psi_6(a_g t_g, ^3T_g, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\alpha_g \mu_g}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\mu_g}|}{2}$$

$$\Psi_7(a_g t_g, ^3T_g, M=1, \zeta_g) = |\alpha_g \zeta_g|$$

$$\Psi_8(a_g t_g, ^3T_g, M=1, \eta_g) = |\alpha_g \eta_g|$$

$$\Psi_9(a_g t_g, ^3T_g, M=1, \mu_g) = |\alpha_g \mu_g|$$

 $a_u t_u$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \zeta_u \zeta_u \rangle + \langle \alpha_u \zeta_u || \alpha_u \zeta_u \rangle}$$

$$\Psi_{10}(a_u t_u, ^3T_g, M=-1, \mu_g) = |\overline{\alpha_u \zeta_u}|$$

$$\Psi_{11}(a_u t_u, ^3T_g, M=-1, \zeta_g) = |\overline{\alpha_u \eta_u}|$$

$$\Psi_{12}(a_u t_u, ^3T_g, M=-1, \eta_g) = |\overline{\alpha_u \mu_u}|$$

$$\Psi_{13}(a_u t_u, ^3T_g, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\alpha_u \zeta_u}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\zeta_u}|}{2}$$

$$\Psi_{14}(a_u t_u, ^3T_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\alpha_u \eta_u}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\eta_u}|}{2}$$

$$\Psi_{15}(a_u t_u, ^3T_g, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\alpha_u \mu_u}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\mu_u}|}{2}$$

$$\Psi_{16}(a_u t_u, ^3T_g, M=1, \mu_g) = |\alpha_u \zeta_u|$$

$$\Psi_{17}(a_u t_u, ^3T_g, M=1, \zeta_g) = |\alpha_u \eta_u|$$

$$\Psi_{18}(a_u t_u, ^3T_g, M=1, \eta_g) = |\alpha_u \mu_u|$$

 $e_u^1 t_u$

$$\boxed{\Delta E = \langle \beta_u \zeta_u || \beta_u \zeta_u \rangle}$$

$$\Psi_{19}(e_u^1 t_u, ^3T_g, M=-1, \mu_g) = \frac{i(\sqrt{3}+i)|\overline{\beta_u \zeta_u}|}{2}$$

$$\Psi_{20}(e_u^1 t_u, ^3T_g, M=-1, \zeta_g) = |\overline{\beta_u \eta_u}|$$

$$\Psi_{21}(e_u^1 t_u, ^3T_g, M=-1, \eta_g) = -\frac{i(\sqrt{3}-i)|\overline{\beta_u \mu_u}|}{2}$$

$$\Psi_{22}(e_u^1 t_u, ^3T_g, M=0, \mu_g) = \frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\beta_u \zeta_u}|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\beta_u \overline{\zeta_u}|}{4}$$

$$\Psi_{23}(e_u^1 t_u, ^3T_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_u \eta_u}|}{2} + \frac{\sqrt{2}|\beta_u \overline{\eta_u}|}{2}$$

$$\Psi_{24}(e_u^1 t_u, ^3T_g, M=0, \eta_g) = -\frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\beta_u \mu_u}|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\beta_u \overline{\mu_u}|}{4}$$

$$\Psi_{25}(e_u^1 t_u, ^3T_g, M=1, \mu_g) = \frac{i(\sqrt{3}+i)|\beta_u \zeta_u|}{2}$$

$$\Psi_{26}(e_u^1 t_u, ^3T_g, M=1, \zeta_g) = |\beta_u \eta_u|$$

$$\Psi_{27}(e_u^1 t_u, ^3T_g, M=1, \eta_g) = -\frac{i(\sqrt{3}-i)|\beta_u \mu_u|}{2}$$

 $e_u^2 t_u$

$$\boxed{\Delta E = \langle \gamma_u \zeta_u || \gamma_u \zeta_u \rangle}$$

$$\Psi_{28}(e_u^2 t_u, ^3T_g, M=-1, \mu_g) = -\frac{i(\sqrt{3}-i)|\overline{\gamma_u \zeta_u}|}{2}$$

$$\Psi_{29}(e_u^2 t_u, ^3T_g, M=-1, \zeta_g) = |\overline{\gamma_u \eta_u}|$$

$$\Psi_{30}(e_u^2 t_u, ^3T_g, M=-1, \eta_g) = \frac{i(\sqrt{3}+i)|\overline{\gamma_u \mu_u}|}{2}$$

$$\frac{\Psi_{31}(e_u^2 t_u, ^3T_g, M=0, \mu_g)}{-\frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\gamma_u \zeta_u}|}{4}} - \frac{\sqrt{2}i(\sqrt{3}-i)|\gamma_u \overline{\zeta_u}|}{4}$$

$$\Psi_{32}(e_u^2 t_u, ^3T_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\gamma_u \eta_u}|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\eta_u}|}{2}$$

$$\frac{\Psi_{33}(e_u^2 t_u, ^3T_g, M=0, \eta_g)}{\frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\gamma_u \mu_u}|}{4}} + \frac{\sqrt{2}i(\sqrt{3}+i)|\gamma_u \overline{\mu_u}|}{4}$$

$$\Psi_{34}(e_u^2 t_u, ^3T_g, M=1, \mu_g) = -\frac{i(\sqrt{3}-i)|\gamma_u \zeta_u|}{2}$$

$$\Psi_{35}(e_u^2 t_u, ^3T_g, M=1, \zeta_g) = |\gamma_u \eta_u|$$

$$\Psi_{36}(e_u^2 t_u, ^3T_g, M=1, \eta_g) = \frac{i(\sqrt{3}+i)|\gamma_u \mu_u|}{2}$$

 $e_g^2 t_g$

$$\boxed{\Delta E = \langle \gamma_g \zeta_g || \gamma_g \zeta_g \rangle}$$

$$\Psi_{37}(e_g^2 t_g, ^3T_g, M=-1, \zeta_g) = |\overline{\gamma_g \zeta_g}|$$

$$\Psi_{38}(e_g^2 t_g, ^3T_g, M=-1, \eta_g) = \frac{i(\sqrt{3}+i)|\overline{\gamma_g \eta_g}|}{2}$$

$$\Psi_{39}(e_g^2 t_g, ^3T_g, M=-1, \mu_g) = -\frac{i(\sqrt{3}-i)|\overline{\gamma_g \mu_g}|}{2}$$

$$\Psi_{40}(e_g^2 t_g, ^3T_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\gamma_g \zeta_g}|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\zeta_g}|}{2}$$

$$\frac{\Psi_{41}(e_g^2 t_g, ^3T_g, M=0, \eta_g)}{\frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\gamma_g \eta_g}|}{4}} + \frac{\sqrt{2}i(\sqrt{3}+i)|\gamma_g \overline{\eta_g}|}{4}$$

$$\frac{\Psi_{42}(e_g^2 t_g, ^3T_g, M=0, \mu_g)}{-\frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\gamma_g \mu_g}|}{4}} - \frac{\sqrt{2}i(\sqrt{3}-i)|\gamma_g \overline{\mu_g}|}{4}$$

$$\Psi_{43}(e_g^2 t_g, ^3T_g, M=1, \zeta_g) = |\gamma_g \zeta_g|$$

$$\Psi_{44}(e_g^2 t_g, ^3T_g, M=1, \eta_g) = \frac{i(\sqrt{3}+i)|\gamma_g \eta_g|}{2}$$

$$\Psi_{45}(e_g^2 t_g, ^3T_g, M=1, \mu_g) = -\frac{i(\sqrt{3}-i)|\gamma_g \mu_g|}{2}$$

 $e_g^1 t_g$

$$\boxed{\Delta E = \langle \beta_g \zeta_g || \beta_g \zeta_g \rangle}$$

$$\Psi_{46}(e_g^1 t_g, ^3T_g, M=-1, \zeta_g) = |\overline{\beta_g \zeta_g}|$$

$$\Psi_{47}(e_g^1 t_g, ^3T_g, M=-1, \eta_g) = -\frac{i(\sqrt{3}-i)|\overline{\beta_g \eta_g}|}{2}$$

$$\Psi_{48}(e_g^1 t_g, ^3T_g, M=-1, \mu_g) = \frac{i(\sqrt{3}+i)|\overline{\beta_g \mu_g}|}{2}$$

$$\Psi_{49}(e_g^1 t_g, ^3T_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_g \zeta_g}|}{2} + \frac{\sqrt{2}|\beta_g \overline{\zeta_g}|}{2}$$

$$\frac{\Psi_{50}(e_g^1 t_g, ^3T_g, M=0, \eta_g)}{-\frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\beta_g \eta_g}|}{4}} - \frac{\sqrt{2}i(\sqrt{3}-i)|\beta_g \overline{\eta_g}|}{4}$$

$$\begin{aligned}\Psi_{51}(e_g^1 t_g, {}^3T_g, M=0, \mu_g) &= \\ \frac{\sqrt{2}i(\sqrt{3}+i)|\beta_g \mu_g|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\beta_g \mu_g|}{4} \\ \Psi_{52}(e_g^1 t_g, {}^3T_g, M=1, \zeta_g) &= |\beta_g \zeta_g| \\ \Psi_{53}(e_g^1 t_g, {}^3T_g, M=1, \eta_g) &= -\frac{i(\sqrt{3}-i)|\beta_g \eta_g|}{2} \\ \Psi_{54}(e_g^1 t_g, {}^3T_g, M=1, \mu_g) &= \frac{i(\sqrt{3}+i)|\beta_g \mu_g|}{2}\end{aligned}$$

 t_g^2

$$\Delta E = \langle \zeta_g \mu_g || \zeta_g \mu_g \rangle - \langle \zeta_g \zeta_g || \zeta_g \zeta_g \rangle$$

$$\begin{aligned}\Psi_{55}(t_g^2, {}^3T_g, M=-1, \eta_g) &= |\overline{\zeta_g} \overline{\mu_g}| \\ \Psi_{56}(t_g^2, {}^3T_g, M=-1, \mu_g) &= |\overline{\eta_g} \overline{\zeta_g}| \\ \Psi_{57}(t_g^2, {}^3T_g, M=-1, \zeta_g) &= |\overline{\mu_g} \eta_g| \\ \Psi_{58}(t_g^2, {}^3T_g, M=0, \eta_g) &= \frac{\sqrt{2}|\overline{\zeta_g} \mu_g|}{2} + \frac{\sqrt{2}|\zeta_g \overline{\mu_g}|}{2} \\ \Psi_{59}(t_g^2, {}^3T_g, M=0, \mu_g) &= \frac{\sqrt{2}|\overline{\eta_g} \zeta_g|}{2} + \frac{\sqrt{2}|\eta_g \overline{\zeta_g}|}{2} \\ \Psi_{60}(t_g^2, {}^3T_g, M=0, \zeta_g) &= \frac{\sqrt{2}|\overline{\mu_g} \eta_g|}{2} + \frac{\sqrt{2}|\mu_g \overline{\eta_g}|}{2} \\ \Psi_{61}(t_g^2, {}^3T_g, M=1, \eta_g) &= |\zeta_g \mu_g| \\ \Psi_{62}(t_g^2, {}^3T_g, M=1, \mu_g) &= |\eta_g \zeta_g| \\ \Psi_{63}(t_g^2, {}^3T_g, M=1, \zeta_g) &= |\mu_g \eta_g|\end{aligned}$$

 t_u^2

$$\Delta E = \langle \zeta_u \eta_u || \zeta_u \eta_u \rangle - \langle \zeta_u \zeta_u || \zeta_u \zeta_u \rangle$$

$$\begin{aligned}\Psi_{64}(t_u^2, {}^3T_g, M=-1, \eta_g) &= |\overline{\zeta_u} \overline{\eta_u}| \\ \Psi_{65}(t_u^2, {}^3T_g, M=-1, \mu_g) &= |\overline{\eta_u} \overline{\mu_u}| \\ \Psi_{66}(t_u^2, {}^3T_g, M=-1, \zeta_g) &= |\overline{\mu_u} \overline{\zeta_u}| \\ \Psi_{67}(t_u^2, {}^3T_g, M=0, \eta_g) &= \frac{\sqrt{2}|\overline{\zeta_u} \eta_u|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\eta_u}|}{2} \\ \Psi_{68}(t_u^2, {}^3T_g, M=0, \mu_g) &= \frac{\sqrt{2}|\overline{\eta_u} \mu_u|}{2} + \frac{\sqrt{2}|\eta_u \overline{\mu_u}|}{2} \\ \Psi_{69}(t_u^2, {}^3T_g, M=0, \zeta_g) &= \frac{\sqrt{2}|\overline{\mu_u} \zeta_u|}{2} + \frac{\sqrt{2}|\mu_u \overline{\zeta_u}|}{2} \\ \Psi_{70}(t_u^2, {}^3T_g, M=1, \eta_g) &= |\zeta_u \eta_u| \\ \Psi_{71}(t_u^2, {}^3T_g, M=1, \mu_g) &= |\eta_u \mu_u| \\ \Psi_{72}(t_u^2, {}^3T_g, M=1, \zeta_g) &= |\mu_u \zeta_u|\end{aligned}$$

2.29.13 1T_g $a_g t_g$

$$\Delta E = \langle \alpha_g \alpha_g || \zeta_g \zeta_g \rangle + \langle \alpha_g \zeta_g || \alpha_g \zeta_g \rangle$$

$$\begin{aligned}\Psi_1(a_g t_g, {}^1T_g, M=0, \zeta_g) &= -\frac{\sqrt{2}|\overline{\alpha_g} \zeta_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\zeta_g}|}{2} \\ \Psi_2(a_g t_g, {}^1T_g, M=0, \eta_g) &= -\frac{\sqrt{2}|\overline{\alpha_g} \eta_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\eta_g}|}{2} \\ \Psi_3(a_g t_g, {}^1T_g, M=0, \mu_g) &= -\frac{\sqrt{2}|\overline{\alpha_g} \mu_g|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\mu_g}|}{2}\end{aligned}$$

 $a_u t_u$

$$\Delta E = \langle \alpha_u \alpha_u || \zeta_u \zeta_u \rangle + \langle \alpha_u \zeta_u || \alpha_u \zeta_u \rangle$$

$$\Psi_4(a_u t_u, {}^1T_g, M=0, \mu_g) = -\frac{\sqrt{2}|\overline{\alpha_u} \zeta_u|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\zeta_u}|}{2}$$

$$\Psi_5(a_u t_u, {}^1T_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\alpha_u} \eta_u|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\eta_u}|}{2}$$

$$\Psi_6(a_u t_u, {}^1T_g, M=0, \eta_g) = -\frac{\sqrt{2}|\overline{\alpha_u} \mu_u|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\mu_u}|}{2}$$

 $e_u^1 t_u$

$$\Delta E = \langle \beta_u \zeta_u || \beta_u \zeta_u \rangle$$

$$\begin{aligned}\Psi_7(e_u^1 t_u, {}^1T_g, M=0, \mu_g) &= \\ -\frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\beta_u} \zeta_u|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\beta_u \overline{\zeta_u}|}{4}\end{aligned}$$

$$\Psi_8(e_u^1 t_u, {}^1T_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\beta_u} \eta_u|}{2} + \frac{\sqrt{2}|\beta_u \overline{\eta_u}|}{2}$$

$$\begin{aligned}\Psi_9(e_u^1 t_u, {}^1T_g, M=0, \eta_g) &= \\ \frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\beta_u} \mu_u|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\beta_u \overline{\mu_u}|}{4}\end{aligned}$$

 $e_u^2 t_u$

$$\Delta E = \langle \gamma_u \zeta_u || \gamma_u \zeta_u \rangle$$

$$\begin{aligned}\Psi_{10}(e_u^2 t_u, {}^1T_g, M=0, \mu_g) &= \\ \frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\gamma_u} \zeta_u|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\gamma_u \overline{\zeta_u}|}{4}\end{aligned}$$

$$\Psi_{11}(e_u^2 t_u, {}^1T_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\gamma_u} \eta_u|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\eta_u}|}{2}$$

$$\begin{aligned}\Psi_{12}(e_u^2 t_u, {}^1T_g, M=0, \eta_g) &= \\ -\frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\gamma_u} \mu_u|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\gamma_u \overline{\mu_u}|}{4}\end{aligned}$$

 $e_g^2 t_g$

$$\Delta E = \langle \gamma_g \zeta_g || \gamma_g \zeta_g \rangle$$

$$\Psi_{13}(e_g^2 t_g, {}^1T_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\gamma_g} \zeta_g|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\zeta_g}|}{2}$$

$$\begin{aligned}\Psi_{14}(e_g^2 t_g, {}^1T_g, M=0, \eta_g) &= \\ -\frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\gamma_g} \eta_g|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\gamma_g \overline{\eta_g}|}{4}\end{aligned}$$

$$\begin{aligned}\Psi_{15}(e_g^2 t_g, {}^1T_g, M=0, \mu_g) &= \\ \frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\gamma_g} \mu_g|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\gamma_g \overline{\mu_g}|}{4}\end{aligned}$$

 $e_g^1 t_g$

$$\Delta E = \langle \beta_g \zeta_g || \beta_g \zeta_g \rangle$$

$$\Psi_{16}(e_g^1 t_g, {}^1T_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\beta_g} \zeta_g|}{2} + \frac{\sqrt{2}|\beta_g \overline{\zeta_g}|}{2}$$

$$\begin{aligned}\Psi_{17}(e_g^1 t_g, {}^1T_g, M=0, \eta_g) &= \\ \frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\beta_g} \eta_g|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\beta_g \overline{\eta_g}|}{4}\end{aligned}$$

$$\begin{aligned}\Psi_{18}(e_g^1 t_g, {}^1T_g, M=0, \mu_g) &= \\ -\frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\beta_g} \mu_g|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\beta_g \overline{\mu_g}|}{4}\end{aligned}$$

 t_g^2

$$\Psi_{18}(a_u t_g, {}^3T_u, M=1, \zeta_u) = |\alpha_u \mu_g|$$

$\Delta E = \langle \zeta_g \mu_g || \zeta_g \mu_g \rangle + \langle \zeta_g \zeta_g || \zeta_g \zeta_g \rangle$

$\Psi_{19}(t_g^2, {}^1T_g, M=0, \eta_g) = -\frac{\sqrt{2}|\zeta_g \mu_g|}{2} + \frac{\sqrt{2}|\zeta_g \mu_g|}{2}$
 $\Psi_{20}(t_g^2, {}^1T_g, M=0, \mu_g) = -\frac{\sqrt{2}|\eta_g \zeta_g|}{2} + \frac{\sqrt{2}|\eta_g \zeta_g|}{2}$
 $\Psi_{21}(t_g^2, {}^1T_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\mu_g \eta_g|}{2} + \frac{\sqrt{2}|\mu_g \eta_g|}{2}$

$e_u^1 t_g$

$\Delta E = \langle \beta_u \zeta_g || \beta_u \zeta_g \rangle$

$\Psi_{22}(t_u^2, {}^1T_g, M=0, \eta_g) = -\frac{\sqrt{2}|\zeta_u \eta_u|}{2} + \frac{\sqrt{2}|\zeta_u \eta_u|}{2}$
 $\Psi_{23}(t_u^2, {}^1T_g, M=0, \mu_g) = -\frac{\sqrt{2}|\eta_u \mu_u|}{2} + \frac{\sqrt{2}|\eta_u \mu_u|}{2}$
 $\Psi_{24}(t_u^2, {}^1T_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\mu_u \zeta_u|}{2} + \frac{\sqrt{2}|\mu_u \zeta_u|}{2}$

$e_u^1 t_g, {}^3T_u, M=-1, \eta_u$
 $e_u^1 t_g, {}^3T_u, M=-1, \mu_u$
 $e_u^1 t_g, {}^3T_u, M=-1, \zeta_u$
 $e_u^1 t_g, {}^3T_u, M=0, \eta_u$
 $e_u^1 t_g, {}^3T_u, M=0, \mu_u$
 $e_u^1 t_g, {}^3T_u, M=0, \zeta_u$

2.29.14 3T_u

$a_g t_u$

$\Delta E = -\langle \alpha_g \alpha_g || \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u || \alpha_g \zeta_u \rangle$

$\Psi_1(a_g t_u, {}^3T_u, M=-1, \zeta_u) = |\overline{\alpha_g \zeta_u}|$
 $\Psi_2(a_g t_u, {}^3T_u, M=-1, \eta_u) = |\overline{\alpha_g \eta_u}|$
 $\Psi_3(a_g t_u, {}^3T_u, M=-1, \mu_u) = |\overline{\alpha_g \mu_u}|$
 $\Psi_4(a_g t_u, {}^3T_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_g \zeta_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\zeta_u}|}{2}$
 $\Psi_5(a_g t_u, {}^3T_u, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\alpha_g \eta_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\eta_u}|}{2}$
 $\Psi_6(a_g t_u, {}^3T_u, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\alpha_g \mu_u}|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\mu_u}|}{2}$
 $\Psi_7(a_g t_u, {}^3T_u, M=1, \zeta_u) = |\alpha_g \zeta_u|$
 $\Psi_8(a_g t_u, {}^3T_u, M=1, \eta_u) = |\alpha_g \eta_u|$
 $\Psi_9(a_g t_u, {}^3T_u, M=1, \mu_u) = |\alpha_g \mu_u|$

$a_u t_g$

$\Delta E = -\langle \alpha_u \alpha_u || \zeta_g \zeta_g \rangle + \langle \alpha_u \zeta_g || \alpha_u \zeta_g \rangle$

$\Psi_{10}(a_u t_g, {}^3T_u, M=-1, \eta_u) = |\overline{\alpha_u \zeta_g}|$
 $\Psi_{11}(a_u t_g, {}^3T_u, M=-1, \mu_u) = |\overline{\alpha_u \eta_g}|$
 $\Psi_{12}(a_u t_g, {}^3T_u, M=-1, \zeta_u) = |\overline{\alpha_u \mu_g}|$
 $\Psi_{13}(a_u t_g, {}^3T_u, M=0, \eta_u) = \frac{\sqrt{2}|\overline{\alpha_u \zeta_g}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\zeta_g}|}{2}$
 $\Psi_{14}(a_u t_g, {}^3T_u, M=0, \mu_u) = \frac{\sqrt{2}|\overline{\alpha_u \eta_g}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\eta_g}|}{2}$
 $\Psi_{15}(a_u t_g, {}^3T_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_u \mu_g}|}{2} + \frac{\sqrt{2}|\alpha_u \overline{\mu_g}|}{2}$
 $\Psi_{16}(a_u t_g, {}^3T_u, M=1, \eta_u) = |\alpha_u \zeta_g|$
 $\Psi_{17}(a_u t_g, {}^3T_u, M=1, \mu_u) = |\alpha_u \eta_g|$

$e_u^2 t_g$

$\Delta E = \langle \gamma_u \zeta_g || \gamma_u \zeta_g \rangle$

$\Psi_{28}(e_u^2 t_g, {}^3T_u, M=-1, \eta_u) = \frac{i(\sqrt{3}+i)|\overline{\gamma_u \zeta_g}|}{2}$
 $\Psi_{29}(e_u^2 t_g, {}^3T_u, M=-1, \mu_u) = -\frac{i(\sqrt{3}-i)|\overline{\gamma_u \eta_g}|}{2}$
 $\Psi_{30}(e_u^2 t_g, {}^3T_u, M=-1, \zeta_u) = |\overline{\gamma_u \mu_g}|$
 $\Psi_{31}(e_u^2 t_g, {}^3T_u, M=0, \eta_u) = \frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\gamma_u \zeta_g}|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\gamma_u \overline{\zeta_g}|}{4}$
 $\Psi_{32}(e_u^2 t_g, {}^3T_u, M=0, \mu_u) = -\frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\gamma_u \eta_g}|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\gamma_u \overline{\eta_g}|}{4}$
 $\Psi_{33}(e_u^2 t_g, {}^3T_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\gamma_u \mu_g}|}{2} + \frac{\sqrt{2}|\gamma_u \overline{\mu_g}|}{2}$
 $\Psi_{34}(e_u^2 t_g, {}^3T_u, M=1, \eta_u) = \frac{i(\sqrt{3}+i)|\gamma_u \zeta_g|}{2}$
 $\Psi_{35}(e_u^2 t_g, {}^3T_u, M=1, \mu_u) = -\frac{i(\sqrt{3}-i)|\gamma_u \eta_g|}{2}$
 $\Psi_{36}(e_u^2 t_g, {}^3T_u, M=1, \zeta_u) = |\gamma_u \mu_g|$

$e_g^2 t_u$

$\Delta E = \langle \gamma_g \zeta_u || \gamma_g \zeta_u \rangle$

$\Psi_{37}(e_g^2 t_u, {}^3T_u, M=-1, \zeta_u) = |\overline{\gamma_g \zeta_u}|$
 $\Psi_{38}(e_g^2 t_u, {}^3T_u, M=-1, \eta_u) = \frac{i(\sqrt{3}+i)|\overline{\gamma_g \eta_u}|}{2}$
 $\Psi_{39}(e_g^2 t_u, {}^3T_u, M=-1, \mu_u) = -\frac{i(\sqrt{3}-i)|\overline{\gamma_g \mu_u}|}{2}$
 $\Psi_{40}(e_g^2 t_u, {}^3T_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\gamma_g \zeta_u}|}{2} + \frac{\sqrt{2}|\gamma_g \overline{\zeta_u}|}{2}$
 $\Psi_{41}(e_g^2 t_u, {}^3T_u, M=0, \eta_u) = \frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\gamma_g \eta_u}|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\gamma_g \overline{\eta_u}|}{4}$

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$$\begin{aligned} \Psi_{42}(e_g^2 t_u, {}^3T_u, M=0, \mu_u) &= -\frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\alpha_g}\mu_u|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\gamma_g\mu_u|}{4} \\ \Psi_{43}(e_g^2 t_u, {}^3T_u, M=1, \zeta_u) &= |\gamma_g\zeta_u| \\ \Psi_{44}(e_g^2 t_u, {}^3T_u, M=1, \eta_u) &= \frac{i(\sqrt{3}+i)|\gamma_g\eta_u|}{2} \\ \Psi_{45}(e_g^2 t_u, {}^3T_u, M=1, \mu_u) &= -\frac{i(\sqrt{3}-i)|\gamma_g\mu_u|}{2} \\ e_g^1 t_u \\ \boxed{\Delta E = \langle \beta_g \zeta_u || \beta_g \zeta_u \rangle} \\ \Psi_{46}(e_g^1 t_u, {}^3T_u, M=-1, \zeta_u) &= |\overline{\beta_g}\zeta_u| \\ \Psi_{47}(e_g^1 t_u, {}^3T_u, M=-1, \eta_u) &= -\frac{i(\sqrt{3}-i)|\overline{\beta_g}\eta_u|}{2} \\ \Psi_{48}(e_g^1 t_u, {}^3T_u, M=-1, \mu_u) &= \frac{i(\sqrt{3}+i)|\overline{\beta_g}\mu_u|}{2} \\ \Psi_{49}(e_g^1 t_u, {}^3T_u, M=0, \zeta_u) &= \frac{\sqrt{2}|\overline{\beta_g}\zeta_u|}{2} + \frac{\sqrt{2}|\beta_g\zeta_u|}{2} \\ \Psi_{50}(e_g^1 t_u, {}^3T_u, M=0, \eta_u) &= -\frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\beta_g}\eta_u|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\beta_g\eta_u|}{4} \\ \Psi_{51}(e_g^1 t_u, {}^3T_u, M=0, \mu_u) &= \frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\beta_g}\mu_u|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\beta_g\mu_u|}{4} \\ \Psi_{52}(e_g^1 t_u, {}^3T_u, M=1, \zeta_u) &= |\beta_g\zeta_u| \\ \Psi_{53}(e_g^1 t_u, {}^3T_u, M=1, \eta_u) &= -\frac{i(\sqrt{3}-i)|\beta_g\eta_u|}{2} \\ \Psi_{54}(e_g^1 t_u, {}^3T_u, M=1, \mu_u) &= \frac{i(\sqrt{3}+i)|\beta_g\mu_u|}{2} \\ t_g t_u \\ \boxed{\Delta E = -\langle \zeta_g \zeta_g || \zeta_u \zeta_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle} \\ \Psi_{55}(t_g t_u, {}^3T_u, M=-1, \mu_u) &= |\overline{\zeta_g}\zeta_u| \\ \Psi_{56}(t_g t_u, {}^3T_u, M=-1, \zeta_u) &= |\overline{\eta_g}\eta_u| \\ \Psi_{57}(t_g t_u, {}^3T_u, M=-1, \eta_u) &= |\overline{\mu_g}\mu_u| \\ \Psi_{58}(t_g t_u, {}^3T_u, M=0, \mu_u) &= \frac{\sqrt{2}|\overline{\zeta_g}\zeta_u|}{2} + \frac{\sqrt{2}|\zeta_g\zeta_u|}{2} \\ \Psi_{59}(t_g t_u, {}^3T_u, M=0, \zeta_u) &= \frac{\sqrt{2}|\overline{\eta_g}\eta_u|}{2} + \frac{\sqrt{2}|\eta_g\eta_u|}{2} \\ \Psi_{60}(t_g t_u, {}^3T_u, M=0, \eta_u) &= \frac{\sqrt{2}|\overline{\mu_g}\mu_u|}{2} + \frac{\sqrt{2}|\mu_g\mu_u|}{2} \\ \Psi_{61}(t_g t_u, {}^3T_u, M=1, \mu_u) &= |\zeta_g\zeta_u| \\ \Psi_{62}(t_g t_u, {}^3T_u, M=1, \zeta_u) &= |\eta_g\eta_u| \\ \Psi_{63}(t_g t_u, {}^3T_u, M=1, \eta_u) &= |\mu_g\mu_u| \end{aligned}$$

2.29.15 1T_u

$$a_g t_u$$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \zeta_u \zeta_u \rangle + \langle \alpha_g \zeta_u || \alpha_g \zeta_u \rangle}$$

$$\Psi_1(a_g t_u, {}^1T_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\zeta_u|}{2} + \frac{\sqrt{2}|\alpha_g\zeta_u|}{2}$$

$$\begin{aligned} \Psi_2(a_g t_u, {}^1T_u, M=0, \eta_u) &= -\frac{\sqrt{2}|\overline{\alpha_g}\eta_u|}{2} + \frac{\sqrt{2}|\alpha_g\eta_u|}{2} \\ \Psi_3(a_g t_u, {}^1T_u, M=0, \mu_u) &= -\frac{\sqrt{2}|\overline{\alpha_g}\mu_u|}{2} + \frac{\sqrt{2}|\alpha_g\mu_u|}{2} \\ e_u^1 t_g \\ \boxed{\Delta E = \langle \alpha_u \alpha_u || \zeta_g \zeta_g \rangle + \langle \alpha_u \zeta_g || \alpha_u \zeta_g \rangle} \\ \Psi_4(a_u t_g, {}^1T_u, M=0, \eta_u) &= -\frac{\sqrt{2}|\overline{\alpha_u}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_u\zeta_g|}{2} \\ \Psi_5(a_u t_g, {}^1T_u, M=0, \mu_u) &= -\frac{\sqrt{2}|\overline{\alpha_u}\eta_g|}{2} + \frac{\sqrt{2}|\alpha_u\eta_g|}{2} \\ \Psi_6(a_u t_g, {}^1T_u, M=0, \zeta_u) &= -\frac{\sqrt{2}|\overline{\alpha_u}\mu_g|}{2} + \frac{\sqrt{2}|\alpha_u\mu_g|}{2} \\ e_u^1 t_g \\ \boxed{\Delta E = \langle \beta_u \zeta_g || \beta_u \zeta_g \rangle} \\ \Psi_7(e_u^1 t_g, {}^1T_u, M=0, \eta_u) &= \frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\beta_u}\zeta_g|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\beta_u\zeta_g|}{4} \\ \Psi_8(e_u^1 t_g, {}^1T_u, M=0, \mu_u) &= -\frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\beta_u}\eta_g|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\beta_u\eta_g|}{4} \\ \Psi_9(e_u^1 t_g, {}^1T_u, M=0, \zeta_u) &= -\frac{\sqrt{2}|\overline{\beta_u}\mu_g|}{2} + \frac{\sqrt{2}|\beta_u\mu_g|}{2} \\ e_u^2 t_g \\ \boxed{\Delta E = \langle \gamma_u \zeta_g || \gamma_u \zeta_g \rangle} \\ \Psi_{10}(e_u^2 t_g, {}^1T_u, M=0, \eta_u) &= -\frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\gamma_u}\zeta_g|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\gamma_u\zeta_g|}{4} \\ \Psi_{11}(e_u^2 t_g, {}^1T_u, M=0, \mu_u) &= \frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\gamma_u}\eta_g|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\gamma_u\eta_g|}{4} \\ \Psi_{12}(e_u^2 t_g, {}^1T_u, M=0, \zeta_u) &= -\frac{\sqrt{2}|\overline{\gamma_u}\mu_g|}{2} + \frac{\sqrt{2}|\gamma_u\mu_g|}{2} \\ e_g^2 t_u \\ \boxed{\Delta E = \langle \gamma_g \zeta_u || \gamma_g \zeta_u \rangle} \\ \Psi_{13}(e_g^2 t_u, {}^1T_u, M=0, \zeta_u) &= -\frac{\sqrt{2}|\overline{\gamma_g}\zeta_u|}{2} + \frac{\sqrt{2}|\gamma_g\zeta_u|}{2} \\ \Psi_{14}(e_g^2 t_u, {}^1T_u, M=0, \eta_u) &= -\frac{\sqrt{2}i(\sqrt{3}+i)|\overline{\gamma_g}\eta_u|}{4} + \frac{\sqrt{2}i(\sqrt{3}+i)|\gamma_g\eta_u|}{4} \\ \Psi_{15}(e_g^2 t_u, {}^1T_u, M=0, \mu_u) &= \frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\gamma_g}\mu_u|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\gamma_g\mu_u|}{4} \\ e_g^1 t_u \\ \boxed{\Delta E = \langle \beta_g \zeta_u || \beta_g \zeta_u \rangle} \\ \Psi_{16}(e_g^1 t_u, {}^1T_u, M=0, \zeta_u) &= -\frac{\sqrt{2}|\overline{\beta_g}\zeta_u|}{2} + \frac{\sqrt{2}|\beta_g\zeta_u|}{2} \\ \Psi_{17}(e_g^1 t_u, {}^1T_u, M=0, \eta_u) &= \frac{\sqrt{2}i(\sqrt{3}-i)|\overline{\beta_g}\eta_u|}{4} - \frac{\sqrt{2}i(\sqrt{3}-i)|\beta_g\eta_u|}{4} \end{aligned}$$

$$\Psi_{18}(e_g^1 t_u, {}^1T_u, M=0, \mu_u) = -\frac{\sqrt{2}i(\sqrt{3+i})|\beta_g \mu_u|}{4} + \frac{\sqrt{2}i(\sqrt{3+i})|\beta_g \mu_u|}{4}$$

$$\boxed{\Delta E = 0}$$

$$\Delta E = \langle \zeta_g \zeta_g || \zeta_u \zeta_u \rangle + \langle \zeta_g \zeta_u || \zeta_g \zeta_u \rangle$$

$$\Psi_{19}(t_g t_u, {}^1T_u, M=0, \mu_u) = -\frac{\sqrt{2}|\zeta_g \zeta_u|}{2} + \frac{\sqrt{2}|\zeta_g \zeta_u|}{2}$$

$$\Psi_{20}(t_g t_u, {}^1T_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\eta_g \eta_u|}{2} + \frac{\sqrt{2}|\eta_g \eta_u|}{2}$$

$$\Psi_{21}(t_g t_u, {}^1T_u, M=0, \eta_u) = -\frac{\sqrt{2}|\mu_g \mu_u|}{2} + \frac{\sqrt{2}|\mu_g \mu_u|}{2}$$

2.29.16 3A_g

$e_u^1 e_u^2$

$$\Psi_1(e_u^1 e_u^2, {}^3A_g, M=-1, \alpha_g) = |\overline{\beta_u} \gamma_u|$$

$$\boxed{\Delta E = 0}$$

$$\Psi_2(e_u^1 e_u^2, {}^3A_g, M=0, \alpha_g) = \frac{\sqrt{2}|\overline{\beta_u} \gamma_u|}{2} + \frac{\sqrt{2}|\beta_u \gamma_u|}{2}$$

$$\Psi_3(e_u^1 e_u^2, {}^3A_g, M=1, \alpha_g) = |\beta_u \gamma_u|$$

$$\boxed{e_g^1 e_g^2}$$

$$\boxed{\Delta E = 0}$$

$$\Psi_4(e_g^1 e_g^2, {}^3A_g, M=-1, \alpha_g) = |\overline{\gamma_g} \beta_g|$$

$$\Psi_5(e_g^1 e_g^2, {}^3A_g, M=0, \alpha_g) = \frac{\sqrt{2}|\overline{\gamma_g} \beta_g|}{2} + \frac{\sqrt{2}|\gamma_g \beta_g|}{2}$$

$$\Psi_6(e_g^1 e_g^2, {}^3A_g, M=1, \alpha_g) = |\gamma_g \beta_g|$$

2.30 Group O Component labels

$A_1 : \{\alpha\} \longrightarrow A_2 : \{\beta\} \longrightarrow E : \{\gamma, \zeta\} \longrightarrow T_1 : \{\eta, \mu, \nu\} \longrightarrow T_2 : \{\xi, \phi, \chi\}$

$\Psi_5(t_2^2, {}^1A_1, M=0, \alpha) = -\frac{\sqrt{3}|\bar{\chi}\chi|}{3} - \frac{\sqrt{3}|\bar{\phi}\phi|}{3} - \frac{\sqrt{3}|\bar{\xi}\xi|}{3}$

2.30.1 1A_1

a_1^2

$\boxed{\Delta E = \langle \alpha\alpha || \alpha\alpha \rangle}$

$\Psi_1(a_1^2, {}^1A_1, M=0, \alpha) = -|\overline{\alpha}\alpha|$

2.30.2 3A_2

$a_1 a_2$

$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$

$\Psi_1(a_1 a_2, {}^3A_2, M=-1, \beta) = |\overline{\alpha}\beta|$

$\Psi_2(a_1 a_2, {}^3A_2, M=0, \beta) = \frac{\sqrt{2}|\overline{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\overline{\beta}|}{2}$

$\Psi_3(a_1 a_2, {}^3A_2, M=1, \beta) = |\alpha\beta|$

e^2

$\boxed{\Delta E = \langle \zeta\zeta || \gamma\gamma \rangle + \langle \zeta\zeta || \zeta\zeta \rangle}$

$\boxed{\Delta E = -3\langle \zeta\zeta || \gamma\gamma \rangle + \langle \zeta\zeta || \zeta\zeta \rangle}$

$\Psi_4(e^2, {}^3A_2, M=-1, \beta) = -|\overline{\gamma}\zeta|$

$\Psi_5(e^2, {}^3A_2, M=0, \beta) = -\frac{\sqrt{2}|\overline{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\zeta\overline{\gamma}|}{2}$

$\Psi_6(e^2, {}^3A_2, M=1, \beta) = -|\gamma\zeta|$

$t_1 t_2$

$\boxed{\Delta E = -\langle \nu\nu || \phi\phi \rangle + \langle \nu\phi || \nu\phi \rangle + 2\langle \nu\xi || \mu\phi \rangle - 2\langle \nu\mu || \xi\phi \rangle}$

$\Psi_3(e^2, {}^1A_1, M=0, \alpha) = -\frac{\sqrt{2}|\bar{\gamma}\gamma|}{2} - \frac{\sqrt{2}|\bar{\zeta}\zeta|}{2}$

t_1^2

$\boxed{\Delta E = 2\langle \nu\nu || \mu\mu \rangle + \langle \nu\nu || \nu\nu \rangle}$

$\Psi_4(t_1^2, {}^1A_1, M=0, \alpha) = -\frac{\sqrt{3}|\bar{\eta}\eta|}{3} - \frac{\sqrt{3}|\bar{\mu}\mu|}{3} - \frac{\sqrt{3}|\bar{\nu}\nu|}{3}$

t_2^2

$\boxed{\Delta E = 2\langle \xi\xi || \phi\phi \rangle + \langle \xi\xi || \xi\xi \rangle}$

$\Psi_7(t_1 t_2, {}^3A_2, M=-1, \beta) = \frac{\sqrt{3}|\bar{\eta}\chi|}{3} + \frac{\sqrt{3}|\bar{\mu}\xi|}{3} + \frac{\sqrt{3}|\bar{\nu}\phi|}{3}$

$$\begin{aligned}\Psi_8(t_1t_2, {}^3A_2, M=0, \beta) &= \frac{\sqrt{6}|\bar{\eta}\chi|}{6} + \frac{\sqrt{6}|\bar{\mu}\xi|}{6} + \frac{\sqrt{6}|\bar{\nu}\phi|}{6} + \frac{\sqrt{6}|\eta\bar{\chi}|}{6} + \frac{\sqrt{6}|\mu\bar{\xi}|}{6} + \frac{\sqrt{6}|\nu\bar{\phi}|}{6} \\ \Psi_9(t_1t_2, {}^3A_2, M=1, \beta) &= \frac{\sqrt{3}|\eta\chi|}{3} + \frac{\sqrt{3}|\mu\xi|}{3} + \frac{\sqrt{3}|\nu\phi|}{3}\end{aligned}$$

2.30.3 1A_2 *a₁a₂*

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\begin{aligned}\Psi_1(a_1a_2, {}^1A_2, M=0, \beta) &= -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2} \\ t_1t_2\end{aligned}$$

$$\begin{aligned}\Delta E &= \langle \nu\nu || \phi\phi \rangle + \langle \nu\phi || \nu\phi \rangle + 2\langle \nu\xi || \mu\phi \rangle \\ &\quad + 2\langle \nu\mu || \xi\phi \rangle\end{aligned}$$

$$\begin{aligned}\Psi_2(t_1t_2, {}^1A_2, M=0, \beta) &= -\frac{\sqrt{6}|\bar{\eta}\chi|}{6} - \frac{\sqrt{6}|\bar{\mu}\xi|}{6} - \frac{\sqrt{6}|\bar{\nu}\phi|}{6} + \frac{\sqrt{6}|\eta\bar{\chi}|}{6} + \frac{\sqrt{6}|\mu\bar{\xi}|}{6} + \frac{\sqrt{6}|\nu\bar{\phi}|}{6}\end{aligned}$$

2.30.4 3E *a₁e*

$$\boxed{\Delta E = -\langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\begin{aligned}\Psi_1(a_1e, {}^3E, M=-1, \gamma) &= |\bar{\alpha}\gamma| \\ \Psi_2(a_1e, {}^3E, M=-1, \zeta) &= |\bar{\alpha}\bar{\zeta}|\end{aligned}$$

$$\Psi_3(a_1e, {}^3E, M=0, \gamma) = \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_4(a_1e, {}^3E, M=0, \zeta) = \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

$$\Psi_5(a_1e, {}^3E, M=1, \gamma) = |\alpha\gamma|$$

$$\Psi_6(a_1e, {}^3E, M=1, \zeta) = |\alpha\zeta|$$

a₂e

$$\boxed{\Delta E = -\langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle}$$

$$\Psi_7(a_2e, {}^3E, M=-1, \zeta) = -|\bar{\beta}\bar{\gamma}|$$

$$\Psi_8(a_2e, {}^3E, M=-1, \gamma) = |\bar{\beta}\bar{\zeta}|$$

$$\Psi_9(a_2e, {}^3E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} - \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_{10}(a_2e, {}^3E, M=0, \gamma) = \frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

$$\Psi_{11}(a_2e, {}^3E, M=1, \zeta) = -|\beta\gamma|$$

$$\Psi_{12}(a_2e, {}^3E, M=1, \gamma) = |\beta\zeta|$$

t₁t₂

$$\boxed{\begin{aligned}\Delta E &= -\langle \nu\nu || \phi\phi \rangle + \langle \nu\phi || \nu\phi \rangle - \langle \nu\xi || \mu\phi \rangle \\ &\quad + \langle \nu\mu || \xi\phi \rangle\end{aligned}}$$

$$\Psi_{13}(t_1t_2, {}^3E, M=-1, \gamma) = -\frac{\sqrt{2}|\bar{\eta}\chi|}{2} + \frac{\sqrt{2}|\bar{\nu}\phi|}{2}$$

$$\Psi_{14}(t_1t_2, {}^3E, M=-1, \zeta) = \frac{\sqrt{6}|\bar{\eta}\chi|}{6} - \frac{\sqrt{6}|\bar{\mu}\xi|}{3} + \frac{\sqrt{6}|\bar{\nu}\phi|}{6}$$

$$\Psi_{15}(t_1t_2, {}^3E, M=0, \gamma) = -\frac{|\bar{\eta}\chi|}{2} + \frac{|\bar{\nu}\phi|}{2} - \frac{|\eta\bar{\chi}|}{2} + \frac{|\nu\bar{\phi}|}{2}$$

$$\begin{aligned}\Psi_{16}(t_1t_2, {}^3E, M=0, \zeta) &= \frac{\sqrt{3}|\bar{\eta}\chi|}{6} - \frac{\sqrt{3}|\bar{\mu}\xi|}{3} + \frac{\sqrt{3}|\bar{\nu}\phi|}{6} + \frac{\sqrt{3}|\mu\bar{\xi}|}{3} - \frac{\sqrt{3}|\nu\bar{\phi}|}{6} \\ \Psi_{17}(t_1t_2, {}^3E, M=1, \gamma) &= -\frac{\sqrt{2}|\bar{\eta}\chi|}{2} + \frac{\sqrt{2}|\bar{\nu}\phi|}{2}\end{aligned}$$

$$\begin{aligned}\Psi_{18}(t_1t_2, {}^3E, M=1, \zeta) &= \frac{\sqrt{6}|\eta\chi|}{6} - \frac{\sqrt{6}|\mu\xi|}{3} + \frac{\sqrt{6}|\nu\phi|}{6}\end{aligned}$$

2.30.5 1E *a₁e*

$$\boxed{\Delta E = \langle \alpha\alpha || \zeta\zeta \rangle + \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1e, {}^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_2(a_1e, {}^1E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

a₂e

$$\boxed{\Delta E = \langle \beta\beta || \zeta\zeta \rangle + \langle \beta\zeta || \beta\zeta \rangle}$$

$$\Psi_3(a_2e, {}^1E, M=0, \zeta) = \frac{\sqrt{2}|\bar{\beta}\gamma|}{2} - \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_4(a_2e, {}^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\beta}\zeta|}{2} + \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

e²

$$\boxed{\Delta E = -\langle \zeta\zeta || \gamma\gamma \rangle + \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\Psi_5(e^2, {}^1E, M=0, \gamma) = \frac{\sqrt{2}|\bar{\gamma}\gamma|}{2} - \frac{\sqrt{2}|\gamma\bar{\gamma}|}{2}$$

$$\Psi_6(e^2, {}^1E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} - \frac{\sqrt{2}|\zeta\bar{\gamma}|}{2}$$

t₁²

$$\boxed{\Delta E = -\langle \nu\nu || \mu\mu \rangle + \langle \nu\nu || \nu\nu \rangle}$$

$$\Psi_7(t_1^2, {}^1E, M=0, \gamma) = -\frac{\sqrt{6}|\bar{\eta}\eta|}{6} + \frac{\sqrt{6}|\bar{\mu}\mu|}{3} - \frac{\sqrt{6}|\bar{\nu}\nu|}{6}$$

$$\Psi_8(t_1^2, {}^1E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\eta}\eta|}{2} + \frac{\sqrt{2}|\bar{\nu}\nu|}{2}$$

t₁t₂

$$\boxed{\begin{aligned}\Delta E &= \langle \nu\nu || \phi\phi \rangle + \langle \nu\phi || \nu\phi \rangle - \langle \nu\xi || \mu\phi \rangle \\ &\quad - \langle \nu\mu || \xi\phi \rangle\end{aligned}}$$

$$\Psi_9(t_1t_2, {}^1E, M=0, \gamma) = \frac{|\bar{\eta}\chi|}{2} - \frac{|\bar{\nu}\phi|}{2} - \frac{|\eta\bar{\chi}|}{2} + \frac{|\nu\bar{\phi}|}{2}$$

$$\begin{aligned}
& -\frac{\sqrt{3}|\bar{\eta}\chi|}{6} + \frac{\sqrt{3}|\bar{\mu}\xi|}{3} - \frac{\sqrt{3}|\bar{\nu}\phi|}{6} + \frac{\sqrt{3}|\eta\bar{\chi}|}{6} - \frac{\sqrt{3}|\mu\bar{\xi}|}{3} + \frac{\sqrt{3}|\nu\bar{\phi}|}{6} \\
& \quad t_2^2 \\
& \boxed{\Delta E = -\langle\xi\xi||\phi\phi\rangle + \langle\xi\xi||\xi\xi\rangle} \\
\Psi_{11}(t_2^2, {}^1E, M=0, \gamma) &= -\frac{\sqrt{6}|\bar{\chi}\chi|}{6} - \frac{\sqrt{6}|\bar{\phi}\phi|}{6} + \frac{\sqrt{6}|\bar{\xi}\xi|}{3} \\
\Psi_{12}(t_2^2, {}^1E, M=0, \zeta) &= -\frac{\sqrt{2}|\bar{\chi}\chi|}{2} + \frac{\sqrt{2}|\bar{\phi}\phi|}{2}
\end{aligned}$$

2.30.6 3T_1 *a₁t₁*

$$\boxed{\Delta E = -\langle\alpha\alpha||\nu\nu\rangle + \langle\alpha\nu||\alpha\nu\rangle}$$

$$\begin{aligned}
\Psi_1(a_1t_1, {}^3T_1, M=-1, \eta) &= |\bar{\alpha}\eta| \\
\Psi_2(a_1t_1, {}^3T_1, M=-1, \mu) &= |\bar{\alpha}\mu| \\
\Psi_3(a_1t_1, {}^3T_1, M=-1, \nu) &= |\bar{\alpha}\nu| \\
\Psi_4(a_1t_1, {}^3T_1, M=0, \eta) &= \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2} \\
\Psi_5(a_1t_1, {}^3T_1, M=0, \mu) &= \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2} \\
\Psi_6(a_1t_1, {}^3T_1, M=0, \nu) &= \frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2} \\
\Psi_7(a_1t_1, {}^3T_1, M=1, \eta) &= |\alpha\eta| \\
\Psi_8(a_1t_1, {}^3T_1, M=1, \mu) &= |\alpha\mu| \\
\Psi_9(a_1t_1, {}^3T_1, M=1, \nu) &= |\alpha\nu|
\end{aligned}$$

a₂t₂

$$\boxed{\Delta E = -\langle\beta\beta||\xi\xi\rangle + \langle\beta\xi||\beta\xi\rangle}$$

$$\begin{aligned}
\Psi_{10}(a_2t_2, {}^3T_1, M=-1, \mu) &= |\bar{\beta}\xi| \\
\Psi_{11}(a_2t_2, {}^3T_1, M=-1, \nu) &= |\bar{\beta}\phi| \\
\Psi_{12}(a_2t_2, {}^3T_1, M=-1, \eta) &= |\bar{\beta}\chi| \\
\Psi_{13}(a_2t_2, {}^3T_1, M=0, \mu) &= \frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2} \\
\Psi_{14}(a_2t_2, {}^3T_1, M=0, \nu) &= \frac{\sqrt{2}|\bar{\beta}\phi|}{2} + \frac{\sqrt{2}|\beta\bar{\phi}|}{2} \\
\Psi_{15}(a_2t_2, {}^3T_1, M=0, \eta) &= \frac{\sqrt{2}|\bar{\beta}\chi|}{2} + \frac{\sqrt{2}|\beta\bar{\chi}|}{2} \\
\Psi_{16}(a_2t_2, {}^3T_1, M=1, \mu) &= |\beta\xi| \\
\Psi_{17}(a_2t_2, {}^3T_1, M=1, \nu) &= |\beta\phi| \\
\Psi_{18}(a_2t_2, {}^3T_1, M=1, \eta) &= |\beta\chi|
\end{aligned}$$

et₁

$$\begin{aligned}
\Delta E = & -\frac{\sqrt{3}\langle\zeta\nu||\gamma\nu\rangle}{3} + \langle\zeta\nu||\zeta\nu\rangle + \frac{\langle\zeta\zeta||\mu\mu\rangle}{3} \\
& -\frac{4\langle\zeta\zeta||\nu\nu\rangle}{3}
\end{aligned}$$

$$\begin{aligned}
\Psi_{19}(et_1, {}^3T_1, M=-1, \eta) &= \frac{|\bar{\gamma}\eta|}{2} + \frac{\sqrt{3}|\bar{\zeta}\eta|}{2} \\
\Psi_{20}(et_1, {}^3T_1, M=-1, \mu) &= -|\bar{\gamma}\mu| \\
\Psi_{21}(et_1, {}^3T_1, M=-1, \nu) &= \frac{|\bar{\gamma}\nu|}{2} - \frac{\sqrt{3}|\bar{\zeta}\nu|}{2} \\
\Psi_{22}(et_1, {}^3T_1, M=0, \eta) &= \frac{\sqrt{2}|\bar{\gamma}\eta|}{4} + \frac{\sqrt{6}|\bar{\zeta}\eta|}{4} + \frac{\sqrt{2}|\bar{\gamma}\eta|}{4} + \frac{\sqrt{6}|\zeta\bar{\eta}|}{4} \\
\Psi_{23}(et_1, {}^3T_1, M=0, \mu) &= -\frac{\sqrt{2}|\bar{\gamma}\mu|}{2} - \frac{\sqrt{2}|\gamma\bar{\mu}|}{2} \\
\Psi_{24}(et_1, {}^3T_1, M=0, \nu) &= \frac{\sqrt{2}|\bar{\gamma}\nu|}{4} - \frac{\sqrt{6}|\bar{\zeta}\nu|}{4} + \frac{\sqrt{2}|\gamma\bar{\nu}|}{4} - \frac{\sqrt{6}|\zeta\bar{\nu}|}{4} \\
\Psi_{25}(et_1, {}^3T_1, M=1, \eta) &= \frac{|\gamma\eta|}{2} + \frac{\sqrt{3}|\zeta\eta|}{2} \\
\Psi_{26}(et_1, {}^3T_1, M=1, \mu) &= -|\gamma\mu| \\
\Psi_{27}(et_1, {}^3T_1, M=1, \nu) &= \frac{|\gamma\nu|}{2} - \frac{\sqrt{3}|\zeta\nu|}{2}
\end{aligned}$$

et₂

$$\boxed{\Delta E = \langle\zeta\xi||\zeta\xi\rangle - \langle\zeta\zeta||\xi\xi\rangle}$$

$$\begin{aligned}
\Psi_{28}(et_2, {}^3T_1, M=-1, \nu) &= \frac{\sqrt{3}|\bar{\gamma}\phi|}{2} + \frac{|\bar{\zeta}\phi|}{2} \\
\Psi_{29}(et_2, {}^3T_1, M=-1, \eta) &= -\frac{\sqrt{3}|\bar{\gamma}\chi|}{2} + \frac{|\bar{\zeta}\chi|}{2} \\
\Psi_{30}(et_2, {}^3T_1, M=-1, \mu) &= -|\bar{\zeta}\xi| \\
\Psi_{31}(et_2, {}^3T_1, M=0, \nu) &= \frac{\sqrt{6}|\bar{\gamma}\phi|}{4} + \frac{\sqrt{2}|\bar{\zeta}\phi|}{4} + \frac{\sqrt{6}|\gamma\bar{\phi}|}{4} + \frac{\sqrt{2}|\zeta\bar{\phi}|}{4} \\
\Psi_{32}(et_2, {}^3T_1, M=0, \eta) &= -\frac{\sqrt{6}|\bar{\gamma}\chi|}{4} + \frac{\sqrt{2}|\bar{\zeta}\chi|}{4} - \frac{\sqrt{6}|\gamma\bar{\chi}|}{4} + \frac{\sqrt{2}|\zeta\bar{\chi}|}{4} \\
\Psi_{33}(et_2, {}^3T_1, M=0, \mu) &= -\frac{\sqrt{2}|\bar{\zeta}\xi|}{2} - \frac{\sqrt{2}|\zeta\bar{\xi}|}{2} \\
\Psi_{34}(et_2, {}^3T_1, M=1, \nu) &= \frac{\sqrt{3}|\bar{\gamma}\phi|}{2} + \frac{|\bar{\zeta}\phi|}{2} \\
\Psi_{35}(et_2, {}^3T_1, M=1, \eta) &= -\frac{\sqrt{3}|\bar{\gamma}\chi|}{2} + \frac{|\bar{\zeta}\chi|}{2} \\
\Psi_{36}(et_2, {}^3T_1, M=1, \mu) &= -|\zeta\xi|
\end{aligned}$$

t₁²

$$\boxed{\Delta E = \langle\nu\mu||\nu\mu\rangle - \langle\nu\nu||\mu\mu\rangle}$$

$$\begin{aligned}
\Psi_{37}(t_1^2, {}^3T_1, M=-1, \nu) &= -|\bar{\eta}\mu| \\
\Psi_{38}(t_1^2, {}^3T_1, M=-1, \mu) &= |\bar{\eta}\nu| \\
\Psi_{39}(t_1^2, {}^3T_1, M=-1, \eta) &= -|\mu\nu| \\
\Psi_{40}(t_1^2, {}^3T_1, M=0, \nu) &= -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} + \frac{\sqrt{2}|\bar{\mu}\eta|}{2} \\
\Psi_{41}(t_1^2, {}^3T_1, M=0, \mu) &= \frac{\sqrt{2}|\bar{\eta}\nu|}{2} - \frac{\sqrt{2}|\bar{\nu}\eta|}{2} \\
\Psi_{42}(t_1^2, {}^3T_1, M=0, \eta) &= -\frac{\sqrt{2}|\bar{\mu}\nu|}{2} + \frac{\sqrt{2}|\bar{\nu}\mu|}{2} \\
\Psi_{43}(t_1^2, {}^3T_1, M=1, \nu) &= -|\eta\mu| \\
\Psi_{44}(t_1^2, {}^3T_1, M=1, \mu) &= |\eta\nu| \\
\Psi_{45}(t_1^2, {}^3T_1, M=1, \eta) &= -|\mu\nu|
\end{aligned}$$

t₁t₂

$$\boxed{\Delta E = -\langle \nu\nu || \xi\xi \rangle + \langle \nu\xi || \mu\phi \rangle + \langle \nu\xi || \nu\xi \rangle - \langle \nu\mu || \phi\xi \rangle}$$

$$\begin{aligned}\Psi_{46}(t_1 t_2, {}^3T_1, M=-1, \nu) &= \frac{\sqrt{2}|\bar{\eta}\bar{\xi}|}{2} + \frac{\sqrt{2}|\bar{\mu}\bar{\chi}|}{2} \\ \Psi_{47}(t_1 t_2, {}^3T_1, M=-1, \mu) &= \frac{\sqrt{2}|\bar{\eta}\bar{\phi}|}{2} + \frac{\sqrt{2}|\bar{\nu}\bar{\chi}|}{2} \\ \Psi_{48}(t_1 t_2, {}^3T_1, M=-1, \eta) &= \frac{\sqrt{2}|\bar{\mu}\bar{\phi}|}{2} + \frac{\sqrt{2}|\bar{\nu}\bar{\xi}|}{2} \\ \Psi_{49}(t_1 t_2, {}^3T_1, M=0, \nu) &= \frac{|\bar{\eta}\bar{\xi}|}{2} + \frac{|\bar{\mu}\bar{\chi}|}{2} + \frac{|\bar{\eta}\bar{\xi}|}{2} + \frac{|\bar{\mu}\bar{\chi}|}{2} \\ \Psi_{50}(t_1 t_2, {}^3T_1, M=0, \mu) &= \frac{|\bar{\eta}\bar{\phi}|}{2} + \frac{|\bar{\nu}\bar{\chi}|}{2} + \frac{|\bar{\eta}\bar{\phi}|}{2} + \frac{|\bar{\nu}\bar{\chi}|}{2} \\ \Psi_{51}(t_1 t_2, {}^3T_1, M=0, \eta) &= \frac{|\bar{\mu}\bar{\phi}|}{2} + \frac{|\bar{\nu}\bar{\xi}|}{2} + \frac{|\bar{\mu}\bar{\phi}|}{2} + \frac{|\bar{\nu}\bar{\xi}|}{2} \\ \Psi_{52}(t_1 t_2, {}^3T_1, M=1, \nu) &= \frac{\sqrt{2}|\eta\xi|}{2} + \frac{\sqrt{2}|\mu\chi|}{2} \\ \Psi_{53}(t_1 t_2, {}^3T_1, M=1, \mu) &= \frac{\sqrt{2}|\eta\phi|}{2} + \frac{\sqrt{2}|\nu\chi|}{2} \\ \Psi_{54}(t_1 t_2, {}^3T_1, M=1, \eta) &= \frac{\sqrt{2}|\mu\phi|}{2} + \frac{\sqrt{2}|\nu\xi|}{2}\end{aligned}$$

 t_2^2

$$\boxed{\Delta E = \langle \xi\phi || \xi\phi \rangle - \langle \xi\xi || \phi\phi \rangle}$$

$$\Psi_{55}(t_2^2, {}^3T_1, M=-1, \eta) = -|\bar{\xi}\bar{\phi}|$$

$$\Psi_{56}(t_2^2, {}^3T_1, M=-1, \nu) = |\bar{\xi}\bar{\chi}|$$

$$\Psi_{57}(t_2^2, {}^3T_1, M=-1, \mu) = -|\bar{\phi}\bar{\chi}|$$

$$\Psi_{58}(t_2^2, {}^3T_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\phi}\xi|}{2} - \frac{\sqrt{2}|\bar{\xi}\phi|}{2}$$

$$\Psi_{59}(t_2^2, {}^3T_1, M=0, \nu) = -\frac{\sqrt{2}|\bar{\chi}\xi|}{2} + \frac{\sqrt{2}|\bar{\xi}\chi|}{2}$$

$$\Psi_{60}(t_2^2, {}^3T_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\chi}\phi|}{2} - \frac{\sqrt{2}|\bar{\phi}\chi|}{2}$$

$$\Psi_{61}(t_2^2, {}^3T_1, M=1, \eta) = -|\xi\phi|$$

$$\Psi_{62}(t_2^2, {}^3T_1, M=1, \nu) = |\xi\chi|$$

$$\Psi_{63}(t_2^2, {}^3T_1, M=1, \mu) = -|\phi\chi|$$

2.30.7 1T_1 $a_1 t_1$

$$\boxed{\Delta E = \langle \alpha\alpha || \nu\nu \rangle + \langle \alpha\nu || \alpha\nu \rangle}$$

$$\Psi_1(a_1 t_1, {}^1T_1, M=0, \eta) = -\frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_2(a_1 t_1, {}^1T_1, M=0, \mu) = -\frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_3(a_1 t_1, {}^1T_1, M=0, \nu) = -\frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2}$$

 $a_2 t_2$

$$\boxed{\Delta E = \langle \beta\beta || \xi\xi \rangle + \langle \beta\xi || \beta\xi \rangle}$$

$$\begin{aligned}\Psi_4(a_2 t_2, {}^1T_1, M=0, \mu) &= -\frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2} \\ \Psi_5(a_2 t_2, {}^1T_1, M=0, \nu) &= -\frac{\sqrt{2}|\bar{\beta}\phi|}{2} + \frac{\sqrt{2}|\beta\bar{\phi}|}{2} \\ \Psi_6(a_2 t_2, {}^1T_1, M=0, \eta) &= -\frac{\sqrt{2}|\bar{\beta}\chi|}{2} + \frac{\sqrt{2}|\beta\bar{\chi}|}{2}\end{aligned}$$

 et_1

$$\boxed{\Delta E = -\frac{\sqrt{3}\langle \zeta\nu || \gamma\nu \rangle}{3} + \langle \zeta\nu || \zeta\nu \rangle - \frac{\langle \zeta\zeta || \mu\mu \rangle}{3} + \frac{4\langle \zeta\zeta || \nu\nu \rangle}{3}}$$

$$\begin{aligned}\Psi_7(et_1, {}^1T_1, M=0, \eta) &= -\frac{\sqrt{2}|\bar{\gamma}\eta|}{4} - \frac{\sqrt{6}|\bar{\zeta}\eta|}{4} + \frac{\sqrt{2}|\gamma\bar{\eta}|}{4} + \frac{\sqrt{6}|\zeta\bar{\eta}|}{4} \\ \Psi_8(et_1, {}^1T_1, M=0, \mu) &= \frac{\sqrt{2}|\bar{\gamma}\mu|}{2} - \frac{\sqrt{2}|\gamma\bar{\mu}|}{2} \\ \Psi_9(et_1, {}^1T_1, M=0, \nu) &= -\frac{\sqrt{2}|\bar{\gamma}\nu|}{4} + \frac{\sqrt{6}|\bar{\zeta}\nu|}{4} + \frac{\sqrt{2}|\gamma\bar{\nu}|}{4} - \frac{\sqrt{6}|\zeta\bar{\nu}|}{4}\end{aligned}$$

 et_2

$$\boxed{\Delta E = \langle \zeta\xi || \zeta\xi \rangle + \langle \zeta\zeta || \xi\xi \rangle}$$

$$\begin{aligned}\Psi_{10}(et_2, {}^1T_1, M=0, \nu) &= -\frac{\sqrt{6}|\bar{\gamma}\phi|}{4} - \frac{\sqrt{2}|\bar{\zeta}\phi|}{4} + \frac{\sqrt{6}|\gamma\bar{\phi}|}{4} + \frac{\sqrt{2}|\zeta\bar{\phi}|}{4} \\ \Psi_{11}(et_2, {}^1T_1, M=0, \eta) &= \frac{\sqrt{6}|\bar{\gamma}\chi|}{4} - \frac{\sqrt{2}|\bar{\zeta}\chi|}{4} - \frac{\sqrt{6}|\gamma\bar{\chi}|}{4} + \frac{\sqrt{2}|\zeta\bar{\chi}|}{4} \\ \Psi_{12}(et_2, {}^1T_1, M=0, \mu) &= \frac{\sqrt{2}|\bar{\zeta}\xi|}{2} - \frac{\sqrt{2}|\zeta\bar{\xi}|}{2}\end{aligned}$$

 $t_1 t_2$

$$\boxed{\Delta E = \langle \nu\nu || \xi\xi \rangle + \langle \nu\xi || \mu\phi \rangle + \langle \nu\xi || \nu\xi \rangle + \langle \nu\mu || \phi\xi \rangle}$$

$$\Psi_{13}(t_1 t_2, {}^1T_1, M=0, \nu) = -\frac{|\bar{\eta}\xi|}{2} - \frac{|\bar{\mu}\chi|}{2} + \frac{|\bar{\eta}\xi|}{2} + \frac{|\mu\bar{\chi}|}{2}$$

$$\Psi_{14}(t_1 t_2, {}^1T_1, M=0, \mu) = -\frac{|\bar{\eta}\phi|}{2} - \frac{|\bar{\nu}\chi|}{2} + \frac{|\bar{\eta}\phi|}{2} + \frac{|\nu\bar{\chi}|}{2}$$

$$\Psi_{15}(t_1 t_2, {}^1T_1, M=0, \eta) = -\frac{|\bar{\mu}\phi|}{2} - \frac{|\bar{\nu}\xi|}{2} + \frac{|\bar{\mu}\phi|}{2} + \frac{|\nu\bar{\xi}|}{2}$$

2.30.8 3T_2 $a_1 t_2$

$$\boxed{\Delta E = -\langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle}$$

$$\Psi_1(a_1 t_2, {}^3T_2, M=-1, \xi) = |\bar{\alpha}\bar{\xi}|$$

$$\Psi_2(a_1 t_2, {}^3T_2, M=-1, \phi) = |\bar{\alpha}\bar{\phi}|$$

$$\Psi_3(a_1 t_2, {}^3T_2, M=-1, \chi) = |\bar{\alpha}\bar{\chi}|$$

$$\Psi_4(a_1 t_2, {}^3T_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\alpha}\xi|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2}$$

$$\Psi_5(a_1 t_2, {}^3T_2, M=0, \phi) = \frac{\sqrt{2}|\bar{\alpha}\phi|}{2} + \frac{\sqrt{2}|\alpha\bar{\phi}|}{2}$$

$$\Psi_6(a_1 t_2, {}^3T_2, M=0, \chi) = \frac{\sqrt{2}|\bar{\alpha}\chi|}{2} + \frac{\sqrt{2}|\alpha\bar{\chi}|}{2}$$

$$\Psi_7(a_1 t_2, {}^3T_2, M=1, \xi) = |\alpha\xi|$$

$$\Psi_8(a_1 t_2, {}^3T_2, M=1, \phi) = |\alpha\phi|$$

$$\Psi_9(a_1 t_2, {}^3T_2, M=1, \chi) = |\alpha\chi|$$

a₂t₁

$$\boxed{\Delta E = -\langle \beta\beta || \nu\nu \rangle + \langle \beta\nu || \beta\nu \rangle}$$

$$\Psi_{10}(a_2 t_1, {}^3T_2, M=-1, \chi) = |\bar{\beta}\bar{\eta}|$$

$$\Psi_{11}(a_2 t_1, {}^3T_2, M=-1, \xi) = |\bar{\beta}\bar{\mu}|$$

$$\Psi_{12}(a_2 t_1, {}^3T_2, M=-1, \phi) = |\bar{\beta}\bar{\nu}|$$

$$\Psi_{13}(a_2 t_1, {}^3T_2, M=0, \chi) = \frac{\sqrt{2}|\bar{\beta}\eta|}{2} + \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_{14}(a_2 t_1, {}^3T_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_{15}(a_2 t_1, {}^3T_2, M=0, \phi) = \frac{\sqrt{2}|\bar{\beta}\nu|}{2} + \frac{\sqrt{2}|\beta\bar{\nu}|}{2}$$

$$\Psi_{16}(a_2 t_1, {}^3T_2, M=1, \chi) = |\beta\eta|$$

$$\Psi_{17}(a_2 t_1, {}^3T_2, M=1, \xi) = |\beta\mu|$$

$$\Psi_{18}(a_2 t_1, {}^3T_2, M=1, \phi) = |\beta\nu|$$

et₁

$$\boxed{\Delta E = \sqrt{3} \langle \zeta\nu || \gamma\nu \rangle + \langle \zeta\nu || \zeta\nu \rangle - \langle \zeta\zeta || \mu\mu \rangle}$$

$$\Psi_{19}(et_1, {}^3T_2, M=-1, \chi) = \frac{\sqrt{3}|\bar{\gamma}\bar{\eta}|}{2} - \frac{|\bar{\zeta}\bar{\eta}|}{2}$$

$$\Psi_{20}(et_1, {}^3T_2, M=-1, \phi) = -\frac{\sqrt{3}|\bar{\gamma}\bar{\nu}|}{2} - \frac{|\bar{\zeta}\bar{\nu}|}{2}$$

$$\Psi_{21}(et_1, {}^3T_2, M=-1, \xi) = |\bar{\zeta}\bar{\mu}|$$

$$\Psi_{22}(et_1, {}^3T_2, M=0, \chi) = \frac{\sqrt{6}|\bar{\gamma}\eta|}{4} - \frac{\sqrt{2}|\bar{\zeta}\eta|}{4} + \frac{\sqrt{6}|\gamma\bar{\eta}|}{4} - \frac{\sqrt{2}|\zeta\bar{\eta}|}{4}$$

$$\Psi_{23}(et_1, {}^3T_2, M=0, \phi) = -\frac{\sqrt{6}|\bar{\gamma}\nu|}{4} - \frac{\sqrt{2}|\bar{\zeta}\nu|}{4} - \frac{\sqrt{6}|\gamma\bar{\nu}|}{4} - \frac{\sqrt{2}|\zeta\bar{\nu}|}{4}$$

$$\Psi_{24}(et_1, {}^3T_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\zeta}\mu|}{2} + \frac{\sqrt{2}|\zeta\bar{\mu}|}{2}$$

$$\Psi_{25}(et_1, {}^3T_2, M=1, \chi) = \frac{\sqrt{3}|\gamma\eta|}{2} - \frac{|\zeta\eta|}{2}$$

$$\Psi_{26}(et_1, {}^3T_2, M=1, \phi) = -\frac{\sqrt{3}|\gamma\nu|}{2} - \frac{|\zeta\nu|}{2}$$

$$\Psi_{27}(et_1, {}^3T_2, M=1, \xi) = |\zeta\mu|$$

et₂

$$\boxed{\Delta E = \frac{4 \langle \zeta\phi || \zeta\phi \rangle}{3} - \frac{\langle \zeta\xi || \zeta\xi \rangle}{3} - \frac{4 \langle \zeta\zeta || \phi\phi \rangle}{3} + \frac{\langle \zeta\zeta || \xi\xi \rangle}{3}}$$

$$\Psi_{28}(et_2, {}^3T_2, M=-1, \xi) = |\bar{\gamma}\bar{\xi}|$$

$$\Psi_{29}(et_2, {}^3T_2, M=-1, \phi) = -\frac{|\bar{\gamma}\bar{\phi}|}{2} + \frac{\sqrt{3}|\bar{\zeta}\bar{\phi}|}{2}$$

$$\Psi_{30}(et_2, {}^3T_2, M=-1, \chi) = -\frac{|\bar{\gamma}\bar{\chi}|}{2} - \frac{\sqrt{3}|\bar{\zeta}\bar{\chi}|}{2}$$

$$\Psi_{31}(et_2, {}^3T_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\gamma}\xi|}{2} + \frac{\sqrt{2}|\gamma\bar{\xi}|}{2}$$

$$\Psi_{32}(et_2, {}^3T_2, M=0, \phi) = -\frac{\sqrt{2}|\bar{\gamma}\phi|}{4} + \frac{\sqrt{6}|\bar{\zeta}\phi|}{4} - \frac{\sqrt{2}|\gamma\bar{\phi}|}{4} + \frac{\sqrt{6}|\zeta\bar{\phi}|}{4}$$

$$\Psi_{33}(et_2, {}^3T_2, M=0, \chi) = -\frac{\sqrt{2}|\bar{\gamma}\chi|}{4} - \frac{\sqrt{6}|\bar{\zeta}\chi|}{4} - \frac{\sqrt{2}|\gamma\bar{\chi}|}{4} - \frac{\sqrt{6}|\zeta\bar{\chi}|}{4}$$

$$\Psi_{34}(et_2, {}^3T_2, M=1, \xi) = |\gamma\xi|$$

$$\Psi_{35}(et_2, {}^3T_2, M=1, \phi) = -\frac{|\gamma\phi|}{2} + \frac{\sqrt{3}|\zeta\phi|}{2}$$

$$\Psi_{36}(et_2, {}^3T_2, M=1, \chi) = -\frac{|\gamma\chi|}{2} - \frac{\sqrt{3}|\zeta\chi|}{2}$$

t₁t₂

$$\boxed{\Delta E = -\langle \nu\nu || \xi\xi \rangle - \langle \nu\xi || \mu\phi \rangle + \langle \nu\xi || \nu\xi \rangle + \langle \nu\mu || \phi\xi \rangle}$$

$$\Psi_{37}(t_1 t_2, {}^3T_2, M=-1, \phi) = \frac{\sqrt{2}|\bar{\eta}\bar{\xi}|}{2} - \frac{\sqrt{2}|\bar{\mu}\bar{\chi}|}{2}$$

$$\Psi_{38}(t_1 t_2, {}^3T_2, M=-1, \xi) = -\frac{\sqrt{2}|\bar{\eta}\bar{\phi}|}{2} + \frac{\sqrt{2}|\bar{\nu}\bar{\chi}|}{2}$$

$$\Psi_{39}(t_1 t_2, {}^3T_2, M=-1, \chi) = \frac{\sqrt{2}|\bar{\mu}\bar{\phi}|}{2} - \frac{\sqrt{2}|\bar{\nu}\bar{\xi}|}{2}$$

$$\Psi_{40}(t_1 t_2, {}^3T_2, M=0, \phi) = \frac{|\bar{\eta}\xi|}{2} - \frac{|\bar{\mu}\chi|}{2} + \frac{|\eta\bar{\xi}|}{2} - \frac{|\mu\bar{\chi}|}{2}$$

$$\Psi_{41}(t_1 t_2, {}^3T_2, M=0, \xi) = -\frac{|\bar{\eta}\phi|}{2} + \frac{|\bar{\nu}\chi|}{2} - \frac{|\eta\bar{\phi}|}{2} + \frac{|\nu\bar{\chi}|}{2}$$

$$\Psi_{42}(t_1 t_2, {}^3T_2, M=0, \chi) = \frac{|\bar{\mu}\phi|}{2} - \frac{|\bar{\nu}\xi|}{2} + \frac{|\mu\bar{\phi}|}{2} - \frac{|\nu\bar{\xi}|}{2}$$

$$\Psi_{43}(t_1 t_2, {}^3T_2, M=1, \phi) = \frac{\sqrt{2}|\eta\xi|}{2} - \frac{\sqrt{2}|\mu\chi|}{2}$$

$$\Psi_{44}(t_1 t_2, {}^3T_2, M=1, \xi) = -\frac{\sqrt{2}|\eta\phi|}{2} + \frac{\sqrt{2}|\nu\chi|}{2}$$

$$\Psi_{45}(t_1 t_2, {}^3T_2, M=1, \chi) = \frac{\sqrt{2}|\mu\phi|}{2} - \frac{\sqrt{2}|\nu\xi|}{2}$$

2.30.9 ¹T₂

a₁t₂

$$\boxed{\Delta E = \langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle}$$

$$\Psi_1(a_1 t_2, {}^1T_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\alpha}\xi|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2}$$

$$\Psi_2(a_1 t_2, {}^1T_2, M=0, \phi) = -\frac{\sqrt{2}|\bar{\alpha}\phi|}{2} + \frac{\sqrt{2}|\alpha\bar{\phi}|}{2}$$

$$\Psi_3(a_1 t_2, {}^1T_2, M=0, \chi) = -\frac{\sqrt{2}|\bar{\alpha}\chi|}{2} + \frac{\sqrt{2}|\alpha\bar{\chi}|}{2}$$

a₂t₁

$$\boxed{\Delta E = \langle \beta\beta || \nu\nu \rangle + \langle \beta\nu || \beta\nu \rangle}$$

$$\Psi_4(a_2 t_1, {}^1T_2, M=0, \chi) = -\frac{\sqrt{2}|\bar{\beta}\eta|}{2} + \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_5(a_2 t_1, {}^1T_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_6(a_2 t_1, {}^1T_2, M=0, \phi) = -\frac{\sqrt{2}|\bar{\beta}\nu|}{2} + \frac{\sqrt{2}|\beta\bar{\nu}|}{2}$$

et₁

$$\boxed{\Delta E = \sqrt{3} \langle \zeta \nu | \gamma \nu \rangle + \langle \zeta \nu | \zeta \nu \rangle + \langle \zeta \zeta | \mu \mu \rangle}$$

$$\Psi_7(e t_1, {}^1 T_2, M=0, \chi) = -\frac{\sqrt{6} |\bar{\gamma} \eta|}{4} + \frac{\sqrt{2} |\bar{\zeta} \eta|}{4} + \frac{\sqrt{6} |\gamma \bar{\eta}|}{4} - \frac{\sqrt{2} |\zeta \bar{\eta}|}{4}$$

$$\Psi_8(e t_1, {}^1 T_2, M=0, \phi) = \frac{\sqrt{6} |\bar{\gamma} \nu|}{4} + \frac{\sqrt{2} |\bar{\zeta} \nu|}{4} - \frac{\sqrt{6} |\gamma \bar{\nu}|}{4} - \frac{\sqrt{2} |\zeta \bar{\nu}|}{4}$$

$$\Psi_9(e t_1, {}^1 T_2, M=0, \xi) = -\frac{\sqrt{2} |\bar{\zeta} \mu|}{2} + \frac{\sqrt{2} |\zeta \bar{\mu}|}{2}$$

$$\boxed{\Delta E = \frac{4 \langle \zeta \phi | \zeta \phi \rangle}{3} - \frac{\langle \zeta \xi | \zeta \xi \rangle}{3} + \frac{4 \langle \zeta \zeta | \phi \phi \rangle}{3} - \frac{\langle \zeta \zeta | \xi \xi \rangle}{3}}$$

$$\Psi_{10}(e t_2, {}^1 T_2, M=0, \xi) = -\frac{\sqrt{2} |\bar{\gamma} \xi|}{2} + \frac{\sqrt{2} |\gamma \bar{\xi}|}{2}$$

$$\Psi_{11}(e t_2, {}^1 T_2, M=0, \phi) = \frac{\sqrt{2} |\bar{\gamma} \phi|}{4} - \frac{\sqrt{6} |\bar{\zeta} \phi|}{4} - \frac{\sqrt{2} |\gamma \bar{\phi}|}{4} + \frac{\sqrt{6} |\zeta \bar{\phi}|}{4}$$

$$\Psi_{12}(e t_2, {}^1 T_2, M=0, \chi) = \frac{\sqrt{2} |\bar{\gamma} \chi|}{4} + \frac{\sqrt{6} |\bar{\zeta} \chi|}{4} - \frac{\sqrt{2} |\gamma \bar{\chi}|}{4} - \frac{\sqrt{6} |\zeta \bar{\chi}|}{4}$$

t_1^2

$$\boxed{\Delta E = \langle \nu \mu | \nu \mu \rangle + \langle \nu \nu | \mu \mu \rangle}$$

$$\Psi_{13}(t_1^2, {}^1 T_2, M=0, \phi) = -\frac{\sqrt{2} |\bar{\eta} \mu|}{2} - \frac{\sqrt{2} |\bar{\mu} \eta|}{2}$$

$$\Psi_{14}(t_1^2, {}^1 T_2, M=0, \xi) = -\frac{\sqrt{2} |\bar{\eta} \nu|}{2} - \frac{\sqrt{2} |\bar{\nu} \eta|}{2}$$

$$\Psi_{15}(t_1^2, {}^1 T_2, M=0, \chi) = -\frac{\sqrt{2} |\bar{\mu} \nu|}{2} - \frac{\sqrt{2} |\bar{\nu} \mu|}{2}$$

$t_1 t_2$

$$\boxed{\Delta E = \langle \nu \nu | \xi \xi \rangle - \langle \nu \xi | \mu \phi \rangle + \langle \nu \xi | \nu \xi \rangle - \langle \nu \mu | \phi \xi \rangle}$$

$$\Psi_{16}(t_1 t_2, {}^1 T_2, M=0, \phi) = -\frac{|\bar{\eta} \xi|}{2} + \frac{|\bar{\mu} \chi|}{2} + \frac{|\eta \bar{\xi}|}{2} - \frac{|\mu \bar{\chi}|}{2}$$

$$\Psi_{17}(t_1 t_2, {}^1 T_2, M=0, \xi) = \frac{|\bar{\eta} \phi|}{2} - \frac{|\bar{\nu} \chi|}{2} - \frac{|\eta \bar{\phi}|}{2} + \frac{|\nu \bar{\chi}|}{2}$$

$$\Psi_{18}(t_1 t_2, {}^1 T_2, M=0, \chi) = -\frac{|\bar{\mu} \phi|}{2} + \frac{|\bar{\nu} \xi|}{2} + \frac{|\mu \bar{\phi}|}{2} - \frac{|\nu \bar{\xi}|}{2}$$

t_2^2

$$\boxed{\Delta E = \langle \xi \phi | \xi \phi \rangle + \langle \xi \xi | \phi \phi \rangle}$$

$$\Psi_{19}(t_2^2, {}^1 T_2, M=0, \chi) = -\frac{\sqrt{2} |\bar{\phi} \xi|}{2} - \frac{\sqrt{2} |\bar{\xi} \phi|}{2}$$

$$\Psi_{20}(t_2^2, {}^1 T_2, M=0, \phi) = -\frac{\sqrt{2} |\bar{\chi} \xi|}{2} - \frac{\sqrt{2} |\bar{\xi} \chi|}{2}$$

$$\Psi_{21}(t_2^2, {}^1 T_2, M=0, \xi) = -\frac{\sqrt{2} |\bar{\chi} \phi|}{2} - \frac{\sqrt{2} |\bar{\phi} \chi|}{2}$$

2.31 Group T_d

Component labels

$$A_1 : \{\alpha\} \longrightarrow A_2 : \{\beta\} \longrightarrow E : \{\gamma, \zeta\} \longrightarrow T_2 : \{\xi, \phi, \chi\} \longrightarrow T_1 : \{\eta, \mu, \nu\}$$

$$\boxed{\Psi_3(e^2, {}^1 A_1, M=0, \alpha) = -\frac{\sqrt{2} |\bar{\gamma} \zeta|}{2} - \frac{\sqrt{2} |\bar{\zeta} \gamma|}{2}}$$

2.31.1 ${}^1 A_1$

t_2^2

a_1^2

$$\boxed{\Delta E = \langle \alpha \alpha | \alpha \alpha \rangle}$$

$$\Psi_1(a_1^2, {}^1 A_1, M=0, \alpha) = -|\bar{\alpha} \alpha|$$

a_2^2

$$\boxed{\Delta E = \langle \beta \beta | \beta \beta \rangle}$$

$$\Psi_2(a_2^2, {}^1 A_1, M=0, \alpha) = -|\bar{\beta} \beta|$$

e^2

$$\boxed{\Delta E = \langle \zeta \gamma | \zeta \gamma \rangle}$$

$$\boxed{\Delta E = 2 \langle \xi \xi | \phi \phi \rangle + \langle \xi \xi | \xi \xi \rangle}$$

$$\Psi_4(t_2^2, {}^1 A_1, M=0, \alpha) = -\frac{\sqrt{3} |\bar{\chi} \chi|}{3} - \frac{\sqrt{3} |\bar{\phi} \phi|}{3} - \frac{\sqrt{3} |\bar{\xi} \xi|}{3}$$

t_1^2

$$\boxed{\Delta E = 2 \langle \nu \nu | \mu \mu \rangle + \langle \nu \nu | \nu \nu \rangle}$$

$$\Psi_5(t_1^2, {}^1 A_1, M=0, \alpha) = -\frac{\sqrt{3} |\bar{\eta} \eta|}{3} - \frac{\sqrt{3} |\bar{\mu} \mu|}{3} - \frac{\sqrt{3} |\bar{\nu} \nu|}{3}$$

2.31.2 3A_2 **$a_1 a_2$**

$$\boxed{\Delta E = -\langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\begin{aligned}\Psi_1(a_1 a_2, ^3A_2, M=-1, \beta) &= |\bar{\alpha}\bar{\beta}| \\ \Psi_2(a_1 a_2, ^3A_2, M=0, \beta) &= \frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2} \\ \Psi_3(a_1 a_2, ^3A_2, M=1, \beta) &= |\alpha\beta|\end{aligned}$$

 e^2

$$\boxed{\Delta E = \langle \zeta\gamma || \zeta\gamma \rangle}$$

$$\begin{aligned}\Psi_4(e^2, ^3A_2, M=-1, \beta) &= -|\bar{\gamma}\bar{\zeta}| \\ \Psi_5(e^2, ^3A_2, M=0, \beta) &= -\frac{\sqrt{2}|\bar{\gamma}\zeta|}{2} + \frac{\sqrt{2}|\bar{\zeta}\gamma|}{2} \\ \Psi_6(e^2, ^3A_2, M=1, \beta) &= -|\gamma\zeta|\end{aligned}$$

 $t_1 t_2$

$$\boxed{\Delta E = 2\langle \xi\eta || \phi\mu \rangle + \langle \xi\eta || \xi\eta \rangle - \langle \xi\xi || \eta\eta \rangle - 2\langle \xi\phi || \mu\eta \rangle}$$

$$\begin{aligned}\Psi_7(t_1 t_2, ^3A_2, M=-1, \beta) &= \frac{\sqrt{3}|\bar{\chi}\nu|}{3} + \frac{\sqrt{3}|\bar{\phi}\mu|}{3} + \frac{\sqrt{3}|\bar{\xi}\eta|}{3} \\ \Psi_8(t_1 t_2, ^3A_2, M=0, \beta) &= \frac{\sqrt{6}|\bar{\chi}\nu|}{6} + \frac{\sqrt{6}|\bar{\phi}\mu|}{6} + \frac{\sqrt{6}|\bar{\xi}\eta|}{6} + \frac{\sqrt{6}|\chi\nu|}{6} + \frac{\sqrt{6}|\phi\mu|}{6} + \frac{\sqrt{6}|\xi\eta|}{6} \\ \Psi_9(t_1 t_2, ^3A_2, M=1, \beta) &= \frac{\sqrt{3}|\chi\nu|}{3} + \frac{\sqrt{3}|\phi\mu|}{3} + \frac{\sqrt{3}|\xi\eta|}{3}\end{aligned}$$

2.31.3 1A_2 **$a_1 a_2$**

$$\boxed{\Delta E = \langle \alpha\alpha || \beta\beta \rangle + \langle \alpha\beta || \alpha\beta \rangle}$$

$$\Psi_1(a_1 a_2, ^1A_2, M=0, \beta) = -\frac{\sqrt{2}|\bar{\alpha}\beta|}{2} + \frac{\sqrt{2}|\alpha\bar{\beta}|}{2}$$

 $t_1 t_2$

$$\boxed{\Delta E = 2\langle \xi\eta || \phi\mu \rangle + \langle \xi\eta || \xi\eta \rangle + \langle \xi\xi || \eta\eta \rangle + 2\langle \xi\phi || \mu\eta \rangle}$$

$$\begin{aligned}\Psi_2(t_1 t_2, ^1A_2, M=0, \beta) &= -\frac{\sqrt{6}|\bar{\chi}\nu|}{6} - \frac{\sqrt{6}|\bar{\phi}\mu|}{6} - \frac{\sqrt{6}|\bar{\xi}\eta|}{6} + \frac{\sqrt{6}|\chi\nu|}{6} + \frac{\sqrt{6}|\phi\mu|}{6} + \frac{\sqrt{6}|\xi\eta|}{6}\end{aligned}$$

2.31.4 3E **$a_1 e$**

$$\boxed{\Delta E = \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\begin{aligned}\Psi_1(a_1 e, ^3E, M=-1, \gamma) &= |\bar{\alpha}\bar{\gamma}| \\ \Psi_2(a_1 e, ^3E, M=-1, \zeta) &= |\bar{\alpha}\bar{\zeta}| \\ \Psi_3(a_1 e, ^3E, M=0, \gamma) &= \frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2} \\ \Psi_4(a_1 e, ^3E, M=0, \zeta) &= \frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2} \\ \Psi_5(a_1 e, ^3E, M=1, \gamma) &= |\alpha\gamma| \\ \Psi_6(a_1 e, ^3E, M=1, \zeta) &= |\alpha\zeta|\end{aligned}$$

 $a_2 e$

$$\boxed{\Delta E = \langle \beta\zeta || \beta\zeta \rangle}$$

$$\begin{aligned}\Psi_7(a_2 e, ^3E, M=-1, \gamma) &= |\bar{\beta}\bar{\gamma}| \\ \Psi_8(a_2 e, ^3E, M=-1, \zeta) &= -|\bar{\beta}\bar{\zeta}| \\ \Psi_9(a_2 e, ^3E, M=0, \gamma) &= \frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2} \\ \Psi_{10}(a_2 e, ^3E, M=0, \zeta) &= -\frac{\sqrt{2}|\bar{\beta}\zeta|}{2} - \frac{\sqrt{2}|\beta\bar{\zeta}|}{2} \\ \Psi_{11}(a_2 e, ^3E, M=1, \gamma) &= |\beta\gamma| \\ \Psi_{12}(a_2 e, ^3E, M=1, \zeta) &= -|\beta\zeta|\end{aligned}$$

 $t_1 t_2$

$$\boxed{\Delta E = -\langle \xi\eta || \phi\mu \rangle + \langle \xi\eta || \xi\eta \rangle - \langle \xi\xi || \eta\eta \rangle + \langle \xi\phi || \mu\eta \rangle}$$

$$\begin{aligned}\Psi_{13}(t_1 t_2, ^3E, M=-1, \gamma) &= \frac{\sqrt{3}|\bar{\chi}\nu|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\bar{\phi}\bar{\mu}| + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\bar{\xi}\bar{\eta}| \\ \Psi_{14}(t_1 t_2, ^3E, M=-1, \zeta) &= \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\bar{\chi}\nu| - \frac{\sqrt{3}|\bar{\phi}\bar{\mu}|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\bar{\xi}\bar{\eta}| \\ \Psi_{15}(t_1 t_2, ^3E, M=0, \gamma) &= \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\phi}\bar{\mu}|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\bar{\xi}\bar{\eta}|}{6} + \frac{\sqrt{6}|\chi\nu|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\phi\bar{\mu}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\xi\bar{\eta}|}{2} \\ \Psi_{16}(t_1 t_2, ^3E, M=0, \zeta) &= \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\bar{\chi}\nu|}{2} - \frac{\sqrt{6}|\bar{\phi}\bar{\mu}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\xi}\bar{\eta}|}{2} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\chi}\nu|}{2} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\chi\nu|}{2} - \frac{\sqrt{6}|\phi\bar{\mu}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\xi\bar{\eta}|}{2} \\ \Psi_{17}(t_1 t_2, ^3E, M=1, \gamma) &= \frac{\sqrt{3}|\chi\nu|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\phi\mu| + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\xi\eta| \\ \Psi_{18}(t_1 t_2, ^3E, M=1, \zeta) &= \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\chi\nu| - \frac{\sqrt{3}|\phi\mu|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\xi\eta|\end{aligned}$$

2.31.5 1E **a_1e**

$$\boxed{\Delta E = \langle \alpha\zeta || \alpha\zeta \rangle}$$

$$\Psi_1(a_1e, ^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\alpha}\gamma|}{2} + \frac{\sqrt{2}|\alpha\bar{\gamma}|}{2}$$

$$\Psi_2(a_1e, ^1E, M=0, \zeta) = -\frac{\sqrt{2}|\bar{\alpha}\zeta|}{2} + \frac{\sqrt{2}|\alpha\bar{\zeta}|}{2}$$

 a_2e

$$\boxed{\Delta E = \langle \beta\zeta || \beta\zeta \rangle}$$

$$\Psi_3(a_2e, ^1E, M=0, \gamma) = -\frac{\sqrt{2}|\bar{\beta}\gamma|}{2} + \frac{\sqrt{2}|\beta\bar{\gamma}|}{2}$$

$$\Psi_4(a_2e, ^1E, M=0, \zeta) = \frac{\sqrt{2}|\bar{\beta}\zeta|}{2} - \frac{\sqrt{2}|\beta\bar{\zeta}|}{2}$$

 e^2

$$\boxed{\Delta E = \langle \zeta\zeta || \zeta\zeta \rangle}$$

$$\Psi_5(e^2, ^1E, M=0, \zeta) = -|\bar{\gamma}\gamma|$$

$$\Psi_6(e^2, ^1E, M=0, \gamma) = -|\bar{\zeta}\zeta|$$

 t_2^2

$$\boxed{\Delta E = -\langle \xi\xi || \phi\phi \rangle + \langle \xi\xi || \xi\xi \rangle}$$

$$\Psi_7(t_2^2, ^1E, M=0, \gamma) = -\frac{\sqrt{3}|\bar{\chi}\chi|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\bar{\phi}\phi| + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\xi}\xi|$$

$$\Psi_8(t_2^2, ^1E, M=0, \zeta) = \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\bar{\chi}\chi| - \frac{\sqrt{3}|\bar{\phi}\phi|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\xi}\xi|$$

 t_1t_2

$$\boxed{\Delta E = -\langle \xi\eta || \phi\mu \rangle + \langle \xi\eta || \xi\eta \rangle + \langle \xi\xi || \eta\eta \rangle - \langle \xi\phi || \mu\eta \rangle}$$

$$\Psi_9(t_1t_2, ^1E, M=0, \gamma) = -\frac{\sqrt{6}|\bar{\chi}\nu|}{6} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\phi}\mu|}{2} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\bar{\xi}\eta|}{2} + \frac{\sqrt{6}|\chi\bar{\nu}|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\phi\bar{\mu}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\xi\bar{\eta}|}{2}$$

$$\Psi_{10}(t_1t_2, ^1E, M=0, \zeta) = -\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\bar{\chi}\nu|}{2} + \frac{\sqrt{6}|\bar{\phi}\mu|}{6} - \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\xi}\eta|}{2} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\chi\bar{\nu}|}{2} - \frac{\sqrt{6}|\phi\bar{\mu}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\xi\bar{\eta}|}{2}$$

 t_1^2

$$\boxed{\Delta E = -\langle \nu\nu || \mu\mu \rangle + \langle \nu\nu || \nu\nu \rangle}$$

$$\Psi_{11}(t_1^2, ^1E, M=0, \gamma) = \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\eta}\eta| + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\bar{\mu}\mu| - \frac{\sqrt{3}|\bar{\nu}\nu|}{3}$$

$$\Psi_{12}(t_1^2, ^1E, M=0, \zeta) = \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\bar{\eta}\eta| - \frac{\sqrt{3}|\bar{\mu}\mu|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\bar{\nu}\nu|$$

2.31.6 3T_2 **a_1t_2**

$$\boxed{\Delta E = -\langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle}$$

$$\Psi_1(a_1t_2, ^3T_2, M=-1, \xi) = |\bar{\alpha}\bar{\xi}|$$

$$\Psi_2(a_1t_2, ^3T_2, M=-1, \phi) = |\bar{\alpha}\bar{\phi}|$$

$$\Psi_3(a_1t_2, ^3T_2, M=-1, \chi) = |\bar{\alpha}\bar{\chi}|$$

$$\Psi_4(a_1t_2, ^3T_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\alpha}\xi|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2}$$

$$\Psi_5(a_1t_2, ^3T_2, M=0, \phi) = \frac{\sqrt{2}|\bar{\alpha}\phi|}{2} + \frac{\sqrt{2}|\alpha\bar{\phi}|}{2}$$

$$\Psi_6(a_1t_2, ^3T_2, M=0, \chi) = \frac{\sqrt{2}|\bar{\alpha}\chi|}{2} + \frac{\sqrt{2}|\alpha\bar{\chi}|}{2}$$

$$\Psi_7(a_1t_2, ^3T_2, M=1, \xi) = |\alpha\xi|$$

$$\Psi_8(a_1t_2, ^3T_2, M=1, \phi) = |\alpha\phi|$$

$$\Psi_9(a_1t_2, ^3T_2, M=1, \chi) = |\alpha\chi|$$

 a_2t_1

$$\boxed{\Delta E = -\langle \beta\beta || \nu\nu \rangle + \langle \beta\nu || \beta\nu \rangle}$$

$$\Psi_{10}(a_2t_1, ^3T_2, M=-1, \xi) = |\bar{\beta}\bar{\eta}|$$

$$\Psi_{11}(a_2t_1, ^3T_2, M=-1, \phi) = |\bar{\beta}\bar{\mu}|$$

$$\Psi_{12}(a_2t_1, ^3T_2, M=-1, \chi) = |\bar{\beta}\bar{\nu}|$$

$$\Psi_{13}(a_2t_1, ^3T_2, M=0, \xi) = \frac{\sqrt{2}|\bar{\beta}\eta|}{2} + \frac{\sqrt{2}|\beta\bar{\eta}|}{2}$$

$$\Psi_{14}(a_2t_1, ^3T_2, M=0, \phi) = \frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2}$$

$$\Psi_{15}(a_2t_1, ^3T_2, M=0, \chi) = \frac{\sqrt{2}|\bar{\beta}\nu|}{2} + \frac{\sqrt{2}|\beta\bar{\nu}|}{2}$$

$$\Psi_{16}(a_2t_1, ^3T_2, M=1, \xi) = |\beta\eta|$$

$$\Psi_{17}(a_2t_1, ^3T_2, M=1, \phi) = |\beta\mu|$$

$$\Psi_{18}(a_2t_1, ^3T_2, M=1, \chi) = |\beta\nu|$$

 et_2

$$\boxed{\Delta E = \langle \zeta\xi || \zeta\xi \rangle}$$

$$\Psi_{19}(et_2, ^3T_2, M=-1, \xi) = \frac{\sqrt{2}|\bar{\gamma}\bar{\xi}|}{2} + \frac{\sqrt{2}|\zeta\bar{\xi}|}{2}$$

$$\Psi_{20}(et_2, ^3T_2, M=-1, \phi) = \frac{(-1)^{\frac{3}{2}}\sqrt{2}|\bar{\gamma}\bar{\phi}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta\bar{\phi}|}{2}$$

$$\Psi_{21}(et_2, ^3T_2, M=-1, \chi) = -\frac{\sqrt[3]{-1}\sqrt{2}|\bar{\gamma}\bar{\chi}|}{2} + \frac{(-1)^{\frac{3}{2}}\sqrt{2}|\zeta\bar{\chi}|}{2}$$

$$\Psi_{22}(et_2, ^3T_2, M=0, \xi) = \frac{|\bar{\gamma}\xi|}{2} + \frac{|\bar{\zeta}\xi|}{2} + \frac{|\bar{\gamma}\bar{\xi}|}{2} + \frac{|\zeta\bar{\xi}|}{2}$$

$$\Psi_{23}(et_2, ^3T_2, M=0, \phi) = \frac{(-1)^{\frac{3}{2}}|\bar{\gamma}\phi|}{2} - \frac{\sqrt[3]{-1}|\bar{\zeta}\phi|}{2} + \frac{(-1)^{\frac{3}{2}}|\gamma\bar{\phi}|}{2} - \frac{\sqrt[3]{-1}|\zeta\bar{\phi}|}{2}$$

$$\Psi_{24}(et_2, ^3T_2, M=0, \chi) = -\frac{\sqrt[3]{-1}|\bar{\gamma}\chi|}{2} + \frac{(-1)^{\frac{3}{2}}|\bar{\zeta}\chi|}{2} - \frac{\sqrt[3]{-1}|\gamma\bar{\chi}|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta\bar{\chi}|}{2}$$

$$\begin{aligned}\Psi_{25}(et_2, {}^3T_2, M=1, \xi) &= \frac{\sqrt{2}|\gamma\xi|}{2} + \frac{\sqrt{2}|\zeta\xi|}{2} \\ \Psi_{26}(et_2, {}^3T_2, M=1, \phi) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma\phi|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta\phi|}{2} \\ \Psi_{27}(et_2, {}^3T_2, M=1, \chi) &= -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma\chi|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta\chi|}{2}\end{aligned}$$

et₁

$$\boxed{\Delta E = \langle \zeta\nu || \zeta\nu \rangle}$$

$$\begin{aligned}\Psi_{28}(et_1, {}^3T_2, M=-1, \xi) &= -\frac{\sqrt{2}|\bar{\gamma}\bar{\eta}|}{2} + \frac{\sqrt{2}|\bar{\zeta}\bar{\eta}|}{2} \\ \Psi_{29}(et_1, {}^3T_2, M=-1, \phi) &= -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\bar{\gamma}\bar{\mu}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\bar{\zeta}\bar{\mu}|}{2} \\ \Psi_{30}(et_1, {}^3T_2, M=-1, \chi) &= \frac{\sqrt[3]{-1}\sqrt{2}|\bar{\gamma}\bar{\nu}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\bar{\zeta}\bar{\nu}|}{2} \\ \Psi_{31}(et_1, {}^3T_2, M=0, \xi) &= -\frac{|\bar{\gamma}\eta|}{2} + \frac{|\bar{\zeta}\eta|}{2} - \frac{|\bar{\gamma}\bar{\eta}|}{2} + \frac{|\zeta\bar{\eta}|}{2} \\ \Psi_{32}(et_1, {}^3T_2, M=0, \phi) &= -\frac{(-1)^{\frac{2}{3}}|\bar{\gamma}\mu|}{2} - \frac{\sqrt[3]{-1}|\bar{\zeta}\mu|}{2} - \frac{(-1)^{\frac{2}{3}}|\gamma\bar{\mu}|}{2} - \frac{\sqrt[3]{-1}|\zeta\bar{\mu}|}{2} \\ \Psi_{33}(et_1, {}^3T_2, M=0, \chi) &= \frac{\sqrt[3]{-1}|\bar{\gamma}\nu|}{2} + \frac{(-1)^{\frac{2}{3}}|\bar{\zeta}\nu|}{2} + \frac{\sqrt[3]{-1}|\gamma\bar{\nu}|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta\bar{\nu}|}{2} \\ \Psi_{34}(et_1, {}^3T_2, M=1, \xi) &= -\frac{\sqrt{2}|\gamma\eta|}{2} + \frac{\sqrt{2}|\zeta\eta|}{2} \\ \Psi_{35}(et_1, {}^3T_2, M=1, \phi) &= -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma\mu|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta\mu|}{2} \\ \Psi_{36}(et_1, {}^3T_2, M=1, \chi) &= \frac{\sqrt[3]{-1}\sqrt{2}|\gamma\nu|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta\nu|}{2}\end{aligned}$$

t₁t₂

$$\boxed{\Delta E = -\langle \xi\eta || \phi\mu \rangle + \langle \xi\nu || \xi\nu \rangle - \langle \xi\xi || \nu\nu \rangle + \langle \xi\phi || \eta\mu \rangle}$$

$$\begin{aligned}\Psi_{37}(t_1t_2, {}^3T_2, M=-1, \chi) &= \frac{\sqrt{2}|\bar{\phi}\bar{\eta}|}{2} - \frac{\sqrt{2}|\bar{\xi}\bar{\mu}|}{2} \\ \Psi_{38}(t_1t_2, {}^3T_2, M=-1, \phi) &= -\frac{\sqrt{2}|\bar{\chi}\bar{\eta}|}{2} + \frac{\sqrt{2}|\bar{\xi}\bar{\nu}|}{2} \\ \Psi_{39}(t_1t_2, {}^3T_2, M=-1, \xi) &= \frac{\sqrt{2}|\bar{\chi}\bar{\mu}|}{2} - \frac{\sqrt{2}|\bar{\phi}\bar{\nu}|}{2} \\ \Psi_{40}(t_1t_2, {}^3T_2, M=0, \chi) &= \frac{|\bar{\phi}\eta|}{2} - \frac{|\bar{\xi}\mu|}{2} + \frac{|\bar{\phi}\bar{\eta}|}{2} - \frac{|\xi\bar{\mu}|}{2} \\ \Psi_{41}(t_1t_2, {}^3T_2, M=0, \phi) &= -\frac{|\bar{\chi}\eta|}{2} + \frac{|\bar{\xi}\nu|}{2} - \frac{|\chi\bar{\eta}|}{2} + \frac{|\xi\bar{\nu}|}{2} \\ \Psi_{42}(t_1t_2, {}^3T_2, M=0, \xi) &= \frac{|\bar{\chi}\mu|}{2} - \frac{|\bar{\phi}\nu|}{2} + \frac{|\chi\bar{\mu}|}{2} - \frac{|\phi\bar{\nu}|}{2} \\ \Psi_{43}(t_1t_2, {}^3T_2, M=1, \chi) &= \frac{\sqrt{2}|\bar{\phi}\eta|}{2} - \frac{\sqrt{2}|\xi\mu|}{2} \\ \Psi_{44}(t_1t_2, {}^3T_2, M=1, \phi) &= -\frac{\sqrt{2}|\chi\eta|}{2} + \frac{\sqrt{2}|\xi\nu|}{2} \\ \Psi_{45}(t_1t_2, {}^3T_2, M=1, \xi) &= \frac{\sqrt{2}|\chi\mu|}{2} - \frac{\sqrt{2}|\phi\nu|}{2}\end{aligned}$$

2.31.7 ¹T₂*a₁t₂*

$$\boxed{\Delta E = \langle \alpha\alpha || \xi\xi \rangle + \langle \alpha\xi || \alpha\xi \rangle}$$

$$\begin{aligned}\Psi_1(a_1t_2, {}^1T_2, M=0, \xi) &= -\frac{\sqrt{2}|\bar{\alpha}\bar{\xi}|}{2} + \frac{\sqrt{2}|\alpha\bar{\xi}|}{2} \\ \Psi_2(a_1t_2, {}^1T_2, M=0, \phi) &= -\frac{\sqrt{2}|\bar{\alpha}\phi|}{2} + \frac{\sqrt{2}|\alpha\bar{\phi}|}{2} \\ \Psi_3(a_1t_2, {}^1T_2, M=0, \chi) &= -\frac{\sqrt{2}|\bar{\alpha}\chi|}{2} + \frac{\sqrt{2}|\alpha\bar{\chi}|}{2}\end{aligned}$$

a₂t₁

$$\boxed{\Delta E = \langle \beta\beta || \nu\nu \rangle + \langle \beta\nu || \beta\nu \rangle}$$

$$\begin{aligned}\Psi_4(a_2t_1, {}^1T_2, M=0, \xi) &= -\frac{\sqrt{2}|\bar{\beta}\eta|}{2} + \frac{\sqrt{2}|\beta\bar{\eta}|}{2} \\ \Psi_5(a_2t_1, {}^1T_2, M=0, \phi) &= -\frac{\sqrt{2}|\bar{\beta}\mu|}{2} + \frac{\sqrt{2}|\beta\bar{\mu}|}{2} \\ \Psi_6(a_2t_1, {}^1T_2, M=0, \chi) &= -\frac{\sqrt{2}|\bar{\beta}\nu|}{2} + \frac{\sqrt{2}|\beta\bar{\nu}|}{2}\end{aligned}$$

et₂

$$\boxed{\Delta E = \langle \zeta\xi || \zeta\xi \rangle}$$

$$\begin{aligned}\Psi_7(et_2, {}^1T_2, M=0, \xi) &= -\frac{|\bar{\gamma}\xi|}{2} - \frac{|\bar{\zeta}\xi|}{2} + \frac{|\gamma\bar{\xi}|}{2} + \frac{|\zeta\bar{\xi}|}{2} \\ \Psi_8(et_2, {}^1T_2, M=0, \phi) &= -\frac{(-1)^{\frac{2}{3}}|\bar{\gamma}\phi|}{2} + \frac{\sqrt[3]{-1}|\bar{\zeta}\phi|}{2} + \frac{(-1)^{\frac{2}{3}}|\gamma\bar{\phi}|}{2} - \frac{\sqrt[3]{-1}|\zeta\bar{\phi}|}{2} \\ \Psi_9(et_2, {}^1T_2, M=0, \chi) &= \frac{\sqrt[3]{-1}|\bar{\gamma}\chi|}{2} - \frac{(-1)^{\frac{2}{3}}|\bar{\zeta}\chi|}{2} - \frac{\sqrt[3]{-1}|\gamma\bar{\chi}|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta\bar{\chi}|}{2}\end{aligned}$$

et₁

$$\boxed{\Delta E = \langle \zeta\nu || \zeta\nu \rangle}$$

$$\begin{aligned}\Psi_{10}(et_1, {}^1T_2, M=0, \xi) &= \frac{|\bar{\gamma}\eta|}{2} - \frac{|\bar{\zeta}\eta|}{2} - \frac{|\gamma\bar{\eta}|}{2} + \frac{|\zeta\bar{\eta}|}{2} \\ \Psi_{11}(et_1, {}^1T_2, M=0, \phi) &= \frac{(-1)^{\frac{2}{3}}|\bar{\gamma}\mu|}{2} + \frac{\sqrt[3]{-1}|\bar{\zeta}\mu|}{2} - \frac{(-1)^{\frac{2}{3}}|\gamma\bar{\mu}|}{2} - \frac{\sqrt[3]{-1}|\zeta\bar{\mu}|}{2} \\ \Psi_{12}(et_1, {}^1T_2, M=0, \chi) &= -\frac{\sqrt[3]{-1}|\bar{\gamma}\nu|}{2} - \frac{(-1)^{\frac{2}{3}}|\bar{\zeta}\nu|}{2} + \frac{\sqrt[3]{-1}|\gamma\bar{\nu}|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta\bar{\nu}|}{2}\end{aligned}$$

t₂²

$$\boxed{\Delta E = \langle \xi\phi || \xi\phi \rangle + \langle \xi\xi || \phi\phi \rangle}$$

$$\begin{aligned}\Psi_{13}(t_2^2, {}^1T_2, M=0, \chi) &= -\frac{\sqrt{2}|\bar{\phi}\xi|}{2} - \frac{\sqrt{2}|\bar{\xi}\phi|}{2} \\ \Psi_{14}(t_2^2, {}^1T_2, M=0, \phi) &= -\frac{\sqrt{2}|\bar{\chi}\xi|}{2} - \frac{\sqrt{2}|\bar{\xi}\chi|}{2} \\ \Psi_{15}(t_2^2, {}^1T_2, M=0, \xi) &= -\frac{\sqrt{2}|\bar{\chi}\phi|}{2} - \frac{\sqrt{2}|\bar{\phi}\chi|}{2}\end{aligned}$$

t₁t₂

$$\boxed{\Delta E = -\langle \xi\eta || \phi\mu \rangle + \langle \xi\nu || \xi\nu \rangle + \langle \xi\xi || \nu\nu \rangle - \langle \xi\phi || \eta\mu \rangle}$$

$$\begin{aligned}\Psi_{16}(t_1t_2, {}^1T_2, M=0, \chi) &= -\frac{|\bar{\phi}\eta|}{2} + \frac{|\bar{\xi}\mu|}{2} + \frac{|\phi\bar{\eta}|}{2} - \frac{|\xi\bar{\mu}|}{2} \\ \Psi_{17}(t_1t_2, {}^1T_2, M=0, \phi) &= \frac{|\bar{\chi}\eta|}{2} - \frac{|\bar{\xi}\nu|}{2} - \frac{|\chi\bar{\eta}|}{2} + \frac{|\xi\bar{\nu}|}{2}\end{aligned}$$

$$\Psi_{18}(t_1 t_2, {}^1T_2, M=0, \xi) = -\frac{|\bar{x}\mu|}{2} + \frac{|\bar{\phi}\nu|}{2} + \frac{|x\bar{\mu}|}{2} - \frac{|\phi\bar{\nu}|}{2}$$

$$t_1^2$$

$$\boxed{\Delta E = \langle \nu\mu || \nu\mu \rangle + \langle \nu\nu || \mu\mu \rangle}$$

$$\Psi_{19}(t_1^2, {}^1T_2, M=0, \chi) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} - \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

$$\Psi_{20}(t_1^2, {}^1T_2, M=0, \phi) = -\frac{\sqrt{2}|\bar{\eta}\nu|}{2} - \frac{\sqrt{2}|\bar{\nu}\eta|}{2}$$

$$\Psi_{21}(t_1^2, {}^1T_2, M=0, \xi) = -\frac{\sqrt{2}|\bar{\mu}\nu|}{2} - \frac{\sqrt{2}|\bar{\nu}\mu|}{2}$$

2.31.8 3T_1 $a_1 t_1$

$$\boxed{\Delta E = -\langle \alpha\alpha || \nu\nu \rangle + \langle \alpha\nu || \alpha\nu \rangle}$$

$$\Psi_1(a_1 t_1, {}^3T_1, M=-1, \eta) = |\bar{\alpha}\eta|$$

$$\Psi_2(a_1 t_1, {}^3T_1, M=-1, \mu) = |\bar{\alpha}\mu|$$

$$\Psi_3(a_1 t_1, {}^3T_1, M=-1, \nu) = |\bar{\alpha}\nu|$$

$$\Psi_4(a_1 t_1, {}^3T_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\Psi_5(a_1 t_1, {}^3T_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2}$$

$$\Psi_6(a_1 t_1, {}^3T_1, M=0, \nu) = \frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2}$$

$$\Psi_7(a_1 t_1, {}^3T_1, M=1, \eta) = |\alpha\eta|$$

$$\Psi_8(a_1 t_1, {}^3T_1, M=1, \mu) = |\alpha\mu|$$

$$\Psi_9(a_1 t_1, {}^3T_1, M=1, \nu) = |\alpha\nu|$$

 $a_2 t_2$

$$\boxed{\Delta E = -\langle \beta\beta || \xi\xi \rangle + \langle \beta\xi || \beta\xi \rangle}$$

$$\Psi_{10}(a_2 t_2, {}^3T_1, M=-1, \eta) = |\bar{\beta}\xi|$$

$$\Psi_{11}(a_2 t_2, {}^3T_1, M=-1, \mu) = |\bar{\beta}\phi|$$

$$\Psi_{12}(a_2 t_2, {}^3T_1, M=-1, \nu) = |\bar{\beta}\chi|$$

$$\Psi_{13}(a_2 t_2, {}^3T_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2}$$

$$\Psi_{14}(a_2 t_2, {}^3T_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\beta}\phi|}{2} + \frac{\sqrt{2}|\beta\bar{\phi}|}{2}$$

$$\Psi_{15}(a_2 t_2, {}^3T_1, M=0, \nu) = \frac{\sqrt{2}|\bar{\beta}\chi|}{2} + \frac{\sqrt{2}|\beta\bar{\chi}|}{2}$$

$$\Psi_{16}(a_2 t_2, {}^3T_1, M=1, \eta) = |\beta\xi|$$

$$\Psi_{17}(a_2 t_2, {}^3T_1, M=1, \mu) = |\beta\phi|$$

$$\Psi_{18}(a_2 t_2, {}^3T_1, M=1, \nu) = |\beta\chi|$$

 et_2

$$\boxed{\Delta E = \langle \zeta\xi || \zeta\xi \rangle}$$

$$\Psi_{19}(et_2, {}^3T_1, M=-1, \eta) = -\frac{\sqrt{2}|\bar{\gamma}\xi|}{2} + \frac{\sqrt{2}|\bar{\zeta}\xi|}{2}$$

$$\Psi_{20}(et_2, {}^3T_1, M=-1, \mu) = -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\bar{\gamma}\phi|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\bar{\zeta}\phi|}{2}$$

$$\Psi_{21}(et_2, {}^3T_1, M=-1, \nu) = \frac{\sqrt[3]{-1}\sqrt{2}|\bar{\gamma}\chi|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\bar{\zeta}\chi|}{2}$$

$$\Psi_{22}(et_2, {}^3T_1, M=0, \eta) = -\frac{|\bar{\gamma}\xi|}{2} + \frac{|\bar{\zeta}\xi|}{2} - \frac{|\gamma\bar{\xi}|}{2} + \frac{|\zeta\bar{\xi}|}{2}$$

$$\Psi_{23}(et_2, {}^3T_1, M=0, \mu) = -\frac{(-1)^{\frac{2}{3}}|\bar{\gamma}\phi|}{2} - \frac{\sqrt[3]{-1}|\bar{\zeta}\phi|}{2} - \frac{(-1)^{\frac{2}{3}}|\gamma\bar{\phi}|}{2} - \frac{\sqrt[3]{-1}|\zeta\bar{\phi}|}{2}$$

$$\Psi_{24}(et_2, {}^3T_1, M=0, \nu) = \frac{\sqrt[3]{-1}|\bar{\gamma}\chi|}{2} + \frac{(-1)^{\frac{2}{3}}|\bar{\zeta}\chi|}{2} + \frac{\sqrt[3]{-1}|\gamma\bar{\chi}|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta\bar{\chi}|}{2}$$

$$\Psi_{25}(et_2, {}^3T_1, M=1, \eta) = -\frac{\sqrt{2}|\gamma\xi|}{2} + \frac{\sqrt{2}|\zeta\xi|}{2}$$

$$\Psi_{26}(et_2, {}^3T_1, M=1, \mu) = -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma\phi|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta\phi|}{2}$$

$$\Psi_{27}(et_2, {}^3T_1, M=1, \nu) = \frac{\sqrt[3]{-1}\sqrt{2}|\gamma\chi|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta\chi|}{2}$$

 et_1

$$\boxed{\Delta E = \langle \zeta\nu || \zeta\nu \rangle}$$

$$\Psi_{28}(et_1, {}^3T_1, M=-1, \eta) = \frac{\sqrt{2}|\bar{\gamma}\eta|}{2} + \frac{\sqrt{2}|\bar{\zeta}\eta|}{2}$$

$$\Psi_{29}(et_1, {}^3T_1, M=-1, \mu) = \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\bar{\gamma}\mu|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\bar{\zeta}\mu|}{2}$$

$$\Psi_{30}(et_1, {}^3T_1, M=-1, \nu) = -\frac{\sqrt[3]{-1}\sqrt{2}|\bar{\gamma}\nu|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\bar{\zeta}\nu|}{2}$$

$$\Psi_{31}(et_1, {}^3T_1, M=0, \eta) = \frac{|\bar{\gamma}\eta|}{2} + \frac{|\bar{\zeta}\eta|}{2} + \frac{|\gamma\bar{\eta}|}{2} + \frac{|\zeta\bar{\eta}|}{2}$$

$$\Psi_{32}(et_1, {}^3T_1, M=0, \mu) = -\frac{(-1)^{\frac{2}{3}}|\bar{\gamma}\mu|}{2} - \frac{\sqrt[3]{-1}|\bar{\zeta}\mu|}{2} + \frac{(-1)^{\frac{2}{3}}|\gamma\bar{\mu}|}{2} - \frac{\sqrt[3]{-1}|\zeta\bar{\mu}|}{2}$$

$$\Psi_{33}(et_1, {}^3T_1, M=0, \nu) = -\frac{\sqrt[3]{-1}|\bar{\gamma}\nu|}{2} + \frac{(-1)^{\frac{2}{3}}|\bar{\zeta}\nu|}{2} - \frac{\sqrt[3]{-1}|\gamma\bar{\nu}|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta\bar{\nu}|}{2}$$

$$\Psi_{34}(et_1, {}^3T_1, M=1, \eta) = \frac{\sqrt{2}|\gamma\eta|}{2} + \frac{\sqrt{2}|\zeta\eta|}{2}$$

$$\Psi_{35}(et_1, {}^3T_1, M=1, \mu) = \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma\mu|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta\mu|}{2}$$

$$\Psi_{36}(et_1, {}^3T_1, M=1, \nu) = -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma\nu|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta\nu|}{2}$$

 t_2^2

$$\boxed{\Delta E = \langle \xi\phi || \xi\phi \rangle - \langle \xi\xi || \phi\phi \rangle}$$

$$\Psi_{37}(t_2^2, {}^3T_1, M=-1, \nu) = -|\bar{\xi}\phi|$$

$$\Psi_{38}(t_2^2, {}^3T_1, M=-1, \mu) = |\bar{\xi}\bar{\chi}|$$

$$\Psi_{39}(t_2^2, {}^3T_1, M=-1, \eta) = -|\bar{\phi}\bar{\chi}|$$

$$\Psi_{40}(t_2^2, {}^3T_1, M=0, \nu) = \frac{\sqrt{2}|\bar{\phi}\xi|}{2} - \frac{\sqrt{2}|\bar{\xi}\phi|}{2}$$

$$\Psi_{41}(t_2^2, {}^3T_1, M=0, \mu) = -\frac{\sqrt{2}|\bar{\chi}\xi|}{2} + \frac{\sqrt{2}|\bar{\xi}\chi|}{2}$$

$$\Psi_{42}(t_2^2, {}^3T_1, M=0, \eta) = \frac{\sqrt{2}|\bar{\chi}\phi|}{2} - \frac{\sqrt{2}|\bar{\phi}\chi|}{2}$$

$$\Psi_{43}(t_2^2, {}^3T_1, M=1, \nu) = -|\xi\phi|$$

$$\Psi_{44}(t_2^2, {}^3T_1, M=1, \mu) = |\xi\chi|$$

$$\Psi_{45}(t_2^2, {}^3T_1, M=1, \eta) = -|\phi\chi|$$

$t_1 t_2$

$$\Delta E = \langle \xi\eta || \phi\mu \rangle + \langle \xi\nu || \xi\nu \rangle - \langle \xi\xi || \nu\nu \rangle - \langle \xi\phi || \eta\mu \rangle$$

$$\begin{aligned}\Psi_{46}(t_1 t_2, {}^3T_1, M=-1, \nu) &= \frac{\sqrt{2}|\bar{\phi}\bar{\eta}|}{2} + \frac{\sqrt{2}|\bar{\xi}\bar{\mu}|}{2} \\ \Psi_{47}(t_1 t_2, {}^3T_1, M=-1, \mu) &= \frac{\sqrt{2}|\bar{x}\bar{\eta}|}{2} + \frac{\sqrt{2}|\bar{\xi}\bar{\nu}|}{2} \\ \Psi_{48}(t_1 t_2, {}^3T_1, M=-1, \eta) &= \frac{\sqrt{2}|\bar{x}\bar{\mu}|}{2} + \frac{\sqrt{2}|\bar{\phi}\bar{\nu}|}{2} \\ \Psi_{49}(t_1 t_2, {}^3T_1, M=0, \nu) &= \frac{|\bar{\phi}\eta|}{2} + \frac{|\bar{\xi}\mu|}{2} + \frac{|\phi\bar{\eta}|}{2} + \frac{|\xi\bar{\mu}|}{2} \\ \Psi_{50}(t_1 t_2, {}^3T_1, M=0, \mu) &= \frac{|\bar{x}\eta|}{2} + \frac{|\bar{\xi}\nu|}{2} + \frac{|\chi\bar{\eta}|}{2} + \frac{|\xi\bar{\nu}|}{2} \\ \Psi_{51}(t_1 t_2, {}^3T_1, M=0, \eta) &= \frac{|\bar{x}\mu|}{2} + \frac{|\bar{\phi}\nu|}{2} + \frac{|\chi\bar{\mu}|}{2} + \frac{|\phi\bar{\nu}|}{2} \\ \Psi_{52}(t_1 t_2, {}^3T_1, M=1, \nu) &= \frac{\sqrt{2}|\bar{\phi}\eta|}{2} + \frac{\sqrt{2}|\xi\mu|}{2} \\ \Psi_{53}(t_1 t_2, {}^3T_1, M=1, \mu) &= \frac{\sqrt{2}|\bar{x}\eta|}{2} + \frac{\sqrt{2}|\xi\nu|}{2} \\ \Psi_{54}(t_1 t_2, {}^3T_1, M=1, \eta) &= \frac{\sqrt{2}|\bar{x}\mu|}{2} + \frac{\sqrt{2}|\phi\nu|}{2}\end{aligned}$$

 t_1^2

$$\Delta E = \langle \nu\mu || \nu\mu \rangle - \langle \nu\nu || \mu\mu \rangle$$

$$\Psi_{55}(t_1^2, {}^3T_1, M=-1, \nu) = -|\bar{\eta}\bar{\mu}|$$

$$\Psi_{56}(t_1^2, {}^3T_1, M=-1, \mu) = |\bar{\eta}\bar{\nu}|$$

$$\Psi_{57}(t_1^2, {}^3T_1, M=-1, \eta) = -|\bar{\mu}\bar{\nu}|$$

$$\Psi_{58}(t_1^2, {}^3T_1, M=0, \nu) = -\frac{\sqrt{2}|\bar{\eta}\mu|}{2} + \frac{\sqrt{2}|\bar{\mu}\eta|}{2}$$

$$\Psi_{59}(t_1^2, {}^3T_1, M=0, \mu) = \frac{\sqrt{2}|\bar{\eta}\nu|}{2} - \frac{\sqrt{2}|\bar{\nu}\eta|}{2}$$

$$\Psi_{60}(t_1^2, {}^3T_1, M=0, \eta) = -\frac{\sqrt{2}|\bar{\mu}\nu|}{2} + \frac{\sqrt{2}|\bar{\nu}\mu|}{2}$$

$$\Psi_{61}(t_1^2, {}^3T_1, M=1, \nu) = -|\eta\mu|$$

$$\Psi_{62}(t_1^2, {}^3T_1, M=1, \mu) = |\eta\nu|$$

$$\Psi_{63}(t_1^2, {}^3T_1, M=1, \eta) = -|\mu\nu|$$

2.31.9 1T_1

 $a_1 t_1$

$$\Delta E = \langle \alpha\alpha || \nu\nu \rangle + \langle \alpha\nu || \alpha\nu \rangle$$

$$\Psi_1(a_1 t_1, {}^1T_1, M=0, \eta) = -\frac{\sqrt{2}|\bar{\alpha}\eta|}{2} + \frac{\sqrt{2}|\alpha\bar{\eta}|}{2}$$

$$\begin{aligned}\Psi_2(a_1 t_1, {}^1T_1, M=0, \mu) &= -\frac{\sqrt{2}|\bar{\alpha}\mu|}{2} + \frac{\sqrt{2}|\alpha\bar{\mu}|}{2} \\ \Psi_3(a_1 t_1, {}^1T_1, M=0, \nu) &= -\frac{\sqrt{2}|\bar{\alpha}\nu|}{2} + \frac{\sqrt{2}|\alpha\bar{\nu}|}{2}\end{aligned}$$

 $a_2 t_2$

$$\Delta E = \langle \beta\beta || \xi\xi \rangle + \langle \beta\xi || \beta\xi \rangle$$

$$\begin{aligned}\Psi_4(a_2 t_2, {}^1T_1, M=0, \eta) &= -\frac{\sqrt{2}|\bar{\beta}\xi|}{2} + \frac{\sqrt{2}|\beta\bar{\xi}|}{2} \\ \Psi_5(a_2 t_2, {}^1T_1, M=0, \mu) &= -\frac{\sqrt{2}|\bar{\beta}\phi|}{2} + \frac{\sqrt{2}|\beta\bar{\phi}|}{2} \\ \Psi_6(a_2 t_2, {}^1T_1, M=0, \nu) &= -\frac{\sqrt{2}|\bar{\beta}\chi|}{2} + \frac{\sqrt{2}|\beta\bar{\chi}|}{2}\end{aligned}$$

 et_2

$$\Delta E = \langle \zeta\xi || \zeta\xi \rangle$$

$$\begin{aligned}\Psi_7(et_2, {}^1T_1, M=0, \eta) &= \frac{|\bar{\gamma}\xi|}{2} - \frac{|\bar{\zeta}\xi|}{2} - \frac{|\gamma\bar{\xi}|}{2} + \frac{|\zeta\bar{\xi}|}{2} \\ \Psi_8(et_2, {}^1T_1, M=0, \mu) &= \\ \frac{(-1)^{\frac{3}{2}}|\bar{\gamma}\phi|}{2} + \frac{\sqrt[3]{-1}|\bar{\zeta}\phi|}{2} &- \frac{(-1)^{\frac{3}{2}}|\gamma\bar{\phi}|}{2} - \frac{\sqrt[3]{-1}|\zeta\bar{\phi}|}{2} \\ \Psi_9(et_2, {}^1T_1, M=0, \nu) &= \\ -\frac{\sqrt[3]{-1}|\bar{\gamma}\chi|}{2} - \frac{(-1)^{\frac{3}{2}}|\bar{\zeta}\chi|}{2} &+ \frac{\sqrt[3]{-1}|\gamma\bar{\chi}|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta\bar{\chi}|}{2}\end{aligned}$$

 et_1

$$\Delta E = \langle \zeta\nu || \zeta\nu \rangle$$

$$\begin{aligned}\Psi_{10}(et_1, {}^1T_1, M=0, \eta) &= -\frac{|\bar{\gamma}\eta|}{2} - \frac{|\bar{\zeta}\eta|}{2} + \frac{|\gamma\bar{\eta}|}{2} + \frac{|\zeta\bar{\eta}|}{2} \\ \Psi_{11}(et_1, {}^1T_1, M=0, \mu) &= \\ -\frac{(-1)^{\frac{3}{2}}|\bar{\gamma}\mu|}{2} + \frac{\sqrt[3]{-1}|\bar{\zeta}\mu|}{2} &+ \frac{(-1)^{\frac{3}{2}}|\gamma\bar{\mu}|}{2} - \frac{\sqrt[3]{-1}|\zeta\bar{\mu}|}{2} \\ \Psi_{12}(et_1, {}^1T_1, M=0, \nu) &= \\ \frac{\sqrt[3]{-1}|\bar{\gamma}\nu|}{2} - \frac{(-1)^{\frac{3}{2}}|\bar{\zeta}\nu|}{2} &- \frac{\sqrt[3]{-1}|\gamma\bar{\nu}|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta\bar{\nu}|}{2}\end{aligned}$$

 $t_1 t_2$

$$\Delta E = \langle \xi\eta || \phi\mu \rangle + \langle \xi\nu || \xi\nu \rangle + \langle \xi\xi || \nu\nu \rangle + \langle \xi\phi || \eta\mu \rangle$$

$$\Psi_{13}(t_1 t_2, {}^1T_1, M=0, \nu) = -\frac{|\bar{\phi}\eta|}{2} - \frac{|\bar{\xi}\mu|}{2} + \frac{|\phi\bar{\eta}|}{2} + \frac{|\xi\bar{\mu}|}{2}$$

$$\Psi_{14}(t_1 t_2, {}^1T_1, M=0, \mu) = -\frac{|\bar{x}\eta|}{2} - \frac{|\bar{\xi}\nu|}{2} + \frac{|\chi\bar{\eta}|}{2} + \frac{|\xi\bar{\nu}|}{2}$$

$$\Psi_{15}(t_1 t_2, {}^1T_1, M=0, \eta) = -\frac{|\bar{x}\mu|}{2} - \frac{|\bar{\phi}\nu|}{2} + \frac{|\chi\bar{\mu}|}{2} + \frac{|\phi\bar{\nu}|}{2}$$

2.32 Group O_h

Component labels

$$\begin{aligned}A_{1g} : \{\alpha_g\} &\longrightarrow A_{2u} : \{\beta_u\} \longrightarrow A_{1u} : \{\alpha_u\} \longrightarrow A_{2g} : \{\beta_g\} \longrightarrow E_u : \{\gamma_u, \zeta_u\} \longrightarrow E_g : \{\gamma_g, \zeta_g\} \longrightarrow \\ T_{1g} : \{\eta_g, \mu_g, \nu_g\} &\longrightarrow T_{2g} : \{\xi_g, \phi_g, \chi_g\} \longrightarrow T_{1u} : \{\eta_u, \mu_u, \nu_u\} \longrightarrow T_{2u} : \{\xi_u, \phi_u, \chi_u\}\end{aligned}$$

	$\Psi_9(t_{1u}^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{3} \eta_u\eta_u }{3} - \frac{\sqrt{3} \mu_u\mu_u }{3} - \frac{\sqrt{3} \nu_u\nu_u }{3}$
2.32.1	${}^1A_{1g}$
	a_{1g}^2
	$\boxed{\Delta E = \langle \alpha_g \alpha_g \alpha_g \alpha_g \rangle}$
$\Psi_1(a_{1g}^2, {}^1A_{1g}, M=0, \alpha_g) = - \overline{\alpha_g} \alpha_g $	
	a_{2u}^2
	$\boxed{\Delta E = \langle \beta_u \beta_u \beta_u \beta_u \rangle}$
$\Psi_2(a_{2u}^2, {}^1A_{1g}, M=0, \alpha_g) = - \overline{\beta_u} \beta_u $	2.32.2
	a_{1u}^2
	$\boxed{\Delta E = \langle \alpha_u \alpha_u \alpha_u \alpha_u \rangle}$
$\Psi_3(a_{1u}^2, {}^1A_{1g}, M=0, \alpha_g) = - \overline{\alpha_u} \alpha_u $	
	a_{2g}^2
	$\boxed{\Delta E = \langle \beta_g \beta_g \beta_g \beta_g \rangle}$
$\Psi_4(a_{2g}^2, {}^1A_{1g}, M=0, \alpha_g) = - \overline{\beta_g} \beta_g $	
	e_u^2
	$\boxed{\Delta E = 0}$
$\varepsilon_u^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{2} \gamma_u\zeta_u }{2} - \frac{\sqrt{2} \zeta_u\gamma_u }{2}$	
	e_g^2
	$\boxed{\Delta E = 0}$
$e_g^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{2} \gamma_g\zeta_g }{2} - \frac{\sqrt{2} \zeta_g\gamma_g }{2}$	
	t_{1g}^2
	$\boxed{\Delta E = 3 \langle \nu_g \nu_g \nu_g \nu_g \rangle}$
$\Psi_7(t_{1g}^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{3} \eta_g\eta_g }{3} - \frac{\sqrt{3} \mu_g\mu_g }{3} - \frac{\sqrt{3} \nu_g\nu_g }{3}$	
	t_{2g}^2
	$\boxed{\Delta E = 3 \langle \xi_g \xi_g \xi_g \xi_g \rangle}$
$\Psi_8(t_{2g}^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{3} \chi_g\chi_g }{3} - \frac{\sqrt{3} \phi_g\phi_g }{3} - \frac{\sqrt{3} \xi_g\xi_g }{3}$	
	t_{1u}^2
	$\boxed{\Delta E = 3 \langle \nu_u \nu_u \nu_u \nu_u \rangle}$
	t_{2u}^2
	$\boxed{\Delta E = 3 \langle \xi_u \xi_u \xi_u \xi_u \rangle}$
	$\Psi_{10}(t_{2u}^2, {}^1A_{1g}, M=0, \alpha_g) = -\frac{\sqrt{3} \chi_u\chi_u }{3} - \frac{\sqrt{3} \phi_u\phi_u }{3} - \frac{\sqrt{3} \xi_u\xi_u }{3}$
	$a_{1g} a_{2u}$
	$\boxed{\Delta E = -\langle \alpha_g \alpha_g \beta_u \beta_u \rangle + \langle \alpha_g \beta_u \alpha_g \beta_u \rangle}$
$\Psi_1(a_{1g} a_{2u}, {}^3A_{2u}, M=-1, \beta_u) = \overline{\alpha_g} \overline{\beta_u} $	
	$\Psi_2(a_{1g} a_{2u}, {}^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2} \overline{\alpha_g} \beta_u }{2} + \frac{\sqrt{2} \alpha_g \overline{\beta_u} }{2}$
$\Psi_3(a_{1g} a_{2u}, {}^3A_{2u}, M=1, \beta_u) = \alpha_g \beta_u $	
	$a_{1u} a_{2g}$
	$\boxed{\Delta E = -\langle \alpha_u \alpha_u \beta_g \beta_g \rangle + \langle \alpha_u \beta_g \alpha_u \beta_g \rangle}$
$\Psi_4(a_{1u} a_{2g}, {}^3A_{2u}, M=-1, \beta_u) = \overline{\alpha_u} \overline{\beta_g} $	
	$\Psi_5(a_{1u} a_{2g}, {}^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{2} \overline{\alpha_u} \beta_g }{2} + \frac{\sqrt{2} \alpha_u \overline{\beta_g} }{2}$
$\Psi_6(a_{1u} a_{2g}, {}^3A_{2u}, M=1, \beta_u) = \alpha_u \beta_g $	
	$e_g e_u$
	$\boxed{\Delta E = 0}$
$\Psi_7(e_g e_u, {}^3A_{2u}, M=-1, \beta_u) = -\frac{\sqrt{2} \overline{\gamma_u} \zeta_g }{2} + \frac{\sqrt{2} \overline{\zeta_u} \overline{\gamma_g} }{2}$	
	$\Psi_8(e_g e_u, {}^3A_{2u}, M=0, \beta_u) = -\frac{ \overline{\gamma_u} \zeta_g }{2} + \frac{ \overline{\zeta_u} \gamma_g }{2} - \frac{ \gamma_u \overline{\zeta_g} }{2} + \frac{ \zeta_u \overline{\gamma_g} }{2}$
$\Psi_9(e_g e_u, {}^3A_{2u}, M=1, \beta_u) = -\frac{\sqrt{2} \gamma_u \zeta_g }{2} + \frac{\sqrt{2} \zeta_u \gamma_g }{2}$	
	$t_{1g} t_{2u}$
	$\boxed{\Delta E = 3 \langle \nu_g \chi_u \nu_g \chi_u \rangle - 3 \langle \nu_g \nu_g \chi_u \chi_u \rangle}$
$\Psi_{10}(t_{1g} t_{2u}, {}^3A_{2u}, M=-1, \beta_u) = \frac{\sqrt{3} \overline{\eta_g} \xi_u }{3} + \frac{\sqrt{3} \overline{\mu_g} \phi_u }{3} + \frac{\sqrt{3} \overline{\nu_g} \chi_u }{3}$	
	$\Psi_{11}(t_{1g} t_{2u}, {}^3A_{2u}, M=0, \beta_u) = \frac{\sqrt{6} \overline{\eta_g} \xi_u }{6} + \frac{\sqrt{6} \overline{\mu_g} \phi_u }{6} + \frac{\sqrt{6} \overline{\nu_g} \chi_u }{6}$
	$\Psi_{12}(t_{1g} t_{2u}, {}^3A_{2u}, M=1, \beta_u) = \frac{\sqrt{3} \eta_g \xi_u }{3} + \frac{\sqrt{3} \mu_g \phi_u }{3} + \frac{\sqrt{3} \nu_g \chi_u }{3}$
	$t_{1u} t_{2g}$
	$\boxed{\Delta E = 3 \langle \xi_g \eta_u \xi_g \eta_u \rangle - 3 \langle \xi_g \xi_g \eta_u \eta_u \rangle}$

$$\begin{aligned}\Psi_{13}(t_{1u}t_{2g}, {}^3A_{2u}, M=-1, \beta_u) &= \frac{\sqrt{3}|\chi_g\nu_u|}{3} + \frac{\sqrt{3}|\phi_g\mu_u|}{3} + \frac{\sqrt{3}|\xi_g\eta_u|}{3} \\ \Psi_{14}(t_{1u}t_{2g}, {}^3A_{2u}, M=0, \beta_u) &= \frac{\sqrt{6}|\chi_g\nu_u|}{6} + \frac{\sqrt{6}|\phi_g\mu_u|}{6} + \\ &\quad \frac{\sqrt{6}|\xi_g\eta_u|}{6} + \frac{\sqrt{6}|\chi_g\nu_u|}{6} + \frac{\sqrt{6}|\phi_g\mu_u|}{6} + \frac{\sqrt{6}|\xi_g\eta_u|}{6} \\ \Psi_{15}(t_{1u}t_{2g}, {}^3A_{2u}, M=1, \beta_u) &= \frac{\sqrt{3}|\chi_g\nu_u|}{3} + \frac{\sqrt{3}|\phi_g\mu_u|}{3} + \frac{\sqrt{3}|\xi_g\eta_u|}{3}\end{aligned}$$

2.32.3 ${}^1A_{2u}$ $a_{1g}a_{2u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_u \beta_u \rangle + \langle \alpha_g \beta_u || \alpha_g \beta_u \rangle}$$

$$\begin{aligned}\Psi_1(a_{1g}a_{2u}, {}^1A_{2u}, M=0, \beta_u) &= -\frac{\sqrt{2}|\alpha_g\beta_u|}{2} + \frac{\sqrt{2}|\alpha_g\beta_u|}{2} \\ &\quad a_{1u}a_{2g}\end{aligned}$$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \beta_g \beta_g \rangle + \langle \alpha_u \beta_g || \alpha_u \beta_g \rangle}$$

$$\Psi_2(a_{1u}a_{2g}, {}^1A_{2u}, M=0, \beta_u) = -\frac{\sqrt{2}|\alpha_u\beta_g|}{2} + \frac{\sqrt{2}|\alpha_u\beta_g|}{2}$$

 $e_g e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(e_g e_u, {}^1A_{2u}, M=0, \beta_u) = \frac{|\gamma_u \zeta_g|}{2} - \frac{|\zeta_u \gamma_g|}{2} - \frac{|\gamma_u \bar{\zeta}_g|}{2} + \frac{|\zeta_u \bar{\gamma}_g|}{2}$$

 $t_{1g}t_{2u}$

$$\boxed{\Delta E = 3 \langle \nu_g \chi_u || \nu_g \chi_u \rangle + 3 \langle \nu_g \nu_g || \chi_u \chi_u \rangle}$$

$$\begin{aligned}\Psi_4(t_{1g}t_{2u}, {}^1A_{2u}, M=0, \beta_u) &= -\frac{\sqrt{6}|\eta_g\xi_u|}{6} - \frac{\sqrt{6}|\mu_g\phi_u|}{6} - \\ &\quad \frac{\sqrt{6}|\nu_g\chi_u|}{6} + \frac{\sqrt{6}|\eta_g\bar{\xi}_u|}{6} + \frac{\sqrt{6}|\mu_g\bar{\phi}_u|}{6} + \frac{\sqrt{6}|\nu_g\bar{\chi}_u|}{6}\end{aligned}$$

 $t_{1u}t_{2g}$

$$\boxed{\Delta E = 3 \langle \xi_g \eta_u || \xi_g \eta_u \rangle + 3 \langle \xi_g \xi_g || \eta_u \eta_u \rangle}$$

$$\begin{aligned}\Psi_5(t_{1u}t_{2g}, {}^1A_{2u}, M=0, \beta_u) &= -\frac{\sqrt{6}|\chi_g\nu_u|}{6} - \frac{\sqrt{6}|\phi_g\mu_u|}{6} - \\ &\quad \frac{\sqrt{6}|\xi_g\eta_u|}{6} + \frac{\sqrt{6}|\chi_g\nu_u|}{6} + \frac{\sqrt{6}|\phi_g\mu_u|}{6} + \frac{\sqrt{6}|\xi_g\eta_u|}{6}\end{aligned}$$

2.32.4 ${}^3A_{1u}$ $a_{1g}a_{1u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\begin{aligned}\Psi_1(a_{1g}a_{1u}, {}^3A_{1u}, M=-1, \alpha_u) &= |\overline{\alpha_g \alpha_u}| \\ \Psi_2(a_{1g}a_{1u}, {}^3A_{1u}, M=0, \alpha_u) &= \frac{\sqrt{2}|\overline{\alpha_g} \alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g \overline{\alpha_u}|}{2} \\ \Psi_3(a_{1g}a_{1u}, {}^3A_{1u}, M=1, \alpha_u) &= |\alpha_g \alpha_u| \\ &\quad a_{2g}a_{2u}\end{aligned}$$

$$\boxed{\Delta E = \langle \beta_u \beta_g || \beta_u \beta_g \rangle - \langle \beta_u \beta_u || \beta_g \beta_g \rangle}$$

$$\Psi_4(a_{2g}a_{2u}, {}^3A_{1u}, M=-1, \alpha_u) = |\overline{\beta_u \beta_g}|$$

$$\begin{aligned}\Psi_5(a_{2g}a_{2u}, {}^3A_{1u}, M=0, \alpha_u) &= \frac{\sqrt{2}|\overline{\beta_u} \beta_g|}{2} + \frac{\sqrt{2}|\beta_u \overline{\beta_g}|}{2} \\ \Psi_6(a_{2g}a_{2u}, {}^3A_{1u}, M=1, \alpha_u) &= |\beta_u \beta_g|\end{aligned}$$

 $e_g e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(e_g e_u, {}^3A_{1u}, M=-1, \alpha_u) = \frac{\sqrt{2}|\overline{\gamma_u} \zeta_g|}{2} + \frac{\sqrt{2}|\zeta_u \overline{\gamma_g}|}{2}$$

$$\Psi_8(e_g e_u, {}^3A_{1u}, M=0, \alpha_u) = \frac{|\overline{\gamma_u} \zeta_g|}{2} + \frac{|\gamma_u \overline{\zeta_g}|}{2} + \frac{|\zeta_u \overline{\gamma_g}|}{2}$$

$$\Psi_9(e_g e_u, {}^3A_{1u}, M=1, \alpha_u) = \frac{\sqrt{2}|\gamma_u \zeta_g|}{2} + \frac{\sqrt{2}|\zeta_u \gamma_g|}{2}$$

 $t_{1g}t_{1u}$

$$\boxed{\Delta E = -3 \langle \nu_g \nu_g || \nu_u \nu_u \rangle + 3 \langle \nu_g \nu_u || \nu_g \nu_u \rangle}$$

$$\Psi_{10}(t_{1g}t_{1u}, {}^3A_{1u}, M=-1, \alpha_u) = \frac{\sqrt{3}|\overline{\eta_g} \eta_u|}{3} + \frac{\sqrt{3}|\mu_g \mu_u|}{3} + \frac{\sqrt{3}|\overline{\nu_g} \nu_u|}{3}$$

$$\Psi_{11}(t_{1g}t_{1u}, {}^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{6}|\overline{\eta_g} \eta_u|}{6} + \frac{\sqrt{6}|\mu_g \mu_u|}{6} + \frac{\sqrt{6}|\overline{\nu_g} \nu_u|}{6} + \frac{\sqrt{6}|\eta_g \overline{\nu_u}|}{6} + \frac{\sqrt{6}|\eta_g \overline{\eta_u}|}{6} + \frac{\sqrt{6}|\mu_g \overline{\mu_u}|}{6} + \frac{\sqrt{6}|\nu_g \overline{\nu_u}|}{6}$$

$$\Psi_{12}(t_{1g}t_{1u}, {}^3A_{1u}, M=1, \alpha_u) = \frac{\sqrt{3}|\overline{\eta_g} \eta_u|}{3} + \frac{\sqrt{3}|\mu_g \mu_u|}{3} + \frac{\sqrt{3}|\nu_g \nu_u|}{3}$$

 $t_{2g}t_{2u}$

$$\boxed{\Delta E = -3 \langle \xi_g \xi_g || \xi_u \xi_u \rangle + 3 \langle \xi_g \xi_u || \xi_g \xi_u \rangle}$$

$$\Psi_{13}(t_{2g}t_{2u}, {}^3A_{1u}, M=-1, \alpha_u) = \frac{\sqrt{3}|\overline{\chi_g} \chi_u|}{3} + \frac{\sqrt{3}|\phi_g \phi_u|}{3} + \frac{\sqrt{3}|\xi_g \xi_u|}{3}$$

$$\Psi_{14}(t_{2g}t_{2u}, {}^3A_{1u}, M=0, \alpha_u) = \frac{\sqrt{6}|\overline{\chi_g} \chi_u|}{6} + \frac{\sqrt{6}|\phi_g \phi_u|}{6} + \frac{\sqrt{6}|\overline{\xi_g} \xi_u|}{6} + \frac{\sqrt{6}|\chi_g \overline{\chi_u}|}{6} + \frac{\sqrt{6}|\phi_g \overline{\phi_u}|}{6} + \frac{\sqrt{6}|\xi_g \overline{\xi_u}|}{6}$$

$$\Psi_{15}(t_{2g}t_{2u}, {}^3A_{1u}, M=1, \alpha_u) = \frac{\sqrt{3}|\overline{\chi_g} \chi_u|}{3} + \frac{\sqrt{3}|\phi_g \phi_u|}{3} + \frac{\sqrt{3}|\xi_g \xi_u|}{3}$$

2.32.5 $^1A_{1u}$ $a_{1g}a_{1u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \alpha_u \alpha_u \rangle + \langle \alpha_g \alpha_u || \alpha_g \alpha_u \rangle}$$

$$\Psi_1(a_{1g}a_{1u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\alpha_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\alpha_u}|}{2}$$

 $a_{2g}a_{2u}$

$$\boxed{\Delta E = \langle \beta_u \beta_g || \beta_u \beta_g \rangle + \langle \beta_u \beta_u || \beta_g \beta_g \rangle}$$

$$\Psi_2(a_{2g}a_{2u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{2}|\overline{\beta_u}\beta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\beta_g}|}{2}$$

 $e_g e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(e_g e_u, ^1A_{1u}, M=0, \alpha_u) = -\frac{|\overline{\gamma_u}\zeta_g|}{2} - \frac{|\zeta_u\overline{\gamma_g}|}{2} + \frac{|\gamma_u\overline{\zeta_g}|}{2} + \frac{|\zeta_u\overline{\gamma_g}|}{2}$$

 $t_{1g}t_{1u}$

$$\boxed{\Delta E = 3 \langle \nu_g \nu_g || \nu_u \nu_u \rangle + 3 \langle \nu_g \nu_u || \nu_g \nu_u \rangle}$$

$$\Psi_4(t_{1g}t_{1u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{6}|\overline{\eta_g}\eta_u|}{6} - \frac{\sqrt{6}|\overline{\mu_g}\mu_u|}{6} - \frac{\sqrt{6}|\overline{\nu_g}\nu_u|}{6} + \frac{\sqrt{6}|\eta_g\overline{\eta_u}|}{6} + \frac{\sqrt{6}|\mu_g\overline{\mu_u}|}{6} + \frac{\sqrt{6}|\nu_g\overline{\nu_u}|}{6}$$

 $t_{2g}t_{2u}$

$$\boxed{\Delta E = 3 \langle \xi_g \xi_g || \xi_u \xi_u \rangle + 3 \langle \xi_g \xi_u || \xi_g \xi_u \rangle}$$

$$\Psi_5(t_{2g}t_{2u}, ^1A_{1u}, M=0, \alpha_u) = -\frac{\sqrt{6}|\overline{\chi_g}\chi_u|}{6} - \frac{\sqrt{6}|\overline{\phi_g}\phi_u|}{6} - \frac{\sqrt{6}|\overline{\xi_g}\xi_u|}{6} + \frac{\sqrt{6}|\chi_g\overline{\chi_u}|}{6} + \frac{\sqrt{6}|\phi_g\overline{\phi_u}|}{6} + \frac{\sqrt{6}|\xi_g\overline{\xi_u}|}{6}$$

2.32.6 $^3A_{2g}$ $a_{1g}a_{2g}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_{1g}a_{2g}, ^3A_{2g}, M=-1, \beta_g) = |\overline{\alpha_g}\beta_g|$$

$$\Psi_2(a_{1g}a_{2g}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\alpha_g}\beta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\beta_g}|}{2}$$

$$\Psi_3(a_{1g}a_{2g}, ^3A_{2g}, M=1, \beta_g) = |\alpha_g\beta_g|$$

 $a_{1u}a_{2u}$

$$\boxed{\Delta E = \langle \beta_u \alpha_u || \beta_u \alpha_u \rangle - \langle \beta_u \beta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_4(a_{1u}a_{2u}, ^3A_{2g}, M=-1, \beta_g) = |\overline{\beta_u}\alpha_u|$$

$$\Psi_5(a_{1u}a_{2u}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{2}|\overline{\beta_u}\alpha_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\alpha_u}|}{2}$$

$$\Psi_6(a_{1u}a_{2u}, ^3A_{2g}, M=1, \beta_g) = |\beta_u\alpha_u|$$

 e_u^2

$$\boxed{\Delta E = 0}$$

$$\Psi_7(e_u^2, ^3A_{2g}, M=-1, \beta_g) = -|\overline{\gamma_u}\zeta_u|$$

$$\Psi_8(e_u^2, ^3A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\gamma_u}\zeta_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\gamma_u}|}{2}$$

$$\Psi_9(e_u^2, ^3A_{2g}, M=1, \beta_g) = -|\gamma_u\zeta_u|$$

 e_g^2

$$\boxed{\Delta E = 0}$$

$$\Psi_{10}(e_g^2, ^3A_{2g}, M=-1, \beta_g) = -|\overline{\gamma_g}\zeta_g|$$

$$\Psi_{11}(e_g^2, ^3A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\gamma_g}\zeta_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\gamma_g}|}{2}$$

$$\Psi_{12}(e_g^2, ^3A_{2g}, M=1, \beta_g) = -|\gamma_g\zeta_g|$$

 $t_{1g}t_{2g}$

$$\boxed{\Delta E = 3 \langle \nu_g \chi_g || \nu_g \chi_g \rangle - 3 \langle \nu_g \nu_g || \chi_g \chi_g \rangle}$$

$$\Psi_{13}(t_{1g}t_{2g}, ^3A_{2g}, M=-1, \beta_g) = \frac{\sqrt{3}|\overline{\eta_g}\zeta_g|}{3} + \frac{\sqrt{3}|\mu_g\overline{\phi_g}|}{3} + \frac{\sqrt{3}|\nu_g\overline{\chi_g}|}{3}$$

$$\Psi_{14}(t_{1g}t_{2g}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{6}|\overline{\eta_g}\xi_g|}{6} + \frac{\sqrt{6}|\overline{\mu_g}\phi_g|}{6} + \frac{\sqrt{6}|\overline{\nu_g}\chi_g|}{6} + \frac{\sqrt{6}|\eta_g\overline{\xi_g}|}{6} + \frac{\sqrt{6}|\mu_g\overline{\phi_g}|}{6} + \frac{\sqrt{6}|\nu_g\overline{\chi_g}|}{6}$$

$$\Psi_{15}(t_{1g}t_{2g}, ^3A_{2g}, M=1, \beta_g) = \frac{\sqrt{3}|\eta_g\xi_g|}{3} + \frac{\sqrt{3}|\mu_g\phi_g|}{3} + \frac{\sqrt{3}|\nu_g\chi_g|}{3}$$

 $t_{1u}t_{2u}$

$$\boxed{\Delta E = 3 \langle \nu_u \chi_u || \nu_u \chi_u \rangle - 3 \langle \nu_u \nu_u || \chi_u \chi_u \rangle}$$

$$\Psi_{16}(t_{1u}t_{2u}, ^3A_{2g}, M=-1, \beta_g) = \frac{\sqrt{3}|\overline{\eta_u}\xi_u|}{3} + \frac{\sqrt{3}|\overline{\mu_u}\phi_u|}{3} + \frac{\sqrt{3}|\overline{\nu_u}\chi_u|}{3}$$

$$\Psi_{17}(t_{1u}t_{2u}, ^3A_{2g}, M=0, \beta_g) = \frac{\sqrt{6}|\overline{\eta_u}\xi_u|}{6} + \frac{\sqrt{6}|\overline{\mu_u}\phi_u|}{6} + \frac{\sqrt{6}|\overline{\nu_u}\chi_u|}{6} + \frac{\sqrt{6}|\eta_u\overline{\xi_u}|}{6} + \frac{\sqrt{6}|\mu_u\overline{\phi_u}|}{6} + \frac{\sqrt{6}|\nu_u\overline{\chi_u}|}{6}$$

$$\Psi_{18}(t_{1u}t_{2u}, ^3A_{2g}, M=1, \beta_g) = \frac{\sqrt{3}|\eta_u\xi_u|}{3} + \frac{\sqrt{3}|\mu_u\phi_u|}{3} + \frac{\sqrt{3}|\nu_u\chi_u|}{3}$$

2.32.7 $^1A_{2g}$ $a_{1g}a_{2g}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \beta_g \beta_g \rangle + \langle \alpha_g \beta_g || \alpha_g \beta_g \rangle}$$

$$\Psi_1(a_{1g}a_{2g}, ^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\beta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\beta_g}|}{2}$$

 $a_{1u}a_{2u}$

$$\boxed{\Delta E = \langle \beta_u \alpha_u || \beta_u \alpha_u \rangle + \langle \beta_u \beta_u || \alpha_u \alpha_u \rangle}$$

$$\Psi_2(a_{1u}a_{2u}, {}^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{2}|\beta_u\alpha_u|}{2} + \frac{\sqrt{2}|\beta_u\bar{\alpha}_u|}{2}$$

$t_{1g}t_{2g}$

$$\boxed{\Delta E = 3 \langle \nu_g \chi_g | \nu_g \chi_g \rangle + 3 \langle \nu_g \nu_g | \chi_g \chi_g \rangle}$$

$$\Psi_3(t_{1g}t_{2g}, {}^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{6}|\eta_g\xi_g|}{6} - \frac{\sqrt{6}|\mu_g\phi_g|}{6} -$$

$t_{1u}t_{2u}$

$$\boxed{\Delta E = 3 \langle \nu_u \chi_u | \nu_u \chi_u \rangle + 3 \langle \nu_u \nu_u | \chi_u \chi_u \rangle}$$

$$\Psi_4(t_{1u}t_{2u}, {}^1A_{2g}, M=0, \beta_g) = -\frac{\sqrt{6}|\eta_u\xi_u|}{6} - \frac{\sqrt{6}|\mu_u\phi_u|}{6} -$$

$$\frac{\sqrt{6}|\nu_u\chi_u|}{6} + \frac{\sqrt{6}|\eta_u\bar{\xi}_u|}{6} + \frac{\sqrt{6}|\mu_u\bar{\phi}_u|}{6} + \frac{\sqrt{6}|\nu_u\bar{\chi}_u|}{6}$$

2.32.8 3E_u

$a_{1g}e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(a_{1g}e_u, {}^3E_u, M=-1, \gamma_u) = |\overline{\alpha_g}\gamma_u|$$

$$\Psi_2(a_{1g}e_u, {}^3E_u, M=-1, \zeta_u) = |\overline{\alpha_g}\zeta_u|$$

$$\Psi_3(a_{1g}e_u, {}^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_g}\gamma_u|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\gamma}_u|}{2}$$

$$\Psi_4(a_{1g}e_u, {}^3E_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_g}\zeta_u|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\zeta}_u|}{2}$$

$$\Psi_5(a_{1g}e_u, {}^3E_u, M=1, \gamma_u) = |\alpha_g\gamma_u|$$

$$\Psi_6(a_{1g}e_u, {}^3E_u, M=1, \zeta_u) = |\alpha_g\zeta_u|$$

$a_{2u}e_g$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(a_{2u}e_g, {}^3E_u, M=-1, \gamma_u) = |\overline{\beta_u}\gamma_g|$$

$$\Psi_8(a_{2u}e_g, {}^3E_u, M=-1, \zeta_u) = -|\overline{\beta_u}\zeta_g|$$

$$\Psi_9(a_{2u}e_g, {}^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\beta_u}\gamma_g|}{2} + \frac{\sqrt{2}|\beta_u\bar{\gamma}_g|}{2}$$

$$\Psi_{10}(a_{2u}e_g, {}^3E_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\beta_u}\zeta_g|}{2} - \frac{\sqrt{2}|\beta_u\bar{\zeta}_g|}{2}$$

$$\Psi_{11}(a_{2u}e_g, {}^3E_u, M=1, \gamma_u) = |\beta_u\gamma_g|$$

$$\Psi_{12}(a_{2u}e_g, {}^3E_u, M=1, \zeta_u) = -|\beta_u\zeta_g|$$

$a_{1u}e_g$

$$\boxed{\Delta E = 0}$$

$$\Psi_{13}(a_{1u}e_g, {}^3E_u, M=-1, \gamma_u) = |\overline{\alpha_u}\gamma_g|$$

$$\Psi_{14}(a_{1u}e_g, {}^3E_u, M=-1, \zeta_u) = |\overline{\alpha_u}\zeta_g|$$

$$\Psi_{15}(a_{1u}e_g, {}^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\alpha_u}\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\gamma}_g|}{2}$$

$$\Psi_{16}(a_{1u}e_g, {}^3E_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\alpha_u}\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\zeta}_g|}{2}$$

$$\Psi_{17}(a_{1u}e_g, {}^3E_u, M=1, \gamma_u) = |\alpha_u\gamma_g|$$

$$\Psi_{18}(a_{1u}e_g, {}^3E_u, M=1, \zeta_u) = |\alpha_u\zeta_g|$$

$a_{2g}e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_{19}(a_{2g}e_u, {}^3E_u, M=-1, \gamma_u) = |\overline{\beta_g}\gamma_u|$$

$$\Psi_{20}(a_{2g}e_u, {}^3E_u, M=-1, \zeta_u) = -|\overline{\beta_g}\zeta_u|$$

$$\Psi_{21}(a_{2g}e_u, {}^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\beta_g}\gamma_u|}{2} + \frac{\sqrt{2}|\beta_g\bar{\gamma}_u|}{2}$$

$$\Psi_{22}(a_{2g}e_u, {}^3E_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\beta_g}\zeta_u|}{2} - \frac{\sqrt{2}|\beta_g\bar{\zeta}_u|}{2}$$

$$\Psi_{23}(a_{2g}e_u, {}^3E_u, M=1, \gamma_u) = |\beta_g\gamma_u|$$

$$\Psi_{24}(a_{2g}e_u, {}^3E_u, M=1, \zeta_u) = -|\beta_g\zeta_u|$$

$e_g e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_{25}(e_g e_u, {}^3E_u, M=-1, \zeta_u) = |\overline{\gamma_u}\gamma_g|$$

$$\Psi_{26}(e_g e_u, {}^3E_u, M=-1, \gamma_u) = |\overline{\zeta_u}\zeta_g|$$

$$\Psi_{27}(e_g e_u, {}^3E_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\gamma_u}\gamma_g|}{2} + \frac{\sqrt{2}|\gamma_u\bar{\gamma}_g|}{2}$$

$$\Psi_{28}(e_g e_u, {}^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}|\overline{\zeta_u}\zeta_g|}{2} + \frac{\sqrt{2}|\zeta_u\bar{\zeta}_g|}{2}$$

$$\Psi_{29}(e_g e_u, {}^3E_u, M=1, \zeta_u) = |\gamma_u\gamma_g|$$

$$\Psi_{30}(e_g e_u, {}^3E_u, M=1, \gamma_u) = |\zeta_u\zeta_g|$$

$t_{1g}t_{1u}$

$$\boxed{\Delta E = 0}$$

$$\Psi_{31}(t_{1g}t_{1u}, {}^3E_u, M=-1, \gamma_u) = \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta_g}\eta_u| + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\mu_g}\mu_u| + \frac{\sqrt{3}|\overline{\nu_g}\nu_u|}{3}$$

$$\Psi_{32}(t_{1g}t_{1u}, {}^3E_u, M=-1, \zeta_u) = \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta_g}\eta_u| + \frac{\sqrt{3}|\overline{\mu_g}\mu_u|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\nu_g}\nu_u|$$

$$\Psi_{33}(t_{1g}t_{1u}, {}^3E_u, M=0, \gamma_u) = \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta_g}\eta_u|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\mu_g}\mu_u|}{2} + \frac{\sqrt{6}|\overline{\nu_g}\nu_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\eta_g\bar{\eta}_u|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\mu_g\bar{\mu}_u|}{2} + \frac{\sqrt{6}|\nu_g\bar{\nu}_u|}{6}$$

$$\Psi_{34}(t_{1g}t_{1u}, {}^3E_u, M=0, \zeta_u) = \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta_g}\eta_u|}{2} + \frac{\sqrt{6}|\overline{\mu_g}\mu_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\nu_g}\nu_u|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\eta_g\bar{\eta}_u|}{2} + \frac{\sqrt{6}|\mu_g\bar{\mu}_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\nu_g\bar{\nu}_u|}{2}$$

$$\Psi_{35}(t_{1g}t_{1u}, {}^3E_u, M=1, \gamma_u) = \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\eta_g\eta_u| + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\mu_g\mu_u| + \frac{\sqrt{3}|\nu_g\nu_u|}{3}$$

$$\Psi_{36}(t_{1g}t_{1u}, {}^3E_u, M=1, \zeta_u) = \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\eta_g\eta_u| + \frac{\sqrt{3}|\mu_g\mu_u|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\nu_g\nu_u|$$

$t_{1g}t_{2u}$

$$\boxed{\Delta E = 0}$$

$$\begin{aligned} \Psi_{37}(t_{1g}t_{2u}, {}^3E_u, M=-1, \gamma_u) &= \\ \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta_g\xi_u}| + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\mu_g\phi_u}| + \frac{\sqrt{3}|\overline{\nu_g\chi_u}|}{3} \\ \Psi_{38}(t_{1g}t_{2u}, {}^3E_u, M=-1, \zeta_u) &= \\ \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\eta_g\xi_u}| - \frac{\sqrt{3}|\overline{\mu_g\phi_u}|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\nu_g\chi_u}| \\ \Psi_{39}(t_{1g}t_{2u}, {}^3E_u, M=0, \gamma_u) &= \\ \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\eta_g\xi_u}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\mu_g\phi_u}|}{2} + \frac{\sqrt{6}|\overline{\nu_g\chi_u}|}{6} + \\ \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\eta_g\xi_u}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\mu_g\phi_u}|}{2} + \frac{\sqrt{6}|\overline{\nu_g\chi_u}|}{6} \\ \Psi_{40}(t_{1g}t_{2u}, {}^3E_u, M=0, \zeta_u) &= \\ \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_g\xi_u}|}{2} - \frac{\sqrt{6}|\overline{\mu_g\phi_u}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\nu_g\chi_u}|}{2} + \\ \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_g\xi_u}|}{2} - \frac{\sqrt{6}|\overline{\mu_g\phi_u}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\nu_g\chi_u}|}{2} \\ \Psi_{41}(t_{1g}t_{2u}, {}^3E_u, M=1, \gamma_u) &= \\ \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\eta_g\xi_u| + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\mu_g\phi_u| + \frac{\sqrt{3}|\nu_g\chi_u|}{3} \\ \Psi_{42}(t_{1g}t_{2u}, {}^3E_u, M=1, \zeta_u) &= \\ \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\eta_g\xi_u| - \frac{\sqrt{3}|\mu_g\phi_u|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\nu_g\chi_u| \end{aligned}$$

 $t_{1u}t_{2g}$

$$\boxed{\Delta E = 0}$$

$$\begin{aligned} \Psi_{43}(t_{1u}t_{2g}, {}^3E_u, M=-1, \gamma_u) &= \\ \frac{\sqrt{3}|\overline{\chi_g\nu_u}|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\phi_g\mu_u}| + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\xi_g\eta_u}| \\ \Psi_{44}(t_{1u}t_{2g}, {}^3E_u, M=-1, \zeta_u) &= \\ \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\chi_g\nu_u}| - \frac{\sqrt{3}|\overline{\phi_g\mu_u}|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\xi_g\eta_u}| \\ \Psi_{45}(t_{1u}t_{2g}, {}^3E_u, M=0, \gamma_u) &= \\ \frac{\sqrt{6}|\overline{\chi_g\nu_u}|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\phi_g\mu_u}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\xi_g\eta_u}|}{2} + \\ \frac{\sqrt{6}|\overline{\chi_g\nu_u}|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\phi_g\mu_u}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\xi_g\eta_u}|}{2} \\ \Psi_{46}(t_{1u}t_{2g}, {}^3E_u, M=0, \zeta_u) &= \\ \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\chi_g\nu_u}|}{2} - \frac{\sqrt{6}|\overline{\phi_g\mu_u}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\xi_g\eta_u}|}{2} + \\ \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\chi_g\nu_u}|}{2} - \frac{\sqrt{6}|\overline{\phi_g\mu_u}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\xi_g\eta_u}|}{2} \\ \Psi_{47}(t_{1u}t_{2g}, {}^3E_u, M=1, \gamma_u) &= \\ \frac{\sqrt{3}|\overline{\chi_g\nu_u}|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\phi_g\mu_u}| + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\xi_g\eta_u}| \\ \Psi_{48}(t_{1u}t_{2g}, {}^3E_u, M=1, \zeta_u) &= \\ \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\chi_g\nu_u| - \frac{\sqrt{3}|\phi_g\mu_u|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\xi_g\eta_u| \end{aligned}$$

 $t_{2g}t_{2u}$

$$\boxed{\Delta E = 0}$$

$$\begin{aligned} \Psi_{49}(t_{2g}t_{2u}, {}^3E_u, M=-1, \gamma_u) &= \\ \frac{\sqrt{3}|\overline{\chi_g\chi_u}|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\phi_g\phi_u}| + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\xi_g\xi_u}| \\ \Psi_{50}(t_{2g}t_{2u}, {}^3E_u, M=-1, \zeta_u) &= \\ \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\chi_g\chi_u}| + \frac{\sqrt{3}|\overline{\phi_g\phi_u}|}{3} + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\xi_g\xi_u}| \end{aligned}$$

$$\begin{aligned} \Psi_{51}(t_{2g}t_{2u}, {}^3E_u, M=0, \gamma_u) &= \\ \frac{\sqrt{6}|\overline{\chi_g\chi_u}|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\phi_g\phi_u}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\xi_g\xi_u}|}{2} + \\ \frac{\sqrt{6}|\overline{\chi_g\chi_u}|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\phi_g\phi_u}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\xi_g\xi_u}|}{2} \\ \Psi_{52}(t_{2g}t_{2u}, {}^3E_u, M=0, \zeta_u) &= \\ \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\chi_g\chi_u}|}{2} + \frac{\sqrt{6}|\overline{\phi_g\phi_u}|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\xi_g\xi_u}|}{2} + \\ \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\chi_g\chi_u}|}{2} + \frac{\sqrt{6}|\overline{\phi_g\phi_u}|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\xi_g\xi_u}|}{2} \\ \Psi_{53}(t_{2g}t_{2u}, {}^3E_u, M=1, \gamma_u) &= \\ \frac{\sqrt{3}|\overline{\chi_g\chi_u}|}{3} + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\phi_g\phi_u}| + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\xi_g\xi_u}| \\ \Psi_{54}(t_{2g}t_{2u}, {}^3E_u, M=1, \zeta_u) &= \\ \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\chi_g\chi_u| + \frac{\sqrt{3}|\phi_g\phi_u|}{3} + \left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\xi_g\xi_u| \end{aligned}$$

2.32.9 1E_u $a_{1g}e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(a_{1g}e_u, {}^1E_u, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\alpha_g\gamma_u}|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\gamma_u}|}{2}$$

$$\Psi_2(a_{1g}e_u, {}^1E_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_g\zeta_u}|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\zeta_u}|}{2}$$

 $a_{2u}e_g$

$$\boxed{\Delta E = 0}$$

$$\Psi_3(a_{2u}e_g, {}^1E_u, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\beta_u\gamma_g}|}{2} + \frac{\sqrt{2}|\beta_u\overline{\gamma_g}|}{2}$$

$$\Psi_4(a_{2u}e_g, {}^1E_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\beta_u\zeta_g}|}{2} - \frac{\sqrt{2}|\beta_u\overline{\zeta_g}|}{2}$$

 $a_{1u}e_g$

$$\boxed{\Delta E = 0}$$

$$\Psi_5(a_{1u}e_g, {}^1E_u, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\alpha_u\gamma_g}|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\gamma_g}|}{2}$$

$$\Psi_6(a_{1u}e_g, {}^1E_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\alpha_u\zeta_g}|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\zeta_g}|}{2}$$

 $a_{2g}e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(a_{2g}e_u, {}^1E_u, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\beta_g\gamma_u}|}{2} + \frac{\sqrt{2}|\beta_g\overline{\gamma_u}|}{2}$$

$$\Psi_8(a_{2g}e_u, {}^1E_u, M=0, \zeta_u) = \frac{\sqrt{2}|\overline{\beta_g\zeta_u}|}{2} - \frac{\sqrt{2}|\beta_g\overline{\zeta_u}|}{2}$$

 $e_g e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_9(e_g e_u, {}^1E_u, M=0, \zeta_u) = -\frac{\sqrt{2}|\overline{\gamma_u\gamma_g}|}{2} + \frac{\sqrt{2}|\gamma_u\overline{\gamma_g}|}{2}$$

$$\Psi_{10}(e_g e_u, {}^1E_u, M=0, \gamma_u) = -\frac{\sqrt{2}|\overline{\zeta_u\zeta_g}|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\zeta_g}|}{2}$$

$t_{1g}t_{1u}$

$$\boxed{\Delta E = 0}$$

$$\begin{aligned} \Psi_{11}(t_{1g}t_{1u}, ^1E_u, M=0, \gamma_u) = \\ -\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\eta_g\eta_u|}{2} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\mu_g\mu_u|}{2} - \frac{\sqrt{6}|\nu_g\nu_u|}{6} + \\ -\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\eta_g\bar{\eta}_u|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\mu_g\bar{\mu}_u|}{2} + \frac{\sqrt{6}|\nu_g\bar{\nu}_u|}{6} \end{aligned}$$

$$\begin{aligned} \Psi_{12}(t_{1g}t_{1u}, ^1E_u, M=0, \zeta_u) = \\ -\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\eta_g\eta_u|}{2} - \frac{\sqrt{6}|\mu_g\mu_u|}{6} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\nu_g\nu_u|}{2} + \\ -\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\eta_g\bar{\eta}_u|}{2} + \frac{\sqrt{6}|\mu_g\bar{\mu}_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\nu_g\bar{\nu}_u|}{2} \end{aligned}$$

 $t_{1g}t_{2u}$

$$\boxed{\Delta E = 0}$$

$$\begin{aligned} \Psi_{13}(t_{1g}t_{2u}, ^1E_u, M=0, \gamma_u) = \\ -\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\eta_g\xi_u|}{2} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\mu_g\phi_u|}{2} - \frac{\sqrt{6}|\nu_g\chi_u|}{6} + \\ -\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\eta_g\bar{\xi}_u|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\mu_g\bar{\phi}_u|}{2} + \frac{\sqrt{6}|\nu_g\bar{\chi}_u|}{6} \end{aligned}$$

$$\begin{aligned} \Psi_{14}(t_{1g}t_{2u}, ^1E_u, M=0, \zeta_u) = \\ -\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\eta_g\xi_u|}{2} + \frac{\sqrt{6}|\mu_g\phi_u|}{6} - \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\nu_g\chi_u|}{2} + \\ -\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\eta_g\bar{\xi}_u|}{2} - \frac{\sqrt{6}|\mu_g\bar{\phi}_u|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\nu_g\bar{\chi}_u|}{2} \end{aligned}$$

 $t_{1u}t_{2g}$

$$\boxed{\Delta E = 0}$$

$$\begin{aligned} \Psi_{15}(t_{1u}t_{2g}, ^1E_u, M=0, \gamma_u) = \\ -\frac{\sqrt{6}|\chi_g\nu_u|}{6} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\phi_g\mu_u|}{2} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\xi_g\eta_u|}{2} + \\ -\frac{\sqrt{6}|\chi_g\bar{\nu}_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\phi_g\bar{\mu}_u|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\xi_g\bar{\eta}_u|}{2} \end{aligned}$$

$$\begin{aligned} \Psi_{16}(t_{1u}t_{2g}, ^1E_u, M=0, \zeta_u) = \\ -\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\chi_g\nu_u|}{2} + \frac{\sqrt{6}|\phi_g\mu_u|}{6} - \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\xi_g\eta_u|}{2} + \\ -\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\chi_g\bar{\nu}_u|}{2} - \frac{\sqrt{6}|\phi_g\bar{\mu}_u|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\xi_g\bar{\eta}_u|}{2} \end{aligned}$$

 $t_{2g}t_{2u}$

$$\boxed{\Delta E = 0}$$

$$\begin{aligned} \Psi_{17}(t_{2g}t_{2u}, ^1E_u, M=0, \gamma_u) = \\ -\frac{\sqrt{6}|\chi_g\chi_u|}{6} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\phi_g\phi_u|}{2} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\xi_g\xi_u|}{2} + \\ -\frac{\sqrt{6}|\chi_g\bar{\chi}_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\phi_g\bar{\phi}_u|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\xi_g\bar{\xi}_u|}{2} \end{aligned}$$

$$\begin{aligned} \Psi_{18}(t_{2g}t_{2u}, ^1E_u, M=0, \zeta_u) = \\ -\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\chi_g\chi_u|}{2} - \frac{\sqrt{6}|\phi_g\phi_u|}{6} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\xi_g\bar{\xi}_u|}{2} + \\ -\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}+\frac{i}{2}\right)|\chi_g\bar{\chi}_u|}{2} + \frac{\sqrt{6}|\phi_g\bar{\phi}_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6}-\frac{i}{2}\right)|\xi_g\xi_u|}{2} \end{aligned}$$

2.32.10 3E_g $a_{1g}e_g$

$$\boxed{\Delta E = 0}$$

$$\Psi_1(a_{1g}e_g, ^3E_g, M=-1, \gamma_g) = |\alpha_g\gamma_g|$$

$$\Psi_2(a_{1g}e_g, ^3E_g, M=-1, \zeta_g) = |\alpha_g\zeta_g|$$

$$\Psi_3(a_{1g}e_g, ^3E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\alpha_g\gamma_g|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\gamma}_g|}{2}$$

$$\Psi_4(a_{1g}e_g, ^3E_g, M=0, \zeta_g) = \frac{\sqrt{2}|\alpha_g\zeta_g|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\zeta}_g|}{2}$$

$$\Psi_5(a_{1g}e_g, ^3E_g, M=1, \gamma_g) = |\alpha_g\gamma_g|$$

$$\Psi_6(a_{1g}e_g, ^3E_g, M=1, \zeta_g) = |\alpha_g\zeta_g|$$

 $a_{2u}e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_7(a_{2u}e_u, ^3E_g, M=-1, \gamma_g) = |\beta_u\gamma_u|$$

$$\Psi_8(a_{2u}e_u, ^3E_g, M=-1, \zeta_u) = -|\beta_u\zeta_u|$$

$$\Psi_9(a_{2u}e_u, ^3E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\beta_u\gamma_u|}{2} + \frac{\sqrt{2}|\beta_u\bar{\gamma}_u|}{2}$$

$$\Psi_{10}(a_{2u}e_u, ^3E_g, M=0, \zeta_u) = -\frac{\sqrt{2}|\beta_u\zeta_u|}{2} - \frac{\sqrt{2}|\beta_u\bar{\zeta}_u|}{2}$$

$$\Psi_{11}(a_{2u}e_u, ^3E_g, M=1, \gamma_u) = |\beta_u\gamma_u|$$

$$\Psi_{12}(a_{2u}e_u, ^3E_g, M=1, \zeta_u) = -|\beta_u\zeta_u|$$

 $a_{1u}e_u$

$$\boxed{\Delta E = 0}$$

$$\Psi_{13}(a_{1u}e_u, ^3E_g, M=-1, \gamma_g) = |\alpha_u\gamma_u|$$

$$\Psi_{14}(a_{1u}e_u, ^3E_g, M=-1, \zeta_u) = |\alpha_u\zeta_u|$$

$$\Psi_{15}(a_{1u}e_u, ^3E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\alpha_u\gamma_u|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\gamma}_u|}{2}$$

$$\Psi_{16}(a_{1u}e_u, ^3E_g, M=0, \zeta_u) = \frac{\sqrt{2}|\alpha_u\zeta_u|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\zeta}_u|}{2}$$

$$\Psi_{17}(a_{1u}e_u, ^3E_g, M=1, \gamma_u) = |\alpha_u\gamma_u|$$

$$\Psi_{18}(a_{1u}e_u, ^3E_g, M=1, \zeta_u) = |\alpha_u\zeta_u|$$

 $a_{2g}e_g$

$$\boxed{\Delta E = 0}$$

$$\Psi_{19}(a_{2g}e_g, ^3E_g, M=-1, \gamma_g) = |\beta_g\gamma_g|$$

$$\Psi_{20}(a_{2g}e_g, ^3E_g, M=-1, \zeta_g) = -|\beta_g\zeta_g|$$

$$\Psi_{21}(a_{2g}e_g, ^3E_g, M=0, \gamma_g) = \frac{\sqrt{2}|\beta_g\gamma_g|}{2} + \frac{\sqrt{2}|\beta_g\bar{\gamma}_g|}{2}$$

$$\Psi_{22}(a_{2g}e_g, ^3E_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\beta_g\zeta_g|}{2} - \frac{\sqrt{2}|\beta_g\bar{\zeta}_g|}{2}$$

$$\Psi_{23}(a_{2g}e_g, ^3E_g, M=1, \gamma_g) = |\beta_g\gamma_g|$$

$$\Psi_{24}(a_{2g}e_g, ^3E_g, M=1, \zeta_g) = -|\beta_g\zeta_g|$$

 $t_{1g}t_{2g}$

$$\boxed{\Delta E = 0}$$

$$\begin{aligned}
\Psi_{25}(t_{1g}t_{2g}, {}^3E_g, M=-1, \gamma_g) &= \\
\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta_g\xi_g}| + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\mu_g\phi_g}| + \frac{\sqrt{3}|\nu_g\chi_g|}{3} & \\
\Psi_{26}(t_{1g}t_{2g}, {}^3E_g, M=-1, \zeta_g) = \\
\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\eta_g\xi_g}| - \frac{\sqrt{3}|\overline{\mu_g\phi_g}|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\nu_g\chi_g}| & \\
\Psi_{27}(t_{1g}t_{2g}, {}^3E_g, M=0, \gamma_g) = \\
\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\eta_g\xi_g}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\mu_g\phi_g}|}{2} + \frac{\sqrt{6}|\overline{\nu_g\chi_g}|}{6} + \\
\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\eta_g\xi_g}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\mu_g\phi_g}|}{2} + \frac{\sqrt{6}|\overline{\nu_g\chi_g}|}{6} & \\
\Psi_{28}(t_{1g}t_{2g}, {}^3E_g, M=0, \zeta_g) = \\
\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_g\xi_g}|}{2} - \frac{\sqrt{6}|\overline{\mu_g\phi_g}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\nu_g\chi_g}|}{2} + \\
\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_g\xi_g}|}{2} - \frac{\sqrt{6}|\overline{\mu_g\phi_g}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\nu_g\chi_g}|}{2} & \\
\Psi_{29}(t_{1g}t_{2g}, {}^3E_g, M=1, \gamma_g) = \\
\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\eta_g\xi_g| + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\mu_g\phi_g| + \frac{\sqrt{3}|\nu_g\chi_g|}{3} & \\
\Psi_{30}(t_{1g}t_{2g}, {}^3E_g, M=1, \zeta_g) = \\
\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\eta_g\xi_g| - \frac{\sqrt{3}|\mu_g\phi_g|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\nu_g\chi_g| & \\
t_{1u}t_{2u} \\
\boxed{\Delta E = 0} &
\end{aligned}$$

$$\begin{aligned}
\Psi_{31}(t_{1u}t_{2u}, {}^3E_g, M=-1, \gamma_g) &= \\
\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\eta_u\xi_u}| + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\mu_u\phi_u}| + \frac{\sqrt{3}|\overline{\nu_u\chi_u}|}{3} & \\
\Psi_{32}(t_{1u}t_{2u}, {}^3E_g, M=-1, \zeta_g) = \\
\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\eta_u\xi_u}| - \frac{\sqrt{3}|\overline{\mu_u\phi_u}|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\nu_u\chi_u}| & \\
\Psi_{33}(t_{1u}t_{2u}, {}^3E_g, M=0, \gamma_g) = \\
\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\eta_u\xi_u}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\mu_u\phi_u}|}{2} + \frac{\sqrt{6}|\overline{\nu_u\chi_u}|}{6} + \\
\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\eta_u\xi_u}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\mu_u\phi_u}|}{2} + \frac{\sqrt{6}|\overline{\nu_u\chi_u}|}{6} & \\
\Psi_{34}(t_{1u}t_{2u}, {}^3E_g, M=0, \zeta_g) = \\
\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_u\xi_u}|}{2} - \frac{\sqrt{6}|\overline{\mu_u\phi_u}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\nu_u\chi_u}|}{2} + \\
\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_u\xi_u}|}{2} - \frac{\sqrt{6}|\overline{\mu_u\phi_u}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\nu_u\chi_u}|}{2} & \\
\Psi_{35}(t_{1u}t_{2u}, {}^3E_g, M=1, \gamma_g) = \\
\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\eta_u\xi_u| + \left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\mu_u\phi_u| + \frac{\sqrt{3}|\nu_u\chi_u|}{3} & \\
\Psi_{36}(t_{1u}t_{2u}, {}^3E_g, M=1, \zeta_g) = \\
\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\eta_u\xi_u| - \frac{\sqrt{3}|\mu_u\phi_u|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\nu_u\chi_u| &
\end{aligned}$$

2.32.11 1E_g

$$\begin{aligned}
a_{1g}e_g \\
\boxed{\Delta E = 0} & \\
\Psi_1(a_{1g}e_g, {}^1E_g, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\alpha_g\gamma_g}|}{2} + \frac{\sqrt{2}|\overline{\alpha_g\gamma_g}|}{2} &
\end{aligned}$$

$$\begin{aligned}
\Psi_2(a_{1g}e_g, {}^1E_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\alpha_g\zeta_g}|}{2} + \frac{\sqrt{2}|\overline{\alpha_g\zeta_g}|}{2} \\
a_{2u}e_u \\
\boxed{\Delta E = 0} & \\
\Psi_3(a_{2u}e_u, {}^1E_g, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\beta_u\gamma_u}|}{2} + \frac{\sqrt{2}|\beta_u\gamma_u|}{2} \\
\Psi_4(a_{2u}e_u, {}^1E_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_u\zeta_u}|}{2} - \frac{\sqrt{2}|\beta_u\zeta_u|}{2} \\
a_{1u}e_u \\
\boxed{\Delta E = 0} & \\
\Psi_5(a_{1u}e_u, {}^1E_g, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\alpha_u\gamma_u}|}{2} + \frac{\sqrt{2}|\alpha_u\gamma_u|}{2} \\
\Psi_6(a_{1u}e_u, {}^1E_g, M=0, \zeta_g) = -\frac{\sqrt{2}|\overline{\alpha_u\zeta_u}|}{2} + \frac{\sqrt{2}|\alpha_u\zeta_u|}{2} \\
a_{2g}e_g \\
\boxed{\Delta E = 0} & \\
\Psi_7(a_{2g}e_g, {}^1E_g, M=0, \gamma_g) = -\frac{\sqrt{2}|\overline{\beta_g\gamma_g}|}{2} + \frac{\sqrt{2}|\beta_g\gamma_g|}{2} \\
\Psi_8(a_{2g}e_g, {}^1E_g, M=0, \zeta_g) = \frac{\sqrt{2}|\overline{\beta_g\zeta_g}|}{2} - \frac{\sqrt{2}|\beta_g\zeta_g|}{2} \\
e_u^2 \\
\boxed{\Delta E = 0} & \\
\Psi_9(e_u^2, {}^1E_g, M=0, \zeta_g) = -|\overline{\gamma_u\gamma_u}| \\
\Psi_{10}(e_u^2, {}^1E_g, M=0, \gamma_g) = -|\overline{\zeta_u\zeta_u}| & \\
e_g^2 \\
\boxed{\Delta E = 0} & \\
\Psi_{11}(e_g^2, {}^1E_g, M=0, \zeta_g) = -|\overline{\gamma_g\gamma_g}| \\
\Psi_{12}(e_g^2, {}^1E_g, M=0, \gamma_g) = -|\overline{\zeta_g\zeta_g}| \\
t_{1g}^2 \\
\boxed{\Delta E = 0} & \\
\Psi_{13}(t_{1g}^2, {}^1E_g, M=0, \gamma_g) = \\
\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\eta_g\eta_g}| + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\mu_g\mu_g}| - \frac{\sqrt{3}|\overline{\nu_g\nu_g}|}{3} & \\
\Psi_{14}(t_{1g}^2, {}^1E_g, M=0, \zeta_g) = \\
\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right) |\overline{\eta_g\eta_g}| - \frac{\sqrt{3}|\overline{\mu_g\mu_g}|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right) |\overline{\nu_g\nu_g}| & \\
t_{1g}t_{2g} \\
\boxed{\Delta E = 0} & \\
\Psi_{15}(t_{1g}t_{2g}, {}^1E_g, M=0, \gamma_g) = \\
-\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\eta_g\xi_g}|}{2} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\mu_g\phi_g}|}{2} - \frac{\sqrt{6}|\overline{\nu_g\chi_g}|}{6} + \\
-\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\eta_g\xi_g}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\mu_g\phi_g}|}{2} + \frac{\sqrt{6}|\overline{\nu_g\chi_g}|}{6} &
\end{aligned}$$

$$\Psi_{16}(t_{1g}t_{2g}, {}^1E_g, M=0, \zeta_g) = -\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_g}\xi_g|}{2} + \frac{\sqrt{6}|\overline{\mu_g}\phi_g|}{6} - \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\nu_g}\chi_g|}{2} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\eta_g\overline{\xi_g}|}{2} - \frac{\sqrt{6}|\mu_g\overline{\phi_g}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\nu_g\overline{\chi_g}|}{2}$$

 t_{2g}^2

$$\boxed{\Delta E = 0}$$

$$\Psi_{17}(t_{2g}^2, {}^1E_g, M=0, \gamma_g) = -\frac{\sqrt{3}|\overline{\chi_g}\chi_g|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\phi_g}\phi_g| + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\xi_g}\xi_g|$$

$$\Psi_{18}(t_{2g}^2, {}^1E_g, M=0, \zeta_g) =$$

$$\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\chi_g}\chi_g| - \frac{\sqrt{3}|\overline{\phi_g}\phi_g|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\xi_g}\xi_g|$$

 t_{1u}^2

$$\boxed{\Delta E = 0}$$

$$\Psi_{19}(t_{1u}^2, {}^1E_g, M=0, \gamma_g) = \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_u}\eta_u| + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\mu_u}\mu_u| - \frac{\sqrt{3}|\overline{\nu_u}\nu_u|}{3}$$

$$\Psi_{20}(t_{1u}^2, {}^1E_g, M=0, \zeta_g) =$$

$$\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_u}\eta_u| - \frac{\sqrt{3}|\overline{\mu_u}\mu_u|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\nu_u}\nu_u|$$

 $t_{1u}t_{2u}$

$$\boxed{\Delta E = 0}$$

$$\Psi_{21}(t_{1u}t_{2u}, {}^1E_g, M=0, \gamma_g) = -\frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\eta_u}\xi_u|}{2} - \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\mu_u}\phi_u|}{2} - \frac{\sqrt{6}|\overline{\nu_u}\chi_u|}{6} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\eta_u\overline{\xi_u}|}{2} + \frac{\sqrt{2}\left(-\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\mu_u\overline{\phi_u}|}{2} + \frac{\sqrt{6}|\nu_u\overline{\chi_u}|}{6}$$

$$\Psi_{22}(t_{1u}t_{2u}, {}^1E_g, M=0, \zeta_g) =$$

$$-\frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\eta_u}\xi_u|}{2} + \frac{\sqrt{6}|\overline{\mu_u}\phi_u|}{6} - \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\nu_u}\chi_u|}{2} - \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\eta_u\overline{\xi_u}|}{2} - \frac{\sqrt{6}|\mu_u\overline{\phi_u}|}{6} + \frac{\sqrt{2}\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\nu_u\overline{\chi_u}|}{2}$$

 t_{2u}^2

$$\boxed{\Delta E = 0}$$

$$\Psi_{23}(t_{2u}^2, {}^1E_g, M=0, \gamma_g) = -\frac{\sqrt{3}|\overline{\chi_u}\chi_u|}{3} + \left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\phi_u}\phi_u| + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\xi_u}\xi_u|$$

$$\Psi_{24}(t_{2u}^2, {}^1E_g, M=0, \zeta_g) =$$

$$\left(\frac{\sqrt{3}}{6} - \frac{i}{2}\right)|\overline{\chi_u}\chi_u| - \frac{\sqrt{3}|\overline{\phi_u}\phi_u|}{3} + \left(\frac{\sqrt{3}}{6} + \frac{i}{2}\right)|\overline{\xi_u}\xi_u|$$

2.32.12 ${}^3T_{1g}$

 $a_{1g}t_{1g}$

$$\boxed{\Delta E = -\langle \alpha_g\alpha_g || \nu_g\nu_g \rangle + \langle \alpha_g\nu_g || \alpha_g\nu_g \rangle}$$

$$\Psi_1(a_{1g}t_{1g}, {}^3T_{1g}, M=-1, \eta_g) = |\overline{\alpha_g}\eta_g|$$

$$\Psi_2(a_{1g}t_{1g}, {}^3T_{1g}, M=-1, \mu_g) = |\overline{\alpha_g}\mu_g|$$

$$\Psi_3(a_{1g}t_{1g}, {}^3T_{1g}, M=-1, \nu_g) = |\overline{\alpha_g}\nu_g|$$

$$\Psi_4(a_{1g}t_{1g}, {}^3T_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\alpha_g}\eta_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\eta_g}|}{2}$$

$$\Psi_5(a_{1g}t_{1g}, {}^3T_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\alpha_g}\mu_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\mu_g}|}{2}$$

$$\Psi_6(a_{1g}t_{1g}, {}^3T_{1g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\alpha_g}\nu_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\nu_g}|}{2}$$

$$\Psi_7(a_{1g}t_{1g}, {}^3T_{1g}, M=1, \eta_g) = |\alpha_g\eta_g|$$

$$\Psi_8(a_{1g}t_{1g}, {}^3T_{1g}, M=1, \mu_g) = |\alpha_g\mu_g|$$

$$\Psi_9(a_{1g}t_{1g}, {}^3T_{1g}, M=1, \nu_g) = |\alpha_g\nu_g|$$

 $a_{2u}t_{2u}$

$$\boxed{\Delta E = -\langle \beta_u\beta_u || \xi_u\xi_u \rangle + \langle \beta_u\xi_u || \beta_u\xi_u \rangle}$$

$$\Psi_{10}(a_{2u}t_{2u}, {}^3T_{1g}, M=-1, \eta_g) = |\overline{\beta_u}\xi_u|$$

$$\Psi_{11}(a_{2u}t_{2u}, {}^3T_{1g}, M=-1, \mu_g) = |\overline{\beta_u}\phi_u|$$

$$\Psi_{12}(a_{2u}t_{2u}, {}^3T_{1g}, M=-1, \nu_g) = |\overline{\beta_u}\chi_u|$$

$$\Psi_{13}(a_{2u}t_{2u}, {}^3T_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\beta_u}\xi_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\xi_u}|}{2}$$

$$\Psi_{14}(a_{2u}t_{2u}, {}^3T_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\beta_u}\phi_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\phi_u}|}{2}$$

$$\Psi_{15}(a_{2u}t_{2u}, {}^3T_{1g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\beta_u}\chi_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\chi_u}|}{2}$$

$$\Psi_{16}(a_{2u}t_{2u}, {}^3T_{1g}, M=1, \eta_g) = |\beta_u\xi_u|$$

$$\Psi_{17}(a_{2u}t_{2u}, {}^3T_{1g}, M=1, \mu_g) = |\beta_u\phi_u|$$

$$\Psi_{18}(a_{2u}t_{2u}, {}^3T_{1g}, M=1, \nu_g) = |\beta_u\chi_u|$$

 $a_{1u}t_{1u}$

$$\boxed{\Delta E = -\langle \alpha_u\alpha_u || \nu_u\nu_u \rangle + \langle \alpha_u\nu_u || \alpha_u\nu_u \rangle}$$

$$\Psi_{19}(a_{1u}t_{1u}, {}^3T_{1g}, M=-1, \eta_g) = |\overline{\alpha_u}\eta_u|$$

$$\Psi_{20}(a_{1u}t_{1u}, {}^3T_{1g}, M=-1, \mu_g) = |\overline{\alpha_u}\mu_u|$$

$$\Psi_{21}(a_{1u}t_{1u}, {}^3T_{1g}, M=-1, \nu_g) = |\overline{\alpha_u}\nu_u|$$

$$\Psi_{22}(a_{1u}t_{1u}, {}^3T_{1g}, M=0, \eta_g) = \frac{\sqrt{2}|\overline{\alpha_u}\eta_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\eta_u}|}{2}$$

$$\Psi_{23}(a_{1u}t_{1u}, {}^3T_{1g}, M=0, \mu_g) = \frac{\sqrt{2}|\overline{\alpha_u}\mu_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\mu_u}|}{2}$$

$$\Psi_{24}(a_{1u}t_{1u}, {}^3T_{1g}, M=0, \nu_g) = \frac{\sqrt{2}|\overline{\alpha_u}\nu_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\nu_u}|}{2}$$

$$\Psi_{25}(a_{1u}t_{1u}, {}^3T_{1g}, M=1, \eta_g) = |\alpha_u\eta_u|$$

$$\Psi_{26}(a_{1u}t_{1u}, {}^3T_{1g}, M=1, \mu_g) = |\alpha_u\mu_u|$$

$$\Psi_{27}(a_{1u}t_{1u}, {}^3T_{1g}, M=1, \nu_g) = |\alpha_u\nu_u|$$

 $a_{2g}t_{2g}$

$$\boxed{\Delta E = -\langle \beta_g\beta_g || \xi_g\xi_g \rangle + \langle \beta_g\xi_g || \beta_g\xi_g \rangle}$$

$$\Psi_{28}(a_{2g}t_{2g}, {}^3T_{1g}, M=-1, \eta_g) = |\overline{\beta_g}\xi_g|$$

$$\Psi_{29}(a_{2g}t_{2g}, {}^3T_{1g}, M=-1, \mu_g) = |\overline{\beta_g}\phi_g|$$

$$\Psi_{30}(a_{2g}t_{2g}, {}^3T_{1g}, M=-1, \nu_g) = |\overline{\beta_g}\chi_g|$$

$$\begin{aligned}\Psi_{31}(a_{2g}t_{2g}, {}^3T_{1g}, M=0, \eta_g) &= \frac{\sqrt{2}|\beta_g\xi_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\xi}_g|}{2} \\ \Psi_{32}(a_{2g}t_{2g}, {}^3T_{1g}, M=0, \mu_g) &= \frac{\sqrt{2}|\beta_g\phi_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\phi}_g|}{2} \\ \Psi_{33}(a_{2g}t_{2g}, {}^3T_{1g}, M=0, \nu_g) &= \frac{\sqrt{2}|\beta_g\chi_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\chi}_g|}{2} \\ \Psi_{34}(a_{2g}t_{2g}, {}^3T_{1g}, M=1, \eta_g) &= |\beta_g\xi_g| \\ \Psi_{35}(a_{2g}t_{2g}, {}^3T_{1g}, M=1, \mu_g) &= |\beta_g\phi_g| \\ \Psi_{36}(a_{2g}t_{2g}, {}^3T_{1g}, M=1, \nu_g) &= |\beta_g\chi_g|\end{aligned}$$

 $e_u t_{1u}$

$$\boxed{\Delta E = \langle \zeta_u \nu_u | \zeta_u \nu_u \rangle}$$

$$\begin{aligned}\Psi_{37}(e_u t_{1u}, {}^3T_{1g}, M=-1, \eta_g) &= \frac{\sqrt{2}|\gamma_u\eta_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\eta}_u|}{2} \\ \Psi_{38}(e_u t_{1u}, {}^3T_{1g}, M=-1, \mu_g) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_u\mu_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_u\overline{\mu}_u|}{2} \\ \Psi_{39}(e_u t_{1u}, {}^3T_{1g}, M=-1, \nu_g) &= -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma_u\nu_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_u\overline{\nu}_u|}{2} \\ \Psi_{40}(e_u t_{1u}, {}^3T_{1g}, M=0, \eta_g) &= \frac{|\gamma_u\eta_u|}{2} + \frac{|\zeta_u\overline{\eta}_u|}{2} + \frac{|\gamma_u\overline{\eta}_u|}{2} + \frac{|\zeta_u\overline{\eta}_u|}{2} \\ \Psi_{41}(e_u t_{1u}, {}^3T_{1g}, M=0, \mu_g) &= \frac{(-1)^{\frac{2}{3}}|\gamma_u\mu_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\overline{\mu}_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\gamma_u\overline{\mu}_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\overline{\mu}_u|}{2} \\ \Psi_{42}(e_u t_{1u}, {}^3T_{1g}, M=0, \nu_g) &= -\frac{\sqrt[3]{-1}|\gamma_u\nu_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_u\overline{\nu}_u|}{2} - \frac{\sqrt[3]{-1}|\gamma_u\overline{\nu}_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_u\nu_u|}{2} \\ \Psi_{43}(e_u t_{1u}, {}^3T_{1g}, M=1, \eta_g) &= \frac{\sqrt{2}|\gamma_u\eta_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\eta}_u|}{2} \\ \Psi_{44}(e_u t_{1u}, {}^3T_{1g}, M=1, \mu_g) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_u\mu_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_u\overline{\mu}_u|}{2} \\ \Psi_{45}(e_u t_{1u}, {}^3T_{1g}, M=1, \nu_g) &= -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma_u\nu_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_u\overline{\nu}_u|}{2}\end{aligned}$$

 $e_u t_{2u}$

$$\boxed{\Delta E = \langle \zeta_u \xi_u | \zeta_u \xi_u \rangle}$$

$$\begin{aligned}\Psi_{46}(e_u t_{2u}, {}^3T_{1g}, M=-1, \eta_g) &= -\frac{\sqrt{2}|\gamma_u\overline{\xi}_u|}{2} + \frac{\sqrt{2}|\zeta_u\xi_u|}{2} \\ \Psi_{47}(e_u t_{2u}, {}^3T_{1g}, M=-1, \mu_g) &= -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_u\overline{\phi}_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_u\overline{\phi}_u|}{2} \\ \Psi_{48}(e_u t_{2u}, {}^3T_{1g}, M=-1, \nu_g) &= \frac{\sqrt[3]{-1}\sqrt{2}|\gamma_u\overline{\chi}_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_u\overline{\chi}_u|}{2} \\ \Psi_{49}(e_u t_{2u}, {}^3T_{1g}, M=0, \eta_g) &= -\frac{|\gamma_u\xi_u|}{2} + \frac{|\zeta_u\overline{\xi}_u|}{2} - \frac{|\gamma_u\overline{\xi}_u|}{2} + \frac{|\zeta_u\xi_u|}{2} \\ \Psi_{50}(e_u t_{2u}, {}^3T_{1g}, M=0, \mu_g) &= -\frac{(-1)^{\frac{2}{3}}|\gamma_u\overline{\phi}_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\overline{\phi}_u|}{2} - \frac{(-1)^{\frac{2}{3}}|\gamma_u\overline{\phi}_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\overline{\phi}_u|}{2} \\ \Psi_{51}(e_u t_{2u}, {}^3T_{1g}, M=0, \nu_g) &= \frac{\sqrt[3]{-1}|\gamma_u\overline{\chi}_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_u\overline{\chi}_u|}{2} + \frac{\sqrt[3]{-1}|\gamma_u\overline{\chi}_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_u\overline{\chi}_u|}{2}\end{aligned}$$

$$\Psi_{52}(e_u t_{2u}, {}^3T_{1g}, M=1, \eta_g) = -\frac{\sqrt{2}|\gamma_u\xi_u|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\xi}_u|}{2}$$

$$\begin{aligned}\Psi_{53}(e_u t_{2u}, {}^3T_{1g}, M=1, \mu_g) &= -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_u\phi_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_u\overline{\phi}_u|}{2} \\ \Psi_{54}(e_u t_{2u}, {}^3T_{1g}, M=1, \nu_g) &= \frac{\sqrt[3]{-1}\sqrt{2}|\gamma_u\chi_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_u\overline{\chi}_u|}{2}\end{aligned}$$

 $e_g t_{1g}$

$$\boxed{\Delta E = \langle \zeta_g \nu_g | \zeta_g \nu_g \rangle}$$

$$\Psi_{55}(e_g t_{1g}, {}^3T_{1g}, M=-1, \eta_g) = \frac{\sqrt{2}|\gamma_g\eta_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\eta}_g|}{2}$$

$$\begin{aligned}\Psi_{56}(e_g t_{1g}, {}^3T_{1g}, M=-1, \mu_g) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_g\mu_g|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_g\overline{\mu}_g|}{2} \\ \Psi_{57}(e_g t_{1g}, {}^3T_{1g}, M=-1, \nu_g) &= -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma_g\nu_g|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_g\overline{\nu}_g|}{2} \\ \Psi_{58}(e_g t_{1g}, {}^3T_{1g}, M=0, \eta_g) &= \frac{|\gamma_g\eta_g|}{2} + \frac{|\zeta_g\overline{\eta}_g|}{2} + \frac{|\gamma_g\overline{\eta}_g|}{2} + \frac{|\zeta_g\eta_g|}{2} \\ \Psi_{59}(e_g t_{1g}, {}^3T_{1g}, M=0, \mu_g) &= \frac{(-1)^{\frac{2}{3}}|\gamma_g\mu_g|}{2} - \frac{\sqrt[3]{-1}|\zeta_g\mu_g|}{2} + \frac{(-1)^{\frac{2}{3}}|\gamma_g\overline{\mu}_g|}{2} - \frac{\sqrt[3]{-1}|\zeta_g\overline{\mu}_g|}{2} \\ \Psi_{60}(e_g t_{1g}, {}^3T_{1g}, M=0, \nu_g) &= -\frac{\sqrt[3]{-1}|\gamma_g\nu_g|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_g\overline{\nu}_g|}{2} - \frac{\sqrt[3]{-1}|\gamma_g\overline{\nu}_g|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_g\nu_g|}{2}\end{aligned}$$

$$\Psi_{61}(e_g t_{1g}, {}^3T_{1g}, M=1, \eta_g) = \frac{\sqrt{2}|\gamma_g\eta_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\eta}_g|}{2}$$

$$\begin{aligned}\Psi_{62}(e_g t_{1g}, {}^3T_{1g}, M=1, \mu_g) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_g\mu_g|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_g\overline{\mu}_g|}{2} \\ \Psi_{63}(e_g t_{1g}, {}^3T_{1g}, M=1, \nu_g) &= -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma_g\nu_g|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_g\overline{\nu}_g|}{2}\end{aligned}$$

 $e_g t_{2g}$

$$\boxed{\Delta E = \langle \zeta_g \xi_g | \zeta_g \xi_g \rangle}$$

$$\Psi_{64}(e_g t_{2g}, {}^3T_{1g}, M=-1, \eta_g) = -\frac{\sqrt{2}|\gamma_g\overline{\xi}_g|}{2} + \frac{\sqrt{2}|\zeta_g\xi_g|}{2}$$

$$\begin{aligned}\Psi_{65}(e_g t_{2g}, {}^3T_{1g}, M=-1, \mu_g) &= -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_g\overline{\phi}_g|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_g\overline{\phi}_g|}{2} \\ \Psi_{66}(e_g t_{2g}, {}^3T_{1g}, M=-1, \nu_g) &= \frac{\sqrt[3]{-1}\sqrt{2}|\gamma_g\overline{\chi}_g|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_g\overline{\chi}_g|}{2} \\ \Psi_{67}(e_g t_{2g}, {}^3T_{1g}, M=0, \eta_g) &= -\frac{|\gamma_g\xi_g|}{2} + \frac{|\zeta_g\overline{\xi}_g|}{2} - \frac{|\gamma_g\overline{\xi}_g|}{2} + \frac{|\zeta_g\xi_g|}{2} \\ \Psi_{68}(e_g t_{2g}, {}^3T_{1g}, M=0, \mu_g) &= -\frac{(-1)^{\frac{2}{3}}|\gamma_g\overline{\phi}_g|}{2} - \frac{\sqrt[3]{-1}|\zeta_g\overline{\phi}_g|}{2} - \frac{(-1)^{\frac{2}{3}}|\gamma_g\overline{\phi}_g|}{2} - \frac{\sqrt[3]{-1}|\zeta_g\overline{\phi}_g|}{2} \\ \Psi_{69}(e_g t_{2g}, {}^3T_{1g}, M=0, \nu_g) &= \frac{\sqrt[3]{-1}|\gamma_g\overline{\chi}_g|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_g\overline{\chi}_g|}{2} + \frac{\sqrt[3]{-1}|\gamma_g\overline{\chi}_g|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_g\overline{\chi}_g|}{2}\end{aligned}$$

$$\Psi_{70}(e_g t_{2g}, {}^3T_{1g}, M=1, \eta_g) = -\frac{\sqrt{2}|\gamma_g\xi_g|}{2} + \frac{\sqrt{2}|\zeta_g\overline{\xi}_g|}{2}$$

$$\Psi_{71}(e_g t_{2g}, {}^3T_{1g}, M=1, \mu_g) = -\frac{(-1)^{\frac{2}{3}} \sqrt{2} |\gamma_g \phi_g|}{2} - \frac{\sqrt[3]{-1} \sqrt{2} |\zeta_g \phi_g|}{2}$$

$$\Psi_{72}(e_g t_{2g}, {}^3T_{1g}, M=1, \nu_g) = \frac{\sqrt[3]{-1} \sqrt{2} |\gamma_g \chi_g|}{2} + \frac{(-1)^{\frac{2}{3}} \sqrt{2} |\zeta_g \chi_g|}{2}$$

 t_{1g}^2

$$\boxed{\Delta E = \langle \nu_g \mu_g | | \nu_g \mu_g \rangle - \langle \nu_g \nu_g | | \nu_g \nu_g \rangle}$$

$$\Psi_{73}(t_{1g}^2, {}^3T_{1g}, M=-1, \nu_g) = -|\eta_g \mu_g|$$

$$\Psi_{74}(t_{1g}^2, {}^3T_{1g}, M=-1, \mu_g) = |\eta_g \nu_g|$$

$$\Psi_{75}(t_{1g}^2, {}^3T_{1g}, M=-1, \eta_g) = -|\mu_g \nu_g|$$

$$\Psi_{76}(t_{1g}^2, {}^3T_{1g}, M=0, \nu_g) = -\frac{\sqrt{2} |\eta_g \mu_g|}{2} + \frac{\sqrt{2} |\mu_g \eta_g|}{2}$$

$$\Psi_{77}(t_{1g}^2, {}^3T_{1g}, M=0, \mu_g) = \frac{\sqrt{2} |\eta_g \nu_g|}{2} - \frac{\sqrt{2} |\nu_g \eta_g|}{2}$$

$$\Psi_{78}(t_{1g}^2, {}^3T_{1g}, M=0, \eta_g) = -\frac{\sqrt{2} |\mu_g \nu_g|}{2} + \frac{\sqrt{2} |\nu_g \mu_g|}{2}$$

$$\Psi_{79}(t_{1g}^2, {}^3T_{1g}, M=1, \nu_g) = -|\eta_g \mu_g|$$

$$\Psi_{80}(t_{1g}^2, {}^3T_{1g}, M=1, \mu_g) = |\eta_g \nu_g|$$

$$\Psi_{81}(t_{1g}^2, {}^3T_{1g}, M=1, \eta_g) = -|\mu_g \nu_g|$$

 $t_{1g} t_{2g}$

$$\boxed{\Delta E = \langle \nu_g \chi_g | | \nu_g \chi_g \rangle - \langle \nu_g \nu_g | | \xi_g \xi_g \rangle + \langle \nu_g \xi_g | | \nu_g \xi_g \rangle - \langle \nu_g \mu_g | | \chi_g \phi_g \rangle}$$

$$\Psi_{82}(t_{1g} t_{2g}, {}^3T_{1g}, M=-1, \nu_g) = \frac{\sqrt{2} |\eta_g \phi_g|}{2} + \frac{\sqrt{2} |\mu_g \xi_g|}{2}$$

$$\Psi_{83}(t_{1g} t_{2g}, {}^3T_{1g}, M=-1, \mu_g) = \frac{\sqrt{2} |\eta_g \chi_g|}{2} + \frac{\sqrt{2} |\xi_g \xi_g|}{2}$$

$$\Psi_{84}(t_{1g} t_{2g}, {}^3T_{1g}, M=-1, \eta_g) = \frac{\sqrt{2} |\mu_g \chi_g|}{2} + \frac{\sqrt{2} |\nu_g \phi_g|}{2}$$

$$\Psi_{85}(t_{1g} t_{2g}, {}^3T_{1g}, M=0, \nu_g) = \frac{|\eta_g \phi_g|}{2} + \frac{|\mu_g \xi_g|}{2} + \frac{|\eta_g \phi_g|}{2} + \frac{|\mu_g \xi_g|}{2}$$

$$\Psi_{86}(t_{1g} t_{2g}, {}^3T_{1g}, M=0, \mu_g) = \frac{|\eta_g \chi_g|}{2} + \frac{|\nu_g \xi_g|}{2} + \frac{|\eta_g \chi_g|}{2} + \frac{|\nu_g \xi_g|}{2}$$

$$\Psi_{87}(t_{1g} t_{2g}, {}^3T_{1g}, M=0, \eta_g) = \frac{|\mu_g \chi_g|}{2} + \frac{|\nu_g \phi_g|}{2} + \frac{|\mu_g \chi_g|}{2} + \frac{|\nu_g \phi_g|}{2}$$

$$\Psi_{88}(t_{1g} t_{2g}, {}^3T_{1g}, M=1, \nu_g) = \frac{\sqrt{2} |\eta_g \phi_g|}{2} + \frac{\sqrt{2} |\mu_g \xi_g|}{2}$$

$$\Psi_{89}(t_{1g} t_{2g}, {}^3T_{1g}, M=1, \mu_g) = \frac{\sqrt{2} |\eta_g \chi_g|}{2} + \frac{\sqrt{2} |\nu_g \xi_g|}{2}$$

$$\Psi_{90}(t_{1g} t_{2g}, {}^3T_{1g}, M=1, \eta_g) = \frac{\sqrt{2} |\mu_g \chi_g|}{2} + \frac{\sqrt{2} |\nu_g \phi_g|}{2}$$

 t_{2g}^2

$$\boxed{\Delta E = \langle \xi_g \phi_g | | \xi_g \phi_g \rangle - \langle \xi_g \xi_g | | \xi_g \xi_g \rangle}$$

$$\Psi_{91}(t_{2g}^2, {}^3T_{1g}, M=-1, \nu_g) = -|\xi_g \phi_g|$$

$$\Psi_{92}(t_{2g}^2, {}^3T_{1g}, M=-1, \mu_g) = |\overline{\xi_g} \overline{\chi_g}|$$

$$\Psi_{93}(t_{2g}^2, {}^3T_{1g}, M=-1, \eta_g) = -|\overline{\phi_g} \overline{\chi_g}|$$

$$\Psi_{94}(t_{2g}^2, {}^3T_{1g}, M=0, \nu_g) = \frac{\sqrt{2} |\overline{\phi_g} \xi_g|}{2} - \frac{\sqrt{2} |\overline{\xi_g} \phi_g|}{2}$$

$$\Psi_{95}(t_{2g}^2, {}^3T_{1g}, M=0, \mu_g) = -\frac{\sqrt{2} |\overline{\chi_g} \xi_g|}{2} + \frac{\sqrt{2} |\overline{\xi_g} \chi_g|}{2}$$

$$\Psi_{96}(t_{2g}^2, {}^3T_{1g}, M=0, \eta_g) = \frac{\sqrt{2} |\overline{\chi_g} \phi_g|}{2} - \frac{\sqrt{2} |\overline{\phi_g} \chi_g|}{2}$$

$$\Psi_{97}(t_{2g}^2, {}^3T_{1g}, M=1, \nu_g) = -|\xi_g \phi_g|$$

$$\Psi_{98}(t_{2g}^2, {}^3T_{1g}, M=1, \mu_g) = |\xi_g \chi_g|$$

$$\Psi_{99}(t_{2g}^2, {}^3T_{1g}, M=1, \eta_g) = -|\phi_g \chi_g|$$

 t_{1u}^2

$$\boxed{\Delta E = \langle \nu_u \mu_u | | \nu_u \mu_u \rangle - \langle \nu_u \nu_u | | \nu_u \nu_u \rangle}$$

$$\Psi_{100}(t_{1u}^2, {}^3T_{1g}, M=-1, \nu_g) = -|\overline{\eta_u} \mu_u|$$

$$\Psi_{101}(t_{1u}^2, {}^3T_{1g}, M=-1, \mu_g) = |\overline{\eta_u} \nu_u|$$

$$\Psi_{102}(t_{1u}^2, {}^3T_{1g}, M=-1, \eta_g) = -|\overline{\mu_u} \nu_u|$$

$$\Psi_{103}(t_{1u}^2, {}^3T_{1g}, M=0, \nu_g) = -\frac{\sqrt{2} |\overline{\eta_u} \mu_u|}{2} + \frac{\sqrt{2} |\overline{\mu_u} \eta_u|}{2}$$

$$\Psi_{104}(t_{1u}^2, {}^3T_{1g}, M=0, \mu_g) = \frac{\sqrt{2} |\overline{\eta_u} \nu_u|}{2} - \frac{\sqrt{2} |\overline{\nu_u} \eta_u|}{2}$$

$$\Psi_{105}(t_{1u}^2, {}^3T_{1g}, M=0, \eta_g) = -\frac{\sqrt{2} |\overline{\mu_u} \nu_u|}{2} + \frac{\sqrt{2} |\overline{\nu_u} \mu_u|}{2}$$

$$\Psi_{106}(t_{1u}^2, {}^3T_{1g}, M=1, \nu_g) = -|\eta_u \mu_u|$$

$$\Psi_{107}(t_{1u}^2, {}^3T_{1g}, M=1, \mu_g) = |\eta_u \nu_u|$$

$$\Psi_{108}(t_{1u}^2, {}^3T_{1g}, M=1, \eta_g) = -|\mu_u \nu_u|$$

 $t_{1u} t_{2u}$

$$\boxed{\Delta E = \langle \nu_u \chi_u | | \nu_u \chi_u \rangle - \langle \nu_u \nu_u | | \xi_u \xi_u \rangle + \langle \nu_u \xi_u | | \nu_u \xi_u \rangle - \langle \nu_u \mu_u | | \chi_u \phi_u \rangle}$$

$$\Psi_{109}(t_{1u} t_{2u}, {}^3T_{1g}, M=-1, \nu_g) = \frac{\sqrt{2} |\overline{\eta_u} \phi_u|}{2} + \frac{\sqrt{2} |\overline{\mu_u} \xi_u|}{2}$$

$$\Psi_{110}(t_{1u} t_{2u}, {}^3T_{1g}, M=-1, \mu_g) = \frac{\sqrt{2} |\overline{\eta_u} \chi_u|}{2} + \frac{\sqrt{2} |\overline{\nu_u} \xi_u|}{2}$$

$$\Psi_{111}(t_{1u} t_{2u}, {}^3T_{1g}, M=-1, \eta_g) = \frac{\sqrt{2} |\overline{\mu_u} \chi_u|}{2} + \frac{\sqrt{2} |\overline{\nu_u} \phi_u|}{2}$$

$$\Psi_{112}(t_{1u} t_{2u}, {}^3T_{1g}, M=0, \nu_g) = \frac{|\overline{\eta_u} \phi_u|}{2} + \frac{|\overline{\mu_u} \xi_u|}{2} + \frac{|\overline{\eta_u} \phi_u|}{2} + \frac{|\overline{\mu_u} \xi_u|}{2}$$

$$\Psi_{113}(t_{1u} t_{2u}, {}^3T_{1g}, M=0, \mu_g) = \frac{|\overline{\eta_u} \chi_u|}{2} + \frac{|\overline{\nu_u} \xi_u|}{2} + \frac{|\overline{\eta_u} \chi_u|}{2} + \frac{|\overline{\nu_u} \xi_u|}{2}$$

$$\Psi_{114}(t_{1u} t_{2u}, {}^3T_{1g}, M=0, \eta_g) = \frac{|\overline{\mu_u} \chi_u|}{2} + \frac{|\overline{\nu_u} \phi_u|}{2} + \frac{|\overline{\mu_u} \chi_u|}{2} + \frac{|\overline{\nu_u} \phi_u|}{2}$$

$$\Psi_{115}(t_{1u} t_{2u}, {}^3T_{1g}, M=1, \nu_g) = \frac{\sqrt{2} |\overline{\eta_u} \phi_u|}{2} + \frac{\sqrt{2} |\overline{\mu_u} \xi_u|}{2}$$

$$\Psi_{116}(t_{1u} t_{2u}, {}^3T_{1g}, M=1, \mu_g) = \frac{\sqrt{2} |\overline{\eta_u} \chi_u|}{2} + \frac{\sqrt{2} |\overline{\nu_u} \xi_u|}{2}$$

$$\Psi_{117}(t_{1u} t_{2u}, {}^3T_{1g}, M=1, \eta_g) = \frac{\sqrt{2} |\overline{\mu_u} \chi_u|}{2} + \frac{\sqrt{2} |\overline{\nu_u} \phi_u|}{2}$$

 t_{2u}^2

$$\boxed{\Delta E = \langle \xi_u \phi_u | | \xi_u \phi_u \rangle - \langle \xi_u \xi_u | | \xi_u \xi_u \rangle}$$

$$\Psi_{118}(t_{2u}^2, {}^3T_{1g}, M=-1, \nu_g) = -|\overline{\xi_u} \phi_u|$$

$$\Psi_{119}(t_{2u}^2, {}^3T_{1g}, M=-1, \mu_g) = |\overline{\xi_u} \overline{\chi_u}|$$

$$\Psi_{120}(t_{2u}^2, {}^3T_{1g}, M=-1, \eta_g) = -|\overline{\phi_u} \overline{\chi_u}|$$

$$\begin{aligned}\Psi_{121}(t_{2u}^2, {}^3T_{1g}, M=0, \nu_g) &= \frac{\sqrt{2}|\phi_u\xi_u|}{2} - \frac{\sqrt{2}|\xi_u\phi_u|}{2} \\ \Psi_{122}(t_{2u}^2, {}^3T_{1g}, M=0, \mu_g) &= -\frac{\sqrt{2}|\chi_u\xi_u|}{2} + \frac{\sqrt{2}|\xi_u\chi_u|}{2} \\ \Psi_{123}(t_{2u}^2, {}^3T_{1g}, M=0, \eta_g) &= \frac{\sqrt{2}|\bar{\chi}_u\phi_u|}{2} - \frac{\sqrt{2}|\bar{\phi}_u\chi_u|}{2} \\ \Psi_{124}(t_{2u}^2, {}^3T_{1g}, M=1, \nu_g) &= -|\xi_u\phi_u| \\ \Psi_{125}(t_{2u}^2, {}^3T_{1g}, M=1, \mu_g) &= |\xi_u\chi_u| \\ \Psi_{126}(t_{2u}^2, {}^3T_{1g}, M=1, \eta_g) &= -|\phi_u\chi_u|\end{aligned}$$

$$\begin{aligned}\Psi_{13}(e_u t_{1u}, {}^1T_{1g}, M=0, \eta_g) &= -\frac{|\gamma_u\eta_u|}{2} - \frac{|\zeta_u\eta_u|}{2} + \frac{|\gamma_u\bar{\eta}_u|}{2} + \frac{|\zeta_u\bar{\eta}_u|}{2} \\ \Psi_{14}(e_u t_{1u}, {}^1T_{1g}, M=0, \mu_g) &= -\frac{(-1)^{\frac{3}{2}}|\gamma_u\mu_u|}{2} + \frac{\sqrt[3]{-1}|\zeta_u\mu_u|}{2} + \frac{(-1)^{\frac{3}{2}}|\gamma_u\bar{\mu}_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\bar{\mu}_u|}{2} \\ \Psi_{15}(e_u t_{1u}, {}^1T_{1g}, M=0, \nu_g) &= \frac{\sqrt[3]{-1}|\gamma_u\nu_u|}{2} - \frac{(-1)^{\frac{3}{2}}|\zeta_u\nu_u|}{2} - \frac{\sqrt[3]{-1}|\gamma_u\bar{\nu}_u|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta_u\bar{\nu}_u|}{2}\end{aligned}$$

2.32.13 ${}^1T_{1g}$ **$a_{1g}t_{1g}$**

$$\boxed{\Delta E = \langle \alpha_g \alpha_g | |\nu_g \nu_g \rangle + \langle \alpha_g \nu_g | |\alpha_g \nu_g \rangle}$$

$$\begin{aligned}\Psi_1(a_{1g}t_{1g}, {}^1T_{1g}, M=0, \eta_g) &= -\frac{\sqrt{2}|\bar{\alpha}_g\eta_g|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\eta}_g|}{2} \\ \Psi_2(a_{1g}t_{1g}, {}^1T_{1g}, M=0, \mu_g) &= -\frac{\sqrt{2}|\bar{\alpha}_g\mu_g|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\mu}_g|}{2} \\ \Psi_3(a_{1g}t_{1g}, {}^1T_{1g}, M=0, \nu_g) &= -\frac{\sqrt{2}|\bar{\alpha}_g\nu_g|}{2} + \frac{\sqrt{2}|\alpha_g\bar{\nu}_g|}{2}\end{aligned}$$

 $a_{2u}t_{2u}$

$$\boxed{\Delta E = \langle \beta_u \beta_u | |\xi_u \xi_u \rangle + \langle \beta_u \xi_u | |\beta_u \xi_u \rangle}$$

$$\begin{aligned}\Psi_4(a_{2u}t_{2u}, {}^1T_{1g}, M=0, \eta_g) &= -\frac{\sqrt{2}|\bar{\beta}_u\xi_u|}{2} + \frac{\sqrt{2}|\beta_u\bar{\xi}_u|}{2} \\ \Psi_5(a_{2u}t_{2u}, {}^1T_{1g}, M=0, \mu_g) &= -\frac{\sqrt{2}|\bar{\beta}_u\phi_u|}{2} + \frac{\sqrt{2}|\beta_u\bar{\phi}_u|}{2} \\ \Psi_6(a_{2u}t_{2u}, {}^1T_{1g}, M=0, \nu_g) &= -\frac{\sqrt{2}|\bar{\beta}_u\chi_u|}{2} + \frac{\sqrt{2}|\beta_u\bar{\chi}_u|}{2}\end{aligned}$$

 $a_{1u}t_{1u}$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u | |\nu_u \nu_u \rangle + \langle \alpha_u \nu_u | |\alpha_u \nu_u \rangle}$$

$$\begin{aligned}\Psi_7(a_{1u}t_{1u}, {}^1T_{1g}, M=0, \eta_g) &= -\frac{\sqrt{2}|\bar{\alpha}_u\eta_u|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\eta}_u|}{2} \\ \Psi_8(a_{1u}t_{1u}, {}^1T_{1g}, M=0, \mu_g) &= -\frac{\sqrt{2}|\bar{\alpha}_u\mu_u|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\mu}_u|}{2} \\ \Psi_9(a_{1u}t_{1u}, {}^1T_{1g}, M=0, \nu_g) &= -\frac{\sqrt{2}|\bar{\alpha}_u\nu_u|}{2} + \frac{\sqrt{2}|\alpha_u\bar{\nu}_u|}{2}\end{aligned}$$

 $a_{2g}t_{2g}$

$$\boxed{\Delta E = \langle \beta_g \beta_g | |\xi_g \xi_g \rangle + \langle \beta_g \xi_g | |\beta_g \xi_g \rangle}$$

$$\begin{aligned}\Psi_{10}(a_{2g}t_{2g}, {}^1T_{1g}, M=0, \eta_g) &= -\frac{\sqrt{2}|\bar{\beta}_g\xi_g|}{2} + \frac{\sqrt{2}|\beta_g\bar{\xi}_g|}{2} \\ \Psi_{11}(a_{2g}t_{2g}, {}^1T_{1g}, M=0, \mu_g) &= -\frac{\sqrt{2}|\bar{\beta}_g\phi_g|}{2} + \frac{\sqrt{2}|\beta_g\bar{\phi}_g|}{2} \\ \Psi_{12}(a_{2g}t_{2g}, {}^1T_{1g}, M=0, \nu_g) &= -\frac{\sqrt{2}|\bar{\beta}_g\chi_g|}{2} + \frac{\sqrt{2}|\beta_g\bar{\chi}_g|}{2}\end{aligned}$$

 $e_u t_{1u}$

$$\boxed{\Delta E = \langle \zeta_u \nu_u | |\zeta_u \nu_u \rangle}$$

 $e_u t_{2u}$

$$\boxed{\Delta E = \langle \zeta_u \xi_u | |\zeta_u \xi_u \rangle}$$

$$\Psi_{16}(e_u t_{2u}, {}^1T_{1g}, M=0, \eta_g) = \frac{|\gamma_u\xi_u|}{2} - \frac{|\zeta_u\xi_u|}{2} - \frac{|\gamma_u\bar{\xi}_u|}{2} + \frac{|\zeta_u\bar{\xi}_u|}{2}$$

$$\begin{aligned}\Psi_{17}(e_u t_{2u}, {}^1T_{1g}, M=0, \mu_g) &= \frac{(-1)^{\frac{3}{2}}|\gamma_u\phi_u|}{2} + \frac{\sqrt[3]{-1}|\zeta_u\phi_u|}{2} - \frac{(-1)^{\frac{3}{2}}|\gamma_u\bar{\phi}_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\bar{\phi}_u|}{2} \\ \Psi_{18}(e_u t_{2u}, {}^1T_{1g}, M=0, \nu_g) &= -\frac{\sqrt[3]{-1}|\gamma_u\chi_u|}{2} - \frac{(-1)^{\frac{3}{2}}|\zeta_u\chi_u|}{2} + \frac{\sqrt[3]{-1}|\gamma_u\bar{\chi}_u|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta_u\bar{\chi}_u|}{2}\end{aligned}$$

 $e_g t_{1g}$

$$\boxed{\Delta E = \langle \zeta_g \nu_g | |\zeta_g \nu_g \rangle}$$

$$\Psi_{19}(e_g t_{1g}, {}^1T_{1g}, M=0, \eta_g) = -\frac{|\gamma_g\eta_g|}{2} - \frac{|\zeta_g\eta_g|}{2} + \frac{|\gamma_g\bar{\eta}_g|}{2} + \frac{|\zeta_g\bar{\eta}_g|}{2}$$

$$\begin{aligned}\Psi_{20}(e_g t_{1g}, {}^1T_{1g}, M=0, \mu_g) &= -\frac{(-1)^{\frac{3}{2}}|\gamma_g\mu_g|}{2} + \frac{\sqrt[3]{-1}|\zeta_g\mu_g|}{2} + \frac{(-1)^{\frac{3}{2}}|\gamma_g\bar{\mu}_g|}{2} - \frac{\sqrt[3]{-1}|\zeta_g\bar{\mu}_g|}{2} \\ \Psi_{21}(e_g t_{1g}, {}^1T_{1g}, M=0, \nu_g) &= \frac{\sqrt[3]{-1}|\gamma_g\nu_g|}{2} - \frac{(-1)^{\frac{3}{2}}|\zeta_g\nu_g|}{2} - \frac{\sqrt[3]{-1}|\gamma_g\bar{\nu}_g|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta_g\bar{\nu}_g|}{2}\end{aligned}$$

 $e_g t_{2g}$

$$\boxed{\Delta E = \langle \zeta_g \xi_g | |\zeta_g \xi_g \rangle}$$

$$\Psi_{22}(e_g t_{2g}, {}^1T_{1g}, M=0, \eta_g) = \frac{|\gamma_g\xi_g|}{2} - \frac{|\zeta_g\xi_g|}{2} - \frac{|\gamma_g\bar{\xi}_g|}{2} + \frac{|\zeta_g\bar{\xi}_g|}{2}$$

$$\begin{aligned}\Psi_{23}(e_g t_{2g}, {}^1T_{1g}, M=0, \mu_g) &= \frac{(-1)^{\frac{3}{2}}|\gamma_g\phi_g|}{2} + \frac{\sqrt[3]{-1}|\zeta_g\phi_g|}{2} - \frac{(-1)^{\frac{3}{2}}|\gamma_g\bar{\phi}_g|}{2} - \frac{\sqrt[3]{-1}|\zeta_g\bar{\phi}_g|}{2} \\ \Psi_{24}(e_g t_{2g}, {}^1T_{1g}, M=0, \nu_g) &= -\frac{\sqrt[3]{-1}|\gamma_g\chi_g|}{2} - \frac{(-1)^{\frac{3}{2}}|\zeta_g\chi_g|}{2} + \frac{\sqrt[3]{-1}|\gamma_g\bar{\chi}_g|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta_g\bar{\chi}_g|}{2}\end{aligned}$$

 $t_{1g}t_{2g}$

$$\boxed{\Delta E = \langle \nu_g \chi_g | |\nu_g \chi_g \rangle + \langle \nu_g \nu_g | |\xi_g \xi_g \rangle + \langle \nu_g \xi_g | |\nu_g \xi_g \rangle + \langle \nu_g \mu_g | |\chi_g \phi_g \rangle}$$

$$\Psi_{25}(t_{1g}t_{2g}, {}^1T_{1g}, M=0, \nu_g) = -\frac{|\bar{\eta}_g\phi_g|}{2} - \frac{|\bar{\mu}_g\xi_g|}{2} + \frac{|\eta_g\bar{\phi}_g|}{2} + \frac{|\mu_g\bar{\xi}_g|}{2}$$

$$\Psi_{26}(t_{1g}t_{2g}, {}^1T_{1g}, M=0, \mu_g) = -\frac{|\bar{\eta}_g\chi_g|}{2} - \frac{|\bar{\nu}_g\xi_g|}{2} + \frac{|\eta_g\bar{\chi}_g|}{2} + \frac{|\nu_g\bar{\xi}_g|}{2}$$

$$\Psi_{27}(t_{1g}t_{2g}, {}^1T_{1g}, M=0, \eta_g) = -\frac{|\mu_g\chi_g|}{2} - \frac{|\nu_g\phi_g|}{2} + \frac{|\mu_g\bar{\chi}_g|}{2} + \frac{|\nu_g\bar{\phi}_g|}{2}$$

a_{1u}t_{2u}

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \xi_u \xi_u \rangle + \langle \alpha_u \xi_u || \alpha_u \xi_u \rangle}$$

t_{1u}t_{2u}

$$\Delta E = \langle \nu_u \chi_u || \nu_u \chi_u \rangle + \langle \nu_u \nu_u || \xi_u \xi_u \rangle + \langle \nu_u \xi_u || \nu_u \xi_u \rangle + \langle \nu_u \mu_u || \chi_u \phi_u \rangle$$

$$\Psi_{28}(t_{1u}t_{2u}, {}^1T_{1g}, M=0, \nu_g) = -\frac{|\eta_u\phi_u|}{2} - \frac{|\mu_u\xi_u|}{2} + \frac{|\eta_u\bar{\phi}_u|}{2} + \frac{|\mu_u\bar{\xi}_u|}{2}$$

$$\Psi_{29}(t_{1u}t_{2u}, {}^1T_{1g}, M=0, \mu_g) = -\frac{|\eta_u\chi_u|}{2} - \frac{|\nu_u\xi_u|}{2} + \frac{|\eta_u\bar{\chi}_u|}{2} + \frac{|\nu_u\bar{\xi}_u|}{2}$$

$$\Psi_{30}(t_{1u}t_{2u}, {}^1T_{1g}, M=0, \eta_g) = -\frac{|\mu_u\chi_u|}{2} - \frac{|\nu_u\phi_u|}{2} + \frac{|\mu_u\bar{\chi}_u|}{2} + \frac{|\nu_u\bar{\phi}_u|}{2}$$

$$\Psi_{19}(a_{1u}t_{2u}, {}^3T_{2g}, M=-1, \xi_g) = |\overline{\alpha_u}\overline{\xi_u}|$$

$$\Psi_{20}(a_{1u}t_{2u}, {}^3T_{2g}, M=-1, \phi_g) = |\overline{\alpha_u}\overline{\phi_u}|$$

$$\Psi_{21}(a_{1u}t_{2u}, {}^3T_{2g}, M=-1, \chi_g) = |\overline{\alpha_u}\overline{\chi_u}|$$

$$\Psi_{22}(a_{1u}t_{2u}, {}^3T_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\alpha_u}\overline{\xi_u}|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\xi_u}|}{2}$$

$$\Psi_{23}(a_{1u}t_{2u}, {}^3T_{2g}, M=0, \phi_g) = \frac{\sqrt{2}|\overline{\alpha_u}\overline{\phi_u}|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\phi_u}|}{2}$$

$$\Psi_{24}(a_{1u}t_{2u}, {}^3T_{2g}, M=0, \chi_g) = \frac{\sqrt{2}|\overline{\alpha_u}\overline{\chi_u}|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\chi_u}|}{2}$$

$$\Psi_{25}(a_{1u}t_{2u}, {}^3T_{2g}, M=1, \xi_g) = |\alpha_u\xi_u|$$

$$\Psi_{26}(a_{1u}t_{2u}, {}^3T_{2g}, M=1, \phi_g) = |\alpha_u\phi_u|$$

$$\Psi_{27}(a_{1u}t_{2u}, {}^3T_{2g}, M=1, \chi_g) = |\alpha_u\chi_u|$$

2.32.14 ${}^3T_{2g}$ *a_{1g}t_{2g}*

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g || \xi_g \xi_g \rangle + \langle \alpha_g \xi_g || \alpha_g \xi_g \rangle}$$

$$\Psi_1(a_{1g}t_{2g}, {}^3T_{2g}, M=-1, \xi_g) = |\overline{\alpha_g}\overline{\xi_g}|$$

$$\Psi_2(a_{1g}t_{2g}, {}^3T_{2g}, M=-1, \phi_g) = |\overline{\alpha_g}\overline{\phi_g}|$$

$$\Psi_3(a_{1g}t_{2g}, {}^3T_{2g}, M=-1, \chi_g) = |\overline{\alpha_g}\overline{\chi_g}|$$

$$\Psi_4(a_{1g}t_{2g}, {}^3T_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\alpha_g}\xi_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\xi}_g|}{2}$$

$$\Psi_5(a_{1g}t_{2g}, {}^3T_{2g}, M=0, \phi_g) = \frac{\sqrt{2}|\overline{\alpha_g}\phi_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\phi}_g|}{2}$$

$$\Psi_6(a_{1g}t_{2g}, {}^3T_{2g}, M=0, \chi_g) = \frac{\sqrt{2}|\overline{\alpha_g}\chi_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\chi}_g|}{2}$$

$$\Psi_7(a_{1g}t_{2g}, {}^3T_{2g}, M=1, \xi_g) = |\alpha_g\xi_g|$$

$$\Psi_8(a_{1g}t_{2g}, {}^3T_{2g}, M=1, \phi_g) = |\alpha_g\phi_g|$$

$$\Psi_9(a_{1g}t_{2g}, {}^3T_{2g}, M=1, \chi_g) = |\alpha_g\chi_g|$$

a_{2u}t_{1u}

$$\boxed{\Delta E = -\langle \beta_u \beta_u || \nu_u \nu_u \rangle + \langle \beta_u \nu_u || \beta_u \nu_u \rangle}$$

$$\Psi_{10}(a_{2u}t_{1u}, {}^3T_{2g}, M=-1, \xi_g) = |\overline{\beta_u}\overline{\eta_u}|$$

$$\Psi_{11}(a_{2u}t_{1u}, {}^3T_{2g}, M=-1, \phi_g) = |\overline{\beta_u}\overline{\mu_u}|$$

$$\Psi_{12}(a_{2u}t_{1u}, {}^3T_{2g}, M=-1, \chi_g) = |\overline{\beta_u}\overline{\nu_u}|$$

$$\Psi_{13}(a_{2u}t_{1u}, {}^3T_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\beta_u}\eta_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\eta}_u|}{2}$$

$$\Psi_{14}(a_{2u}t_{1u}, {}^3T_{2g}, M=0, \phi_g) = \frac{\sqrt{2}|\overline{\beta_u}\mu_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\mu}_u|}{2}$$

$$\Psi_{15}(a_{2u}t_{1u}, {}^3T_{2g}, M=0, \chi_g) = \frac{\sqrt{2}|\overline{\beta_u}\nu_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\nu}_u|}{2}$$

$$\Psi_{16}(a_{2u}t_{1u}, {}^3T_{2g}, M=1, \xi_g) = |\beta_u\eta_u|$$

$$\Psi_{17}(a_{2u}t_{1u}, {}^3T_{2g}, M=1, \phi_g) = |\beta_u\mu_u|$$

$$\Psi_{18}(a_{2u}t_{1u}, {}^3T_{2g}, M=1, \chi_g) = |\beta_u\nu_u|$$

a_{1u}t_{2u}

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u || \xi_u \xi_u \rangle + \langle \alpha_u \xi_u || \alpha_u \xi_u \rangle}$$

$$\Psi_{19}(a_{1u}t_{2u}, {}^3T_{2g}, M=-1, \xi_g) = |\overline{\alpha_u}\overline{\xi_u}|$$

$$\Psi_{20}(a_{1u}t_{2u}, {}^3T_{2g}, M=-1, \phi_g) = |\overline{\alpha_u}\overline{\phi_u}|$$

$$\Psi_{21}(a_{1u}t_{2u}, {}^3T_{2g}, M=-1, \chi_g) = |\overline{\alpha_u}\overline{\chi_u}|$$

$$\Psi_{22}(a_{1u}t_{2u}, {}^3T_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\alpha_u}\overline{\xi_u}|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\xi}_u|}{2}$$

$$\Psi_{23}(a_{1u}t_{2u}, {}^3T_{2g}, M=0, \phi_g) = \frac{\sqrt{2}|\overline{\alpha_u}\overline{\phi_u}|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\phi}_u|}{2}$$

$$\Psi_{24}(a_{1u}t_{2u}, {}^3T_{2g}, M=0, \chi_g) = \frac{\sqrt{2}|\overline{\alpha_u}\overline{\chi_u}|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\chi}_u|}{2}$$

$$\Psi_{25}(a_{1u}t_{2u}, {}^3T_{2g}, M=1, \xi_g) = |\alpha_u\xi_u|$$

$$\Psi_{26}(a_{1u}t_{2u}, {}^3T_{2g}, M=1, \phi_g) = |\alpha_u\phi_u|$$

$$\Psi_{27}(a_{1u}t_{2u}, {}^3T_{2g}, M=1, \chi_g) = |\alpha_u\chi_u|$$

a_{2g}t_{1g}

$$\boxed{\Delta E = -\langle \beta_g \beta_g || \nu_g \nu_g \rangle + \langle \beta_g \nu_g || \beta_g \nu_g \rangle}$$

$$\Psi_{28}(a_{2g}t_{1g}, {}^3T_{2g}, M=-1, \xi_g) = |\overline{\beta_g}\overline{\eta_g}|$$

$$\Psi_{29}(a_{2g}t_{1g}, {}^3T_{2g}, M=-1, \phi_g) = |\overline{\beta_g}\overline{\mu_g}|$$

$$\Psi_{30}(a_{2g}t_{1g}, {}^3T_{2g}, M=-1, \chi_g) = |\overline{\beta_g}\overline{\nu_g}|$$

$$\Psi_{31}(a_{2g}t_{1g}, {}^3T_{2g}, M=0, \xi_g) = \frac{\sqrt{2}|\overline{\beta_g}\eta_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\eta}_g|}{2}$$

$$\Psi_{32}(a_{2g}t_{1g}, {}^3T_{2g}, M=0, \phi_g) = \frac{\sqrt{2}|\overline{\beta_g}\mu_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\mu}_g|}{2}$$

$$\Psi_{33}(a_{2g}t_{1g}, {}^3T_{2g}, M=0, \chi_g) = \frac{\sqrt{2}|\overline{\beta_g}\nu_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\nu}_g|}{2}$$

$$\Psi_{34}(a_{2g}t_{1g}, {}^3T_{2g}, M=1, \xi_g) = |\beta_g\eta_g|$$

$$\Psi_{35}(a_{2g}t_{1g}, {}^3T_{2g}, M=1, \phi_g) = |\beta_g\mu_g|$$

$$\Psi_{36}(a_{2g}t_{1g}, {}^3T_{2g}, M=1, \chi_g) = |\beta_g\nu_g|$$

e_ut_{1u}

$$\boxed{\Delta E = \langle \zeta_u \nu_u || \zeta_u \nu_u \rangle}$$

$$\Psi_{37}(e_{u t_{1u}}, {}^3T_{2g}, M=-1, \xi_g) = -\frac{\sqrt{2}|\overline{\gamma_u}\overline{\eta_u}|}{2} + \frac{\sqrt{2}|\zeta_u\overline{\eta_u}|}{2}$$

$$\Psi_{38}(e_{u t_{1u}}, {}^3T_{2g}, M=-1, \phi_g) = -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u}\mu_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_u\mu_u|}{2}$$

$$\Psi_{39}(e_{u t_{1u}}, {}^3T_{2g}, M=-1, \chi_g) = \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u}\nu_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_u\nu_u|}{2}$$

$$\Psi_{40}(e_{u t_{1u}}, {}^3T_{2g}, M=0, \xi_g) = -\frac{|\overline{\gamma_u}\eta_u|}{2} + \frac{|\zeta_u\eta_u|}{2} - \frac{|\gamma_u\overline{\eta}_u|}{2} + \frac{|\zeta_u\overline{\eta}_u|}{2}$$

$$\Psi_{41}(e_{u t_{1u}}, {}^3T_{2g}, M=0, \phi_g) = -\frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u}\mu_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\mu_u|}{2} - \frac{(-1)^{\frac{2}{3}}|\gamma_u\overline{\mu}_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\overline{\mu}_u|}{2}$$

$$\Psi_{42}(e_{u t_{1u}}, {}^3T_{2g}, M=0, \chi_g) = \frac{\sqrt[3]{-1}|\overline{\gamma_u}\nu_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_u\nu_u|}{2} + \frac{\sqrt[3]{-1}|\gamma_u\overline{\nu}_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_u\overline{\nu}_u|}{2}$$

$$\Psi_{43}(e_{u t_{1u}}, {}^3T_{2g}, M=1, \xi_g) = -\frac{\sqrt{2}|\gamma_u\eta_u|}{2} + \frac{\sqrt{2}|\zeta_u\eta_u|}{2}$$

$$\begin{aligned}\Psi_{44}(e_u t_{1u}, {}^3T_{2g}, M=1, \phi_g) = \\ -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_u \mu_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_u \mu_u|}{2} \\ \Psi_{45}(e_u t_{1u}, {}^3T_{2g}, M=1, \chi_g) = \\ \frac{\sqrt[3]{-1}\sqrt{2}|\gamma_u \nu_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_u \nu_u|}{2}\end{aligned}$$

 $e_u t_{2u}$

$$\boxed{\Delta E = \langle \zeta_u \xi_u | |\zeta_u \xi_u \rangle}$$

$$\begin{aligned}\Psi_{46}(e_u t_{2u}, {}^3T_{2g}, M=-1, \xi_g) = \frac{\sqrt{2}|\overline{\gamma_u \xi_u}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \xi_u}|}{2} \\ \Psi_{47}(e_u t_{2u}, {}^3T_{2g}, M=-1, \phi_g) = \\ \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u \phi_u}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_u \phi_u}|}{2} \\ \Psi_{48}(e_u t_{2u}, {}^3T_{2g}, M=-1, \chi_g) = \\ -\frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u \chi_u}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_u \chi_u}|}{2} \\ \Psi_{49}(e_u t_{2u}, {}^3T_{2g}, M=0, \xi_g) = \\ \frac{|\overline{\gamma_u \xi_u}|}{2} + \frac{|\overline{\zeta_u \xi_u}|}{2} + \frac{|\overline{\gamma_u \xi_u}|}{2} + \frac{|\overline{\zeta_u \xi_u}|}{2} \\ \Psi_{50}(e_u t_{2u}, {}^3T_{2g}, M=0, \phi_g) = \\ \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \phi_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \phi_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \phi_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \phi_u}|}{2} \\ \Psi_{51}(e_u t_{2u}, {}^3T_{2g}, M=0, \chi_g) = \\ -\frac{\sqrt[3]{-1}|\overline{\gamma_u \chi_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \chi_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\gamma_u \chi_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \chi_u}|}{2} \\ \Psi_{52}(e_u t_{2u}, {}^3T_{2g}, M=1, \xi_g) = \frac{\sqrt{2}|\gamma_u \xi_u|}{2} + \frac{\sqrt{2}|\zeta_u \xi_u|}{2} \\ \Psi_{53}(e_u t_{2u}, {}^3T_{2g}, M=1, \phi_g) = \\ \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_u \phi_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_u \phi_u|}{2} \\ \Psi_{54}(e_u t_{2u}, {}^3T_{2g}, M=1, \chi_g) = \\ -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma_u \chi_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_u \chi_u|}{2}\end{aligned}$$

 $e_g t_{1g}$

$$\boxed{\Delta E = \langle \zeta_g \nu_g | |\zeta_g \nu_g \rangle}$$

$$\begin{aligned}\Psi_{55}(e_g t_{1g}, {}^3T_{2g}, M=-1, \xi_g) = -\frac{\sqrt{2}|\overline{\gamma_g \eta_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_g \eta_g}|}{2} \\ \Psi_{56}(e_g t_{1g}, {}^3T_{2g}, M=-1, \phi_g) = \\ -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_g \mu_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_g \mu_g}|}{2} \\ \Psi_{57}(e_g t_{1g}, {}^3T_{2g}, M=-1, \chi_g) = \\ \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_g \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_g \nu_g}|}{2} \\ \Psi_{58}(e_g t_{1g}, {}^3T_{2g}, M=0, \xi_g) = \\ -\frac{|\overline{\gamma_g \eta_g}|}{2} + \frac{|\overline{\zeta_g \eta_g}|}{2} - \frac{|\overline{\gamma_g \eta_g}|}{2} + \frac{|\overline{\zeta_g \eta_g}|}{2} \\ \Psi_{59}(e_g t_{1g}, {}^3T_{2g}, M=0, \phi_g) = \\ -\frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \mu_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \mu_g}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \mu_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \mu_g}|}{2} \\ \Psi_{60}(e_g t_{1g}, {}^3T_{2g}, M=0, \chi_g) = \\ \frac{\sqrt[3]{-1}|\overline{\gamma_g \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g \nu_g}|}{2} + \frac{\sqrt[3]{-1}|\overline{\gamma_g \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g \nu_g}|}{2} \\ \Psi_{61}(e_g t_{1g}, {}^3T_{2g}, M=1, \xi_g) = -\frac{\sqrt{2}|\gamma_g \eta_g|}{2} + \frac{\sqrt{2}|\zeta_g \eta_g|}{2}\end{aligned}$$

$$\begin{aligned}\Psi_{62}(e_g t_{1g}, {}^3T_{2g}, M=1, \phi_g) = \\ -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_g \mu_g|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_g \mu_g|}{2} \\ \Psi_{63}(e_g t_{1g}, {}^3T_{2g}, M=1, \chi_g) = \\ \frac{\sqrt[3]{-1}\sqrt{2}|\gamma_g \nu_g|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_g \nu_g|}{2}\end{aligned}$$

 $e_g t_{2g}$

$$\boxed{\Delta E = \langle \zeta_g \xi_g | |\zeta_g \xi_g \rangle}$$

$$\begin{aligned}\Psi_{64}(e_g t_{2g}, {}^3T_{2g}, M=-1, \xi_g) = \frac{\sqrt{2}|\overline{\gamma_g \xi_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_g \xi_g}|}{2} \\ \Psi_{65}(e_g t_{2g}, {}^3T_{2g}, M=-1, \phi_g) = \\ \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_g \phi_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_g \phi_g}|}{2} \\ \Psi_{66}(e_g t_{2g}, {}^3T_{2g}, M=-1, \chi_g) = \\ -\frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_g \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_g \chi_g}|}{2} \\ \Psi_{67}(e_g t_{2g}, {}^3T_{2g}, M=0, \xi_g) = \\ \frac{|\overline{\gamma_g \xi_g}|}{2} + \frac{|\overline{\zeta_g \xi_g}|}{2} + \frac{|\overline{\gamma_g \xi_g}|}{2} + \frac{|\overline{\zeta_g \xi_g}|}{2} \\ \Psi_{68}(e_g t_{2g}, {}^3T_{2g}, M=0, \phi_g) = \\ \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \phi_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \phi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \phi_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \phi_g}|}{2} \\ \Psi_{69}(e_g t_{2g}, {}^3T_{2g}, M=0, \chi_g) = \\ -\frac{\sqrt[3]{-1}|\overline{\gamma_g \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g \chi_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\gamma_g \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g \chi_g}|}{2} \\ \Psi_{70}(e_g t_{2g}, {}^3T_{2g}, M=1, \xi_g) = \frac{\sqrt{2}|\gamma_g \xi_g|}{2} + \frac{\sqrt{2}|\zeta_g \xi_g|}{2} \\ \Psi_{71}(e_g t_{2g}, {}^3T_{2g}, M=1, \phi_g) = \\ \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_g \phi_g|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_g \phi_g|}{2} \\ \Psi_{72}(e_g t_{2g}, {}^3T_{2g}, M=1, \chi_g) = \\ -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma_g \chi_g|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_g \chi_g|}{2}\end{aligned}$$

 $t_{1g} t_{2g}$

$$\boxed{\Delta E = -\langle \nu_g \chi_g | |\nu_g \chi_g \rangle - \langle \nu_g \nu_g | |\xi_g \xi_g \rangle + \langle \nu_g \xi_g | |\nu_g \xi_g \rangle + \langle \nu_g \mu_g | |\chi_g \phi_g \rangle}$$

$$\begin{aligned}\Psi_{73}(t_{1g} t_{2g}, {}^3T_{2g}, M=-1, \chi_g) = -\frac{\sqrt{2}|\overline{\eta_g \phi_g}|}{2} + \frac{\sqrt{2}|\overline{\mu_g \xi_g}|}{2} \\ \Psi_{74}(t_{1g} t_{2g}, {}^3T_{2g}, M=-1, \phi_g) = \frac{\sqrt{2}|\overline{\eta_g \chi_g}|}{2} - \frac{\sqrt{2}|\overline{\nu_g \xi_g}|}{2} \\ \Psi_{75}(t_{1g} t_{2g}, {}^3T_{2g}, M=-1, \xi_g) = -\frac{\sqrt{2}|\overline{\mu_g \chi_g}|}{2} + \frac{\sqrt{2}|\overline{\nu_g \phi_g}|}{2} \\ \Psi_{76}(t_{1g} t_{2g}, {}^3T_{2g}, M=0, \chi_g) = \\ -\frac{|\overline{\eta_g \phi_g}|}{2} + \frac{|\overline{\mu_g \xi_g}|}{2} - \frac{|\overline{\eta_g \phi_g}|}{2} + \frac{|\overline{\mu_g \xi_g}|}{2} \\ \Psi_{77}(t_{1g} t_{2g}, {}^3T_{2g}, M=0, \phi_g) = \\ \frac{|\overline{\eta_g \chi_g}|}{2} - \frac{|\overline{\nu_g \xi_g}|}{2} + \frac{|\overline{\eta_g \chi_g}|}{2} - \frac{|\overline{\nu_g \xi_g}|}{2} \\ \Psi_{78}(t_{1g} t_{2g}, {}^3T_{2g}, M=0, \xi_g) = \\ -\frac{|\overline{\mu_g \chi_g}|}{2} + \frac{|\overline{\nu_g \phi_g}|}{2} - \frac{|\overline{\mu_g \chi_g}|}{2} + \frac{|\overline{\nu_g \phi_g}|}{2} \\ \Psi_{79}(t_{1g} t_{2g}, {}^3T_{2g}, M=1, \chi_g) = -\frac{\sqrt{2}|\eta_g \phi_g|}{2} + \frac{\sqrt{2}|\mu_g \xi_g|}{2} \\ \Psi_{80}(t_{1g} t_{2g}, {}^3T_{2g}, M=1, \phi_g) = \frac{\sqrt{2}|\eta_g \chi_g|}{2} - \frac{\sqrt{2}|\nu_g \xi_g|}{2}\end{aligned}$$

$$\Psi_{81}(t_{1g}t_{2g}, {}^3T_{2g}, M=1, \xi_g) = -\frac{\sqrt{2}|\mu_g\chi_g|}{2} + \frac{\sqrt{2}|\nu_g\phi_g|}{2}$$

t_{1u}t_{2u}

$$\Delta E = -\langle \nu_u \chi_u || \nu_u \chi_u \rangle - \langle \nu_u \nu_u || \xi_u \xi_u \rangle + \langle \nu_u \xi_u || \nu_u \xi_u \rangle + \langle \nu_u \mu_u || \chi_u \phi_u \rangle$$

$$\Psi_{82}(t_{1u}t_{2u}, {}^3T_{2g}, M=-1, \chi_g) = -\frac{\sqrt{2}|\eta_u\phi_u|}{2} + \frac{\sqrt{2}|\mu_u\xi_u|}{2}$$

$$\Psi_{83}(t_{1u}t_{2u}, {}^3T_{2g}, M=-1, \phi_g) = \frac{\sqrt{2}|\eta_u\chi_u|}{2} - \frac{\sqrt{2}|\nu_u\xi_u|}{2}$$

$$\Psi_{84}(t_{1u}t_{2u}, {}^3T_{2g}, M=-1, \xi_g) = -\frac{\sqrt{2}|\mu_u\chi_u|}{2} + \frac{\sqrt{2}|\nu_u\phi_u|}{2}$$

$$\Psi_{85}(t_{1u}t_{2u}, {}^3T_{2g}, M=0, \chi_g) = -\frac{|\eta_u\phi_u|}{2} + \frac{|\mu_u\xi_u|}{2} - \frac{|\eta_u\phi_u|}{2} + \frac{|\mu_u\xi_u|}{2}$$

$$\Psi_{86}(t_{1u}t_{2u}, {}^3T_{2g}, M=0, \phi_g) = \frac{|\eta_u\chi_u|}{2} - \frac{|\nu_u\xi_u|}{2} + \frac{|\eta_u\chi_u|}{2} - \frac{|\nu_u\xi_u|}{2}$$

$$\Psi_{87}(t_{1u}t_{2u}, {}^3T_{2g}, M=0, \xi_g) = -\frac{|\mu_u\chi_u|}{2} + \frac{|\nu_u\phi_u|}{2} - \frac{|\mu_u\chi_u|}{2} + \frac{|\nu_u\phi_u|}{2}$$

$$\Psi_{88}(t_{1u}t_{2u}, {}^3T_{2g}, M=1, \chi_g) = -\frac{\sqrt{2}|\eta_u\phi_u|}{2} + \frac{\sqrt{2}|\mu_u\xi_u|}{2}$$

$$\Psi_{89}(t_{1u}t_{2u}, {}^3T_{2g}, M=1, \phi_g) = \frac{\sqrt{2}|\eta_u\chi_u|}{2} - \frac{\sqrt{2}|\nu_u\xi_u|}{2}$$

$$\Psi_{90}(t_{1u}t_{2u}, {}^3T_{2g}, M=1, \xi_g) = -\frac{\sqrt{2}|\mu_u\chi_u|}{2} + \frac{\sqrt{2}|\nu_u\phi_u|}{2}$$

2.32.15 ${}^1T_{2g}$

a_{1g}t_{2g}

$$\Delta E = \langle \alpha_g \alpha_g || \xi_g \xi_g \rangle + \langle \alpha_g \xi_g || \alpha_g \xi_g \rangle$$

$$\Psi_1(a_{1g}t_{2g}, {}^1T_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\xi_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\xi_g}|}{2}$$

$$\Psi_2(a_{1g}t_{2g}, {}^1T_{2g}, M=0, \phi_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\phi_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\phi_g}|}{2}$$

$$\Psi_3(a_{1g}t_{2g}, {}^1T_{2g}, M=0, \chi_g) = -\frac{\sqrt{2}|\overline{\alpha_g}\chi_g|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\chi_g}|}{2}$$

a_{2u}t_{1u}

$$\Delta E = \langle \beta_u \beta_u || \nu_u \nu_u \rangle + \langle \beta_u \nu_u || \beta_u \nu_u \rangle$$

$$\Psi_4(a_{2u}t_{1u}, {}^1T_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\beta_u}\eta_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\eta_u}|}{2}$$

$$\Psi_5(a_{2u}t_{1u}, {}^1T_{2g}, M=0, \phi_g) = -\frac{\sqrt{2}|\overline{\beta_u}\mu_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\mu_u}|}{2}$$

$$\Psi_6(a_{2u}t_{1u}, {}^1T_{2g}, M=0, \chi_g) = -\frac{\sqrt{2}|\overline{\beta_u}\nu_u|}{2} + \frac{\sqrt{2}|\beta_u\overline{\nu_u}|}{2}$$

a_{1u}t_{2u}

$$\Delta E = \langle \alpha_u \alpha_u || \xi_u \xi_u \rangle + \langle \alpha_u \xi_u || \alpha_u \xi_u \rangle$$

$$\Psi_7(a_{1u}t_{2u}, {}^1T_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\alpha_u}\xi_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\xi_u}|}{2}$$

$$\Psi_8(a_{1u}t_{2u}, {}^1T_{2g}, M=0, \phi_g) = -\frac{\sqrt{2}|\overline{\alpha_u}\phi_u|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\phi_u}|}{2}$$

a_{2g}t_{1g}

$$\Delta E = \langle \beta_g \beta_g || \nu_g \nu_g \rangle + \langle \beta_g \nu_g || \beta_g \nu_g \rangle$$

$$\Psi_{10}(a_{2g}t_{1g}, {}^1T_{2g}, M=0, \xi_g) = -\frac{\sqrt{2}|\overline{\beta_g}\eta_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\eta_g}|}{2}$$

$$\Psi_{11}(a_{2g}t_{1g}, {}^1T_{2g}, M=0, \phi_g) = -\frac{\sqrt{2}|\overline{\beta_g}\mu_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\mu_g}|}{2}$$

$$\Psi_{12}(a_{2g}t_{1g}, {}^1T_{2g}, M=0, \chi_g) = -\frac{\sqrt{2}|\overline{\beta_g}\nu_g|}{2} + \frac{\sqrt{2}|\beta_g\overline{\nu_g}|}{2}$$

e_ut_{1u}

$$\Delta E = \langle \zeta_u \nu_u || \zeta_u \nu_u \rangle$$

$$\Psi_{13}(e_u t_{1u}, {}^1T_{2g}, M=0, \xi_g) = \frac{|\overline{\gamma_u}\eta_u|}{2} - \frac{|\overline{\zeta_u}\eta_u|}{2} - \frac{|\gamma_u\overline{\eta_u}|}{2} + \frac{|\zeta_u\overline{\eta_u}|}{2}$$

$$\Psi_{14}(e_u t_{1u}, {}^1T_{2g}, M=0, \phi_g) = \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u}\mu_u|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_u}\mu_u|}{2} - \frac{(-1)^{\frac{2}{3}}|\gamma_u\overline{\mu_u}|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\overline{\mu_u}|}{2}$$

$$\Psi_{15}(e_u t_{1u}, {}^1T_{2g}, M=0, \chi_g) = -\frac{\sqrt[3]{-1}|\overline{\gamma_u}\nu_u|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u}\nu_u|}{2} + \frac{\sqrt[3]{-1}|\gamma_u\overline{\nu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_u\overline{\nu_u}|}{2}$$

e_ut_{2u}

$$\Delta E = \langle \zeta_u \xi_u || \zeta_u \xi_u \rangle$$

$$\Psi_{16}(e_u t_{2u}, {}^1T_{2g}, M=0, \xi_g) = -\frac{|\overline{\gamma_u}\xi_u|}{2} - \frac{|\overline{\zeta_u}\xi_u|}{2} + \frac{|\gamma_u\overline{\xi_u}|}{2} + \frac{|\zeta_u\overline{\xi_u}|}{2}$$

$$\Psi_{17}(e_u t_{2u}, {}^1T_{2g}, M=0, \phi_g) = -\frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u}\phi_u|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_u}\phi_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\gamma_u\overline{\phi_u}|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\overline{\phi_u}|}{2}$$

$$\Psi_{18}(e_u t_{2u}, {}^1T_{2g}, M=0, \chi_g) = -\frac{\sqrt[3]{-1}|\overline{\gamma_u}\chi_u|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u}\chi_u|}{2} - \frac{\sqrt[3]{-1}|\gamma_u\overline{\chi_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_u\overline{\chi_u}|}{2}$$

e_gt_{1g}

$$\Delta E = \langle \zeta_g \nu_g || \zeta_g \nu_g \rangle$$

$$\Psi_{19}(e_g t_{1g}, {}^1T_{2g}, M=0, \xi_g) = \frac{|\overline{\gamma_g}\eta_g|}{2} - \frac{|\overline{\zeta_g}\eta_g|}{2} - \frac{|\gamma_g\overline{\eta_g}|}{2} + \frac{|\zeta_g\overline{\eta_g}|}{2}$$

$$\Psi_{20}(e_g t_{1g}, {}^1T_{2g}, M=0, \phi_g) = \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g}\mu_g|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_g}\mu_g|}{2} - \frac{(-1)^{\frac{2}{3}}|\gamma_g\overline{\mu_g}|}{2} - \frac{\sqrt[3]{-1}|\zeta_g\overline{\mu_g}|}{2}$$

$$\Psi_{21}(e_g t_{1g}, {}^1T_{2g}, M=0, \chi_g) = -\frac{\sqrt[3]{-1}|\overline{\gamma_g}\nu_g|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g}\nu_g|}{2} + \frac{\sqrt[3]{-1}|\gamma_g\overline{\nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_g\overline{\nu_g}|}{2}$$

e_gt_{2g}

$$\Delta E = \langle \zeta_g \xi_g || \zeta_g \xi_g \rangle$$

$$\Psi_{22}(e_g t_{2g}, {}^1T_{2g}, M=0, \xi_g) = -\frac{|\overline{\gamma_g}\xi_g|}{2} - \frac{|\overline{\zeta_g}\xi_g|}{2} + \frac{|\gamma_g\overline{\xi_g}|}{2} + \frac{|\zeta_g\overline{\xi_g}|}{2}$$

$$\begin{aligned} \Psi_{23}(e_g t_{2g}, {}^1T_{2g}, M=0, \phi_g) = \\ -\frac{(-1)^{\frac{2}{3}} |\overline{\gamma_g} \phi_g|}{2} + \frac{\sqrt[3]{-1} |\overline{\zeta_g} \phi_g|}{2} + \frac{(-1)^{\frac{2}{3}} |\gamma_g \overline{\phi_g}|}{2} - \frac{\sqrt[3]{-1} |\zeta_g \overline{\phi_g}|}{2} \\ \Psi_{24}(e_g t_{2g}, {}^1T_{2g}, M=0, \chi_g) = \\ \frac{\sqrt[3]{-1} |\overline{\gamma_g} \chi_g|}{2} - \frac{(-1)^{\frac{2}{3}} |\overline{\zeta_g} \chi_g|}{2} - \frac{\sqrt[3]{-1} |\gamma_g \overline{\chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}} |\zeta_g \overline{\chi_g}|}{2} \end{aligned}$$

$$t_{1g}^2$$

$$\boxed{\Delta E = \langle \nu_g \mu_g | \nu_g \mu_g \rangle + \langle \nu_g \nu_g | \nu_g \nu_g \rangle}$$

$$\begin{aligned} \Psi_{25}(t_{1g}^2, {}^1T_{2g}, M=0, \chi_g) &= -\frac{\sqrt{2} |\overline{\eta_g} \mu_g|}{2} - \frac{\sqrt{2} |\overline{\mu_g} \eta_g|}{2} \\ \Psi_{26}(t_{1g}^2, {}^1T_{2g}, M=0, \phi_g) &= -\frac{\sqrt{2} |\overline{\eta_g} \nu_g|}{2} - \frac{\sqrt{2} |\overline{\nu_g} \eta_g|}{2} \\ \Psi_{27}(t_{1g}^2, {}^1T_{2g}, M=0, \xi_g) &= -\frac{\sqrt{2} |\overline{\mu_g} \nu_g|}{2} - \frac{\sqrt{2} |\overline{\nu_g} \mu_g|}{2} \end{aligned}$$

$t_{1g} t_{2g}$

$$\boxed{\Delta E = -\langle \nu_g \chi_g | \nu_g \chi_g \rangle + \langle \nu_g \nu_g | \xi_g \xi_g \rangle + \langle \nu_g \xi_g | \nu_g \xi_g \rangle - \langle \nu_g \mu_g | \chi_g \phi_g \rangle}$$

$$\begin{aligned} \Psi_{28}(t_{1g} t_{2g}, {}^1T_{2g}, M=0, \chi_g) &= \\ \frac{|\overline{\eta_g} \phi_g|}{2} - \frac{|\overline{\mu_g} \xi_g|}{2} - \frac{|\eta_g \overline{\phi_g}|}{2} + \frac{|\mu_g \overline{\xi_g}|}{2} \\ \Psi_{29}(t_{1g} t_{2g}, {}^1T_{2g}, M=0, \phi_g) &= \\ -\frac{|\overline{\eta_g} \chi_g|}{2} + \frac{|\overline{\nu_g} \xi_g|}{2} + \frac{|\eta_g \overline{\chi_g}|}{2} - \frac{|\nu_g \overline{\xi_g}|}{2} \\ \Psi_{30}(t_{1g} t_{2g}, {}^1T_{2g}, M=0, \xi_g) &= \\ \frac{|\overline{\mu_g} \chi_g|}{2} - \frac{|\overline{\nu_g} \phi_g|}{2} - \frac{|\mu_g \overline{\chi_g}|}{2} + \frac{|\nu_g \overline{\phi_g}|}{2} \end{aligned}$$

t_{2g}^2

$$\boxed{\Delta E = \langle \xi_g \phi_g | \xi_g \phi_g \rangle + \langle \xi_g \xi_g | \xi_g \xi_g \rangle}$$

$$\begin{aligned} \Psi_{31}(t_{2g}^2, {}^1T_{2g}, M=0, \chi_g) &= -\frac{\sqrt{2} |\overline{\phi_g} \xi_g|}{2} - \frac{\sqrt{2} |\overline{\xi_g} \phi_g|}{2} \\ \Psi_{32}(t_{2g}^2, {}^1T_{2g}, M=0, \phi_g) &= -\frac{\sqrt{2} |\overline{\chi_g} \xi_g|}{2} - \frac{\sqrt{2} |\overline{\xi_g} \chi_g|}{2} \\ \Psi_{33}(t_{2g}^2, {}^1T_{2g}, M=0, \xi_g) &= -\frac{\sqrt{2} |\overline{\chi_g} \phi_g|}{2} - \frac{\sqrt{2} |\overline{\phi_g} \chi_g|}{2} \end{aligned}$$

t_{1u}^2

$$\boxed{\Delta E = \langle \nu_u \mu_u | \nu_u \mu_u \rangle + \langle \nu_u \nu_u | \nu_u \nu_u \rangle}$$

$$\begin{aligned} \Psi_{34}(t_{1u}^2, {}^1T_{2g}, M=0, \chi_g) &= -\frac{\sqrt{2} |\overline{\eta_u} \mu_u|}{2} - \frac{\sqrt{2} |\overline{\mu_u} \eta_u|}{2} \\ \Psi_{35}(t_{1u}^2, {}^1T_{2g}, M=0, \phi_g) &= -\frac{\sqrt{2} |\overline{\eta_u} \nu_u|}{2} - \frac{\sqrt{2} |\overline{\nu_u} \eta_u|}{2} \\ \Psi_{36}(t_{1u}^2, {}^1T_{2g}, M=0, \xi_g) &= -\frac{\sqrt{2} |\overline{\mu_u} \nu_u|}{2} - \frac{\sqrt{2} |\overline{\nu_u} \mu_u|}{2} \end{aligned}$$

$t_{1u} t_{2u}$

$$\boxed{\Delta E = -\langle \nu_u \chi_u | \nu_u \chi_u \rangle + \langle \nu_u \nu_u | \xi_u \xi_u \rangle + \langle \nu_u \xi_u | \nu_u \xi_u \rangle - \langle \nu_u \mu_u | \chi_u \phi_u \rangle}$$

$$\begin{aligned} \Psi_{37}(t_{1u} t_{2u}, {}^1T_{2g}, M=0, \chi_g) &= \\ \frac{|\overline{\eta_u} \phi_u|}{2} - \frac{|\overline{\mu_u} \xi_u|}{2} - \frac{|\eta_u \overline{\phi_u}|}{2} + \frac{|\mu_u \overline{\xi_u}|}{2} \end{aligned}$$

$$\begin{aligned} \Psi_{38}(t_{1u} t_{2u}, {}^1T_{2g}, M=0, \phi_g) &= \\ -\frac{|\overline{\eta_u} \chi_u|}{2} + \frac{|\overline{\nu_u} \xi_u|}{2} + \frac{|\eta_u \overline{\chi_u}|}{2} - \frac{|\nu_u \overline{\xi_u}|}{2} \\ \Psi_{39}(t_{1u} t_{2u}, {}^1T_{2g}, M=0, \xi_g) &= \\ \frac{|\overline{\mu_u} \chi_u|}{2} - \frac{|\overline{\nu_u} \phi_u|}{2} - \frac{|\mu_u \overline{\chi_u}|}{2} + \frac{|\nu_u \overline{\phi_u}|}{2} \end{aligned}$$

t_{2u}^2

$$\boxed{\Delta E = \langle \xi_u \phi_u | \xi_u \phi_u \rangle + \langle \xi_u \xi_u | \xi_u \xi_u \rangle}$$

$$\begin{aligned} \Psi_{40}(t_{2u}^2, {}^1T_{2g}, M=0, \chi_g) &= -\frac{\sqrt{2} |\overline{\phi_u} \xi_u|}{2} - \frac{\sqrt{2} |\overline{\xi_u} \phi_u|}{2} \\ \Psi_{41}(t_{2u}^2, {}^1T_{2g}, M=0, \phi_g) &= -\frac{\sqrt{2} |\overline{\chi_u} \xi_u|}{2} - \frac{\sqrt{2} |\overline{\xi_u} \chi_u|}{2} \\ \Psi_{42}(t_{2u}^2, {}^1T_{2g}, M=0, \xi_g) &= -\frac{\sqrt{2} |\overline{\chi_u} \phi_u|}{2} - \frac{\sqrt{2} |\overline{\phi_u} \chi_u|}{2} \end{aligned}$$

2.32.16 ${}^3T_{1u}$

$a_{1g} t_{1u}$

$$\boxed{\Delta E = -\langle \alpha_g \alpha_g | \nu_u \nu_u \rangle + \langle \alpha_g \nu_u | \alpha_g \nu_u \rangle}$$

$$\Psi_1(a_{1g} t_{1u}, {}^3T_{1u}, M=-1, \eta_u) = |\overline{\alpha_g} \eta_u|$$

$$\Psi_2(a_{1g} t_{1u}, {}^3T_{1u}, M=-1, \mu_u) = |\overline{\alpha_g} \mu_u|$$

$$\Psi_3(a_{1g} t_{1u}, {}^3T_{1u}, M=-1, \nu_u) = |\overline{\alpha_g} \nu_u|$$

$$\Psi_4(a_{1g} t_{1u}, {}^3T_{1u}, M=0, \eta_u) = \frac{\sqrt{2} |\overline{\alpha_g} \eta_u|}{2} + \frac{\sqrt{2} |\alpha_g \overline{\eta_u}|}{2}$$

$$\Psi_5(a_{1g} t_{1u}, {}^3T_{1u}, M=0, \mu_u) = \frac{\sqrt{2} |\overline{\alpha_g} \mu_u|}{2} + \frac{\sqrt{2} |\alpha_g \overline{\mu_u}|}{2}$$

$$\Psi_6(a_{1g} t_{1u}, {}^3T_{1u}, M=0, \nu_u) = \frac{\sqrt{2} |\overline{\alpha_g} \nu_u|}{2} + \frac{\sqrt{2} |\alpha_g \overline{\nu_u}|}{2}$$

$$\Psi_7(a_{1g} t_{1u}, {}^3T_{1u}, M=1, \eta_u) = |\alpha_g \eta_u|$$

$$\Psi_8(a_{1g} t_{1u}, {}^3T_{1u}, M=1, \mu_u) = |\alpha_g \mu_u|$$

$$\Psi_9(a_{1g} t_{1u}, {}^3T_{1u}, M=1, \nu_u) = |\alpha_g \nu_u|$$

$a_{2u} t_{2g}$

$$\boxed{\Delta E = -\langle \beta_u \beta_u | \xi_g \xi_g \rangle + \langle \beta_u \xi_g | \beta_u \xi_g \rangle}$$

$$\Psi_{10}(a_{2u} t_{2g}, {}^3T_{1u}, M=-1, \eta_u) = |\overline{\beta_u} \xi_g|$$

$$\Psi_{11}(a_{2u} t_{2g}, {}^3T_{1u}, M=-1, \mu_u) = |\overline{\beta_u} \phi_g|$$

$$\Psi_{12}(a_{2u} t_{2g}, {}^3T_{1u}, M=-1, \nu_u) = |\overline{\beta_u} \chi_g|$$

$$\Psi_{13}(a_{2u} t_{2g}, {}^3T_{1u}, M=0, \eta_u) = \frac{\sqrt{2} |\overline{\beta_u} \xi_g|}{2} + \frac{\sqrt{2} |\beta_u \overline{\xi_g}|}{2}$$

$$\Psi_{14}(a_{2u} t_{2g}, {}^3T_{1u}, M=0, \mu_u) = \frac{\sqrt{2} |\overline{\beta_u} \phi_g|}{2} + \frac{\sqrt{2} |\beta_u \overline{\phi_g}|}{2}$$

$$\Psi_{15}(a_{2u} t_{2g}, {}^3T_{1u}, M=0, \nu_u) = \frac{\sqrt{2} |\overline{\beta_u} \chi_g|}{2} + \frac{\sqrt{2} |\beta_u \overline{\chi_g}|}{2}$$

$$\Psi_{16}(a_{2u} t_{2g}, {}^3T_{1u}, M=1, \eta_u) = |\beta_u \xi_g|$$

$$\Psi_{17}(a_{2u} t_{2g}, {}^3T_{1u}, M=1, \mu_u) = |\beta_u \phi_g|$$

$$\Psi_{18}(a_{2u} t_{2g}, {}^3T_{1u}, M=1, \nu_u) = |\beta_u \chi_g|$$

$a_{1u} t_{1g}$

$$\boxed{\Delta E = -\langle \alpha_u \alpha_u | \nu_g \nu_g \rangle + \langle \alpha_u \nu_g | \alpha_u \nu_g \rangle}$$

$$\begin{aligned}
\Psi_{19}(a_{1u}t_{1g}, {}^3T_{1u}, M=-1, \eta_u) &= |\overline{\alpha_u \eta_g}| \\
\Psi_{20}(a_{1u}t_{1g}, {}^3T_{1u}, M=-1, \mu_u) &= |\overline{\alpha_u \mu_g}| \\
\Psi_{21}(a_{1u}t_{1g}, {}^3T_{1u}, M=-1, \nu_u) &= |\overline{\alpha_u \nu_g}| \\
\Psi_{22}(a_{1u}t_{1g}, {}^3T_{1u}, M=0, \eta_u) &= \frac{\sqrt{2}|\overline{\alpha_u \eta_g}|}{2} + \frac{\sqrt{2}|\overline{\alpha_u \bar{\eta}_g}|}{2} \\
\Psi_{23}(a_{1u}t_{1g}, {}^3T_{1u}, M=0, \mu_u) &= \frac{\sqrt{2}|\overline{\alpha_u \mu_g}|}{2} + \frac{\sqrt{2}|\overline{\alpha_u \bar{\mu}_g}|}{2} \\
\Psi_{24}(a_{1u}t_{1g}, {}^3T_{1u}, M=0, \nu_u) &= \frac{\sqrt{2}|\overline{\alpha_u \nu_g}|}{2} + \frac{\sqrt{2}|\overline{\alpha_u \bar{\nu}_g}|}{2} \\
\Psi_{25}(a_{1u}t_{1g}, {}^3T_{1u}, M=1, \eta_u) &= |\alpha_u \eta_g| \\
\Psi_{26}(a_{1u}t_{1g}, {}^3T_{1u}, M=1, \mu_u) &= |\alpha_u \mu_g| \\
\Psi_{27}(a_{1u}t_{1g}, {}^3T_{1u}, M=1, \nu_u) &= |\alpha_u \nu_g| \\
&\quad a_{2g}t_{2u} \\
&\quad \boxed{\Delta E = -\langle \beta_g \beta_g || \xi_u \xi_u \rangle + \langle \beta_g \xi_u || \beta_g \xi_u \rangle} \\
\Psi_{28}(a_{2g}t_{2u}, {}^3T_{1u}, M=-1, \eta_u) &= |\overline{\beta_g \xi_u}| \\
\Psi_{29}(a_{2g}t_{2u}, {}^3T_{1u}, M=-1, \mu_u) &= |\overline{\beta_g \phi_u}| \\
\Psi_{30}(a_{2g}t_{2u}, {}^3T_{1u}, M=-1, \nu_u) &= |\overline{\beta_g \chi_u}| \\
\Psi_{31}(a_{2g}t_{2u}, {}^3T_{1u}, M=0, \eta_u) &= \frac{\sqrt{2}|\overline{\beta_g \xi_u}|}{2} + \frac{\sqrt{2}|\overline{\beta_g \bar{\xi}_u}|}{2} \\
\Psi_{32}(a_{2g}t_{2u}, {}^3T_{1u}, M=0, \mu_u) &= \frac{\sqrt{2}|\overline{\beta_g \phi_u}|}{2} + \frac{\sqrt{2}|\overline{\beta_g \bar{\phi}_u}|}{2} \\
\Psi_{33}(a_{2g}t_{2u}, {}^3T_{1u}, M=0, \nu_u) &= \frac{\sqrt{2}|\overline{\beta_g \chi_u}|}{2} + \frac{\sqrt{2}|\overline{\beta_g \bar{\chi}_u}|}{2} \\
\Psi_{34}(a_{2g}t_{2u}, {}^3T_{1u}, M=1, \eta_u) &= |\beta_g \xi_u| \\
\Psi_{35}(a_{2g}t_{2u}, {}^3T_{1u}, M=1, \mu_u) &= |\beta_g \phi_u| \\
\Psi_{36}(a_{2g}t_{2u}, {}^3T_{1u}, M=1, \nu_u) &= |\beta_g \chi_u| \\
&\quad e_u t_{1g} \\
&\quad \boxed{\Delta E = \langle \zeta_u \nu_g || \zeta_u \nu_g \rangle} \\
\Psi_{37}(e_u t_{1g}, {}^3T_{1u}, M=-1, \eta_u) &= \frac{\sqrt{2}|\overline{\gamma_u \eta_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \eta_g}|}{2} \\
\Psi_{38}(e_u t_{1g}, {}^3T_{1u}, M=-1, \mu_u) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u \mu_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_u \mu_g}|}{2} \\
\Psi_{39}(e_u t_{1g}, {}^3T_{1u}, M=-1, \nu_u) &= -\frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_u \nu_g}|}{2} \\
\Psi_{40}(e_u t_{1g}, {}^3T_{1u}, M=0, \eta_u) &= \frac{|\overline{\gamma_u \eta_g}|}{2} + \frac{|\overline{\zeta_u \eta_g}|}{2} + \frac{|\overline{\gamma_u \bar{\eta}_g}|}{2} + \frac{|\overline{\zeta_u \bar{\eta}_g}|}{2} \\
\Psi_{41}(e_u t_{1g}, {}^3T_{1u}, M=0, \mu_u) &= \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \mu_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \mu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \bar{\mu}_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \bar{\mu}_g}|}{2} \\
\Psi_{42}(e_u t_{1g}, {}^3T_{1u}, M=0, \nu_u) &= -\frac{\sqrt[3]{-1}|\overline{\gamma_u \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \nu_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\gamma_u \bar{\nu}_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \bar{\nu}_g}|}{2} \\
\Psi_{43}(e_u t_{1g}, {}^3T_{1u}, M=1, \eta_u) &= \frac{\sqrt{2}|\overline{\gamma_u \eta_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \eta_g}|}{2} \\
\Psi_{44}(e_u t_{1g}, {}^3T_{1u}, M=1, \mu_u) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u \mu_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_u \mu_g}|}{2} \\
&\quad e_u t_{2g} \\
&\quad \boxed{\Delta E = \langle \zeta_u \xi_g || \zeta_u \xi_g \rangle} \\
\Psi_{45}(e_u t_{1g}, {}^3T_{1u}, M=1, \nu_u) &= -\frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_u \nu_g}|}{2} \\
\Psi_{46}(e_u t_{2g}, {}^3T_{1u}, M=-1, \eta_u) &= -\frac{\sqrt{2}|\overline{\gamma_u \xi_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \xi_g}|}{2} \\
\Psi_{47}(e_u t_{2g}, {}^3T_{1u}, M=-1, \mu_u) &= -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u \phi_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_u \phi_g}|}{2} \\
\Psi_{48}(e_u t_{2g}, {}^3T_{1u}, M=-1, \nu_u) &= \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_u \chi_g}|}{2} \\
\Psi_{49}(e_u t_{2g}, {}^3T_{1u}, M=0, \eta_u) &= -\frac{|\overline{\gamma_u \xi_g}|}{2} + \frac{|\overline{\zeta_u \xi_g}|}{2} - \frac{|\overline{\gamma_u \bar{\xi}_g}|}{2} + \frac{|\overline{\zeta_u \bar{\xi}_g}|}{2} \\
\Psi_{50}(e_u t_{2g}, {}^3T_{1u}, M=0, \mu_u) &= -\frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \phi_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \phi_g}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \bar{\phi}_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \bar{\phi}_g}|}{2} \\
\Psi_{51}(e_u t_{2g}, {}^3T_{1u}, M=0, \nu_u) &= \frac{\sqrt[3]{-1}|\overline{\gamma_u \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \chi_g}|}{2} + \frac{\sqrt[3]{-1}|\overline{\gamma_u \bar{\chi}_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \bar{\chi}_g}|}{2} \\
\Psi_{52}(e_u t_{2g}, {}^3T_{1u}, M=1, \eta_u) &= -\frac{\sqrt{2}|\overline{\gamma_u \xi_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \xi_g}|}{2} \\
\Psi_{53}(e_u t_{2g}, {}^3T_{1u}, M=1, \mu_u) &= -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u \phi_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_u \phi_g}|}{2} \\
\Psi_{54}(e_u t_{2g}, {}^3T_{1u}, M=1, \nu_u) &= \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_u \chi_g}|}{2} \\
&\quad e_g t_{1u} \\
&\quad \boxed{\Delta E = \langle \zeta_g \nu_u || \zeta_g \nu_u \rangle} \\
\Psi_{55}(e_g t_{1u}, {}^3T_{1u}, M=-1, \eta_u) &= \frac{\sqrt{2}|\overline{\gamma_g \eta_u}|}{2} + \frac{\sqrt{2}|\overline{\zeta_g \eta_u}|}{2} \\
\Psi_{56}(e_g t_{1u}, {}^3T_{1u}, M=-1, \mu_u) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_g \mu_u}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_g \mu_u}|}{2} \\
\Psi_{57}(e_g t_{1u}, {}^3T_{1u}, M=-1, \nu_u) &= -\frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_g \nu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_g \nu_u}|}{2} \\
\Psi_{58}(e_g t_{1u}, {}^3T_{1u}, M=0, \eta_u) &= \frac{|\overline{\gamma_g \eta_u}|}{2} + \frac{|\overline{\zeta_g \eta_u}|}{2} + \frac{|\overline{\gamma_g \bar{\eta}_u}|}{2} + \frac{|\overline{\zeta_g \bar{\eta}_u}|}{2} \\
\Psi_{59}(e_g t_{1u}, {}^3T_{1u}, M=0, \mu_u) &= \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \mu_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \mu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \bar{\mu}_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \bar{\mu}_u}|}{2} \\
\Psi_{60}(e_g t_{1u}, {}^3T_{1u}, M=0, \nu_u) &= -\frac{\sqrt[3]{-1}|\overline{\gamma_g \nu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g \nu_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\gamma_g \bar{\nu}_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g \bar{\nu}_u}|}{2} \\
\Psi_{61}(e_g t_{1u}, {}^3T_{1u}, M=1, \eta_u) &= \frac{\sqrt{2}|\overline{\gamma_g \eta_u}|}{2} + \frac{\sqrt{2}|\overline{\zeta_g \eta_u}|}{2} \\
\Psi_{62}(e_g t_{1u}, {}^3T_{1u}, M=1, \mu_u) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_g \mu_u}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_g \mu_u}|}{2}
\end{aligned}$$

$$\Psi_{63}(e_g t_{1u}, {}^3T_{1u}, M=1, \nu_u) = -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma_g \nu_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_g \nu_u|}{2}$$

$$e_g t_{2u}$$

$$\Delta E = \langle \zeta_g \xi_u || \zeta_g \xi_u \rangle$$

$$\Psi_{64}(e_g t_{2u}, {}^3T_{1u}, M=-1, \eta_u) = -\frac{\sqrt{2}|\gamma_g \xi_u|}{2} + \frac{\sqrt{2}|\zeta_g \xi_u|}{2}$$

$$\Psi_{65}(e_g t_{2u}, {}^3T_{1u}, M=-1, \mu_u) = -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_g \phi_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_g \phi_u|}{2}$$

$$\Psi_{66}(e_g t_{2u}, {}^3T_{1u}, M=-1, \nu_u) = \frac{\sqrt[3]{-1}\sqrt{2}|\gamma_g \chi_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_g \chi_u|}{2}$$

$$\Psi_{67}(e_g t_{2u}, {}^3T_{1u}, M=0, \eta_u) = -\frac{|\gamma_g \xi_u|}{2} + \frac{|\zeta_g \xi_u|}{2} - \frac{|\gamma_g \bar{\xi}_u|}{2} + \frac{|\zeta_g \bar{\xi}_u|}{2}$$

$$\Psi_{68}(e_g t_{2u}, {}^3T_{1u}, M=0, \mu_u) = -\frac{(-1)^{\frac{2}{3}}|\gamma_g \phi_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_g \phi_u|}{2} - \frac{(-1)^{\frac{2}{3}}|\gamma_g \bar{\phi}_u|}{2} - \frac{\sqrt[3]{-1}|\zeta_g \bar{\phi}_u|}{2}$$

$$\Psi_{69}(e_g t_{2u}, {}^3T_{1u}, M=0, \nu_u) = \frac{\sqrt[3]{-1}|\gamma_g \chi_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_g \chi_u|}{2} + \frac{\sqrt[3]{-1}|\gamma_g \bar{\chi}_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_g \bar{\chi}_u|}{2}$$

$$\Psi_{70}(e_g t_{2u}, {}^3T_{1u}, M=1, \eta_u) = -\frac{\sqrt{2}|\gamma_g \xi_u|}{2} + \frac{\sqrt{2}|\zeta_g \xi_u|}{2}$$

$$\Psi_{71}(e_g t_{2u}, {}^3T_{1u}, M=1, \mu_u) = -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_g \phi_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_g \phi_u|}{2}$$

$$\Psi_{72}(e_g t_{2u}, {}^3T_{1u}, M=1, \nu_u) = \frac{\sqrt[3]{-1}\sqrt{2}|\gamma_g \chi_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_g \chi_u|}{2}$$

$$t_{1g} t_{1u}$$

$$\Delta E = \langle \nu_g \mu_u || \nu_g \mu_u \rangle - \langle \nu_g \nu_g || \mu_u \mu_u \rangle - \langle \nu_g \nu_u || \nu_g \nu_u \rangle + \langle \nu_g \mu_g || \nu_u \mu_u \rangle$$

$$\Psi_{73}(t_{1g} t_{1u}, {}^3T_{1u}, M=-1, \nu_u) = -\frac{\sqrt{2}|\eta_g \mu_u|}{2} + \frac{\sqrt{2}|\mu_g \eta_u|}{2}$$

$$\Psi_{74}(t_{1g} t_{1u}, {}^3T_{1u}, M=-1, \mu_u) = \frac{\sqrt{2}|\eta_g \nu_u|}{2} - \frac{\sqrt{2}|\nu_g \eta_u|}{2}$$

$$\Psi_{75}(t_{1g} t_{1u}, {}^3T_{1u}, M=-1, \eta_u) = -\frac{\sqrt{2}|\mu_g \nu_u|}{2} + \frac{\sqrt{2}|\nu_g \mu_u|}{2}$$

$$-\frac{|\eta_g \mu_u|}{2} + \frac{|\mu_g \eta_u|}{2} - \frac{|\eta_g \nu_u|}{2} + \frac{|\mu_g \bar{\nu}_u|}{2}$$

$$\Psi_{76}(t_{1g} t_{1u}, {}^3T_{1u}, M=0, \nu_u) = \frac{|\eta_g \nu_u|}{2} - \frac{|\nu_g \eta_u|}{2} + \frac{|\eta_g \bar{\nu}_u|}{2} - \frac{|\nu_g \bar{\eta}_u|}{2}$$

$$\Psi_{77}(t_{1g} t_{1u}, {}^3T_{1u}, M=0, \mu_u) = -\frac{|\eta_g \nu_u|}{2} - \frac{|\nu_g \eta_u|}{2} + \frac{|\eta_g \bar{\nu}_u|}{2} - \frac{|\nu_g \bar{\eta}_u|}{2}$$

$$\Psi_{78}(t_{1g} t_{1u}, {}^3T_{1u}, M=0, \eta_u) = -\frac{|\mu_g \nu_u|}{2} + \frac{|\nu_g \mu_u|}{2} - \frac{|\mu_g \bar{\nu}_u|}{2} + \frac{|\nu_g \bar{\mu}_u|}{2}$$

$$\Psi_{79}(t_{1g} t_{1u}, {}^3T_{1u}, M=1, \nu_u) = -\frac{\sqrt{2}|\eta_g \mu_u|}{2} + \frac{\sqrt{2}|\mu_g \eta_u|}{2}$$

$$\Psi_{80}(t_{1g} t_{1u}, {}^3T_{1u}, M=1, \mu_u) = \frac{\sqrt{2}|\eta_g \nu_u|}{2} - \frac{\sqrt{2}|\nu_g \eta_u|}{2}$$

$$\Psi_{81}(t_{1g} t_{1u}, {}^3T_{1u}, M=1, \eta_u) = -\frac{\sqrt{2}|\mu_g \nu_u|}{2} + \frac{\sqrt{2}|\nu_g \mu_u|}{2}$$

$$t_{1g} t_{2u}$$

$$\Delta E = \langle \nu_g \chi_u || \nu_g \chi_u \rangle - \langle \nu_g \nu_g || \xi_u \xi_u \rangle + \langle \nu_g \xi_u || \nu_g \xi_u \rangle - \langle \nu_g \mu_g || \chi_u \phi_u \rangle$$

$$\Psi_{82}(t_{1g} t_{2u}, {}^3T_{1u}, M=-1, \nu_u) = \frac{\sqrt{2}|\eta_g \phi_u|}{2} + \frac{\sqrt{2}|\mu_g \bar{\xi}_u|}{2}$$

$$\Psi_{83}(t_{1g} t_{2u}, {}^3T_{1u}, M=-1, \mu_u) = \frac{\sqrt{2}|\eta_g \chi_u|}{2} + \frac{\sqrt{2}|\nu_g \bar{\xi}_u|}{2}$$

$$\Psi_{84}(t_{1g} t_{2u}, {}^3T_{1u}, M=-1, \eta_u) = \frac{\sqrt{2}|\mu_g \chi_u|}{2} + \frac{\sqrt{2}|\nu_g \phi_u|}{2}$$

$$\Psi_{85}(t_{1g} t_{2u}, {}^3T_{1u}, M=0, \nu_u) = \frac{|\eta_g \phi_u|}{2} + \frac{|\mu_g \xi_u|}{2} + \frac{|\eta_g \bar{\phi}_u|}{2} + \frac{|\mu_g \bar{\xi}_u|}{2}$$

$$\Psi_{86}(t_{1g} t_{2u}, {}^3T_{1u}, M=0, \mu_u) = \frac{|\eta_g \chi_u|}{2} + \frac{|\nu_g \xi_u|}{2} + \frac{|\eta_g \bar{\chi}_u|}{2} + \frac{|\nu_g \bar{\xi}_u|}{2}$$

$$\Psi_{87}(t_{1g} t_{2u}, {}^3T_{1u}, M=0, \eta_u) = \frac{|\mu_g \chi_u|}{2} + \frac{|\nu_g \phi_u|}{2} + \frac{|\mu_g \bar{\chi}_u|}{2} + \frac{|\nu_g \bar{\phi}_u|}{2}$$

$$\Psi_{88}(t_{1g} t_{2u}, {}^3T_{1u}, M=1, \nu_u) = \frac{\sqrt{2}|\eta_g \phi_u|}{2} + \frac{\sqrt{2}|\mu_g \xi_u|}{2}$$

$$\Psi_{89}(t_{1g} t_{2u}, {}^3T_{1u}, M=1, \mu_u) = \frac{\sqrt{2}|\eta_g \chi_u|}{2} + \frac{\sqrt{2}|\nu_g \xi_u|}{2}$$

$$\Psi_{90}(t_{1g} t_{2u}, {}^3T_{1u}, M=1, \eta_u) = \frac{\sqrt{2}|\mu_g \chi_u|}{2} + \frac{\sqrt{2}|\nu_g \phi_u|}{2}$$

$$t_{1u} t_{2g}$$

$$\Delta E = \langle \xi_g \eta_u || \xi_g \eta_u \rangle + \langle \xi_g \nu_u || \xi_g \nu_u \rangle - \langle \xi_g \xi_g || \nu_u \nu_u \rangle - \langle \xi_g \phi_g || \eta_u \mu_u \rangle$$

$$\Psi_{91}(t_{1u} t_{2g}, {}^3T_{1u}, M=-1, \nu_u) = \frac{\sqrt{2}|\phi_g \bar{\eta}_u|}{2} + \frac{\sqrt{2}|\bar{\xi}_g \mu_u|}{2}$$

$$\Psi_{92}(t_{1u} t_{2g}, {}^3T_{1u}, M=-1, \mu_u) = \frac{\sqrt{2}|\bar{\chi}_g \eta_u|}{2} + \frac{\sqrt{2}|\bar{\xi}_g \nu_u|}{2}$$

$$\Psi_{93}(t_{1u} t_{2g}, {}^3T_{1u}, M=-1, \eta_u) = \frac{\sqrt{2}|\bar{\chi}_g \mu_u|}{2} + \frac{\sqrt{2}|\phi_g \bar{\nu}_u|}{2}$$

$$\Psi_{94}(t_{1u} t_{2g}, {}^3T_{1u}, M=0, \nu_u) = \frac{|\phi_g \eta_u|}{2} + \frac{|\bar{\xi}_g \mu_u|}{2} + \frac{|\phi_g \bar{\eta}_u|}{2} + \frac{|\xi_g \bar{\mu}_u|}{2}$$

$$\Psi_{95}(t_{1u} t_{2g}, {}^3T_{1u}, M=0, \mu_u) = \frac{|\bar{\chi}_g \eta_u|}{2} + \frac{|\bar{\xi}_g \nu_u|}{2} + \frac{|\chi_g \bar{\eta}_u|}{2} + \frac{|\xi_g \bar{\nu}_u|}{2}$$

$$\Psi_{96}(t_{1u} t_{2g}, {}^3T_{1u}, M=0, \eta_u) = \frac{|\bar{\chi}_g \mu_u|}{2} + \frac{|\phi_g \nu_u|}{2} + \frac{|\chi_g \bar{\mu}_u|}{2} + \frac{|\phi_g \bar{\nu}_u|}{2}$$

$$\Psi_{97}(t_{1u} t_{2g}, {}^3T_{1u}, M=1, \nu_u) = \frac{\sqrt{2}|\phi_g \eta_u|}{2} + \frac{\sqrt{2}|\xi_g \mu_u|}{2}$$

$$\Psi_{98}(t_{1u} t_{2g}, {}^3T_{1u}, M=1, \mu_u) = \frac{\sqrt{2}|\chi_g \eta_u|}{2} + \frac{\sqrt{2}|\xi_g \nu_u|}{2}$$

$$\Psi_{99}(t_{1u} t_{2g}, {}^3T_{1u}, M=1, \eta_u) = \frac{\sqrt{2}|\chi_g \mu_u|}{2} + \frac{\sqrt{2}|\phi_g \nu_u|}{2}$$

$$t_{2g} t_{2u}$$

$$\Delta E = \langle \xi_g \phi_u || \xi_g \phi_u \rangle - \langle \xi_g \xi_g || \phi_u \phi_u \rangle - \langle \xi_g \xi_u || \xi_g \xi_u \rangle + \langle \xi_g \phi_g || \xi_u \phi_u \rangle$$

$$\Psi_{100}(t_{2g} t_{2u}, {}^3T_{1u}, M=-1, \nu_u) = \frac{\sqrt{2}|\phi_g \xi_u|}{2} - \frac{\sqrt{2}|\bar{\xi}_g \phi_u|}{2}$$

$$\begin{aligned}\Psi_{101}(t_{2g}t_{2u}, {}^3T_{1u}, M=-1, \mu_u) &= -\frac{\sqrt{2}|\overline{\chi_g\xi_u}|}{2} + \frac{\sqrt{2}|\overline{\xi_g\chi_u}|}{2} \\ \Psi_{102}(t_{2g}t_{2u}, {}^3T_{1u}, M=-1, \eta_u) &= \frac{\sqrt{2}|\overline{\chi_g\phi_u}|}{2} - \frac{\sqrt{2}|\overline{\phi_g\chi_u}|}{2} \\ \Psi_{103}(t_{2g}t_{2u}, {}^3T_{1u}, M=0, \nu_u) &= \frac{|\overline{\phi_g\xi_u}|}{2} - \frac{|\overline{\xi_g\phi_u}|}{2} + \frac{|\overline{\phi_g\xi_u}|}{2} - \frac{|\overline{\xi_g\phi_u}|}{2} \\ \Psi_{104}(t_{2g}t_{2u}, {}^3T_{1u}, M=0, \mu_u) &= -\frac{|\overline{\chi_g\xi_u}|}{2} + \frac{|\overline{\xi_g\chi_u}|}{2} - \frac{|\overline{\chi_g\xi_u}|}{2} + \frac{|\overline{\xi_g\chi_u}|}{2} \\ \Psi_{105}(t_{2g}t_{2u}, {}^3T_{1u}, M=0, \eta_u) &= \frac{|\overline{\chi_g\phi_u}|}{2} - \frac{|\overline{\phi_g\chi_u}|}{2} + \frac{|\overline{\chi_g\phi_u}|}{2} - \frac{|\overline{\phi_g\chi_u}|}{2} \\ \Psi_{106}(t_{2g}t_{2u}, {}^3T_{1u}, M=1, \nu_u) &= \frac{\sqrt{2}|\overline{\phi_g\xi_u}|}{2} - \frac{\sqrt{2}|\overline{\xi_g\phi_u}|}{2} \\ \Psi_{107}(t_{2g}t_{2u}, {}^3T_{1u}, M=1, \mu_u) &= -\frac{\sqrt{2}|\overline{\chi_g\xi_u}|}{2} + \frac{\sqrt{2}|\overline{\xi_g\chi_u}|}{2} \\ \Psi_{108}(t_{2g}t_{2u}, {}^3T_{1u}, M=1, \eta_u) &= \frac{\sqrt{2}|\overline{\chi_g\phi_u}|}{2} - \frac{\sqrt{2}|\overline{\phi_g\chi_u}|}{2}\end{aligned}$$

2.32.17 ${}^1T_{1u}$ $a_{1g}t_{1u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g | |\nu_u \nu_u \rangle + \langle \alpha_g \nu_u | |\alpha_g \nu_u \rangle}$$

$$\begin{aligned}\Psi_1(a_{1g}t_{1u}, {}^1T_{1u}, M=0, \eta_u) &= -\frac{\sqrt{2}|\overline{\alpha_g\eta_u}|}{2} + \frac{\sqrt{2}|\overline{\alpha_g\eta_u}|}{2} \\ \Psi_2(a_{1g}t_{1u}, {}^1T_{1u}, M=0, \mu_u) &= -\frac{\sqrt{2}|\overline{\alpha_g\mu_u}|}{2} + \frac{\sqrt{2}|\overline{\alpha_g\mu_u}|}{2} \\ \Psi_3(a_{1g}t_{1u}, {}^1T_{1u}, M=0, \nu_u) &= -\frac{\sqrt{2}|\overline{\alpha_g\nu_u}|}{2} + \frac{\sqrt{2}|\overline{\alpha_g\nu_u}|}{2}\end{aligned}$$

 $a_{2u}t_{2g}$

$$\boxed{\Delta E = \langle \beta_u \beta_u | |\xi_g \xi_g \rangle + \langle \beta_u \xi_g | |\beta_u \xi_g \rangle}$$

$$\begin{aligned}\Psi_4(a_{2u}t_{2g}, {}^1T_{1u}, M=0, \eta_u) &= -\frac{\sqrt{2}|\overline{\beta_u\xi_g}|}{2} + \frac{\sqrt{2}|\overline{\beta_u\xi_g}|}{2} \\ \Psi_5(a_{2u}t_{2g}, {}^1T_{1u}, M=0, \mu_u) &= -\frac{\sqrt{2}|\overline{\beta_u\phi_g}|}{2} + \frac{\sqrt{2}|\overline{\beta_u\phi_g}|}{2} \\ \Psi_6(a_{2u}t_{2g}, {}^1T_{1u}, M=0, \nu_u) &= -\frac{\sqrt{2}|\overline{\beta_u\chi_g}|}{2} + \frac{\sqrt{2}|\overline{\beta_u\chi_g}|}{2}\end{aligned}$$

 $a_{1u}t_{1g}$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u | |\nu_g \nu_g \rangle + \langle \alpha_u \nu_g | |\alpha_u \nu_g \rangle}$$

$$\begin{aligned}\Psi_7(a_{1u}t_{1g}, {}^1T_{1u}, M=0, \eta_u) &= -\frac{\sqrt{2}|\overline{\alpha_u\eta_g}|}{2} + \frac{\sqrt{2}|\overline{\alpha_u\eta_g}|}{2} \\ \Psi_8(a_{1u}t_{1g}, {}^1T_{1u}, M=0, \mu_u) &= -\frac{\sqrt{2}|\overline{\alpha_u\mu_g}|}{2} + \frac{\sqrt{2}|\overline{\alpha_u\mu_g}|}{2} \\ \Psi_9(a_{1u}t_{1g}, {}^1T_{1u}, M=0, \nu_u) &= -\frac{\sqrt{2}|\overline{\alpha_u\nu_g}|}{2} + \frac{\sqrt{2}|\overline{\alpha_u\nu_g}|}{2}\end{aligned}$$

 $a_{2g}t_{2u}$

$$\boxed{\Delta E = \langle \beta_g \beta_g | |\xi_u \xi_u \rangle + \langle \beta_g \xi_u | |\beta_g \xi_u \rangle}$$

$$\Psi_{10}(a_{2g}t_{2u}, {}^1T_{1u}, M=0, \eta_u) = -\frac{\sqrt{2}|\overline{\beta_g\xi_u}|}{2} + \frac{\sqrt{2}|\overline{\beta_g\xi_u}|}{2}$$

$$\begin{aligned}\Psi_{11}(a_{2g}t_{2u}, {}^1T_{1u}, M=0, \mu_u) &= -\frac{\sqrt{2}|\overline{\beta_g\phi_u}|}{2} + \frac{\sqrt{2}|\overline{\beta_g\phi_u}|}{2} \\ \Psi_{12}(a_{2g}t_{2u}, {}^1T_{1u}, M=0, \nu_u) &= -\frac{\sqrt{2}|\overline{\beta_g\chi_u}|}{2} + \frac{\sqrt{2}|\overline{\beta_g\chi_u}|}{2}\end{aligned}$$

 $e_u t_{1g}$

$$\boxed{\Delta E = \langle \zeta_u \nu_g | |\zeta_u \nu_g \rangle}$$

$$\begin{aligned}\Psi_{13}(e_u t_{1g}, {}^1T_{1u}, M=0, \eta_u) &= -\frac{|\overline{\gamma_u\eta_g}|}{2} - \frac{|\overline{\zeta_u\eta_g}|}{2} + \frac{|\overline{\gamma_u\eta_g}|}{2} + \frac{|\overline{\zeta_u\eta_g}|}{2} \\ \Psi_{14}(e_u t_{1g}, {}^1T_{1u}, M=0, \mu_u) &= -\frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u\mu_g}|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_u\mu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u\mu_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u\mu_g}|}{2} \\ \Psi_{15}(e_u t_{1g}, {}^1T_{1u}, M=0, \nu_u) &= \frac{\sqrt[3]{-1}|\overline{\gamma_u\nu_g}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u\nu_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\gamma_u\nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u\nu_g}|}{2}\end{aligned}$$

 $e_u t_{2g}$

$$\boxed{\Delta E = \langle \zeta_u \xi_g | |\zeta_u \xi_g \rangle}$$

$$\begin{aligned}\Psi_{16}(e_u t_{2g}, {}^1T_{1u}, M=0, \eta_u) &= \frac{|\overline{\gamma_u\xi_g}|}{2} - \frac{|\overline{\zeta_u\xi_g}|}{2} - \frac{|\overline{\gamma_u\xi_g}|}{2} + \frac{|\overline{\zeta_u\xi_g}|}{2} \\ \Psi_{17}(e_u t_{2g}, {}^1T_{1u}, M=0, \mu_u) &= \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u\phi_g}|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_u\phi_g}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u\phi_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u\phi_g}|}{2} \\ \Psi_{18}(e_u t_{2g}, {}^1T_{1u}, M=0, \nu_u) &= -\frac{\sqrt[3]{-1}|\overline{\gamma_u\chi_g}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u\chi_g}|}{2} + \frac{\sqrt[3]{-1}|\overline{\gamma_u\chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u\chi_g}|}{2}\end{aligned}$$

 $e_g t_{1u}$

$$\boxed{\Delta E = \langle \zeta_g \nu_u | |\zeta_g \nu_u \rangle}$$

$$\begin{aligned}\Psi_{19}(e_g t_{1u}, {}^1T_{1u}, M=0, \eta_u) &= -\frac{|\overline{\gamma_g\eta_u}|}{2} - \frac{|\overline{\zeta_g\eta_u}|}{2} + \frac{|\overline{\gamma_g\eta_u}|}{2} + \frac{|\overline{\zeta_g\eta_u}|}{2} \\ \Psi_{20}(e_g t_{1u}, {}^1T_{1u}, M=0, \mu_u) &= -\frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g\mu_u}|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_g\mu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g\mu_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g\mu_u}|}{2} \\ \Psi_{21}(e_g t_{1u}, {}^1T_{1u}, M=0, \nu_u) &= \frac{\sqrt[3]{-1}|\overline{\gamma_g\nu_u}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g\nu_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\gamma_g\nu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g\nu_u}|}{2}\end{aligned}$$

 $e_g t_{2u}$

$$\boxed{\Delta E = \langle \zeta_g \xi_u | |\zeta_g \xi_u \rangle}$$

$$\begin{aligned}\Psi_{22}(e_g t_{2u}, {}^1T_{1u}, M=0, \eta_u) &= \frac{|\overline{\gamma_g\xi_u}|}{2} - \frac{|\overline{\zeta_g\xi_u}|}{2} - \frac{|\overline{\gamma_g\xi_u}|}{2} + \frac{|\overline{\zeta_g\xi_u}|}{2} \\ \Psi_{23}(e_g t_{2u}, {}^1T_{1u}, M=0, \mu_u) &= \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g\phi_u}|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_g\phi_u}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g\phi_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g\phi_u}|}{2} \\ \Psi_{24}(e_g t_{2u}, {}^1T_{1u}, M=0, \nu_u) &= -\frac{\sqrt[3]{-1}|\overline{\gamma_g\chi_u}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g\chi_u}|}{2} + \frac{\sqrt[3]{-1}|\overline{\gamma_g\chi_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g\chi_u}|}{2}\end{aligned}$$

 $t_{1g} t_{1u}$

$$\Delta E = \langle \nu_g \mu_u | \nu_g \mu_u \rangle + \langle \nu_g \nu_g | \mu_u \mu_u \rangle - \langle \nu_g \nu_u | \nu_g \nu_u \rangle - \langle \nu_g \mu_g | \nu_u \mu_u \rangle$$

$$\begin{aligned}\Psi_{25}(t_{1g} t_{1u}, {}^1T_{1u}, M=0, \nu_u) &= \\ \frac{|\eta_g \mu_u|}{2} - \frac{|\mu_g \eta_u|}{2} - \frac{|\eta_g \mu_u|}{2} + \frac{|\mu_g \eta_u|}{2} \\ \Psi_{26}(t_{1g} t_{1u}, {}^1T_{1u}, M=0, \mu_u) &= \\ -\frac{|\eta_g \nu_u|}{2} + \frac{|\nu_g \eta_u|}{2} + \frac{|\eta_g \nu_u|}{2} - \frac{|\nu_g \eta_u|}{2} \\ \Psi_{27}(t_{1g} t_{1u}, {}^1T_{1u}, M=0, \eta_u) &= \\ \frac{|\mu_g \nu_u|}{2} - \frac{|\nu_g \mu_u|}{2} - \frac{|\mu_g \nu_u|}{2} + \frac{|\nu_g \mu_u|}{2}\end{aligned}$$

t_{1g}t_{2u}

$$\Delta E = \langle \nu_g \chi_u | \nu_g \chi_u \rangle + \langle \nu_g \nu_g | \xi_u \xi_u \rangle + \langle \nu_g \xi_u | \nu_g \xi_u \rangle + \langle \nu_g \mu_g | \chi_u \phi_u \rangle$$

$$\begin{aligned}\Psi_{28}(t_{1g} t_{2u}, {}^1T_{1u}, M=0, \nu_u) &= \\ -\frac{|\eta_g \phi_u|}{2} - \frac{|\mu_g \xi_u|}{2} + \frac{|\eta_g \phi_u|}{2} + \frac{|\mu_g \xi_u|}{2} \\ \Psi_{29}(t_{1g} t_{2u}, {}^1T_{1u}, M=0, \mu_u) &= \\ -\frac{|\eta_g \chi_u|}{2} - \frac{|\nu_g \xi_u|}{2} + \frac{|\eta_g \chi_u|}{2} + \frac{|\nu_g \xi_u|}{2} \\ \Psi_{30}(t_{1g} t_{2u}, {}^1T_{1u}, M=0, \eta_u) &= \\ -\frac{|\mu_g \chi_u|}{2} - \frac{|\nu_g \phi_u|}{2} + \frac{|\mu_g \chi_u|}{2} + \frac{|\nu_g \phi_u|}{2}\end{aligned}$$

t_{1u}t_{2g}

$$\Delta E = \langle \xi_g \eta_u | \xi_g \eta_u \rangle + \langle \xi_g \nu_u | \xi_g \nu_u \rangle + \langle \xi_g \xi_g | \nu_u \nu_u \rangle + \langle \xi_g \phi_g | \eta_u \mu_u \rangle$$

$$\begin{aligned}\Psi_{31}(t_{1u} t_{2g}, {}^1T_{1u}, M=0, \nu_u) &= \\ -\frac{|\phi_g \eta_u|}{2} - \frac{|\xi_g \mu_u|}{2} + \frac{|\phi_g \eta_u|}{2} + \frac{|\xi_g \mu_u|}{2} \\ \Psi_{32}(t_{1u} t_{2g}, {}^1T_{1u}, M=0, \mu_u) &= \\ -\frac{|\chi_g \eta_u|}{2} - \frac{|\xi_g \nu_u|}{2} + \frac{|\chi_g \eta_u|}{2} + \frac{|\xi_g \nu_u|}{2} \\ \Psi_{33}(t_{1u} t_{2g}, {}^1T_{1u}, M=0, \eta_u) &= \\ -\frac{|\chi_g \mu_u|}{2} - \frac{|\phi_g \nu_u|}{2} + \frac{|\chi_g \mu_u|}{2} + \frac{|\phi_g \nu_u|}{2}\end{aligned}$$

t_{2g}t_{2u}

$$\Delta E = \langle \xi_g \phi_u | \xi_g \phi_u \rangle + \langle \xi_g \xi_g | \phi_u \phi_u \rangle - \langle \xi_g \xi_u | \xi_g \xi_u \rangle - \langle \xi_g \phi_g | \xi_u \phi_u \rangle$$

$$\begin{aligned}\Psi_{34}(t_{2g} t_{2u}, {}^1T_{1u}, M=0, \nu_u) &= \\ -\frac{|\phi_g \xi_u|}{2} + \frac{|\xi_g \phi_u|}{2} + \frac{|\phi_g \xi_u|}{2} - \frac{|\xi_g \phi_u|}{2} \\ \Psi_{35}(t_{2g} t_{2u}, {}^1T_{1u}, M=0, \mu_u) &= \\ \frac{|\chi_g \xi_u|}{2} - \frac{|\xi_g \chi_u|}{2} - \frac{|\chi_g \xi_u|}{2} + \frac{|\xi_g \chi_u|}{2} \\ \Psi_{36}(t_{2g} t_{2u}, {}^1T_{1u}, M=0, \eta_u) &= \\ -\frac{|\chi_g \phi_u|}{2} + \frac{|\phi_g \chi_u|}{2} + \frac{|\chi_g \phi_u|}{2} - \frac{|\phi_g \chi_u|}{2}\end{aligned}$$

2.32.18 ${}^3T_{2u}$ ***a_{1g}t_{2u}***

$$\Delta E = -\langle \alpha_g \alpha_g | \xi_u \xi_u \rangle + \langle \alpha_g \xi_u | \alpha_g \xi_u \rangle$$

$$\Psi_1(a_{1g} t_{2u}, {}^3T_{2u}, M=-1, \xi_u) = |\overline{\alpha_g \xi_u}|$$

$$\Psi_2(a_{1g} t_{2u}, {}^3T_{2u}, M=-1, \phi_u) = |\overline{\alpha_g \phi_u}|$$

$$\Psi_3(a_{1g} t_{2u}, {}^3T_{2u}, M=-1, \chi_u) = |\overline{\alpha_g \chi_u}|$$

$$\Psi_4(a_{1g} t_{2u}, {}^3T_{2u}, M=0, \xi_u) = \frac{\sqrt{2} |\overline{\alpha_g \xi_u}|}{2} + \frac{\sqrt{2} |\alpha_g \overline{\xi_u}|}{2}$$

$$\Psi_5(a_{1g} t_{2u}, {}^3T_{2u}, M=0, \phi_u) = \frac{\sqrt{2} |\overline{\alpha_g \phi_u}|}{2} + \frac{\sqrt{2} |\alpha_g \overline{\phi_u}|}{2}$$

$$\Psi_6(a_{1g} t_{2u}, {}^3T_{2u}, M=0, \chi_u) = \frac{\sqrt{2} |\overline{\alpha_g \chi_u}|}{2} + \frac{\sqrt{2} |\alpha_g \overline{\chi_u}|}{2}$$

$$\Psi_7(a_{1g} t_{2u}, {}^3T_{2u}, M=1, \xi_u) = |\alpha_g \xi_u|$$

$$\Psi_8(a_{1g} t_{2u}, {}^3T_{2u}, M=1, \phi_u) = |\alpha_g \phi_u|$$

$$\Psi_9(a_{1g} t_{2u}, {}^3T_{2u}, M=1, \chi_u) = |\alpha_g \chi_u|$$

a_{2u}t_{1g}

$$\Delta E = -\langle \beta_u \beta_u | \nu_g \nu_g \rangle + \langle \beta_u \nu_g | \beta_u \nu_g \rangle$$

$$\Psi_{10}(a_{2u} t_{1g}, {}^3T_{2u}, M=-1, \xi_u) = |\overline{\beta_u \eta_g}|$$

$$\Psi_{11}(a_{2u} t_{1g}, {}^3T_{2u}, M=-1, \phi_u) = |\overline{\beta_u \mu_g}|$$

$$\Psi_{12}(a_{2u} t_{1g}, {}^3T_{2u}, M=-1, \chi_u) = |\overline{\beta_u \nu_g}|$$

$$\Psi_{13}(a_{2u} t_{1g}, {}^3T_{2u}, M=0, \xi_u) = \frac{\sqrt{2} |\overline{\beta_u \eta_g}|}{2} + \frac{\sqrt{2} |\beta_u \overline{\eta_g}|}{2}$$

$$\Psi_{14}(a_{2u} t_{1g}, {}^3T_{2u}, M=0, \phi_u) = \frac{\sqrt{2} |\overline{\beta_u \mu_g}|}{2} + \frac{\sqrt{2} |\beta_u \overline{\mu_g}|}{2}$$

$$\Psi_{15}(a_{2u} t_{1g}, {}^3T_{2u}, M=0, \chi_u) = \frac{\sqrt{2} |\overline{\beta_u \nu_g}|}{2} + \frac{\sqrt{2} |\beta_u \overline{\nu_g}|}{2}$$

$$\Psi_{16}(a_{2u} t_{1g}, {}^3T_{2u}, M=1, \xi_u) = |\beta_u \eta_g|$$

$$\Psi_{17}(a_{2u} t_{1g}, {}^3T_{2u}, M=1, \phi_u) = |\beta_u \mu_g|$$

$$\Psi_{18}(a_{2u} t_{1g}, {}^3T_{2u}, M=1, \chi_u) = |\beta_u \nu_g|$$

a_{1u}t_{2g}

$$\Delta E = -\langle \alpha_u \alpha_u | \xi_g \xi_g \rangle + \langle \alpha_u \xi_g | \alpha_u \xi_g \rangle$$

$$\Psi_{19}(a_{1u} t_{2g}, {}^3T_{2u}, M=-1, \xi_u) = |\overline{\alpha_u \xi_g}|$$

$$\Psi_{20}(a_{1u} t_{2g}, {}^3T_{2u}, M=-1, \phi_u) = |\overline{\alpha_u \phi_g}|$$

$$\Psi_{21}(a_{1u} t_{2g}, {}^3T_{2u}, M=-1, \chi_u) = |\overline{\alpha_u \chi_g}|$$

$$\Psi_{22}(a_{1u} t_{2g}, {}^3T_{2u}, M=0, \xi_u) = \frac{\sqrt{2} |\overline{\alpha_u \xi_g}|}{2} + \frac{\sqrt{2} |\alpha_u \overline{\xi_g}|}{2}$$

$$\Psi_{23}(a_{1u} t_{2g}, {}^3T_{2u}, M=0, \phi_u) = \frac{\sqrt{2} |\overline{\alpha_u \phi_g}|}{2} + \frac{\sqrt{2} |\alpha_u \overline{\phi_g}|}{2}$$

$$\Psi_{24}(a_{1u} t_{2g}, {}^3T_{2u}, M=0, \chi_u) = \frac{\sqrt{2} |\overline{\alpha_u \chi_g}|}{2} + \frac{\sqrt{2} |\alpha_u \overline{\chi_g}|}{2}$$

$$\Psi_{25}(a_{1u} t_{2g}, {}^3T_{2u}, M=1, \xi_u) = |\alpha_u \xi_g|$$

$$\Psi_{26}(a_{1u} t_{2g}, {}^3T_{2u}, M=1, \phi_u) = |\alpha_u \phi_g|$$

$$\Psi_{27}(a_{1u} t_{2g}, {}^3T_{2u}, M=1, \chi_u) = |\alpha_u \chi_g|$$

a_{2g}t_{1u}

$$\Delta E = -\langle \beta_g \beta_g | \nu_u \nu_u \rangle + \langle \beta_g \nu_u | \beta_g \nu_u \rangle$$

$$\begin{aligned}
\Psi_{28}(a_{2g}t_{1u}, {}^3T_{2u}, M=-1, \xi_u) &= |\overline{\beta_g \eta_u}| \\
\Psi_{29}(a_{2g}t_{1u}, {}^3T_{2u}, M=-1, \phi_u) &= |\overline{\beta_g \mu_u}| \\
\Psi_{30}(a_{2g}t_{1u}, {}^3T_{2u}, M=-1, \chi_u) &= |\overline{\beta_g \nu_u}| \\
\Psi_{31}(a_{2g}t_{1u}, {}^3T_{2u}, M=0, \xi_u) &= \frac{\sqrt{2}|\overline{\beta_g \eta_u}|}{2} + \frac{\sqrt{2}|\overline{\beta_g \eta_u}|}{2} \\
\Psi_{32}(a_{2g}t_{1u}, {}^3T_{2u}, M=0, \phi_u) &= \frac{\sqrt{2}|\overline{\beta_g \mu_u}|}{2} + \frac{\sqrt{2}|\overline{\beta_g \mu_u}|}{2} \\
\Psi_{33}(a_{2g}t_{1u}, {}^3T_{2u}, M=0, \chi_u) &= \frac{\sqrt{2}|\overline{\beta_g \nu_u}|}{2} + \frac{\sqrt{2}|\overline{\beta_g \nu_u}|}{2} \\
\Psi_{34}(a_{2g}t_{1u}, {}^3T_{2u}, M=1, \xi_u) &= |\beta_g \eta_u| \\
\Psi_{35}(a_{2g}t_{1u}, {}^3T_{2u}, M=1, \phi_u) &= |\beta_g \mu_u| \\
\Psi_{36}(a_{2g}t_{1u}, {}^3T_{2u}, M=1, \chi_u) &= |\beta_g \nu_u|
\end{aligned}$$

 $e_u t_{1g}$

$$\boxed{\Delta E = \langle \zeta_u \nu_g || \zeta_u \nu_g \rangle}$$

$$\begin{aligned}
\Psi_{37}(e_u t_{1g}, {}^3T_{2u}, M=-1, \xi_u) &= -\frac{\sqrt{2}|\overline{\gamma_u \eta_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \eta_g}|}{2} \\
\Psi_{38}(e_u t_{1g}, {}^3T_{2u}, M=-1, \phi_u) &= -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u \mu_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_u \mu_g}|}{2} \\
\Psi_{39}(e_u t_{1g}, {}^3T_{2u}, M=-1, \chi_u) &= \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_u \nu_g}|}{2} \\
\Psi_{40}(e_u t_{1g}, {}^3T_{2u}, M=0, \xi_u) &= -\frac{|\overline{\gamma_u \eta_g}|}{2} + \frac{|\overline{\zeta_u \eta_g}|}{2} - \frac{|\overline{\gamma_u \eta_g}|}{2} + \frac{|\overline{\zeta_u \eta_g}|}{2} \\
\Psi_{41}(e_u t_{1g}, {}^3T_{2u}, M=0, \phi_u) &= -\frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \mu_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \mu_g}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \mu_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \mu_g}|}{2} \\
\Psi_{42}(e_u t_{1g}, {}^3T_{2u}, M=0, \chi_u) &= \frac{\sqrt[3]{-1}|\overline{\gamma_u \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \nu_g}|}{2} + \frac{\sqrt[3]{-1}|\overline{\gamma_u \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \nu_g}|}{2} \\
\Psi_{43}(e_u t_{1g}, {}^3T_{2u}, M=1, \xi_u) &= -\frac{\sqrt{2}|\overline{\gamma_u \eta_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \eta_g}|}{2} \\
\Psi_{44}(e_u t_{1g}, {}^3T_{2u}, M=1, \phi_u) &= -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u \mu_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_u \mu_g}|}{2} \\
\Psi_{45}(e_u t_{1g}, {}^3T_{2u}, M=1, \chi_u) &= \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u \nu_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_u \nu_g}|}{2}
\end{aligned}$$

 $e_u t_{2g}$

$$\boxed{\Delta E = \langle \zeta_u \xi_g || \zeta_u \xi_g \rangle}$$

$$\begin{aligned}
\Psi_{46}(e_u t_{2g}, {}^3T_{2u}, M=-1, \xi_u) &= \frac{\sqrt{2}|\overline{\gamma_u \xi_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \xi_g}|}{2} \\
\Psi_{47}(e_u t_{2g}, {}^3T_{2u}, M=-1, \phi_u) &= \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u \phi_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_u \phi_g}|}{2} \\
\Psi_{48}(e_u t_{2g}, {}^3T_{2u}, M=-1, \chi_u) &= -\frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_u \chi_g}|}{2} \\
\Psi_{49}(e_u t_{2g}, {}^3T_{2u}, M=0, \xi_u) &= \frac{|\overline{\gamma_u \xi_g}|}{2} + \frac{|\overline{\zeta_u \xi_g}|}{2} + \frac{|\overline{\gamma_u \xi_g}|}{2} + \frac{|\overline{\zeta_u \xi_g}|}{2}
\end{aligned}$$

$$\begin{aligned}
\Psi_{50}(e_u t_{2g}, {}^3T_{2u}, M=0, \phi_u) &= \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \phi_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \phi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_u \phi_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_u \phi_g}|}{2} \\
\Psi_{51}(e_u t_{2g}, {}^3T_{2u}, M=0, \chi_u) &= -\frac{\sqrt[3]{-1}|\overline{\gamma_u \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \chi_g}|}{2} - \frac{\sqrt[3]{-1}|\overline{\gamma_u \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_u \chi_g}|}{2}
\end{aligned}$$

$$\Psi_{52}(e_u t_{2g}, {}^3T_{2u}, M=1, \xi_u) = \frac{\sqrt{2}|\overline{\gamma_u \xi_g}|}{2} + \frac{\sqrt{2}|\overline{\zeta_u \xi_g}|}{2}$$

$$\Psi_{53}(e_u t_{2g}, {}^3T_{2u}, M=1, \phi_u) = \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_u \phi_g}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_u \phi_g}|}{2}$$

$$\Psi_{54}(e_u t_{2g}, {}^3T_{2u}, M=1, \chi_u) = -\frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_u \chi_g}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_u \chi_g}|}{2}$$

 $e_g t_{1u}$

$$\boxed{\Delta E = \langle \zeta_g \nu_u || \zeta_g \nu_u \rangle}$$

$$\Psi_{55}(e_g t_{1u}, {}^3T_{2u}, M=-1, \xi_u) = -\frac{\sqrt{2}|\overline{\gamma_g \eta_u}|}{2} + \frac{\sqrt{2}|\overline{\zeta_g \eta_u}|}{2}$$

$$\Psi_{56}(e_g t_{1u}, {}^3T_{2u}, M=-1, \phi_u) = -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_g \mu_u}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_g \mu_u}|}{2}$$

$$\Psi_{57}(e_g t_{1u}, {}^3T_{2u}, M=-1, \chi_u) = \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_g \nu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_g \nu_u}|}{2}$$

$$\Psi_{58}(e_g t_{1u}, {}^3T_{2u}, M=0, \xi_u) = -\frac{|\overline{\gamma_g \eta_u}|}{2} + \frac{|\overline{\zeta_g \eta_u}|}{2} - \frac{|\overline{\gamma_g \eta_u}|}{2} + \frac{|\overline{\zeta_g \eta_u}|}{2}$$

$$\Psi_{59}(e_g t_{1u}, {}^3T_{2u}, M=0, \phi_u) = -\frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \mu_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \mu_u}|}{2} - \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \mu_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \mu_u}|}{2}$$

$$\Psi_{60}(e_g t_{1u}, {}^3T_{2u}, M=0, \chi_u) = \frac{\sqrt[3]{-1}|\overline{\gamma_g \nu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g \nu_u}|}{2} + \frac{\sqrt[3]{-1}|\overline{\gamma_g \nu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\zeta_g \nu_u}|}{2}$$

$$\Psi_{61}(e_g t_{1u}, {}^3T_{2u}, M=1, \xi_u) = -\frac{\sqrt{2}|\overline{\gamma_g \eta_u}|}{2} + \frac{\sqrt{2}|\overline{\zeta_g \eta_u}|}{2}$$

$$\Psi_{62}(e_g t_{1u}, {}^3T_{2u}, M=1, \phi_u) = -\frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_g \mu_u}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_g \mu_u}|}{2}$$

$$\Psi_{63}(e_g t_{1u}, {}^3T_{2u}, M=1, \chi_u) = \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_g \nu_u}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_g \nu_u}|}{2}$$

 $e_g t_{2u}$

$$\boxed{\Delta E = \langle \zeta_g \xi_u || \zeta_g \xi_u \rangle}$$

$$\Psi_{64}(e_g t_{2u}, {}^3T_{2u}, M=-1, \xi_u) = \frac{\sqrt{2}|\overline{\gamma_g \xi_u}|}{2} + \frac{\sqrt{2}|\overline{\zeta_g \xi_u}|}{2}$$

$$\Psi_{65}(e_g t_{2u}, {}^3T_{2u}, M=-1, \phi_u) = \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\gamma_g \phi_u}|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\overline{\zeta_g \phi_u}|}{2}$$

$$\Psi_{66}(e_g t_{2u}, {}^3T_{2u}, M=-1, \chi_u) = -\frac{\sqrt[3]{-1}\sqrt{2}|\overline{\gamma_g \chi_u}|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\overline{\zeta_g \chi_u}|}{2}$$

$$\Psi_{67}(e_g t_{2u}, {}^3T_{2u}, M=0, \xi_u) = \frac{|\overline{\gamma_g \xi_u}|}{2} + \frac{|\overline{\zeta_g \xi_u}|}{2} - \frac{|\overline{\gamma_g \xi_u}|}{2} + \frac{|\overline{\zeta_g \xi_u}|}{2}$$

$$\Psi_{68}(e_g t_{2u}, {}^3T_{2u}, M=0, \phi_u) = \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \phi_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \phi_u}|}{2} + \frac{(-1)^{\frac{2}{3}}|\overline{\gamma_g \phi_u}|}{2} - \frac{\sqrt[3]{-1}|\overline{\zeta_g \phi_u}|}{2}$$

$$\Psi_{69}(e_g t_{2u}, {}^3T_{2u}, M=0, \chi_u) = -\frac{\sqrt[3]{-1}|\gamma_g \chi_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_g \chi_u|}{2} - \frac{\sqrt[3]{-1}|\gamma_g \bar{\chi}_u|}{2} + \frac{(-1)^{\frac{2}{3}}|\zeta_g \bar{\chi}_u|}{2}$$

$$\Psi_{70}(e_g t_{2u}, {}^3T_{2u}, M=1, \xi_u) = \frac{\sqrt{2}|\gamma_g \xi_u|}{2} + \frac{\sqrt{2}|\zeta_g \xi_u|}{2}$$

$$\Psi_{71}(e_g t_{2u}, {}^3T_{2u}, M=1, \phi_u) = \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\gamma_g \phi_u|}{2} - \frac{\sqrt[3]{-1}\sqrt{2}|\zeta_g \phi_u|}{2}$$

$$\Psi_{72}(e_g t_{2u}, {}^3T_{2u}, M=1, \chi_u) = -\frac{\sqrt[3]{-1}\sqrt{2}|\gamma_g \chi_u|}{2} + \frac{(-1)^{\frac{2}{3}}\sqrt{2}|\zeta_g \chi_u|}{2}$$

$t_{1g}t_{1u}$

$$\Delta E = \langle \nu_g \mu_u | \nu_g \mu_u \rangle - \langle \nu_g \nu_g | \mu_u \mu_u \rangle + \langle \nu_g \nu_u | \nu_g \nu_u \rangle - \langle \nu_g \mu_g | \nu_u \mu_u \rangle$$

$$\Psi_{73}(t_{1g}t_{1u}, {}^3T_{2u}, M=-1, \chi_u) = \frac{\sqrt{2}|\eta_g \mu_u|}{2} + \frac{\sqrt{2}|\mu_g \eta_u|}{2}$$

$$\Psi_{74}(t_{1g}t_{1u}, {}^3T_{2u}, M=-1, \phi_u) = \frac{\sqrt{2}|\eta_g \nu_u|}{2} + \frac{\sqrt{2}|\nu_g \eta_u|}{2}$$

$$\Psi_{75}(t_{1g}t_{1u}, {}^3T_{2u}, M=-1, \xi_u) = \frac{\sqrt{2}|\mu_g \nu_u|}{2} + \frac{\sqrt{2}|\nu_g \mu_u|}{2}$$

$$\Psi_{76}(t_{1g}t_{1u}, {}^3T_{2u}, M=0, \chi_u) = \frac{|\eta_g \mu_u|}{2} + \frac{|\mu_g \eta_u|}{2} + \frac{|\eta_g \bar{\mu}_u|}{2} + \frac{|\mu_g \bar{\eta}_u|}{2}$$

$$\Psi_{77}(t_{1g}t_{1u}, {}^3T_{2u}, M=0, \phi_u) = \frac{|\eta_g \nu_u|}{2} + \frac{|\nu_g \eta_u|}{2} + \frac{|\eta_g \bar{\nu}_u|}{2} + \frac{|\nu_g \bar{\eta}_u|}{2}$$

$$\Psi_{78}(t_{1g}t_{1u}, {}^3T_{2u}, M=0, \xi_u) = \frac{|\mu_g \nu_u|}{2} + \frac{|\nu_g \mu_u|}{2} + \frac{|\mu_g \bar{\nu}_u|}{2} + \frac{|\nu_g \bar{\mu}_u|}{2}$$

$$\Psi_{79}(t_{1g}t_{1u}, {}^3T_{2u}, M=1, \chi_u) = \frac{\sqrt{2}|\eta_g \mu_u|}{2} + \frac{\sqrt{2}|\mu_g \eta_u|}{2}$$

$$\Psi_{80}(t_{1g}t_{1u}, {}^3T_{2u}, M=1, \phi_u) = \frac{\sqrt{2}|\eta_g \nu_u|}{2} + \frac{\sqrt{2}|\nu_g \eta_u|}{2}$$

$$\Psi_{81}(t_{1g}t_{1u}, {}^3T_{2u}, M=1, \xi_u) = \frac{\sqrt{2}|\mu_g \nu_u|}{2} + \frac{\sqrt{2}|\nu_g \mu_u|}{2}$$

$t_{1g}t_{2u}$

$$\Delta E = -\langle \nu_g \chi_u | \nu_g \chi_u \rangle - \langle \nu_g \nu_g | \xi_u \xi_u \rangle + \langle \nu_g \xi_u | \nu_g \xi_u \rangle + \langle \nu_g \mu_g | \chi_u \phi_u \rangle$$

$$\Psi_{82}(t_{1g}t_{2u}, {}^3T_{2u}, M=-1, \chi_u) = -\frac{\sqrt{2}|\eta_g \bar{\phi}_u|}{2} + \frac{\sqrt{2}|\mu_g \bar{\xi}_u|}{2}$$

$$\Psi_{83}(t_{1g}t_{2u}, {}^3T_{2u}, M=-1, \phi_u) = \frac{\sqrt{2}|\eta_g \bar{\chi}_u|}{2} - \frac{\sqrt{2}|\nu_g \bar{\xi}_u|}{2}$$

$$\Psi_{84}(t_{1g}t_{2u}, {}^3T_{2u}, M=-1, \xi_u) = -\frac{\sqrt{2}|\mu_g \bar{\chi}_u|}{2} + \frac{\sqrt{2}|\nu_g \bar{\phi}_u|}{2}$$

$$\Psi_{85}(t_{1g}t_{2u}, {}^3T_{2u}, M=0, \chi_u) = -\frac{|\eta_g \bar{\phi}_u|}{2} + \frac{|\mu_g \bar{\xi}_u|}{2} - \frac{|\eta_g \bar{\phi}_u|}{2} + \frac{|\mu_g \bar{\xi}_u|}{2}$$

$$\Psi_{86}(t_{1g}t_{2u}, {}^3T_{2u}, M=0, \phi_u) = \frac{|\eta_g \bar{\chi}_u|}{2} - \frac{|\nu_g \bar{\xi}_u|}{2} + \frac{|\eta_g \bar{\chi}_u|}{2} - \frac{|\nu_g \bar{\xi}_u|}{2}$$

$$\Psi_{87}(t_{1g}t_{2u}, {}^3T_{2u}, M=0, \xi_u) = -\frac{|\mu_g \bar{\chi}_u|}{2} + \frac{|\nu_g \bar{\phi}_u|}{2} - \frac{|\mu_g \bar{\chi}_u|}{2} + \frac{|\nu_g \bar{\phi}_u|}{2}$$

$$\Psi_{88}(t_{1g}t_{2u}, {}^3T_{2u}, M=1, \chi_u) = -\frac{\sqrt{2}|\eta_g \bar{\phi}_u|}{2} + \frac{\sqrt{2}|\mu_g \bar{\xi}_u|}{2}$$

$$\Psi_{89}(t_{1g}t_{2u}, {}^3T_{2u}, M=1, \phi_u) = \frac{\sqrt{2}|\eta_g \bar{\chi}_u|}{2} - \frac{\sqrt{2}|\nu_g \bar{\xi}_u|}{2}$$

$$\Psi_{90}(t_{1g}t_{2u}, {}^3T_{2u}, M=1, \xi_u) = -\frac{\sqrt{2}|\mu_g \chi_u|}{2} + \frac{\sqrt{2}|\nu_g \phi_u|}{2}$$

$t_{1u}t_{2g}$

$$\boxed{\Delta E = -\langle \xi_g \eta_u | \xi_g \eta_u \rangle + \langle \xi_g \nu_u | \xi_g \nu_u \rangle - \langle \xi_g \xi_g | \nu_u \nu_u \rangle + \langle \xi_g \phi_g | \eta_u \mu_u \rangle}$$

$$\Psi_{91}(t_{1u}t_{2g}, {}^3T_{2u}, M=-1, \chi_u) = \frac{\sqrt{2}|\phi_g \bar{\eta}_u|}{2} - \frac{\sqrt{2}|\xi_g \bar{\mu}_u|}{2}$$

$$\Psi_{92}(t_{1u}t_{2g}, {}^3T_{2u}, M=-1, \phi_u) = -\frac{\sqrt{2}|\chi_g \eta_u|}{2} + \frac{\sqrt{2}|\xi_g \nu_u|}{2}$$

$$\Psi_{93}(t_{1u}t_{2g}, {}^3T_{2u}, M=-1, \xi_u) = \frac{\sqrt{2}|\chi_g \mu_u|}{2} - \frac{\sqrt{2}|\phi_g \nu_u|}{2}$$

$$\Psi_{94}(t_{1u}t_{2g}, {}^3T_{2u}, M=0, \chi_u) = \frac{|\phi_g \eta_u|}{2} - \frac{|\xi_g \mu_u|}{2} + \frac{|\phi_g \bar{\eta}_u|}{2} - \frac{|\xi_g \bar{\mu}_u|}{2}$$

$$\Psi_{95}(t_{1u}t_{2g}, {}^3T_{2u}, M=0, \phi_u) = -\frac{|\chi_g \eta_u|}{2} + \frac{|\xi_g \nu_u|}{2} - \frac{|\chi_g \bar{\eta}_u|}{2} + \frac{|\xi_g \bar{\nu}_u|}{2}$$

$$\Psi_{96}(t_{1u}t_{2g}, {}^3T_{2u}, M=0, \xi_u) = \frac{|\chi_g \mu_u|}{2} - \frac{|\phi_g \nu_u|}{2} + \frac{|\chi_g \bar{\mu}_u|}{2} - \frac{|\phi_g \bar{\nu}_u|}{2}$$

$$\Psi_{97}(t_{1u}t_{2g}, {}^3T_{2u}, M=1, \chi_u) = \frac{\sqrt{2}|\phi_g \eta_u|}{2} - \frac{\sqrt{2}|\xi_g \mu_u|}{2}$$

$$\Psi_{98}(t_{1u}t_{2g}, {}^3T_{2u}, M=1, \phi_u) = -\frac{\sqrt{2}|\chi_g \eta_u|}{2} + \frac{\sqrt{2}|\xi_g \nu_u|}{2}$$

$$\Psi_{99}(t_{1u}t_{2g}, {}^3T_{2u}, M=1, \xi_u) = \frac{\sqrt{2}|\chi_g \mu_u|}{2} - \frac{\sqrt{2}|\phi_g \nu_u|}{2}$$

$t_{2g}t_{2u}$

$$\boxed{\Delta E = \langle \xi_g \phi_u | \xi_g \phi_u \rangle - \langle \xi_g \xi_g | \phi_u \phi_u \rangle + \langle \xi_g \xi_u | \xi_g \xi_u \rangle - \langle \xi_g \phi_g | \xi_u \phi_u \rangle}$$

$$\Psi_{100}(t_{2g}t_{2u}, {}^3T_{2u}, M=-1, \chi_u) = \frac{\sqrt{2}|\phi_g \xi_u|}{2} + \frac{\sqrt{2}|\xi_g \phi_u|}{2}$$

$$\Psi_{101}(t_{2g}t_{2u}, {}^3T_{2u}, M=-1, \phi_u) = \frac{\sqrt{2}|\chi_g \bar{\xi}_u|}{2} + \frac{\sqrt{2}|\xi_g \bar{\chi}_u|}{2}$$

$$\Psi_{102}(t_{2g}t_{2u}, {}^3T_{2u}, M=-1, \xi_u) = \frac{\sqrt{2}|\chi_g \bar{\phi}_u|}{2} + \frac{\sqrt{2}|\phi_g \bar{\chi}_u|}{2}$$

$$\Psi_{103}(t_{2g}t_{2u}, {}^3T_{2u}, M=0, \chi_u) = \frac{|\phi_g \xi_u|}{2} + \frac{|\xi_g \phi_u|}{2} + \frac{|\phi_g \bar{\xi}_u|}{2} + \frac{|\xi_g \bar{\phi}_u|}{2}$$

$$\Psi_{104}(t_{2g}t_{2u}, {}^3T_{2u}, M=0, \phi_u) = \frac{|\chi_g \xi_u|}{2} + \frac{|\xi_g \bar{\chi}_u|}{2} + \frac{|\chi_g \bar{\xi}_u|}{2} + \frac{|\xi_g \bar{\phi}_u|}{2}$$

$$\Psi_{105}(t_{2g}t_{2u}, {}^3T_{2u}, M=0, \xi_u) = \frac{|\chi_g \bar{\phi}_u|}{2} + \frac{|\phi_g \bar{\chi}_u|}{2} + \frac{|\chi_g \bar{\phi}_u|}{2} + \frac{|\phi_g \bar{\chi}_u|}{2}$$

$$\Psi_{106}(t_{2g}t_{2u}, {}^3T_{2u}, M=1, \chi_u) = \frac{\sqrt{2}|\phi_g \xi_u|}{2} + \frac{\sqrt{2}|\xi_g \phi_u|}{2}$$

$$\Psi_{107}(t_{2g}t_{2u}, {}^3T_{2u}, M=1, \phi_u) = \frac{\sqrt{2}|\chi_g \xi_u|}{2} + \frac{\sqrt{2}|\xi_g \bar{\chi}_u|}{2}$$

$$\Psi_{108}(t_{2g}t_{2u}, {}^3T_{2u}, M=1, \xi_u) = \frac{\sqrt{2}|\chi_g \bar{\phi}_u|}{2} + \frac{\sqrt{2}|\phi_g \bar{\chi}_u|}{2}$$

2.32.19 $^1T_{2u}$ $a_{1g}t_{2u}$

$$\boxed{\Delta E = \langle \alpha_g \alpha_g || \xi_u \xi_u \rangle + \langle \alpha_g \xi_u || \alpha_g \xi_u \rangle}$$

$$\Psi_1(a_{1g}t_{2u}, ^1T_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\xi_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\xi_u}|}{2}$$

$$\Psi_2(a_{1g}t_{2u}, ^1T_{2u}, M=0, \phi_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\phi_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\phi_u}|}{2}$$

$$\Psi_3(a_{1g}t_{2u}, ^1T_{2u}, M=0, \chi_u) = -\frac{\sqrt{2}|\overline{\alpha_g}\chi_u|}{2} + \frac{\sqrt{2}|\alpha_g\overline{\chi_u}|}{2}$$

 $a_{2u}t_{1g}$

$$\boxed{\Delta E = \langle \beta_u \beta_u || \nu_g \nu_g \rangle + \langle \beta_u \nu_g || \beta_u \nu_g \rangle}$$

$$\Psi_4(a_{2u}t_{1g}, ^1T_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\beta_u}\eta_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\eta_g}|}{2}$$

$$\Psi_5(a_{2u}t_{1g}, ^1T_{2u}, M=0, \phi_u) = -\frac{\sqrt{2}|\overline{\beta_u}\mu_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\mu_g}|}{2}$$

$$\Psi_6(a_{2u}t_{1g}, ^1T_{2u}, M=0, \chi_u) = -\frac{\sqrt{2}|\overline{\beta_u}\nu_g|}{2} + \frac{\sqrt{2}|\beta_u\overline{\nu_g}|}{2}$$

 $a_{1u}t_{2g}$

$$\boxed{\Delta E = \langle \alpha_u \alpha_u || \xi_g \xi_g \rangle + \langle \alpha_u \xi_g || \alpha_u \xi_g \rangle}$$

$$\Psi_7(a_{1u}t_{2g}, ^1T_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\xi_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\xi_g}|}{2}$$

$$\Psi_8(a_{1u}t_{2g}, ^1T_{2u}, M=0, \phi_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\phi_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\phi_g}|}{2}$$

$$\Psi_9(a_{1u}t_{2g}, ^1T_{2u}, M=0, \chi_u) = -\frac{\sqrt{2}|\overline{\alpha_u}\chi_g|}{2} + \frac{\sqrt{2}|\alpha_u\overline{\chi_g}|}{2}$$

 $a_{2g}t_{1u}$

$$\boxed{\Delta E = \langle \beta_g \beta_g || \nu_u \nu_u \rangle + \langle \beta_g \nu_u || \beta_g \nu_u \rangle}$$

$$\Psi_{10}(a_{2g}t_{1u}, ^1T_{2u}, M=0, \xi_u) = -\frac{\sqrt{2}|\overline{\beta_g}\eta_u|}{2} + \frac{\sqrt{2}|\beta_g\overline{\eta_u}|}{2}$$

$$\Psi_{11}(a_{2g}t_{1u}, ^1T_{2u}, M=0, \phi_u) = -\frac{\sqrt{2}|\overline{\beta_g}\mu_u|}{2} + \frac{\sqrt{2}|\beta_g\overline{\mu_u}|}{2}$$

$$\Psi_{12}(a_{2g}t_{1u}, ^1T_{2u}, M=0, \chi_u) = -\frac{\sqrt{2}|\overline{\beta_g}\nu_u|}{2} + \frac{\sqrt{2}|\beta_g\overline{\nu_u}|}{2}$$

 $e_u t_{1g}$

$$\boxed{\Delta E = \langle \zeta_u \nu_g || \zeta_u \nu_g \rangle}$$

$$\Psi_{13}(e_u t_{1g}, ^1T_{2u}, M=0, \xi_u) = \frac{|\overline{\gamma_u}\eta_g|}{2} - \frac{|\overline{\zeta_u}\eta_g|}{2} - \frac{|\gamma_u\overline{\eta_g}|}{2} + \frac{|\zeta_u\overline{\eta_g}|}{2}$$

$$\Psi_{14}(e_u t_{1g}, ^1T_{2u}, M=0, \phi_u) = \frac{(-1)^{\frac{3}{2}}|\overline{\gamma_u}\mu_g|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_u}\mu_g|}{2} - \frac{(-1)^{\frac{3}{2}}|\gamma_u\overline{\mu_g}|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\overline{\mu_g}|}{2}$$

$$\Psi_{15}(e_u t_{1g}, ^1T_{2u}, M=0, \chi_u) = -\frac{\sqrt[3]{-1}|\overline{\gamma_u}\nu_g|}{2} - \frac{(-1)^{\frac{3}{2}}|\overline{\zeta_u}\nu_g|}{2} + \frac{\sqrt[3]{-1}|\gamma_u\overline{\nu_g}|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta_u\overline{\nu_g}|}{2}$$

 $e_u t_{2g}$

$$\boxed{\Delta E = \langle \zeta_u \xi_g || \zeta_u \xi_g \rangle}$$

$$\Psi_{16}(e_u t_{2g}, ^1T_{2u}, M=0, \xi_u) = -\frac{|\overline{\gamma_u}\xi_g|}{2} - \frac{|\overline{\zeta_u}\xi_g|}{2} + \frac{|\gamma_u\overline{\xi_g}|}{2} + \frac{|\zeta_u\overline{\xi_g}|}{2}$$

$$\Psi_{17}(e_u t_{2g}, ^1T_{2u}, M=0, \phi_u) = -\frac{(-1)^{\frac{3}{2}}|\overline{\gamma_u}\phi_g|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_u}\phi_g|}{2} + \frac{(-1)^{\frac{3}{2}}|\gamma_u\overline{\phi_g}|}{2} - \frac{\sqrt[3]{-1}|\zeta_u\overline{\phi_g}|}{2}$$

$$\Psi_{18}(e_u t_{2g}, ^1T_{2u}, M=0, \chi_u) = \frac{\sqrt[3]{-1}|\overline{\gamma_u}\chi_g|}{2} - \frac{(-1)^{\frac{3}{2}}|\overline{\zeta_u}\chi_g|}{2} - \frac{\sqrt[3]{-1}|\gamma_u\overline{\chi_g}|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta_u\overline{\chi_g}|}{2}$$

 $e_g t_{1u}$

$$\boxed{\Delta E = \langle \zeta_g \nu_u || \zeta_g \nu_u \rangle}$$

$$\Psi_{19}(e_g t_{1u}, ^1T_{2u}, M=0, \xi_u) = \frac{|\overline{\gamma_g}\eta_u|}{2} - \frac{|\overline{\zeta_g}\eta_u|}{2} - \frac{|\gamma_g\overline{\eta_u}|}{2} + \frac{|\zeta_g\overline{\eta_u}|}{2}$$

$$\Psi_{20}(e_g t_{1u}, ^1T_{2u}, M=0, \phi_u) = \frac{(-1)^{\frac{3}{2}}|\overline{\gamma_g}\mu_u|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_g}\mu_u|}{2} - \frac{(-1)^{\frac{3}{2}}|\gamma_g\overline{\mu_u}|}{2} - \frac{\sqrt[3]{-1}|\zeta_g\overline{\mu_u}|}{2}$$

$$\Psi_{21}(e_g t_{1u}, ^1T_{2u}, M=0, \chi_u) = -\frac{\sqrt[3]{-1}|\overline{\gamma_g}\nu_u|}{2} - \frac{(-1)^{\frac{3}{2}}|\overline{\zeta_g}\nu_u|}{2} + \frac{\sqrt[3]{-1}|\gamma_g\overline{\nu_u}|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta_g\overline{\nu_u}|}{2}$$

 $e_g t_{2u}$

$$\boxed{\Delta E = \langle \zeta_g \xi_u || \zeta_g \xi_u \rangle}$$

$$\Psi_{22}(e_g t_{2u}, ^1T_{2u}, M=0, \xi_u) = -\frac{|\overline{\gamma_g}\xi_u|}{2} - \frac{|\overline{\zeta_g}\xi_u|}{2} + \frac{|\gamma_g\overline{\xi_u}|}{2} + \frac{|\zeta_g\overline{\xi_u}|}{2}$$

$$\Psi_{23}(e_g t_{2u}, ^1T_{2u}, M=0, \phi_u) = -\frac{(-1)^{\frac{3}{2}}|\overline{\gamma_g}\phi_u|}{2} + \frac{\sqrt[3]{-1}|\overline{\zeta_g}\phi_u|}{2} + \frac{(-1)^{\frac{3}{2}}|\gamma_g\overline{\phi_u}|}{2} - \frac{\sqrt[3]{-1}|\zeta_g\overline{\phi_u}|}{2}$$

$$\Psi_{24}(e_g t_{2u}, ^1T_{2u}, M=0, \chi_u) = \frac{\sqrt[3]{-1}|\overline{\gamma_g}\chi_u|}{2} - \frac{(-1)^{\frac{3}{2}}|\overline{\zeta_g}\chi_u|}{2} - \frac{\sqrt[3]{-1}|\gamma_g\overline{\chi_u}|}{2} + \frac{(-1)^{\frac{3}{2}}|\zeta_g\overline{\chi_u}|}{2}$$

 $t_{1g} t_{1u}$

$$\boxed{\Delta E = \langle \nu_g \mu_u || \nu_g \mu_u \rangle + \langle \nu_g \nu_g || \mu_u \mu_u \rangle + \langle \nu_g \nu_u || \nu_g \nu_u \rangle + \langle \nu_g \mu_g || \nu_u \mu_u \rangle}$$

$$\Psi_{25}(t_{1g} t_{1u}, ^1T_{2u}, M=0, \chi_u) = -\frac{|\overline{\eta_g}\mu_u|}{2} - \frac{|\overline{\mu_g}\eta_u|}{2} + \frac{|\eta_g\overline{\mu_u}|}{2} + \frac{|\mu_g\overline{\eta_u}|}{2}$$

$$\Psi_{26}(t_{1g} t_{1u}, ^1T_{2u}, M=0, \phi_u) = -\frac{|\overline{\eta_g}\nu_u|}{2} - \frac{|\overline{\nu_g}\eta_u|}{2} + \frac{|\eta_g\overline{\nu_u}|}{2} + \frac{|\nu_g\overline{\eta_u}|}{2}$$

$$\Psi_{27}(t_{1g} t_{1u}, ^1T_{2u}, M=0, \xi_u) = -\frac{|\overline{\mu_g}\nu_u|}{2} - \frac{|\overline{\nu_g}\mu_u|}{2} + \frac{|\mu_g\overline{\nu_u}|}{2} + \frac{|\nu_g\overline{\mu_u}|}{2}$$

 $t_{1g} t_{2u}$

$$\boxed{\Delta E = -\langle \nu_g \chi_u || \nu_g \chi_u \rangle + \langle \nu_g \nu_g || \xi_u \xi_u \rangle + \langle \nu_g \xi_u || \nu_g \xi_u \rangle - \langle \nu_g \mu_g || \chi_u \phi_u \rangle}$$

$$\Psi_{28}(t_{1g} t_{2u}, ^1T_{2u}, M=0, \chi_u) = \frac{|\overline{\eta_g}\phi_u|}{2} - \frac{|\overline{\mu_g}\xi_u|}{2} - \frac{|\eta_g\overline{\phi_u}|}{2} + \frac{|\mu_g\overline{\xi_u}|}{2}$$

$$\Psi_{29}(t_{1g}t_{2u}, {}^1T_{2u}, M=0, \phi_u) = -\frac{|\eta_g\chi_u|}{2} + \frac{|\nu_g\xi_u|}{2} + \frac{|\eta_g\bar{\chi}_u|}{2} - \frac{|\nu_g\bar{\xi}_u|}{2}$$

$$\Psi_{30}(t_{1g}t_{2u}, {}^1T_{2u}, M=0, \xi_u) = \frac{|\mu_g\chi_u|}{2} - \frac{|\nu_g\phi_u|}{2} - \frac{|\mu_g\bar{\chi}_u|}{2} + \frac{|\nu_g\bar{\phi}_u|}{2}$$

$t_{1u}t_{2g}$

$$\Delta E = -\langle \xi_g\eta_u || \xi_g\eta_u \rangle + \langle \xi_g\nu_u || \xi_g\nu_u \rangle + \langle \xi_g\xi_g || \nu_u\nu_u \rangle - \langle \xi_g\phi_g || \eta_u\mu_u \rangle$$

$$\Psi_{31}(t_{1u}t_{2g}, {}^1T_{2u}, M=0, \chi_u) = -\frac{|\phi_g\eta_u|}{2} + \frac{|\bar{\xi}_g\mu_u|}{2} + \frac{|\phi_g\bar{\eta}_u|}{2} - \frac{|\xi_g\bar{\mu}_u|}{2}$$

$$\Psi_{32}(t_{1u}t_{2g}, {}^1T_{2u}, M=0, \phi_u) = \frac{|\bar{\chi}_g\eta_u|}{2} - \frac{|\bar{\xi}_g\nu_u|}{2} - \frac{|\chi_g\bar{\eta}_u|}{2} + \frac{|\xi_g\bar{\nu}_u|}{2}$$

$$\Psi_{33}(t_{1u}t_{2g}, {}^1T_{2u}, M=0, \xi_u) = -\frac{|\bar{\chi}_g\mu_u|}{2} + \frac{|\bar{\phi}_g\nu_u|}{2} + \frac{|\chi_g\bar{\mu}_u|}{2} - \frac{|\phi_g\bar{\nu}_u|}{2}$$

$t_{2g}t_{2u}$

$$\Delta E = \langle \xi_g\phi_u || \xi_g\phi_u \rangle + \langle \xi_g\xi_g || \phi_u\phi_u \rangle + \langle \xi_g\xi_u || \xi_g\xi_u \rangle + \langle \xi_g\phi_g || \xi_u\phi_u \rangle$$

$$\Psi_{34}(t_{2g}t_{2u}, {}^1T_{2u}, M=0, \chi_u) = -\frac{|\phi_g\xi_u|}{2} - \frac{|\bar{\xi}_g\phi_u|}{2} + \frac{|\phi_g\bar{\xi}_u|}{2} + \frac{|\xi_g\phi_u|}{2}$$

$$\Psi_{35}(t_{2g}t_{2u}, {}^1T_{2u}, M=0, \phi_u) = -\frac{|\bar{\chi}_g\xi_u|}{2} - \frac{|\bar{\xi}_g\chi_u|}{2} + \frac{|\chi_g\bar{\xi}_u|}{2} + \frac{|\xi_g\bar{\chi}_u|}{2}$$

$$\Psi_{36}(t_{2g}t_{2u}, {}^1T_{2u}, M=0, \xi_u) = -\frac{|\bar{\chi}_g\phi_u|}{2} - \frac{|\phi_g\bar{\chi}_u|}{2} + \frac{|\chi_g\bar{\phi}_u|}{2} + \frac{|\phi_g\bar{\chi}_u|}{2}$$