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Tables Useful for the Calculation of the Molecular Integrals, XI

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Introductory Remarks

In Part X[1] of our series of papers, numerical values of the matrix elements of various operators, for the ground state and lower excited electronic states of the Li_2 and the O_2 molecules were given. Since, in the previous paper, the phase was not fixed in writing the configurations (Table XXXII), these are again drawn up clearly and unambiguously in Table XXXVI following the abbreviations introduced by Kotani and the present authors[2][3]. All the configurations in the framework of the references (2) and (3) are listed here, though some of them are not explicitly considered in Part X and the reference (2). Further, formulae for evaluating the matrix elements of the Hamiltonian, $H_{ij}=(\Phi_i|H|\Phi_j)$, are given in Table XXXVII. This table includes the formulae for the following matrix elements:

(1) for the ground state and lower excited states of the Li_2 molecule and for the ground state of the O_2 molecule, all the matrix elements H_{ij} in the framework stated in the references (2) and (3),

(2) for the lower excited states of the O_2 molecule, matrix elements H_{ij}, which are taken into account explicitly in reference (2) and are given numerically in Part X, and also some other ones picked up for various purposes, for example, for omitting the unimportant configurations. The abbreviations adopted here in expressing H_{ij} are the same as were used in the Appendix of reference (2). For the sake of convenience, these are repeatedly given in the following:

$$(k|h|l)=\int\varphi_k^*(1)\left(-\frac{1}{2}\Delta_1+\frac{Z}{r_{a1}}+\frac{Z}{r_{b1}}\right)\varphi_l(1)d\tau_1\ ,$$

$$h(l)=(l|h|l)\ ,$$

$$(\varphi_i\varphi_k|\varphi_j\varphi_l)=\int\varphi_i^*(1)\varphi_j^*(2)\frac{1}{r_{12}}\varphi_k(1)\varphi_l(2)d\tau_1 d\tau_2\ ,$$

$$J(\varphi_k\varphi_l)=(\varphi_k\varphi_k|\varphi_l\varphi_l)\ ,\qquad \text{(Coulomb Integral)}$$

$$K(\varphi_k\varphi_l)=(\varphi_k\varphi_l|\varphi_l\varphi_k)\ ,\qquad \text{(Exchange Integral)}\ .$$

It must be remarked here that, in conformity with the previous reports,[1][2][3] the nuclear repulsion term $\frac{Z^2}{R}$ is included in the Hamiltonian of the O_2 molecule, whereas this is not included in that of the Li_2 molecule.

The reduction formulae for the matrix elements $(z^2)_{ij}$, $(x^2+y^2)_{ij}$, and $(q_a)_{ij}$ of Part X can be obtained easily from the parts of the one electron integrals in H_{ij} by replacing $(k|h|l)$ by

$$(k|z^2|l)=\int \varphi_k^*(1)z_1^2\varphi_l(1)d\tau_1\,, \qquad (k|x^2+y^2|l)=\int \varphi_k^*(1)(x_1^2+y_1^2)\varphi_l(1)d\tau_1\,,$$

and

$$\left(k\left|\frac{3\cos^2\theta_a-1}{2r_a^3}\right|l\right)=\int \varphi_k^*(1)\frac{3\cos^2\theta_{a1}-1}{2r_{a1}^3}\varphi_l(1)d\tau_1\,,$$

respectively. Accordingly these are not listed here.

The matrix elements q_{ij} and ρ_{ij} of Part X can be represented as $(2F)_{ij}=(\Phi_i(^3\Sigma_g^-)\,|\sum_k f_k\,2S_{kz}\,|\,\Phi_j(^3\Sigma_g^-))$, where, f_k is $\frac{3\cos^2\theta_{ak}-1}{2r_{ak}^3}$ and $\delta(r_{ak})$, and S_{kz} is the z component of the spin angular momentum of the k-th electron. $\Phi_i(^3\Sigma_g^-)$'s are the configurational wave functions for the ground state of the O_2 molecule. The reduction formulae for the non-vanishing elements of F_{ij}, within the 9 and 15 dimensional matrices explained in reference (2) are given in Table XXXVIII.

The reduction formulae for the matrix elements used in calculating an oscillator strength by the dipole velocity method are listed in Table XXXIX. The corresponding ones for the dipole length method can be constructed from this Table easily. It must be mentioned, however, that the reverse is not always allowed, since matrix elements of a length operator can be simplified on account of the Hermitian property of it, contrary to those of a velocity operator.

References

1) E. Ishiguro, K. Kayama, Y. Mizuno, T. Arai, and M. Sakamoto: Natural Science Rep. Ochanomizu Univ. **7**, 63 (1956).
2) M. Kotani, Y. Mizuno, K. Kayama, and E. Ishiguro: J. Phys. Soc. Japan. **12**, 707 (1957).
3) M. Kotani, Y. Mizuno, K. Kayama, and E. Ishiguro: J. Phys. Soc. Japan to be published.

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Table XXXVI. Configuration Tabulation

(i) $^1\Sigma_g{}^+(Li_2)$

	σ_{1g}	σ_{2g}	σ_{3g}	$\pi_g{}^+$	$\pi_g{}^-$	σ_{1u}	σ_{2u}	σ_{3u}	$\pi_u{}^+$	$\pi_u{}^-$
1	2	2				2				
2	2		2			2				
3	2					2	2			
4	2					2		2		
5	2	1	1			2				
6	2					2	1	1		
7	2			1	1	2				
8	2					2			1	1

(ii) $^1\Sigma_u{}^+$ and $^3\Sigma_u{}^+$ (Li_2)

	σ_{1g}	σ_{2g}	σ_{3g}	$\pi_g{}^+$	$\pi_g{}^-$	σ_{1u}	σ_{2u}	σ_{3u}	$\pi_u{}^+$	$\pi_u{}^-$
1	2	1				2	1			
2	2	1				2		1		
3	2		1			2	1			
4	2		1			2		1		
5	2			1		2				1

(iii) $^1\Pi_u(Li_2)$

	σ_{1g}	σ_{2g}	σ_{3g}	$\pi_g{}^+$	$\pi_g{}^-$	σ_{1u}	σ_{2u}	σ_{3u}	$\pi_u{}^+$	$\pi_u{}^-$
1	2	1				2			1	
2	2		1			2			1	
3	2			1		2	1			
4	2			1		2		1		

(iv) $^3\Sigma_g^-$ (O_2)

	π_u^+	π_u^-	π_g^+	π_g^-	σ_{2g}	σ_{2u}	σ_{2u}	σ_{2g}	σ_{1u}	σ_{1g}
A	2	2	1	1	2		2	2	2	2
B	2	2	1	1		2	2	2	2	2
C	1	1	2	2	2		2	2	2	2
D	1	1	2	2		2	2	2	2	2
E_1	$\bar{1}$	$\bar{1}$	$\underline{1}$	$\underline{1}$	2	2	2	2	2	2
E_2	$\underline{1}$	$\underline{1}$	$\bar{1}$	$\bar{1}$	2	2	2	2	2	2
F_1	$\bar{1}$	2	2	$\bar{1}$	$\underline{1}$	$\underline{1}$	2	2	2	2
F_2	$\underline{1}$	2	2	$\underline{1}$	$\bar{1}$	$\bar{1}$	2	2	2	2
F_3	$\bar{1}$	2	2	$\bar{1}$	$\bar{\bar{1}}$	$\bar{\bar{1}}$	2	2	2	2
G	1	1	2	2	2	2		2	2	2
H	2	2	1	1	2	2		2	2	2
I_1	$\bar{1}$	$\bar{1}$	2	2	2	$\underline{1}$	$\underline{1}$	2	2	2
I_3	$\bar{1}$	$\bar{1}$	2	2	2	$\bar{\bar{1}}$	$\bar{\bar{1}}$	2	2	2
J_1	2	2	$\bar{1}$	$\bar{1}$	2	$\underline{1}$	$\underline{1}$	2	2	2
J_3	2	2	$\bar{1}$	$\bar{1}$	2	$\bar{\bar{1}}$	$\bar{\bar{1}}$	2	2	2
K	1	1	2	2	2	2	2		2	2
L	2	2	1	1	2	2	2		2	2
M_1	$\bar{1}$	2	2	$\bar{1}$	2	$\underline{1}$	2	$\underline{1}$	2	2
M_2	$\underline{1}$	2	2	$\underline{1}$	2	$\bar{1}$	2	$\bar{1}$	2	2
M_3	$\bar{1}$	2	2	$\bar{1}$	2	$\bar{\bar{1}}$	2	$\bar{\bar{1}}$	2	2
N_1	$\bar{1}$	$\bar{1}$	2	2	$\underline{1}$	2	2	$\underline{1}$	2	2
N_3	$\bar{1}$	$\bar{1}$	2	2	$\bar{\bar{1}}$	2	2	$\bar{\bar{1}}$	2	2
O_1	2	2	$\bar{1}$	$\bar{1}$	$\underline{1}$	2	2	$\underline{1}$	2	2
O_3	2	2	$\bar{1}$	$\bar{1}$	$\bar{\bar{1}}$	2	2	$\bar{\bar{1}}$	2	2
P_1	$\bar{1}$	2	2	$\bar{1}$	$\underline{1}$	2	$\underline{1}$	2	2	2
P_2	$\underline{1}$	2	2	$\underline{1}$	$\bar{1}$	2	$\bar{1}$	2	2	2
P_3	$\bar{1}$	2	2	$\bar{1}$	$\bar{\bar{1}}$	2	$\bar{\bar{1}}$	2	2	2
Q_1	$\bar{1}$	2	2	$\bar{1}$	2	2	$\underline{1}$	$\underline{1}$	2	2
Q_2	$\underline{1}$	2	2	$\underline{1}$	2	2	$\bar{1}$	$\bar{1}$	2	2
Q_3	$\bar{1}$	2	2	$\bar{1}$	2	2	$\bar{\bar{1}}$	$\bar{\bar{1}}$	2	2

(v) $^3\Sigma_u^+$ and $^3\Sigma_u^-$ (O_2)

	π_g^+	π_g^-	π_u^+	π_u^-	σ_{3g}	σ_{3u}	σ_{2g}	σ_{2u}	σ_{1u}	σ_{1g}
A	1	2	2	1	2		2	2	2	2
B	1	2	2	1		2	2	2	2	2
C	1	2	1		2	2	2	2	2	2
D	1		1	2	2	2	2	2	2	2
(−)E_1	$\bar{1}$	$\bar{1}$	2	2	$\underline{1}$	$\underline{1}$	2	2	2	2
(+)E_2	$\underline{1}$	$\underline{1}$	2	2	$\bar{1}$	$\bar{1}$	2	2	2	2
(−)E_3	$\bar{1}$	$\bar{1}$	2	2	$\bar{\bar{1}}$	$\bar{\bar{1}}$	2	2	2	2
(−)F_1	2	2	$\bar{1}$	$\bar{1}$	$\underline{1}$	$\underline{1}$	2	2	2	2
(+)F_2	2	2	$\underline{1}$	$\underline{1}$	$\bar{1}$	$\bar{1}$	2	2	2	2
(−)F_3	2	2	$\bar{1}$	$\bar{1}$	$\bar{\bar{1}}$	$\bar{\bar{1}}$	2	2	2	2
G	1	2	2	1	2	2	2		2	2
H	1	2	2	1	2	2		2	2	2
I_1	$\bar{1}$	2	2	$\bar{1}$	2	$\underline{1}$	2	$\underline{1}$	2	2
I_2	$\underline{1}$	2	2	$\underline{1}$	2	$\bar{1}$	2	$\bar{1}$	2	2
I_3	$\bar{1}$	2	2	$\bar{1}$	2	$\bar{\bar{1}}$	2	$\bar{\bar{1}}$	2	2
J_1	$\bar{1}$	2	2	$\bar{1}$	$\underline{1}$	2	$\underline{1}$	2	2	2
J_2	$\underline{1}$	2	2	$\underline{1}$	$\bar{1}$	2	$\bar{1}$	2	2	2
J_3	$\bar{1}$	2	2	$\bar{1}$	$\bar{\bar{1}}$	2	$\bar{\bar{1}}$	2	2	2
(−)K_1	2	2	$\bar{1}$	$\bar{1}$	$\underline{1}$	2	2	$\underline{1}$	2	2
(+)K_2	2	2	$\underline{1}$	$\underline{1}$	$\bar{1}$	2	2	$\bar{1}$	2	2
(−)K_3	2	2	$\bar{1}$	$\bar{1}$	$\bar{\bar{1}}$	2	2	$\bar{\bar{1}}$	2	2
(−)L_1	2	2	$\bar{1}$	$\bar{1}$	2	$\underline{1}$	$\underline{1}$	2	2	2
(+)L_2	2	2	$\underline{1}$	$\underline{1}$	2	$\bar{1}$	$\bar{1}$	2	2	2
(−)L_3	2	2	$\bar{1}$	$\bar{1}$	2	$\bar{\bar{1}}$	$\bar{\bar{1}}$	2	2	2
(−)M_1	$\bar{1}$	$\bar{1}$	2	2	$\underline{1}$	2	2	$\underline{1}$	2	2
(+)M_2	$\underline{1}$	$\underline{1}$	2	2	$\bar{1}$	2	2	$\bar{1}$	2	2
(−)M_3	$\bar{1}$	$\bar{1}$	2	2	$\bar{\bar{1}}$	2	2	$\bar{\bar{1}}$	2	2
(−)N_1	$\bar{1}$	$\bar{1}$	2	2	2	$\underline{1}$	$\underline{1}$	2	2	2
(+)N_2	$\underline{1}$	$\underline{1}$	2	2	2	$\bar{1}$	$\bar{1}$	2	2	2
(−)N_3	$\bar{1}$	$\bar{1}$	2	2	2	$\bar{\bar{1}}$	$\bar{\bar{1}}$	2	2	2
(+)O	2	2	2	2	1	1	2		2	2
(+)P	2	2	2	2	1	1		2	2	2

	π_g^+	π_g^-	π_u^+	π_u^-	σ_{3g}	σ_{3u}	σ_{2g}	σ_{2u}	σ_{1u}	σ_{1g}
(+)Q	2	2	2	2	2		1	1	2	2
(+)R	2	2	2	2		2	1	1	2	2

Configurations to which (+) or (−) is attached do not vanish for only $^3\sum_u^+$ or on'y $^3\sum_u^-$ state, respectively.

(vi) $^1\sum_u^+$ and $^1\sum_u^-$ (O_2)

	π_g^+	π_g^-	π_u^+	π_u^-	σ_{3g}	σ_{3u}	σ_{2g}	σ_{2u}	σ_{1u}	σ_{1g}
A	1	2	2	1	2		2	2	2	2
B	1	2	2	1		2	2	2	2	2
C	1	2	1		2	2	2	2	2	2
D	1		1	2	2	2	2	2	2	2
(+)E_1	$\underline{1}$	$\underline{1}$	2	2	$\underline{\underline{1}}$	$\underline{\underline{1}}$	2	2	2	2
(−)E_2	$\overline{1}$	$\overline{1}$	2	2	$\overline{\overline{1}}$	$\overline{\overline{1}}$	2	2	2	2
(+)F_1	2	2	$\underline{1}$	$\underline{1}$	$\underline{\underline{1}}$	$\underline{\underline{1}}$	2	2	2	2
(−)F_2	2	2	$\overline{1}$	$\overline{1}$	$\overline{\overline{1}}$	$\overline{\overline{1}}$	2	2	2	2
G	1	2	2	1	2	2	2		2	2
H	1	2	2	1	2	2		2	2	2
I_1	$\underline{1}$	2	2	$\underline{1}$	2	$\underline{\underline{1}}$	2	$\underline{\underline{1}}$	2	2
I_2	$\overline{1}$	2	2	$\overline{1}$	2	$\overline{\overline{1}}$	2	$\overline{\overline{1}}$	2	2
J_1	$\underline{1}$	2	2	$\underline{1}$	$\underline{\underline{1}}$	2	$\underline{\underline{1}}$	2	2	2
J_2	$\overline{1}$	2	2	$\overline{1}$	$\overline{\overline{1}}$	2	$\overline{\overline{1}}$	2	2	2
(+)K_1	2	2	$\underline{1}$	$\underline{1}$	$\underline{\underline{1}}$	2	2	$\underline{\underline{1}}$	2	2
(−)K_2	2	2	$\overline{1}$	$\overline{1}$	$\overline{\overline{1}}$	2	2	$\overline{\overline{1}}$	2	2
(+)L_1	2	2	$\underline{1}$	$\underline{1}$	2	$\underline{\underline{1}}$	$\underline{\underline{1}}$	2	2	2
(−)L_2	2	2	$\overline{1}$	$\overline{1}$	2	$\overline{\overline{1}}$	$\overline{\overline{1}}$	2	2	2
(+)M_1	$\underline{1}$	$\underline{1}$	2	2	$\underline{\underline{1}}$	2	2	$\underline{\underline{1}}$	2	2
(−)M_2	$\overline{1}$	$\overline{1}$	2	2	$\overline{\overline{1}}$	2	2	$\overline{\overline{1}}$	2	2
(+)N_1	$\underline{1}$	$\underline{1}$	2	2	2	$\underline{\underline{1}}$	$\underline{\underline{1}}$	2	2	2
(−)N_2	$\overline{1}$	$\overline{1}$	2	2	2	$\overline{\overline{1}}$	$\overline{\overline{1}}$	2	2	2
(+)O	2	2	2	2	1	1	2		2	2
(+)P	2	2	2	2	1	1		2	2	2
(+)Q	2	2	2	2	2		1	1	2	2
(+)R	2	2	2	2		2	1	1	2	2

Configurations to which (+) or (−) is attached exist for only $^1\sum_u^+$ or only $^1\sum_u^-$ state, respectively.

(vii) $^1\Delta_g$ (O_2)

	π_g^+	π_g^-	π_u^+	π_u^-	σ_{3u}	σ_{3g}	σ_{2u}	σ_{2g}	σ_{1u}	σ_{1g}
A	2		2	2		2	2	2	2	2
B	1	1	2		2	2	2	2	2	1
C	2	2	2			2	2	2	2	2
D	2		2	2	2		2	2	2	2
E	2		1	1	2	2	2	2	2	2
F	2	2	2		2		2	2	2	2
G_1	2	$\underline{1}$	2	$\underline{1}$	$\underline{\underline{1}}$	$\underline{\underline{1}}$	2	2	2	2
G_2	2	$\overline{1}$	2	$\overline{1}$	$\overline{\overline{1}}$	$\overline{\overline{1}}$	2	2	2	2
H	2		2	2	2	2		2	2	2
I	2	2	2		2	2		2	2	2
J	2		2	2	1	2	1	2	2	2
K	2	2	2		1	2	1	2	2	2
L_1	2	$\underline{1}$	2	$\underline{1}$	2	$\underline{\underline{1}}$	$\underline{\underline{\underline{1}}}$	2	2	2
L_2	2	$\overline{1}$	2	$\overline{1}$	2	$\overline{\overline{1}}$	$\overline{\overline{\overline{1}}}$	2	2	2
M_1	2	$\underline{1}$	2	$\underline{1}$	$\underline{\underline{1}}$	2	2	$\underline{\underline{\underline{1}}}$	2	2
M_2	2	$\overline{1}$	2	$\overline{1}$	$\overline{\overline{1}}$	2	2	$\overline{\overline{\overline{1}}}$	2	2
N	2		2	2	2	1	2	1	2	2
O	2	2	2		2	1	2	1	2	2
P_1	2	$\underline{1}$	2	$\underline{1}$	2	2	$\underline{\underline{\underline{1}}}$	$\underline{\underline{1}}$	2	2
P_2	2	$\overline{1}$	2	$\overline{1}$	2	2	$\overline{\overline{\overline{1}}}$	$\overline{\overline{1}}$	2	2
Q	2		2	2	2	2	2		2	2
R	2	2	2		2	2	2		2	2

(viii) $^1\sum_g{}^+$ (O_2)

	$\pi_g{}^+$	$\pi_g{}^-$	$\pi_u{}^+$	$\pi_u{}^-$	σ_{3u}	σ_{3g}	σ_{2u}	σ_{2g}	σ_{1u}	σ_{1g}
A	1	1	2	2		2	2	2	2	2
B	2	2	1	1		2	2	2	2	2
C	2	2	2	2			2	2	2	2
D			2	2	2	2	2	2	2	2
E	1	1	2	2	2		2	2	2	2
F	2	2	1	1	2		2	2	2	2
G	2	2			2	2	2	2	2	2
H_1	$\underline{1}$	$\underline{1}$	$\underline{\underline{1}}$	$\underline{\underline{1}}$	2	2	2	2	2	2
H_2	$\overline{1}$	$\overline{1}$	$\overline{\overline{1}}$	$\overline{\overline{1}}$	2	2	2	2	2	2
I	2			2	2	2	2	2	2	2
J_1	$\underline{1}$	2	2	$\underline{1}$	$\underline{\underline{1}}$	$\underline{\underline{1}}$	2	2	2	2
J_2	$\overline{1}$	2	2	$\overline{1}$	$\overline{\overline{1}}$	$\overline{\overline{1}}$	2	2	2	2
K	2	2	1	1	2	2		2	2	2
L	1	1	2	2	2	2		2	2	2
M	2	2	2	2		2		2	2	2
N_1	$\underline{1}$	$\underline{1}$	2	2	$\underline{\underline{1}}$	2	$\underline{\underline{1}}$	2	2	2
O_1	2	2	$\underline{1}$	$\underline{1}$	$\underline{\underline{1}}$	2	$\underline{\underline{1}}$	2	2	2
P	2	2	1	1	2	2	2		2	2
Q	1	1	2	2	2	2	2		2	2
R	2	2	2	2		2	2		2	2
S_1	$\underline{1}$	2	2	$\underline{1}$	$\underline{\underline{1}}$	2	2	$\underline{\underline{1}}$	2	2
S_2	$\overline{1}$	2	2	$\overline{1}$	$\overline{\overline{1}}$	2	2	$\overline{\overline{1}}$	2	2
T_1	2	2	$\underline{1}$	$\underline{1}$	2	$\underline{\underline{1}}$	2	$\underline{\underline{1}}$	2	2
U_1	$\underline{1}$	$\underline{1}$	2	2	2	$\underline{\underline{1}}$	2	$\underline{\underline{1}}$	2	2
V	2	2	2	2	2		2		2	2
W	2	2	2	2	2			2	2	2
X_1	$\underline{1}$	2	2	$\underline{1}$	2	$\underline{\underline{1}}$	$\underline{\underline{1}}$	2	2	2
X_2	$\overline{1}$	2	2	$\overline{1}$	2	$\overline{\overline{1}}$	$\overline{\overline{1}}$	2	2	2
Y	2	2	2	2	2	2			2	2
Z_1	$\underline{1}$	2	2	$\underline{1}$	2	2	$\underline{\underline{1}}$	$\underline{\underline{1}}$	2	2
Z_2	$\overline{1}$	2	2	$\overline{1}$	2	2	$\overline{\overline{1}}$	$\overline{\overline{1}}$	2	2

(ix) $^3\Delta_u$ (O_2)

	π_g^+	π_g^-	π_u^+	π_u^-	σ_{3u}	σ_{3g}	σ_{2u}	σ_{2g}	σ_{1u}	σ_{1g}
A	2	1	2	1		2	2	2	2	2
B	2	1	2	1	2		2	2	2	2
C	2		2	2	1	1	2	2	2	2
D	2	2	2		1	1	2	2	2	2
E	1		2	1	2	2	2	2	2	2
F	2	1	1		2	2	2	2	2	2
G_1	2	$\bar{1}$	2	$\bar{1}$	$\underline{1}$	2	$\underline{1}$	2	2	2
G_2	2	$\underline{1}$	2	$\underline{1}$	$\bar{1}$	2	$\bar{1}$	2	2	2
G_3	2	$\bar{1}$	2	$\bar{1}$	$\bar{\bar{1}}$	2	$\bar{\bar{1}}$	2	2	2
H	2	1	2	1	2	2		2	2	2
I_1	2	$\bar{1}$	2	$\bar{1}$	2	$\underline{1}$	2	$\underline{1}$	2	2
I_2	2	$\underline{1}$	2	$\underline{1}$	2	$\bar{1}$	2	$\bar{1}$	2	2
I_3	2	$\bar{1}$	2	$\bar{1}$	2	$\bar{\bar{1}}$	2	$\bar{\bar{1}}$	2	2
J	2	1	2	1	2	2	2		2	2
K	2		2	2	2	1	1	2	2	2
L	2	2	2		2	1	1	2	2	2
M	2		2	2	1	2	2	1	2	2
N	2	2	2		1	2	2	1	2	2
O	2		2	2	2	2	1	1	2	2
P	2	2	2		2	2	1	1	2	2

(X) $^1\Delta_u$ (O_2)

For this state, the primitive functions which give all the non-vanishing configurations within our framework are the same as those of the previous $^3\Delta_u$ state. In case a primitive function contains only one set of unpaired orbitals, only one configuration exists with spin function Θ_1, for the singlet state as well as for the triplet state. Now all the primitive functions of the $^3\Delta_u$ state, except G and I, are of this type, so it will be unnecessary to repeat these configurations here. Hence, we shall here specify only the configurations resulting from primitive functions G and I.

	π_g^+	π_g^-	π_u^+	π_u^-	σ_{3u}	σ_{3g}	σ_{2u}	σ_{2g}	σ_{1u}	σ_{1g}
G_1	2	$\underline{1}$	2	$\underline{1}$	$\underline{\underline{1}}$	2	$\underline{\underline{1}}$	2	2	2
G_2	2	$\bar{1}$	2	$\bar{1}$	$\bar{\bar{1}}$	2	$\bar{\bar{1}}$	2	2	2
I_1	2	$\underline{1}$	2	$\underline{1}$	2	$\underline{\underline{1}}$	2	$\underline{\underline{1}}$	2	2
I_2	2	$\bar{1}$	2	$\bar{1}$	2	$\bar{\bar{1}}$	2	$\bar{\bar{1}}$	2	2

Table XXXVII. Formulae for Evaluating Matrix Elements

a) Li_2 case.

(i) $^1\Sigma_g^+$ (Li_2)

$$\begin{aligned}H_{11}=&2\{h(\sigma_{1g})+h(\sigma_{1u})+h(\sigma_{2g})\}\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{2g},\sigma_{2g})\\&+4\{J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\sigma_{2g})+J(\sigma_{1u},\sigma_{2g})\}\\&-2\{K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{2g})+K(\sigma_{1u},\sigma_{2g})\}\end{aligned}$$

$$\begin{aligned}H_{22}=&2\{h(\sigma_{1g})+h(\sigma_{1u})+h(\sigma_{3g})\}\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{3g},\sigma_{3g})\\&+4\{J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\sigma_{3g})+J(\sigma_{1u},\sigma_{3g})\}\\&-2\{K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{3g})+K(\sigma_{1u},\sigma_{3g})\}\end{aligned}$$

$$\begin{aligned}H_{33}=&2\{h(\sigma_{1g})+h(\sigma_{1u})+h(\sigma_{2u})\}\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{2u},\sigma_{2u})\\&+4\{J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\sigma_{2u})+J(\sigma_{1u},\sigma_{2u})\}\\&-2\{K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{2u})+K(\sigma_{1u},\sigma_{2u})\}\end{aligned}$$

$$\begin{aligned}H_{44}=&2\{h(\sigma_{1g})+h(\sigma_{1u})+h(\sigma_{3u})\}\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{3u},\sigma_{3u})\\&+4\{J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\sigma_{3u})+J(\sigma_{1u},\sigma_{3u})\\&-2\{K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{3u})+K(\sigma_{1u},\sigma_{3u})\}\end{aligned}$$

$$\begin{aligned}H_{55}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{2g})+h(\sigma_{3g})\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{2g},\sigma_{3g})+K(\sigma_{2g},\sigma_{3g})\\&+2\{J(\sigma_{1g},\sigma_{2g})+J(\sigma_{1g},\sigma_{3g})+J(\sigma_{1u},\sigma_{2g})+J(\sigma_{1u},\sigma_{3g})\}\\&+4J(\sigma_{1g},\sigma_{1u})\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{2g})+K(\sigma_{1g},\sigma_{3g})+K(\sigma_{1u},\sigma_{2g})+K(\sigma_{1u},\sigma_{3g})\}\end{aligned}$$

$$\begin{aligned}H_{66}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{2u})+h(\sigma_{3u})\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{2u},\sigma_{3u})+K(\sigma_{2u},\sigma_{3u})\\&+2\{J(\sigma_{1g},\sigma_{2u})+J(\sigma_{1g},\sigma_{3u})+J(\sigma_{1u},\sigma_{2u})+J(\sigma_{1u},\sigma_{3u})\}\\&+4J(\sigma_{1g},\sigma_{1u})\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{2u})+K(\sigma_{1g},\sigma_{3u})+K(\sigma_{1u},\sigma_{2u})+K(\sigma_{1u},\sigma_{3u})\}\end{aligned}$$

$$\begin{aligned}H_{77}=&2\{h(\sigma_{1g})+h(\sigma_{1u})+h(\pi_g^+)\}\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\pi_g^+,\pi_g^-)+K(\pi_g^+,\pi_g^-)\\&+4\{J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\pi_g^+)+J(\sigma_{1u},\pi_g^+)\}\\&-2\{K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\pi_g^+)+K(\sigma_{1u},\pi_g^+)\}\end{aligned}$$

$$\begin{aligned}H_{88}=&2\{h(\sigma_{1g})+h(\sigma_{1u})+h(\pi_u^+)\}\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\pi_u^+,\pi_u^-)+K(\pi_u^+,\pi_u^-)\\&+4\{J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\pi_u^+)+J(\sigma_{1u},\pi_u^+)\}\\&-2\{K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\pi_u^+)+K(\sigma_{1u},\pi_u^+)\}\end{aligned}$$

$H_{12}=(\sigma_{2g}\sigma_{3g}|\sigma_{2g}\sigma_{3g})$ $\qquad$ $H_{14}=(\sigma_{2g}\sigma_{3u}|\sigma_{2g}\sigma_{3u})$

$H_{13}=(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{2u})$

$$\begin{aligned}H_{15}=\sqrt{2}\{&(\sigma_{2g}|h|\sigma_{3g})+(\sigma_{2g}\sigma_{2g}|\sigma_{2g}\sigma_{3g})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2g}\sigma_{3g})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2g}\sigma_{3g})\\&-(\sigma_{1g}\sigma_{2g}|\sigma_{1g}\sigma_{3g})-(\sigma_{2g}\sigma_{1u}|\sigma_{3g}\sigma_{1u})\}\end{aligned}$$

$H_{16}=\sqrt{2}\,(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u})$ $\qquad$ $H_{23}=(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$

$H_{17}=\sqrt{2}\,(\sigma_{2g}\pi_g^+|\sigma_{2g}\pi_g^-)$ $\qquad$ $H_{24}=(\sigma_{3g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})$

$H_{18}=\sqrt{2}\,(\sigma_{3g}\pi_u^+|\sigma_{2g}\pi_u^-)$

$$\begin{aligned}H_{25}=\sqrt{2}\{&(\sigma_{2g}|h|\sigma_{3g})+(\sigma_{2g}\sigma_{3g}|\sigma_{3g}\sigma_{3g})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2g}\sigma_{3g})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2g}\sigma_{3g})\\&-(\sigma_{1g}\sigma_{2g}|\sigma_{1g}\sigma_{3g})-(\sigma_{1u}\sigma_{2g}|\sigma_{1u}\sigma_{3g})\}\end{aligned}$$

$H_{26}=\sqrt{2}\,(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$

$H_{27}=\sqrt{2}\,(\sigma_{3g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)$

$H_{28}=\sqrt{2}\,(\sigma_{3g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-)$

$H_{34}=(\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{3u})$

$H_{35}=\sqrt{2}\,(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{2u})$

$$H_{36}=\sqrt{2}\,\{(\sigma_{2u}|h|\sigma_{3u})+(\sigma_{2u}\sigma_{2u}|\sigma_{2u}\sigma_{3u})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2u}\sigma_{3u})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2u}\sigma_{3u})$$
$$-(\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})-(\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u})\}$$

$H_{37}=\sqrt{2}\,(\sigma_{2u}\pi_g{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{38}=\sqrt{2}\,(\sigma_{2u}\pi_u{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{45}=\sqrt{2}\,(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})$

$$H_{46}=\sqrt{2}\,\{(\sigma_{2u}|h|\sigma_{3u})+(\sigma_{2u}\sigma_{3u}|\sigma_{3u}\sigma_{3u})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2u}\sigma_{3u})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2u}\sigma_{3u})$$
$$-(\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})-(\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u})\}$$

$H_{47}=\sqrt{2}\,(\sigma_{3u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{48}=\sqrt{2}\,(\sigma_{3u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{56}=(\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})+(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{2u})$

$H_{57}=2(\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)$

$H_{58}=2(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-)$

$H_{67}=2(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{68}=2(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{78}=(\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-)+(\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+)$

(ii) $^1\sum_u{}^+$ and $^3\sum_u{}^+$ (Li_2)

$$\begin{aligned}H_{11}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{2g})+h(\sigma_{2u})\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{2g},\sigma_{2u})\\&+2\{J(\sigma_{1g},\sigma_{2g})+J(\sigma_{1g},\sigma_{2u})+J(\sigma_{1u},\sigma_{2g})+J(\sigma_{1u},\sigma_{2u})\}\\&+4J(\sigma_{1g},\sigma_{1u})\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{2g})+K(\sigma_{1g},\sigma_{2u})+K(\sigma_{1u},\sigma_{2g})+K(\sigma_{1u},\sigma_{2u})\}\\&\pm K(\sigma_{2g},\sigma_{2u})\end{aligned}$$

$$\begin{aligned}H_{22}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{2g})+h(\sigma_{3u})\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{2g},\sigma_{3u})\\&+2\{J(\sigma_{1g},\sigma_{2g})+J(\sigma_{1g},\sigma_{3u})+J(\sigma_{1u},\sigma_{2g})+J(\sigma_{1u},\sigma_{3u})\}\\&+4J(\sigma_{1g},\sigma_{1u})\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{2g})+K(\sigma_{1g},\sigma_{3u})+K(\sigma_{1u},\sigma_{2g})+K(\sigma_{1u},\sigma_{3u})\}\\&\pm K(\sigma_{2g},\sigma_{3u})\end{aligned}$$

$$\begin{aligned}H_{33}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{3g})+h(\sigma_{2u})\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{3g},\sigma_{2u})\\&+2\{J(\sigma_{1g},\sigma_{3g})+J(\sigma_{1g},\sigma_{2u})+J(\sigma_{1u},\sigma_{3g})+J(\sigma_{1u},\sigma_{2u})\}\\&+4J(\sigma_{1g},\sigma_{1u})\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{3g})+K(\sigma_{1g},\sigma_{2u})+K(\sigma_{1u},\sigma_{3g})+K(\sigma_{1u},\sigma_{2u})\}\\&\pm K(\sigma_{3g},\sigma_{2u})\end{aligned}$$

$$\begin{aligned}H_{44}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{3g})+h(\sigma_{3u})\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{3g},\sigma_{3u})\\&+2\{J(\sigma_{1g},\sigma_{3g})+J(\sigma_{1g},\sigma_{3u})+J(\sigma_{1u},\sigma_{3g})+J(\sigma_{1u},\sigma_{3u})\}\\&+4J(\sigma_{1g},\sigma_{1u})\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{3g})+K(\sigma_{1g},\sigma_{3u})+K(\sigma_{1u},\sigma_{3g})+K(\sigma_{1u},\sigma_{3u})\}\\&\pm K(\sigma_{3g},\sigma_{3u})\end{aligned}$$

$$\begin{aligned}H_{55}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\pi_g{}^+)+h(\pi_u{}^+)\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\pi_g{}^+,\pi_u{}^-)\\&+2\{J(\sigma_{1g},\pi_g{}^+)+J(\sigma_{1g},\pi_u{}^+)+J(\sigma_{1u},\pi_g{}^+)+J(\sigma_{1u},\pi_u{}^+)\}\\&+4J(\sigma_{1g},\sigma_{1u})\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\pi_g{}^+)+K(\sigma_{1g},\pi_u{}^+)+K(\sigma_{1u},\pi_g{}^+)+K(\sigma_{1u},\pi_u{}^-)\}\\&+(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)\\&\pm\{K(\pi_g{}^+,\pi_u{}^-)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\}\end{aligned}$$

$$H_{12}=(\sigma_{2u}|h|\sigma_{3u})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2u}\sigma_{3u})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2u}\sigma_{3u})+(\sigma_{2g}\sigma_{2g}|\sigma_{2u}\sigma_{3u})$$
$$-\{(\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})+(\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u})\}\pm(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u})$$

$$H_{13}=(\sigma_{2g}|h|\sigma_{3g})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2g}\sigma_{3g})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2g}\sigma_{3g})+(\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{2u})$$
$$-\{(\sigma_{1g}\sigma_{2g}|\sigma_{1g}\sigma_{3g})+(\sigma_{2g}\sigma_{1u}|\sigma_{3g}\sigma_{1u})\}\pm(\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$$

$$H_{14}=(\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{3u})\pm(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{2u})$$
$$H_{15}=\sqrt{2}\{(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\pm(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$$
$$H_{23}=(\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{3u})\pm(\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$$
$$\begin{aligned}H_{24}=&(\sigma_{2g}|h|\sigma_{3g})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2g}\sigma_{3g})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2g}\sigma_{3g})+(\sigma_{2g}\sigma_{3g}|\sigma_{3u}\sigma_{3u})\\&-\{(\sigma_{1g}\sigma_{2g}|\sigma_{1g}\sigma_{3g})+(\sigma_{2g}\sigma_{1u}|\sigma_{3g}\sigma_{1u})\}\pm(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})\end{aligned}$$
$$H_{25}=\sqrt{2}\{(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)\pm(\sigma_{2g}\pi_u{}^-|\sigma_{3u}\pi_g{}^+)\}$$
$$\begin{aligned}H_{34}=&(\sigma_{2u}|h|\sigma_{3u})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2u}\sigma_{3u})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2u}\sigma_{3u})+(\sigma_{3g}\sigma_{3g}|\sigma_{2u}\sigma_{3u})\\&-\{(\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})+(\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u})\}\pm(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})\end{aligned}$$
$$H_{35}=\sqrt{2}\{(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\pm(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$$
$$H_{45}=\sqrt{2}\{(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)\pm(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

In the above formulae the upper or the lower of a double sign corresponds to ${}^1\sum_u{}^+$ or ${}^3\sum_u{}^+$ state, respectively.

(iii) ${}^1\Pi_u$ (Li_2)

$$\begin{aligned}H_{11}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{2g})+h(\pi_u{}^+)\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{2g},\pi_u{}^+)\\&+2\{2J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\sigma_{2g})+J(\sigma_{1g},\pi_u{}^+)+J(\sigma_{1u},\sigma_{2g})++J(\sigma_{1u},\pi_u{}^+)\}\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{2g})+K(\sigma_{1g},\pi_u{}^+)+K(\sigma_{1u},\sigma_{2g})+K(\sigma_{1u},\pi_u{}^+)-K(\sigma_{2g},\pi_u{}^+)\}\end{aligned}$$
$$\begin{aligned}H_{22}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{3g})+h(\pi_u{}^+)\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{3g},\pi_u{}^+)\\&+2\{2J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\sigma_{3g})+J(\sigma_{1g},\pi_u{}^+)+J(\sigma_{1u},\sigma_{3g})+J(\sigma_{1u},\pi_u{}^+)\}\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{3g})+K(\sigma_{1g},\pi_u{}^+)+K(\sigma_{1u},\sigma_{3g})+K(\sigma_{1u},\pi_u{}^+)-K(\sigma_{3g},\pi_u{}^+)\}\end{aligned}$$
$$\begin{aligned}H_{33}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{2u})+h(\pi_g{}^+)\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{2u},\pi_g{}^+)\\&+2\{2J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\sigma_{2u})+J(\sigma_{1g},\pi_g{}^+)+J(\sigma_{1u},\sigma_{2u})+J(\sigma_{1u},\pi_g{}^+)\}\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{2u})+K(\sigma_{1g},\pi_g{}^+)+K(\sigma_{1u},\sigma_{2u})+K(\sigma_{1u},\pi_g{}^+)-K(\sigma_{2u},\pi_g{}^+)\}\end{aligned}$$
$$\begin{aligned}H_{44}=&2\{h(\sigma_{1g})+h(\sigma_{1u})\}+h(\sigma_{3u})+h(\pi_g{}^+)\\&+J(\sigma_{1g},\sigma_{1g})+J(\sigma_{1u},\sigma_{1u})+J(\sigma_{3u},\pi_g{}^+)\\&+2\{2J(\sigma_{1g},\sigma_{1u})+J(\sigma_{1g},\sigma_{3u})+J(\sigma_{1g},\pi_g{}^+)+J(\sigma_{1u},\sigma_{3u})+J(\sigma_{1u},\pi_g{}^+)\}\\&-\{2K(\sigma_{1g},\sigma_{1u})+K(\sigma_{1g},\sigma_{3u})+K(\sigma_{1g},\pi_g{}^+)+K(\sigma_{1u},\sigma_{3u})+K(\sigma_{1u},\pi_g{}^+)-K(\sigma_{3u},\pi_g{}^+)\}\end{aligned}$$
$$\begin{aligned}H_{12}=&(\sigma_{2g}|h|\sigma_{3g})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2g}\sigma_{3g})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2g}\sigma_{3g})+(\sigma_{2g}\sigma_{3g}|\pi_u{}^+\pi_u{}^+)\\&-\{(\sigma_{1g}\sigma_{2g}|\sigma_{1g}\sigma_{3g})+(\sigma_{2g}\sigma_{1u}|\sigma_{3g}\sigma_{1u})-(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-)\}\end{aligned}$$
$$H_{13}=(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\qquad H_{23}=(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$$
$$H_{14}=(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)\qquad H_{24}=(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$$
$$\begin{aligned}H_{34}=&(\sigma_{2u}|h|\sigma_{3u})+2(\sigma_{1g}\sigma_{1g}|\sigma_{2u}\sigma_{3u})+2(\sigma_{1u}\sigma_{1u}|\sigma_{2u3u})+(\sigma_{2u}\sigma_{3u}|\pi_g{}^+\pi_g{}^+)\\&-\{(\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})+(\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u})-(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}\end{aligned}$$

b) O_2 case.

When we write down the formulae for diagonal matrix elements, it is convenient to introduce the following abbreviations:

$$s=4\sum_{\alpha>\beta}J(\alpha,\beta)+\sum_{\alpha}J(\alpha,\alpha),$$
$$t(\gamma)=2\sum_{\alpha}J(\alpha,\gamma),\qquad t=2\sum_{\gamma}t(\gamma),$$
$$f=4\sum_{\alpha>\beta}K(\alpha,\beta),$$
$$g(\gamma)=2\sum_{\alpha}K(\alpha,\gamma),\qquad g=2\sum_{\gamma}g(\gamma).$$

In the above formulae, α, β, and γ are the orbitals which depend on the configuration considered. We show these orbitals for all the configurations used for each state.

Moreover throughout all the configurations we use

$$p=2\{h(\sigma_{1g})+h(\sigma_{1u})+h(\sigma_{2g})+h(\sigma_{2u})+h(\sigma_{3g})+h(\sigma_{3u})+h(\pi_u^+)+h(\pi_u^-)$$
$$+h(\pi_g^+)+h(\pi_g^-)\}+\frac{Z^2}{R}\,.$$

(iv) $^3\Sigma_g^-$ (O_2)

Configurations	$\alpha,\ \beta$	γ
$A,\ B,\ C,\ D,\ E_i,\ F_i$	$\sigma_{1g},\ \sigma_{1u},\ \sigma_{2g},\ \sigma_{2u}$	$\sigma_{3g},\ \sigma_{3u},\ \pi_u^{\pm},\ \pi_g^{\pm}$
$G,\ H,\ I_i,\ J_i$	$\sigma_{1g},\ \sigma_{1u},\ \sigma_{2g},\ \sigma_{3g}$	$\sigma_{2u},\ \sigma_{3u},\ \pi_u^{\pm},\ \pi_g^{\pm}$
$K,\ L,\ M_i$	$\sigma_{1g},\ \sigma_{1u},\ \sigma_{2u},\ \sigma_{3g}$	$\sigma_{2g},\ \sigma_{3u},\ \pi_u^{\pm},\ \pi_g^{\pm}$
$N_i,\ O_i$	$\sigma_{1g},\ \sigma_{1u},\ \sigma_{2u},\ \sigma_{3u}$	$\sigma_{2g},\ \sigma_{3g},\ \pi_u^{\pm},\ \pi_g^{\pm}$
P_i	$\sigma_{1g},\ \sigma_{1u},\ \sigma_{2g},\ \sigma_{3u},\ \pi_u^-,\ \pi_g^+$	$\sigma_{2u},\ \sigma_{3g},\ \pi_u^+,\ \pi_g^-$
Q_i	$\sigma_{1g},\ \sigma_{1u},\ \sigma_{3g},\ \sigma_{3u},\ \pi_u^-,\ \pi_g^+$	$\sigma_{2g},\ \sigma_{2u},\ \pi_u^+,\ \pi_g^-$

$$\begin{aligned}H_{AA}=&\,p-h(\pi_g^+)-h(\pi_g^-)-2h(\sigma_{3u})\\
&+s+t-t(\pi_g^+)-t(\pi_g^-)-2t(\sigma_{3u})\\
&+J(\pi_g^+,\pi_g^-)+2J(\pi_g^+,\sigma_{3g})+2J(\pi_g^+,\pi_u^+)+2J(\pi_g^+,\pi_u^-)\\
&\qquad+2J(\pi_g^-,\sigma_{3g})+2J(\pi_g^-,\pi_u^+)+2J(\pi_g^-,\pi_u^-)\\
&\qquad+J(\sigma_{3g},\sigma_{3g})+4J(\sigma_{3g},\pi_u^+)+4J(\sigma_{3g},\pi_u^-)\\
&\qquad\qquad+J(\pi_u^+,\pi_u^+)+4J(\pi_u^+,\pi_u^-)\\
&\qquad\qquad\qquad+J(\pi_u^-,\pi_u^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_g^+)-g(\pi_g^-)-2g(\sigma_{3u})\\
&\qquad+2K(\pi_g^+,\pi_g^-)+2K(\pi_g^+,\sigma_{3g})+2K(\pi_g^+,\pi_u^+)+2K(\pi_g^+,\pi_u^-)\\
&\qquad\qquad+2K(\pi_g^-,\sigma_{3g})+2K(\pi_g^-,\pi_u^+)+2K(\pi_g^-,\pi_u^-)\\
&\qquad\qquad\qquad+4K(\sigma_{3g},\pi_u^+)+4K(\sigma_{3g},\pi_u^-)\\
&\qquad\qquad\qquad\qquad+4K(\pi_u^+,\pi_u^-)\}\end{aligned}$$

$$\begin{aligned}H_{BB}=&\,p-h(\pi_g^+)-h(\pi_g^-)-2h(\sigma_{3g})\\
&+s+t-t(\pi_g^+)-t(\pi_g^-)-2t(\sigma_{3g})\\
&+J(\pi_g^+,\pi_g^-)+2J(\pi_g^+,\sigma_{3u})+2J(\pi_g^+,\pi_u^+)+2J(\pi_g^+,\pi_u^-)\\
&\qquad+2J(\pi_g^-,\sigma_{3u})+2J(\pi_g^-,\pi_u^+)+2J(\pi_g^-,\pi_u^-)\\
&\qquad+J(\sigma_{3u},\sigma_{3u})+4J(\sigma_{3u},\pi_u^+)+4J(\sigma_{3u},\pi_u^-)\\
&\qquad\qquad+J(\pi_u^+,\pi_u^+)+4J(\pi_u^+,\pi_u^-)\\
&\qquad\qquad\qquad+J(\pi_u^-,\pi_u^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_g^+)-g(\pi_g^-)-2g(\sigma_{3g})\\
&\qquad+2K(\pi_g^+,\pi_g^-)+2K(\pi_g^+,\sigma_{3u})+2K(\pi_g^+,\pi_u^+)+2K(\pi_g^+,\pi_u^-)\\
&\qquad\qquad+2K(\pi_g^-,\sigma_{3u})+2K(\pi_g^-,\pi_u^+)+2K(\pi_g^-,\pi_u^-)\\
&\qquad\qquad\qquad+4K(\sigma_{3u},\pi_u^+)+4K(\sigma_{3u},\pi_u^-)\\
&\qquad\qquad\qquad\qquad+4K(\pi_u^+,\pi_u^-)\}\end{aligned}$$

$$\begin{aligned}H_{CC}=&\,p-h(\pi_u^+)-h(\pi_u^-)-2h(\sigma_{3u})\\
&+s+t-t(\pi_u^+)-t(\pi_u^-)-2t(\sigma_{3u})\\
&+J(\pi_u^+,\pi_u^-)+2J(\pi_u^+,\sigma_{3g})+2J(\pi_u^+,\pi_g^+)+2J(\pi_u^+,\pi_g^-)\\
&\qquad+2J(\pi_u^-,\sigma_{3g})+2J(\pi_u^-,\pi_g^+)+2J(\pi_u^-,\pi_g^-)\\
&\qquad+J(\sigma_{3g},\sigma_{3g})+4J(\sigma_{3g},\pi_g^+)+4J(\sigma_{3g},\pi_g^-)\\
&\qquad\qquad+J(\pi_g^+,\pi_g^+)+4J(\pi_g^+,\pi_g^-)\\
&\qquad\qquad\qquad+J(\pi_g^-,\pi_g^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_u^+)-g(\pi_u^-)-2g(\sigma_{3u})\\
&\qquad+2K(\pi_u^+,\pi_u^-)+2K(\pi_u^+,\sigma_{3g})+2K(\pi_u^+,\pi_g^+)+2K(\pi_u^+,\pi_g^-)\\
&\qquad\qquad+2K(\pi_u^-,\sigma_{3g})+2K(\pi_u^-,\pi_g^+)+2K(\pi_u^-,\pi_g^-)\\
&\qquad\qquad\qquad+4K(\sigma_{3g},\pi_g^+)+4K(\sigma_{3g},\pi_g^-)\\
&\qquad\qquad\qquad\qquad+4K(\pi_g^+,\pi_g^-)\}\end{aligned}$$

$$
\begin{aligned}
H_{DD}=\;& p-h(\pi_u{}^+)-h(\pi_u{}^-)-2h(\sigma_{3g})\\
&+s+t-t(\pi_u{}^+)-t(\pi_u{}^-)-2t(\sigma_{3g})\\
&+J(\pi_u{}^+,\pi_u{}^-)+2J(\pi_u{}^+,\sigma_{3u})+2J(\pi_u{}^+,\pi_g{}^+)+2J(\pi_u{}^+,\pi_g{}^-)\\
&\qquad+2J(\pi_u{}^-,\sigma_{3u})+2J(\pi_u{}^-,\pi_g{}^+)+2J(\pi_u{}^-,\pi_g{}^-)\\
&\qquad+J(\sigma_{3u},\sigma_{3u})+4J(\sigma_{3u},\pi_g{}^+)+4J(\sigma_{3u},\pi_g{}^-)\\
&\qquad\qquad+J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_g{}^-)\\
&\qquad\qquad\qquad+J(\pi_g{}^-,\pi_g{}^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_u{}^+)-g(\pi_u{}^-)-2g(\sigma_{3g})\\
&\quad+2K(\pi_u{}^+,\pi_u{}^-)+2K(\pi_u{}^+,\sigma_{3u})+2K(\pi_u{}^+,\pi_g{}^+)+2K(\pi_u{}^+,\pi_g{}^-)\\
&\qquad+2K(\pi_u{}^-,\sigma_{3u})+2K(\pi_u{}^-,\pi_g{}^+)+2K(\pi_u{}^-,\pi_g{}^-)\\
&\qquad+4K(\sigma_{3u},\pi_g{}^+)+4K(\pi_g{}^+,\pi_g{}^-)\\
&\qquad\qquad+4K(\sigma_{3u},\pi_g{}^-)\}
\end{aligned}
$$

$$
\left.\begin{matrix}H_{E_1E_1}\\ H_{E_2E_2}\end{matrix}\right\}=
\begin{aligned}
&p-h(\pi_u{}^+)-h(\pi_u{}^-)-h(\pi_g{}^+)-h(\pi_g{}^-)\\
&+s+t-t(\pi_u{}^+)-t(\pi_u{}^-)-t(\pi_g{}^+)-t(\pi_g{}^-)\\
&+J(\pi_u{}^+,\pi_u{}^-)+J(\pi_u{}^+,\pi_g{}^+)+J(\pi_u{}^+,\pi_g{}^-)+2J(\pi_u{}^+,\sigma_{3g})+2J(\pi_u{}^+,\sigma_{3u})\\
&\qquad+J(\pi_u{}^-,\pi_g{}^+)+J(\pi_u{}^-,\pi_g{}^-)+2J(\pi_u{}^-,\sigma_{3g})+2J(\pi_u{}^-,\sigma_{3u})\\
&\qquad\qquad+J(\pi_g{}^+,\pi_g{}^-)+2J(\pi_g{}^+,\sigma_{3g})+2J(\pi_g{}^+,\sigma_{3u})\\
&\qquad\qquad\qquad+2J(\pi_g{}^-,\sigma_{3g})+2J(\pi_g{}^-,\sigma_{3u})\\
&\qquad\qquad\qquad+J(\sigma_{3g},\sigma_{3g})+4J(\sigma_{3g},\sigma_{3u})\\
&\qquad\qquad\qquad\qquad+J(\sigma_{3u},\sigma_{3u})\\
&+\tfrac{1}{2}\{f+g-g(\pi_u{}^+)-g(\pi_u{}^-)-g(\pi_g{}^+)-g(\pi_g{}^-)\\
&\quad+2K(\pi_u{}^+,\sigma_{3g})+2K(\pi_u{}^+,\sigma_{3u})+2K(\pi_u{}^-,\sigma_{3g})+2K(\pi_u{}^-,\sigma_{3u})\\
&\quad+2K(\pi_g{}^+,\sigma_{3g})+2K(\pi_g{}^+,\sigma_{3u})+2K(\pi_g{}^-,\sigma_{3g})+2K(\pi_g{}^-,\sigma_{3u})+4K(\sigma_{3g},\sigma_{3u})\}\\
&+\begin{cases}-K(\pi_u{}^+,\pi_u{}^-)-K(\pi_g{}^+,\pi_u{}^+)-K(\pi_g{}^+,\pi_u{}^-)+K(\pi_g{}^+,\pi_g{}^-)\\ +K(\pi_u{}^+,\pi_u{}^-)-K(\pi_g{}^+,\pi_u{}^+)-K(\pi_g{}^+,\pi_u{}^-)-K(\pi_g{}^+,\pi_g{}^-)\end{cases}
\end{aligned}
$$

$$
\left.\begin{matrix}H_{F_1F_1}\\ H_{F_2F_2}\\ H_{F_3F_3}\end{matrix}\right\}=
\begin{aligned}
&p-h(\pi_u{}^+)-h(\pi_g{}^-)-h(\sigma_{3g})-h(\sigma_{3u})\\
&+s+t-t(\pi_u{}^+)-t(\pi_g{}^-)-t(\sigma_{3g})-t(\sigma_{3u})\\
&+J(\pi_u{}^+,\pi_g{}^-)+J(\pi_u{}^+,\sigma_{3g})+J(\pi_u{}^+,\sigma_{3u})+2J(\pi_u{}^+,\pi_g{}^+)+2J(\pi_u{}^+,\pi_u{}^-)\\
&\qquad+J(\pi_g{}^-,\sigma_{3g})+J(\pi_g{}^-,\sigma_{3u})+2J(\pi_g{}^-,\pi_g{}^+)+2J(\pi_g{}^-,\pi_u{}^-)\\
&\qquad\qquad+J(\sigma_{3g},\sigma_{3u})+2J(\sigma_{3g},\pi_g{}^+)+2J(\sigma_{3g},\pi_u{}^-)\\
&\qquad\qquad\qquad+2J(\sigma_{3u},\pi_g{}^+)+2J(\sigma_{3u},\pi_u{}^-)\\
&\qquad\qquad\qquad+J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_u{}^-)\\
&\qquad\qquad\qquad\qquad+J(\pi_u{}^-,\pi_u{}^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_u{}^+)-g(\pi_g{}^-)-g(\sigma_{3g})-g(\sigma_{3u})\\
&\quad+2K(\pi_u{}^+,\pi_g{}^+)+2K(\pi_u{}^+,\pi_u{}^-)+2K(\pi_g{}^-,\pi_g{}^+)+2K(\pi_g{}^-,\pi_u{}^-)\\
&\quad+2K(\sigma_{3g},\pi_g{}^+)+2K(\sigma_{3g},\pi_u{}^-)+2K(\sigma_{3u},\pi_g{}^+)+2K(\sigma_{3u},\pi_u{}^-)+4K(\pi_g{}^+,\pi_u{}^-)\}\\
&+\begin{cases}-K(\pi_g{}^+,\pi_u{}^-)-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{3g})-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{3u})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{3g})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{3u})\\ \qquad+K(\sigma_{3g},\sigma_{3u})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\\ +K(\pi_g{}^+,\pi_u{}^-)-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{3g})-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{3u})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{3g})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{3u})\\ \qquad-K(\sigma_{3g},\sigma_{3u})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)-(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\\ -K(\pi_g{}^+,\pi_u{}^-)-K(\sigma_{3g},\sigma_{3u})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\end{cases}
\end{aligned}
$$

$$
\begin{aligned}
H_{GG}=\;& p-h(\pi_u{}^+)-h(\pi^-)-2h(\sigma_{2u})\\
&+s+t-t(\pi_u{}^+)-t(\pi_u{}^-)-2t(\sigma_{2u})\\
&+J(\pi_u{}^+,\pi_u{}^-)+2J(\pi_u{}^+,\sigma_{3u})+2J(\pi_u{}^+,\pi_g{}^+)+2J(\pi_u{}^+,\pi_g{}^-)\\
&\qquad+2J(\pi_u{}^-,\sigma_{3u})+2J(\pi_u{}^-,\pi_g{}^+)+2J(\pi_u{}^-,\pi_g{}^-)\\
&\qquad+J(\sigma_{3u},\sigma_{3u})+4J(\sigma_{3u},\pi_g{}^+)+4J(\sigma_{3u},\pi_g{}^-)\\
&\qquad\qquad+J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_{g-})\\
&\qquad\qquad\qquad+J(\pi_g{}^-,\pi_g{}^-)
\end{aligned}
$$

$$
\begin{aligned}
&-\tfrac{1}{2}\{f+g-g(\pi_u{}^+)-g(\pi_u{}^-)-2g(\sigma_{2u})\\
&\quad+2K(\pi_u{}^+,\pi_u{}^-)+2K(\pi_u{}^+,\sigma_{3u})+2K(\pi_u{}^+,\pi_g{}^+)+2K(\pi_u{}^+,\pi_g{}^-)\\
&\qquad+2K(\pi_u{}^-,\sigma_{3u})+2K(\pi_u{}^-,\pi_g{}^+)+2K(\pi_u{}^-,\pi_g{}^-)\\
&\qquad\qquad+4K(\sigma_{3u},\pi_g{}^+)+4K(\sigma_{3u},\pi_g{}^-)\\
&\qquad\qquad\qquad+4K(\pi_g{}^+,\pi_g{}^-)\}
\end{aligned}
$$

$$
\begin{aligned}
H_{HH}=\;&p-h(\pi_g{}^+)-h(\pi_g{}^-)-2h(\sigma_{2u})\\
&+s+t-t(\pi_g{}^+)-t(\pi_g{}^-)-2t(\sigma_{2u})\\
&+J(\pi_g{}^+,\pi_g{}^-)+2J(\pi_g{}^+,\sigma_{3u})+2J(\pi_g{}^+,\pi_u{}^+)+2J(\pi_g{}^+,\pi_u{}^-)\\
&\qquad+2J(\pi_g{}^-,\sigma_{3u})+2J(\pi_g{}^-,\pi_u{}^+)+2J(\pi_g{}^-,\pi_u{}^-)\\
&\qquad+J(\sigma_{3u},\sigma_{3u})+4J(\sigma_{3u},\pi_u{}^+)+4J(\sigma_{3u},\pi_u{}^-)\\
&\qquad\qquad+J(\pi_u{}^+,\pi_u{}^+)+4J(\pi_u{}^+,\pi_u{}^-)\\
&\qquad\qquad\qquad+J(\pi_u{}^-,\pi_u{}^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_g{}^-)-2g(\sigma_{2u})\\
&\quad+2K(\pi_g{}^+,\pi_g{}^-)+2K(\pi_g{}^+,\sigma_{3u})+2K(\pi_g{}^+,\pi_u{}^+)+2K(\pi_g{}^+,\pi_u{}^-)\\
&\qquad+2K(\pi_g{}^-,\sigma_{3u})+2K(\pi_g{}^-,\pi_u{}^+)+2K(\pi_g{}^-,\pi_u{}^-)\\
&\qquad\qquad+4K(\sigma_{3u},\pi_u{}^+)+4K(\sigma_{3u},\pi_u{}^-)\\
&\qquad\qquad\qquad+4K(\pi_u{}^+,\pi_u{}^-)\}
\end{aligned}
$$

$$
\left.\begin{matrix}H_{I_1I_1}\\H_{I_3I_3}\end{matrix}\right\}=
\begin{aligned}
&p-h(\pi_u{}^+)-h(\pi_u{}^-)-h(\sigma_{3u})-h(\sigma_{2u})\\
&+s+t-t(\pi_u{}^+)-t(\pi_u{}^-)-t(\sigma_{3u})-t(\sigma_{2u})\\
&+J(\pi_u{}^+,\pi_u{}^-)+J(\pi_u{}^+,\sigma_{3u})+J(\pi_u{}^+,\sigma_{2u})+2J(\pi_u{}^+,\pi_g{}^+)+2J(\pi_u{}^+,\pi_g{}^-)\\
&\qquad+J(\pi_u{}^-,\sigma_{3u})+J(\pi_u{}^-,\sigma_{2u})+2J(\pi_u{}^-,\pi_g{}^+)+2J(\pi_u{}^-,\pi_g{}^-)\\
&\qquad\qquad+J(\sigma_{3u},\sigma_{2u})+2J(\sigma_{3u},\pi_g{}^+)+2J(\sigma_{3u},\pi_g{}^-)\\
&\qquad\qquad\qquad+2J(\sigma_{2u},\pi_g{}^+)+2J(\sigma_{2u},\pi_g{}^-)\\
&\qquad\qquad\qquad+J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_g{}^-)\\
&\qquad\qquad\qquad\qquad+J(\pi_g{}^-,\pi_g{}^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_u{}^+)-g(\pi_u{}^-)-g(\sigma_{3u})-g(\sigma_{2u})\\
&\quad+2K(\pi_u{}^+,\pi_g{}^+)+2K(\pi_u{}^+,\pi_g{}^-)+2K(\pi_u{}^-,\pi_g{}^+)+2K(\pi_u{}^-,\pi_g{}^-)\\
&\quad+2K(\sigma_{3u},\pi_g{}^+)+2K(\sigma_{3u},\pi_g{}^-)+2K(\sigma_{2u},\pi_g{}^+)+2K(\sigma_{2u},\pi_g{}^-)+4K(\pi_g{}^+,\pi_g{}^-)\}\\
&+\begin{cases}-K(\pi_u{}^+,\pi_u{}^-)-K(\pi_u{}^+,\sigma_{3u})-K(\pi_u{}^+,\sigma_{2u})+K(\sigma_{3u},\sigma_{2u})\\-K(\pi_u{}^+,\pi_u{}^-)-K(\sigma_{3u},\sigma_{2u})\end{cases}
\end{aligned}
$$

$$
\left.\begin{matrix}H_{J_1J_1}\\H_{J_3J_3}\end{matrix}\right\}=
\begin{aligned}
&p-h(\pi_g{}^+)-h(\pi_g{}^-)-h(\sigma_{3u})-h(\sigma_{2u})\\
&+s+t-t(\pi_g{}^+)-t(\pi_g{}^-)-t(\sigma_{3u})-t(\sigma_{2u})\\
&+J(\pi_g{}^+,\pi_g{}^-)+J(\pi_g{}^+,\sigma_{3u})+J(\pi_g{}^+,\sigma_{2u})+2J(\pi_g{}^+,\pi_u{}^+)+2J(\pi_g{}^+,\pi_u{}^-)\\
&\qquad+J(\pi_g{}^-,\sigma_{3u})+J(\pi_g{}^-,\sigma_{2u})+2J(\pi_g{}^-,\pi_u{}^+)+2J(\pi_g{}^-,\pi_u{}^-)\\
&\qquad\qquad+J(\sigma_{3u},\sigma_{2u})+2J(\sigma_{3u},\pi_u{}^+)+2J(\sigma_{3u},\pi_u{}^-)\\
&\qquad\qquad\qquad+2J(\sigma_{2u},\pi_u{}^+)+2J(\sigma_{2u},\pi_u{}^-)\\
&\qquad\qquad\qquad+J(\pi_u{}^+,\pi_u{}^+)+4J(\pi_u{}^+,\pi_u{}^-)\\
&\qquad\qquad\qquad\qquad+J(\pi_u{}^-,\pi_u{}^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_g{}^-)-g(\sigma_{3u})-g(\sigma_{2u})\\
&\quad+2K(\pi_g{}^+,\pi_u{}^+)+2K(\pi_g{}^+,\pi_u{}^-)+2K(\pi_g{}^-,\pi_u{}^+)+2K(\pi_g{}^-,\pi_u{}^-)\\
&\quad+2K(\sigma_{3u},\pi_u{}^+)+2K(\sigma_{3u},\pi_u{}^-)+2K(\sigma_{2u},\pi_u{}^+)+2K(\sigma_{2u},\pi_u{}^-)\\
&\qquad\qquad+4K(\pi_u{}^+,\pi_u{}^-)\}\\
&+\begin{cases}-K(\pi_g{}^+,\pi_g{}^-)-K(\pi_g{}^+,\sigma_{3u})-K(\pi_g{}^+,\sigma_{2u})+K(\sigma_{3u},\sigma_{2u})\\-K(\pi_g{}^+,\pi_g{}^-)-K(\sigma_{3u},\sigma_{2u})\end{cases}
\end{aligned}
$$

$$
\begin{aligned}
H_{KK}=\;&p-h(\pi_u{}^+)-h(\pi_u{}^-)-2h(\sigma_{2g})\\
&+s+t-t(\pi_u{}^+)-t(\pi_u{}^-)-2t(\sigma_{2g})\\
&+J(\pi_u{}^+,\pi_u{}^-)+2J(\pi_u{}^+,\sigma_{3u})+2J(\pi_u{}^+,\pi_g{}^+)+2J(\pi_u{}^+,\pi_g{}^-)\\
&\qquad+2J(\pi_u{}^-,\sigma_{3u})+2J(\pi_u{}^-,\pi_g{}^+)+2J(\pi_u{}^-,\pi_g{}^-)\\
&\qquad+J(\sigma_{3u},\sigma_{3u})+4J(\sigma_{3u},\pi_g{}^+)+4J(\sigma_{3u},\pi_g{}^-)\\
&\qquad\qquad+J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_g{}^-)\\
&\qquad\qquad\qquad+J(\pi_g{}^-,\pi_g{}^-)
\end{aligned}
$$

$$
\begin{aligned}
&-\tfrac{1}{2}\{f+g-g(\pi_u{}^+)-g(\pi_u{}^-)-2g(\sigma_{2g})\\
&\quad+2K(\pi_u{}^+,\pi_u{}^-)+2K(\pi_u{}^+,\sigma_{3u})+2K(\pi_u{}^+,\pi_g{}^+)+2K(\pi_u{}^+,\pi_g{}^-)\\
&\qquad+2K(\pi_u{}^-,\sigma_{3u})+2K(\pi_u{}^-,\pi_g{}^+)+2K(\pi_u{}^-,\pi_g{}^-)\\
&\qquad\qquad+4K(\sigma_{3u},\pi_g{}^+)+4K(\sigma_{3u},\pi_g{}^-)\\
&\qquad\qquad\qquad+4K(\pi_g{}^+,\pi_g{}^-)\}
\end{aligned}
$$

$$
\begin{aligned}
H_{LL}=&\,p-h(\pi_g{}^+)-h(\pi_g{}^-)-2h(\sigma_{2g})\\
&+s+t-t(\pi_g{}^+)-t(\pi_g{}^-)-2t(\sigma_{2g})\\
&+J(\pi_g{}^+,\pi_g{}^-)+2J(\pi_g{}^+,\sigma_{3u})+2J(\pi_g{}^+,\pi_u{}^+)+2J(\pi_g{}^+,\pi_u{}^-)\\
&\qquad+2J(\pi_g{}^-,\sigma_{3u})+2J(\pi_g{}^-,\pi_u{}^+)+2J(\pi_g{}^-,\pi_u{}^-)\\
&\qquad+J(\sigma_{3u},\sigma_{3u})+4J(\sigma_{3u},\pi_u{}^+)+4J(\sigma_{3u},\pi_u{}^-)\\
&\qquad\qquad+J(\pi_u{}^+,\pi_u{}^+)+4J(\pi_u{}^+,\pi_u{}^-)\\
&\qquad\qquad\qquad+J(\pi_u{}^-,\pi_u{}^-)
\end{aligned}
$$

$$
\begin{aligned}
&-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_g{}^-)-2g(\sigma_{2g})\\
&\quad+2K(\pi_g{}^+,\pi_g{}^-)+2K(\pi_g{}^+,\sigma_{3u})+2K(\pi_g{}^+,\pi_u{}^+)+2K(\pi_g{}^+,\pi_u{}^-)\\
&\qquad+2K(\pi_g{}^-,\sigma_{3u})+2K(\pi_g{}^-,\pi_u{}^+)+2K(\pi_g{}^-,\pi_u{}^-)\\
&\qquad\qquad+4K(\sigma_{3u},\pi_u{}^+)+4K(\sigma_{3u},\pi_u{}^-)\\
&\qquad\qquad\qquad+4K(\pi_u{}^+,\pi_u{}^-)\}
\end{aligned}
$$

$$
\left.\begin{matrix}H_{M_1M_1}\\H_{M_2M_2}\\H_{M_3M_3}\end{matrix}\right\}=p-h(\pi_g{}^-)-h(\pi_u{}^+)-h(\sigma_{3u})-h(\sigma_{2g})
$$

$$
\begin{aligned}
&+s+t-t(\pi_g{}^-)-t(\pi_u{}^+)-t(\sigma_{3u})-t(\sigma_{2g})\\
&+J(\pi_g{}^-,\pi_u{}^+)+J(\pi_u{}^+,\sigma_{3u})+J(\pi_u{}^+,\sigma_{2g})+2J(\pi_u{}^+,\pi_g{}^+)+2J(\pi_u{}^+,\pi_u{}^-)\\
&\qquad+J(\pi_g{}^-,\sigma_{3u})+J(\pi_g{}^-,\sigma_{2g})+2J(\pi_g{}^-,\pi_g{}^+)+2J(\pi_g{}^-,\pi_u{}^-)\\
&\qquad\qquad+J(\sigma_{3u},\sigma_{2g})+2J(\sigma_{3u},\pi_g{}^+)+2J(\sigma_{3u},\pi_u{}^-)\\
&\qquad\qquad\qquad+2J(\sigma_{2g},\pi_g{}^+)+2J(\sigma_{2g},\pi_u{}^-)\\
&\qquad\qquad\qquad+J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_u{}^-)\\
&\qquad\qquad\qquad\qquad+J(\pi_u{}^-,\pi_u{}^-)
\end{aligned}
$$

$$
\begin{aligned}
&-\tfrac{1}{2}\{f+g-g(\pi_u{}^+)-g(\pi_g{}^-)-g(\sigma_{3u})-g(\sigma_{2g})\\
&\quad+2K(\pi_u{}^+,\pi_g{}^+)+2K(\pi_u{}^+,\pi_u{}^-)+2K(\pi_g{}^-,\pi_g{}^+)+2K(\pi_g{}^-,\pi_u{}^-)\\
&\quad+2K(\sigma_{3u},\pi_g{}^+)+2K(\sigma_{3u},\pi_u{}^-)+2K(\sigma_{2g},\pi_g{}^+)+2K(\sigma_{2g},\pi_u{}^-)\\
&\qquad\qquad\qquad\qquad+4K(\pi_g{}^+,\pi_u{}^-)\}\\
&+\left\{\begin{matrix}
-K(\pi_u{}^+,\pi_g{}^-)-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{3u})-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{2g})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{3u})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{2g})\\
\qquad+K(\sigma_{3u},\sigma_{2g})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\\
+K(\pi_u{}^+,\pi_g{}^-)-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{3u})-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{2g})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{3u})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{2g})\\
\qquad-K(\sigma_{3u},\sigma_{2g})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)-(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\\
-K(\pi_u{}^+,\pi_g{}^-)-K(\sigma_{3u},\sigma_{2g})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)
\end{matrix}\right.
\end{aligned}
$$

$$
\left.\begin{matrix}H_{N_1N_1}\\H_{N_3N_3}\end{matrix}\right\}=p-h(\pi_u{}^+)-h(\pi_u{}^-)-h(\sigma_{3g})-h(\sigma_{2g})
$$

$$
\begin{aligned}
&+s+t-t(\pi_u{}^+)-t(\pi_u{}^-)-t(\sigma_{3g})-t(\sigma_{2g})\\
&+J(\pi_u{}^+,\pi_u{}^-)+J(\pi_u{}^+,\sigma_{3g})+J(\pi_u{}^+,\sigma_{2g})+2J(\pi_u{}^+,\pi_g{}^+)+2J(\pi_u{}^+,\pi_g{}^-)\\
&\qquad+J(\pi_u{}^-,\sigma_{3g})+J(\pi_u{}^-,\sigma_{2g})+2J(\pi_u{}^-,\pi_g{}^+)+2J(\pi_u{}^-,\pi_g{}^-)\\
&\qquad\qquad+J(\sigma_{3g},\sigma_{2g})+2J(\sigma_{3g},\pi_g{}^+)+2J(\sigma_{3g},\pi_g{}^-)\\
&\qquad\qquad\qquad+2J(\sigma_{2g},\pi_g{}^+)+2J(\sigma_{2g},\pi_g{}^-)\\
&\qquad\qquad\qquad+J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_g{}^-)\\
&\qquad\qquad\qquad\qquad+J(\pi_g{}^-,\pi_g{}^-)
\end{aligned}
$$

$$
\begin{aligned}
&-\tfrac{1}{2}\{f+g-g(\pi_u{}^+)-g(\pi_u{}^-)-g(\sigma_{3g})-g(\sigma_{2g})\\
&\quad+2K(\pi_u{}^+,\pi_g{}^+)+2K(\pi_u{}^+,\pi_g{}^-)+2K(\pi_u{}^-,\pi_g{}^+)+2K(\pi_u{}^-,\pi_g{}^-)\\
&\quad+2K(\sigma_{3g},\pi_g{}^+)+2K(\sigma_{3g},\pi_g{}^-)+2K(\sigma_{2g},\pi_g{}^+)+2K(\sigma_{2g},\pi_g{}^-)\\
&\qquad\qquad\qquad\qquad+4K(\pi_g{}^+,\pi_g{}^-)\}\\
&+\left\{\begin{matrix}
-K(\pi_u{}^+,\pi_u{}^-)-K(\pi_u{}^+,\sigma_{3g})-K(\pi_u{}^+,\sigma_{2g})+K(\sigma_{3g},\sigma_{2g})\\
-K(\pi_u{}^+,\pi_u{}^-)-K(\sigma_{3g},\sigma_{2g})
\end{matrix}\right.
\end{aligned}
$$

$$
\left.\begin{matrix} H_{O_1O_1} \\ H_{O_3O_3} \end{matrix}\right\} = p - h(\pi_g{}^+) - h(\pi_g{}^-) - h(\sigma_{3g}) - h(\sigma_{2g})
$$

$$
\begin{aligned}
&+s+t-t(\pi_g{}^+)-t(\pi_g{}^-)-t(\sigma_{3g})-t(\sigma_{2g}) \\
&+J(\pi_g{}^+,\pi_g{}^-)+J(\pi_g{}^+,\sigma_{3g})+J(\pi_g{}^+,\sigma_{2g})+2J(\pi_g{}^+,\pi_u{}^+)+2J(\pi_g{}^+,\pi_u{}^-) \\
&\qquad +J(\pi_g{}^-,\sigma_{3g})+J(\pi_g{}^-,\sigma_{2g})+2J(\pi_g{}^-,\pi_u{}^+)+2J(\pi_g{}^-,\pi_u{}^-) \\
&\qquad\qquad +J(\sigma_{3g},\sigma_{2g})+2J(\sigma_{3g},\pi_u{}^+)+2J(\sigma_{3g},\pi_u{}^-) \\
&\qquad\qquad\qquad +2J(\sigma_{2g},\pi_u{}^+)+2J(\sigma_{2g},\pi_u{}^-) \\
&\qquad\qquad\qquad +J(\pi_u{}^+,\pi_u{}^+)+4J(\pi_u{}^+,\pi_u{}^-) \\
&\qquad\qquad\qquad\qquad +J(\pi_u{}^-,\pi_u{}^-) \\
&-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_g{}^-)-g(\sigma_{3g})-g(\sigma_{2g}) \\
&\quad +2K(\pi_g{}^+,\pi_u{}^+)+2K(\pi_g{}^+,\pi_u{}^-)+2K(\pi_g{}^-,\pi_u{}^+)+2K(\pi_g{}^-,\pi_u{}^-) \\
&\quad +2K(\sigma_{3g},\pi_u{}^+)+2K(\sigma_{3g},\pi_u{}^-)+2K(\sigma_{2g},\pi_u{}^+)+2K(\sigma_{2g},\pi_u{}^-) \\
&\qquad\qquad +4K(\pi_u{}^+,\pi_u{}^-)\} \\
&+\begin{cases} -K(\pi_g{}^+,\pi_g{}^-)-K(\pi_g{}^+,\sigma_{3g})-K(\pi_g{}^+,\sigma_{2g})+K(\sigma_{3g},\sigma_{2g}) \\ -K(\pi_g{}^+,\pi_g{}^-)-K(\sigma_{3g},\sigma_{2g}) \end{cases}
\end{aligned}
$$

$$
\left.\begin{matrix} H_{P_1P_1} \\ H_{P_2P_2} \\ H_{P_3P_3} \end{matrix}\right\} = p - h(\pi_u{}^+) - h(\pi_g{}^-) - h(\sigma_{3g}) - h(\sigma_{2u})
$$

$$
\begin{aligned}
&+s+t+J(\pi_u{}^+,\pi_g{}^-)+J(\pi_u{}^+,\sigma_{3g})+J(\pi_u{}^+,\sigma_{2u}) \\
&\qquad +J(\pi_g{}^-,\sigma_{3g})+J(\pi_g{}^-,\sigma_{2u})+J(\sigma_{3g},\sigma_{2u}) \\
&-\tfrac{1}{2}\{f+g\} \\
&+\begin{cases} -K(\pi_u{}^+,\pi_g{}^-)-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{3g})-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{2u})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{3g})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{2u}) \\ \qquad +K(\sigma_{3g},\sigma_{2u})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+) \\ +K(\pi_u{}^+,\pi_g{}^-)-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{3g})-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{2u})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{3g})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{2u}) \\ \qquad -K(\sigma_{3g},\sigma_{2u})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)-(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+) \\ -K(\pi_u{}^+,\pi_g{}^-)-K(\sigma_{3g},\sigma_{2u})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+) \end{cases}
\end{aligned}
$$

$$
\left.\begin{matrix} H_{Q_1Q_1} \\ H_{Q_2Q_2} \\ H_{Q_3Q_3} \end{matrix}\right\} = p - h(\pi_u{}^+) - h(\pi_g{}^-) - h(\sigma_{2u}) - h(\sigma_{2g})
$$

$$
\begin{aligned}
&+s+t+J(\pi_u{}^+,\pi_g{}^-)+J(\pi_u{}^+,\sigma_{2u})+J(\pi_u{}^+,\sigma_{2g}) \\
&\qquad +J(\pi_g{}^-,\sigma_{2u})+J(\pi_g{}^-,\sigma_{2g})+J(\sigma_{2u},\sigma_{2g}) \\
&-\tfrac{1}{2}\{f+g\} \\
&+\begin{cases} -K(\pi_u{}^+,\pi_g{}^-)-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{2u})-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{2g})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{2u})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{2g}) \\ \qquad +K(\sigma_{2u},\sigma_{2g})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+) \\ +K(\pi_u{}^+,\pi_g{}^-)-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{2u})-\tfrac{1}{2}K(\pi_u{}^+,\sigma_{2g})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{2u})-\tfrac{1}{2}K(\pi_g{}^-,\sigma_{2g}) \\ \qquad -K(\sigma_{2u},\sigma_{2g})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)-(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+) \\ -K(\pi_u{}^+,\pi_g{}^-)-K(\sigma_{2u},\sigma_{2g})-(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+) \end{cases}
\end{aligned}
$$

$$
\begin{aligned}
H_{AB} &= (\sigma_{3g}\sigma_{3u}|\sigma_{3g}\sigma_{3u}) & H_{AF_2} &= (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) \\
H_{AC} &= (\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-)-(\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+) & H_{AF_3} &= -\sqrt{2}\,(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) \\
H_{AD} &= 0 & H_{AG} &= 0 \\
H_{AE_1} &= 0 & H_{AH} &= (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{3u}) \\
H_{AE_2} &= -\sqrt{2}\,(\sigma_{3u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) & H_{AI_1} &= 0 \\
H_{AF_1} &= -2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) & H_{AI_3} &= 0
\end{aligned}
$$

$$
\begin{aligned}
H_{AJ_1} = \sqrt{2}\,[&(\sigma_{2u}|h|\sigma_{3u})+2(\sigma_{2u}\sigma_{3u}|\pi_g{}^+\pi_g{}^+)+(\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{2u}) \\
&+4(\sigma_{2u}\sigma_{3u}|\pi_u{}^+\pi_u{}^+)+2(\sigma_{2u}\sigma_{3u}|\sigma_{3g}\sigma_{3g})+2(\sigma_{2u}\sigma_{3u}|\sigma_{2g}\sigma_{2g})+2(\sigma_{2u}\sigma_{3u}|\sigma_{1u}\sigma_{1u}) \\
&+2(\sigma_{2u}\sigma_{3u}|\sigma_{1g}\sigma_{1g}) \\
&-\{(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)+2(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-)+(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) \\
&+(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u})+(\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u})+(\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})\}\,]
\end{aligned}
$$

$$
\begin{aligned}
H_{AJ_3} &= 2(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-) & H_{AM_1} &= -2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) \\
H_{AK} &= 0 & H_{AM_2} &= -(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) \\
H_{AL} &= (\sigma_{2g}\sigma_{3u}|\sigma_{2g}\sigma_{3u}) & H_{AM_3} &= \sqrt{2}\,(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)
\end{aligned}
$$

$H_{AN_1} = 0$

$H_{AN_3} = 0$

$H_{AO_1} = -\sqrt{2}\,(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})$

$H_{AO_3} = 0$

$H_{AP_1} = 0$

$H_{AP_2} = 0$

$H_{AP_3} = 0$

$H_{AQ_1} = 0$

$H_{AQ_2} = 0$

$H_{AQ_3} = 0$

$H_{BC} = 0$

$H_{BD} = (\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-) - (\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+)$

$H_{BE_1} = 0$

$H_{BE_2} = -\sqrt{2}\,(\sigma_{3g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-)$

$H_{BF_1} = -2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{BF_2} = -(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{BF_3} = \sqrt{2}\,(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{BG} = 0$

$H_{BH} = (\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$

$H_{BI_1} = 0$

$H_{BI_3} = 0$

$H_{BJ_1} = -\sqrt{2}\,(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$

$H_{BJ_3} = 0$

$H_{BK} = 0$

$H_{BL} = (\sigma_{2g}\sigma_{3g}|\sigma_{2g}\sigma_{3g})$

$H_{BM_1} = 0$

$H_{BM_2} = 0$

$H_{BM_3} = 0$

$H_{BN_1} = 0$

$H_{BN_3} = 0$

$$\begin{aligned} H_{BO_1} = \sqrt{2}\,[&(\sigma_{2g}|h|\sigma_{3g}) + 2(\sigma_{2g}\sigma_{3g}|\pi_g{}^+\pi_g{}^+) + (\sigma_{2g}\sigma_{2g}|\sigma_{2g}\sigma_{3g}) + 4(\sigma_{2g}\sigma_{2g}|\pi_u{}^+\pi_u{}^-) \\ &+ 2(\sigma_{2g}\sigma_{3g}|\sigma_{3u}\sigma_{3u}) + 2(\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{2u}) + 2(\sigma_{2g}\sigma_{3g}|\sigma_{1u}\sigma_{1u}) + 2(\sigma_{2g}\sigma_{3g}|\sigma_{1g}\sigma_{1g}) \\ &- \{(\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-) + 2(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) + (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u}) + (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{2u}) \\ &+ (\sigma_{2g}\sigma_{1u}|\sigma_{3g}\sigma_{1u}) + (\sigma_{2g}\sigma_{1g}|\sigma_{3g}\sigma_{1g})\}] \end{aligned}$$

$H_{BO_3} = 2(\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)$

$H_{BP_1} = -2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^+)$

$H_{BP_2} = -(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^+)$

$H_{BP_3} = \sqrt{2}\,(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^+)$

$H_{BQ_1} = 0$

$H_{BQ_2} = 0$

$H_{BQ_3} = 0$

$H_{CD} = (\sigma_{3g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})$

$H_{CE_1} = -\sqrt{2}\,(\sigma_{3u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{CE_2} = 0$

$H_{CF_1} = -2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{C_2F} = -(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{CF_3} = -\sqrt{2}\,(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{CG} = (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{3u})$

$H_{CH} = 0$

$$\begin{aligned} H_{CI_1} = \sqrt{2}\,[&(\sigma_{2u}|h|\sigma_{3u}) + 2(\sigma_{2u}\sigma_{3u}|\pi_u{}^+\pi_u{}^+) + (\sigma_{2u}\sigma_{2u}|\sigma_{2u}\sigma_{3u}) + 4(\sigma_{2u}\sigma_{3u}|\pi_g{}^+\pi_g{}^+) \\ &+ 2(\sigma_{3g}\sigma_{3g}|\sigma_{2u}\sigma_{3u}) + 2(\sigma_{2g}\sigma_{2g}|\sigma_{2u}\sigma_{3u}) + 2(\sigma_{1u}\sigma_{1u}|\sigma_{2u}\sigma_{3u}) + 2(\sigma_{1g}\sigma_{1g}|\sigma_{2u}\sigma_{3u}) \\ &- \{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) + 2(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-) + (\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) \\ &+ (\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u}) + (\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u}) + (\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})\}] \end{aligned}$$

$H_{CI_3} = 2(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{CJ_1} = 0$

$H_{CJ_3} = 0$

$H_{CK} = (\sigma_{2g}\sigma_{3u}|\sigma_{2g}\sigma_{3u})$

$H_{CL} = 0$

$H_{CM_1} = -2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{CM_2} = (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{CM_3} = \sqrt{2}\,(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_J{}^-)$

$H_{CN_1} = -\sqrt{2}\,(\sigma_{2J}\sigma_{3u}|\sigma$

$H_{CN_3} = 0$

$H_{CO_1} = 0$

$H_{CO_3} = 0$

$H_{CP_1} = 0$

$H_{CP_2} = 0$

$H_{CP_3} = 0$

$H_{CQ_1} = 0$

$H_{CQ_2} = 0$

$H_{CQ_3} = 0$

$H_{DE_1} = -\sqrt{2}\,(\sigma_{3J}\pi_J{}^+|\sigma_{3g}\pi_g{}^-)$

$H_{DE_2} = 0$

$H_{DF_1} = -2(\sigma_{3J}\sigma_{3u}|\pi_J{}^+\pi_u{}^+) + (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{DF_2} = (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{DF_3} = \sqrt{2}\,(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{DG} = (\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$

$H_{DH} = 0$

$H_{DI_1} = -\sqrt{2}\,(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})_{3g}\sigma_{3u})$

$H_{DI_3} = 0$

$H_{DJ_1} = 0$

$H_{DJ_3} = 0$

$H_{DK} = (\sigma_{2g}\sigma_{3g}|\sigma_{2g}\sigma_{3g})$

$H_{DL} = 0$

$H_{DM_1} = 0$

$H_{DM_2} = 0$

$H_{DM_3} = 0$

$$H_{DN_1} = \sqrt{2}\,[(\sigma_{2g}|h|\sigma_{3g}) + 2(\sigma_{2g}\sigma_{3g}|\pi_u{}^+\pi_u{}^+) + (\sigma_{2g}\sigma_{2g}|\sigma_{2g3g}) + 4(\sigma_{2g}\sigma_{3g}|\pi_g{}^+\pi_g{}^+) + 2(\sigma_{2g}\sigma_{3g}|\sigma_{3u}\sigma_{3u}) + 2(\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{2u}) + 2(\sigma_{2g}\sigma_{3g}|\sigma_{1u}\sigma_{1u}) + 2(\sigma_{2g}\sigma_{3g}|\sigma_{1g}\sigma_{1g}) - \{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) + 2(\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-) + (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u}) + (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{2u}) + (\sigma_{2g}\sigma_{1u}|\sigma_{3g}\sigma_{1u}) + (\sigma_{1g}\sigma_{2g}|\sigma_{1g}\sigma_{3g})\}]$$

$$H_{DN_3} = 2(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) \qquad H_{DP_3} = \sqrt{2}\,(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$$

$$H_{DO_1} = 0 \qquad H_{DQ_1} = 0$$

$$H_{DO_3} = 0 \qquad H_{DQ_2} = 0$$

$$H_{DP_1} = -2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{DQ_3} = 0$$

$$H_{DP_2} = (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{E_1E_2} = -K(\pi_g{}^+, \pi_u{}^+) + K(\pi_g{}^+, \pi_u{}^-)$$

$$H_{E_1F_1} = -\frac{1}{\sqrt{2}}\{(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) + (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{E_1F_2} = -\frac{1}{\sqrt{2}}\{(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{E_1F_3} = -\{(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{E_1G} = -\sqrt{2}\,(\sigma_{2u}\pi_g{}^+|\sigma_{2u}\pi_g{}^-) \qquad H_{E_1J_1} = 0$$

$$H_{E_1H} = 0 \qquad H_{E_1J_3} = 0$$

$$H_{E_1I_1} = 2(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-) \qquad H_{E_1K} = -\sqrt{2}\,(\sigma_{2g}\pi_g{}^+|\sigma_{2g}\pi_g{}^-)$$

$$H_{E_1I_3} = 0 \qquad H_{E_1L} = 0$$

$$H_{E_1M_1} = -\frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) + (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{E_1M_2} = \frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{E_1M_3} = (\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-) \qquad H_{E_1O_1} = 0$$

$$H_{E_1N_1} = 2(\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-) \qquad H_{E_1O_3} = 0$$

$$H_{E_1N_3} = 0$$

$$H_{E_1P_1} = -\frac{1}{\sqrt{2}}\{(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) + (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$$

$$H_{E_1P_2} = -\frac{1}{\sqrt{2}}\{(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) - (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$$

$$H_{E_1P_3} = -(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) + (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$$

$$H_{E_1Q_1} = -\frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) + (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$$

$$H_{E_1Q_2} = -\frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$$

$$H_{E_1Q_3} = -(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) + (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$$

$$H_{E_2F_1} = -\frac{1}{\sqrt{2}}\{(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) + (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{E_2F_2} = -\frac{1}{\sqrt{2}}\{(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{E_2F_3} = (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-) \qquad H_{E_2J_1} = 2(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-)$$

$$H_{E_2G} = 0 \qquad H_{E_2J_3} = 0$$

$$H_{E_2H} = -\sqrt{2}\,(\sigma_{2u}\pi_u{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{E_2K} = 0$$

$$H_{E_2I_1} = 0 \qquad H_{E_2L} = -\sqrt{2}\,(\sigma_{2g}\pi_u{}^+|\sigma_{2g}\pi_u{}^-)$$

$$H_{E_2I_3} = 0$$

$$H_{E_2M_1} = -\frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) + (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{E_2M_2} = \frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{E_2M_3} = -(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-) + (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-) \qquad H_{E_2O_1} = 2(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-)$$

$$H_{E_2N_1} = 0 \qquad H_{E_2O_3} = 0$$

$$H_{E_2N_3} = 0$$

$$H_{E_2P_1} = -\frac{1}{\sqrt{2}}\{(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) + (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$$

$$H_{E_2P_2} = -\frac{1}{\sqrt{2}}\{(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) - (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$$

$$H_{E_2P_3} = (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) - (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$$

$$H_{E_2Q_1} = -\frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) + (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$$

$$H_{E_2Q_2} = -\frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$$

$$H_{E_2Q_3} = (\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$$

$$H_{F_1F_2} = \frac{1}{2}\{-K(\sigma_{3g}, \pi_u{}^+) + K(\sigma_{3u}, \pi_u{}^+) + K(\sigma_{3g}, \pi_g{}^+) - K(\sigma_{3u}, \pi_g{}^+)\}$$

$$H_{F_1F_3} = \frac{1}{\sqrt{2}}\{K(\sigma_{3g}, \pi_u{}^+) - K(\sigma_{3u}, \pi_u{}^+) + K(\sigma_{3g}, \pi_g{}^+) - K(\sigma_{3u}, \pi_g{}^+)\}$$

$$H_{F_1G} = 0 \qquad H_{F_1H} = 0$$

$$H_{F_1I_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$$

$$H_{F_1I_3} = -(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$$

$$H_{F_1J_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$$

$$H_{F_1J_3} = -(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{F_1L} = 0$$

$$H_{F_1K} = 0$$

$$\begin{aligned} H_{F_1M_1} = -\Big[& (\sigma_{2g}|h|\sigma_{3g}) + 3(\sigma_{2g}\sigma_{3g}|\pi_u{}^+\pi_u{}^+) + 3(\sigma_{2g}\sigma_{3g}|\pi_g{}^+\pi_g{}^+) + (\sigma_{2g}\sigma_{2g}|\sigma_{2g}\sigma_{3g}) \\ & + (\sigma_{2g}\sigma_{3g}|\sigma_{3u}\sigma_{3u}) + (\sigma_{2g}\sigma_{3g}|\sigma_{3g}\sigma_{3g}) + 2(\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{2u}) + 2(\sigma_{2g}\sigma_{3g}|\sigma_{1u}\sigma_{1u}) \\ & + 2(\sigma_{2g}\sigma_{3g}|\sigma_{1g}\sigma_{1g}) \\ & - \Big\{\frac{3}{2}(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) + \frac{3}{2}(\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-) + 2(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u}) \\ & + (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{2u}) + (\sigma_{2g}\sigma_{1u}|\sigma_{3g}\sigma_{1u}) + (\sigma_{1g}\sigma_{2g}|\sigma_{1g}\sigma_{3g})\Big\}\Big] \end{aligned}$$

$$H_{F_1M_2} = \frac{1}{2}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$$

$$H_{F_1M_3} = -\frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) + (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$$

$$H_{F_1N_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)\}$$

$$H_{F_1N_3} = -(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$$

$$H_{F_1O_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{F_1O_3} = -(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$$

$$\begin{aligned} H_{F_1P_1} = -\Big[& (\sigma_{2u}|h|\sigma_{3u}) + 3(\sigma_{2u}\sigma_{3u}|\pi_u{}^+\pi_u{}^+) + 3(\sigma_{2u}\sigma_{3u}|\pi_g{}^+\pi_g{}^+) + (\sigma_{2u}\sigma_{3u}|\sigma_{3g}\sigma_{3g}) \\ & + (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{2u}) + (\sigma_{2u}\sigma_{3u}|\sigma_{3u}\sigma_{3u}) + 2(\sigma_{2u}\sigma_{3u}|\sigma_{2g}\sigma_{2g}) + 2(\sigma_{2u}\sigma_{3u}|\sigma_{1u}\sigma_{1u}) \\ & + 2(\sigma_{2u}\sigma_{3u}|\sigma_{1g}\sigma_{1g}) \\ & - \Big\{\frac{3}{2}(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) + \frac{3}{2}(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-) + 2(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) \\ & + (\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u}) + (\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u}) + (\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})\Big\}\Big] \end{aligned}$$

$$H_{F_1P_2} = \frac{1}{2}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{F_1P_3} = -\frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) + (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{F_1Q_1} = (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{2u}) + (\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{3u}) \qquad H_{F_1Q_3} = 0$$

$$H_{F_1Q_2} = 0$$

$$H_{F_2F_3} = -\frac{1}{\sqrt{2}}\{K(\sigma_{3g}, \pi_u{}^+) + K(\sigma_{3u}, \pi_u{}^+) - K(\sigma_{3g}, \pi_g{}^+) - K(\sigma_{3u}, \pi_g{}^+)\}$$

$$H_{F_2G} = 0 \qquad H_{F_2I_1} = \frac{1}{\sqrt{2}}(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$$

$$H_{F_2H} = 0 \qquad H_{F_2I_3} = -(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$$

$H_{F_2J_1} = -\frac{1}{\sqrt{2}}(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$ $\quad H_{F_2K} = 0$

$H_{F_2J_3} = (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$ $\quad H_{F_2L} = 0$

$H_{F_2M_1} = -\frac{1}{2}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$

$H_{F_2M_2} = -\{H_{F_1M_1} - 2(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})\}$

$H_{F_2M_3} = \frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$

$H_{F_2N_1} = -\frac{1}{\sqrt{2}}(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$ $\quad H_{F_2O_1} = \frac{1}{\sqrt{2}}(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{F_2N_3} = (\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$ $\quad H_{F_2O_3} = -(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{F_2P_1} = \frac{1}{2}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$

$H_{F_2P_2} = H_{F_1P_1} - 2(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$

$H_{F_2P_3} = -\frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$

$H_{F_2Q_1} = 0$ $\quad H_{F_3I_3} = -\sqrt{2}(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)$

$H_{F_2Q_2} = (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{2u}) - (\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{3u})$ $\quad H_{F_3J_1} = (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{F_2Q_3} = 0$ $\quad H_{F_3J_3} = -\sqrt{2}(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)$

$H_{F_3G} = 0$ $\quad H_{F_3K} = 0$

$H_{F_3H} = 0$ $\quad H_{F_3L} = 0$

$H_{F_3I_1} = (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{F_3M_1} = \frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) + (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$

$H_{F_3M_2} = \frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$

$H_{F_3M_3} = -\{H_{F_1M_1} + \frac{1}{2}(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) + \frac{1}{2}(\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-) - 2(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})\}$

$H_{F_3N_1} = -(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$ $\quad H_{F_3O_1} = -(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{F_3N_3} = \sqrt{2}(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)$ $\quad H_{F_3O_3} = \sqrt{2}(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)$

$H_{F_3P_1} = \frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$

$H_{F_3P_2} = -\frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$

$H_{F_3P_3} = H_{F_1P_1} + \frac{1}{2}(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) + \frac{1}{2}(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-) - 2(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$

$H_{F_3Q_1} = 0$ $\quad H_{F_3Q_3} = (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{2u}) - (\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{3u})$

$H_{F_3Q_2} = 0$ $\quad H_{GH} = (\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-) - (\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+)$

$H_{GI_1} = H_{CI_1} + \sqrt{2}\{(\sigma_{2u}\sigma_{3u}|\sigma_{3u}\sigma_{3u}) - (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{2u})\}$

$H_{GI_3} = -2(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-)$ $\quad H_{GO_1} = 0$

$H_{GJ_1} = 0$ $\quad H_{GO_3} = 0$

$H_{GJ_3} = 0$ $\quad H_{GP_1} = -2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{GK} = (\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{2u})$ $\quad H_{GP_2} = -(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{GL} = 0$ $\quad H_{GP_3} = -\sqrt{2}(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{GM_1} = 0$ $\quad H_{GQ_1} = -2(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{GM_2} = 0$ $\quad H_{GQ_2} = (\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{GM_3} = 0$ $\quad H_{GQ_3} = \sqrt{2}(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{GN_1} = -\sqrt{2}(\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$ $\quad H_{HI_1} = 0$

$H_{GN_3} = 0$ $\quad H_{HI_3} = 0$

$H_{HJ_1} = H_{AJ_1} + \sqrt{2}\{(\sigma_{2u}\sigma_{3u}|\sigma_{3u}\sigma_{3u}) - (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{2u})\}$

$H_{HJ_3} = -2(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)$ $\quad H_{HL} = (\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{2u})$

$H_{HK} = 0$ $\quad H_{HM_1} = 0$

$H_{HM_2} = 0$

$H_{HM_3} = 0$

$H_{HN_1} = 0$

$H_{HN_3} = 0$

$H_{HO_1} = -\sqrt{2}\,(\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$

$H_{HO_3} = 0$

$H_{HP_1} = -2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{HP_2} = (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{HP_3} = -\sqrt{2}\,(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{HQ_1} = -2(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{HQ_2} = -(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{HQ_3} = \sqrt{2}\,(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{I_1I_3} = \sqrt{2}\,\{K(\sigma_{3u}, \pi_u{}^+) - K(\sigma_{2u}, \pi_u{}^+)\}$

$H_{I_1J_1} = (\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-)$

$H_{I_1J_3} = 0$

$H_{I_1K} = -\sqrt{2}\,(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u})$

$H_{I_1L} = 0$

$H_{I_1M_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$

$H_{I_1M_2} = -\frac{1}{\sqrt{2}}(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{I_1M_3} = -(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{I_1N_1} = (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) + (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{2u})$

$H_{I_1N_3} = 0$

$H_{I_1O_1} = 0$

$H_{I_1O_3} = 0$

$H_{I_1P_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$

$H_{I_1P_2} = \frac{1}{\sqrt{2}}(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{I_1P_3} = (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{I_1Q_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$

$H_{I_1Q_2} = \frac{1}{\sqrt{2}}(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{I_1Q_3} = (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{I_3J_1} = 0$

$H_{I_3J_3} = (\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-)$

$H_{I_3K} = 0$

$H_{I_3L} = 0$

$H_{I_3M_1} = -(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{I_3M_2} = (\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{I_3M_3} = \sqrt{2}\,(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)$

$H_{I_3N_1} = 0$

$H_{I_3N_3} = (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) - (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{2u})$

$H_{I_3O_1} = 0$

$H_{I_3O_3} = 0$

$H_{I_3P_1} = (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{I_3P_2} = (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{I_3P_3} = \sqrt{2}\,(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)$

$H_{I_3Q_1} = -(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{I_3Q_2} = (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{I_3Q_3} = -\sqrt{2}\,(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)$

$H_{J_1J_3} = \sqrt{2}\,\{K(\sigma_{3u}, \pi_g{}^+) - K(\sigma_{2u}, \pi_g{}^+)\}$

$H_{J_1K} = 0$

$H_{J_1L} = -\sqrt{2}\,(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u})$

$H_{J_1M_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$

$H_{J_1M_2} = \frac{1}{\sqrt{2}}(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{J_1M_3} = -(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{J_1N_1} = 0$

$H_{J_1N_3} = 0$

$H_{J_1O_1} = (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) + (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{2u})$

$H_{J_1O_3} = 0$

$H_{J_1P_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)\}$

$H_{J_1P_2} = -\frac{1}{\sqrt{2}}(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{J_1P_3} = (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{J_1Q_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)\}$

$H_{J_1Q_2} = \frac{1}{\sqrt{2}}(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{J_1Q_3} = -(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{J_3K} = 0$

$H_{J_3L} = 0$

$H_{J_3M_1} = -(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{J_3M_2} = -(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{J_3M_3} = \sqrt{2}\,(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)$

$H_{J_3N_1} = 0$

$H_{J_3N_3} = 0$

$H_{J_3O_1} = 0$

$H_{J_3O_3} = (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) - (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{2u})$

$H_{J_3Q_3} = -\sqrt{2}\,(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)$

$H_{J_3P_1} = (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{KL} = (\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-) - (\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+)$

$H_{J_3P_2} = -(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{KM_1} = -2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{J_3P_3} = \sqrt{2}\,(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)$

$H_{KM_2} = -(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{J_3Q_1} = (\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{KM_3} = -\sqrt{2}\,(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{J_3Q_2} = (\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{KN_1} = H_{DN_1} + \sqrt{2}\,\{(\sigma_{2g}\sigma_{3g}|\sigma_{3g}\sigma_{3g}) - (\sigma_{2g}\sigma_{3g}|\sigma_{2g}\sigma_{2g})\}$

$H_{KN_3} = -2(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-)$

$H_{KQ_2} = -(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{KO_1} = 0$

$H_{KQ_3} = -\sqrt{2}\,(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{KO_3} = 0$

$H_{LM_1} = -2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{KP_1} = 0$

$H_{LM_2} = (\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{KP_2} = 0$

$H_{LM_3} = -\sqrt{2}\,(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{KP_3} = 0$

$H_{LN_1} = 0$

$H_{KQ_1} = -2(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{LN_3} = 0$

$H_{LO_1} = H_{BO_1} + \sqrt{2}\,\{(\sigma_{2g}\sigma_{3g}|\sigma_{3g}\sigma_{3g}) - (\sigma_{2g}\sigma_{3g}|\sigma_{2g}\sigma_{2g})\}$

$H_{LO_3} = -2(\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)$

$H_{LQ_1} = -2(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{LP_1} = 0$

$H_{LQ_2} = (\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{LP_2} = 0$

$H_{LQ_3} = -\sqrt{2}\,(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{LP_3} = 0$

$$H_{M_1M_2} = \frac{1}{2}\{-K(\sigma_{3u}, \pi_u{}^+) + K(\sigma_{2g}, \pi_u{}^+) + K(\sigma_{3u}, \pi_g{}^+) - K(\sigma_{2g}, \pi_g{}^+)\}$$

$$H_{M_1M_3} = \frac{1}{\sqrt{2}}\{K(\sigma_{3u}, \pi_u{}^+) - K(\sigma_{2g}, \pi_u{}^+) + K(\sigma_{3u}, \pi_g{}^+) - K(\sigma_{2g}, \pi_g{}^+)\}$$

$$H_{M_1N_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)\}$$

$H_{M_1N_3} = (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$$H_{M_1O_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$H_{M_1O_3} = (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{M_1P_2} = 0$

$H_{M_1P_1} = (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) + (\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{3u})$

$H_{M_1P_3} = 0$

$H_{M_1Q_1} = H_{F_1P_1} - (\sigma_{2u}\sigma_{3u}|\sigma_{3g}\sigma_{3g}) + (\sigma_{2u}\sigma_{3u}|\sigma_{2g}\sigma_{2g}) + (\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u}) - (\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$

$$H_{M_1Q_2} = -\frac{1}{2}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{M_1Q_3} = \frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) + (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{M_2M_3} = -\frac{1}{\sqrt{2}}\{K(\sigma_{3u}, \pi_u{}^+) + K(\sigma_{2g}, \pi_u{}^+) - K(\sigma_{3u}, \pi_g{}^+) - K(\sigma_{2g}, \pi_g{}^+)\}$$

$H_{M_2N_1} = \frac{1}{\sqrt{2}}(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{M_2P_1} = 0$

$H_{M_2N_3} = (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{M_2P_2} = (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) - (\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{3u})$

$H_{M_2O_1} = -\frac{1}{\sqrt{2}}(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{M_2P_3} = 0$

$H_{M_2O_2} = -(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$$H_{M_2Q_1} = -\frac{1}{2}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$H_{M_2Q_2} = H_{M_1Q_1} - 2(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u})$

$$H_{M_2Q_3} = -\frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$H_{M_3N_1} = (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{M_3O_3} = \sqrt{2}\,(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)$

$H_{M_3N_3} = \sqrt{2}\,(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)$

$H_{M_3P_1} = 0$

$H_{M_3O_1} = (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{M_3P_2} = 0$

$$H_{M_3P_3} = (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) - (\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{3u})$$

$$H_{M_3Q_1} = -\frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) + (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{M_3Q_2} = \frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) - (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\}$$

$$H_{M_3Q_3} = H_{M_1Q_1} + \frac{1}{2}\{(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) + (\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)\} - 2(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u})$$

$$H_{N_1N_3} = \sqrt{2}\{K(\sigma_{3g}, \pi_u{}^+) - K(\sigma_{2g}, \pi_u{}^+)\} \qquad H_{N_1O_3} = 0$$

$$H_{N_1O_1} = (\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-) - (\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+)$$

$$H_{N_1P_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$$

$$H_{N_1P_2} = -\frac{1}{\sqrt{2}}(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{N_1P_3} = -(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$$

$$H_{N_1Q_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$$

$$H_{N_1Q_2} = \frac{1}{\sqrt{2}}(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{N_3P_3} = \sqrt{2}(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)$$

$$H_{N_1Q_3} = (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{N_3Q_1} = (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$$

$$H_{N_3O_1} = 0 \qquad H_{N_3Q_2} = (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$$

$$H_{N_3O_3} = (\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-) - (\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+) \qquad H_{N_3Q_3} = \sqrt{2}(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)$$

$$H_{N_3P_1} = -(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{O_1O_3} = \sqrt{2}\{K(\sigma_{3g}, \pi_g{}^+) - K(\sigma_{2g}, \pi_g{}^+)\}$$

$$H_{N_3P_2} = (\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$$

$$H_{O_1P_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$$

$$H_{O_1P_2} = \frac{1}{\sqrt{2}}(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) \qquad H_{O_1P_3} = -(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$$

$$H_{O_1Q_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$$

$$H_{O_1Q_2} = -\frac{1}{\sqrt{2}}(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) \qquad H_{O_3P_3} = \sqrt{2}(\sigma_{2g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)$$

$$H_{O_1Q_3} = (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) \qquad H_{O_3Q_1} = (\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$$

$$H_{O_3P_1} = -(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) \qquad H_{O_3Q_2} = -(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$$

$$H_{O_3P_2} = -(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-) \qquad H_{O_3Q_3} = \sqrt{2}(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)$$

$$H_{P_1P_2} = \frac{1}{2}\{-K(\sigma_{3g}, \pi_u{}^+) + K(\sigma_{2u}, \pi_u{}^+) + K(\sigma_{3g}, \pi_g{}^+) - K(\sigma_{2u}, \pi_g{}^+)\}$$

$$H_{P_1P_3} = \frac{1}{\sqrt{2}}\{K(\sigma_{3g}, \pi_u{}^+) - K(\sigma_{2u}, \pi_u{}^+) + K(\sigma_{3g}, \pi_g{}^+) - K(\sigma_{2u}, \pi_g{}^+)\}$$

$$H_{P_1Q_1} = H_{F_1M_1} + \{(\sigma_{2g}\sigma_{3g}|\sigma_{2u}\sigma_{2u}) - (\sigma_{2g}\sigma_{3g}|\sigma_{3u}\sigma_{3u}) + (\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{2u}) - (\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})\}$$

$$H_{P_1Q_2} = \frac{1}{2}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$$

$$H_{P_1Q_3} = -\frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) + (\sigma_{3g}\pi_g{}^+|\sigma_{2g}\pi_g{}^-)\}$$

$$H_{P_2P_3} = \frac{1}{\sqrt{2}}\{-K(\sigma_{3g}, \pi_u{}^+) - K(\sigma_{2u}, \pi_u{}^+) + K(\sigma_{3g}, \pi_g{}^+) + K(\sigma_{2u}, \pi_g{}^+)\}$$

$$H_{P_2Q_1} = -\frac{1}{2}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$$

$$H_{P_2Q_2} = -H_{P_1Q_1} + 2(\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$$

$$H_{P_2Q_3} = \frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$$

$$H_{P_3Q_1} = \frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) + (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$$

$$H_{P_3Q_2} = \frac{1}{\sqrt{2}}\{(\sigma_{2g}\pi_u{}^+|\sigma_{3g}\pi_u{}^-) - (\sigma_{2g}\pi_g{}^+|\sigma_{3g}\pi_g{}^-)\}$$

$$H_{P_3Q_3} = -H_{P_1Q_1} - \frac{1}{2}\{(\sigma_{2g}\pi_u^+|\sigma_{3g}\pi_u^-) + (\sigma_{2g}\pi_g^+|\sigma_{3g}\pi_g^-)\} + 2(\sigma_{2g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$$

$$H_{Q_1Q_2} = \frac{1}{2}\{-K(\sigma_{2u}, \pi_u^+) + K(\sigma_{2g}, \pi_u^+) + K(\sigma_{2u}, \pi_g^+) - K(\sigma_{2g}, \pi_g^+)\}$$

$$H_{Q_1Q_3} = \frac{1}{\sqrt{2}}\{K(\sigma_{2u}, \pi_u^+) - K(\sigma_{2g}, \pi_u^+) + K(\sigma_{2u}, \pi_g^+) - K(\sigma_{2g}, \pi_g^+)\}$$

$$H_{Q_2Q_3} = \frac{1}{\sqrt{2}}\{-K(\sigma_{2u}, \pi_u^+) - K(\sigma_{2g}, \pi_u^+) + K(\sigma_{2u}, \pi_g^+) + K(\sigma_{2g}, \pi_g^+)\}$$

(v) $^3\Sigma_u^+$ and $^3\Sigma_u^-$ (O_2)

Configurations used	α, β	γ
A, B, C, D, E_i, F_i	σ_{1g}, σ_{1u}, σ_{2g}, σ_{2u}	σ_{3g}, σ_{3u}, $\pi_u^\pm$, $\pi_g^\pm$
G, M_i, K_i	σ_{1g}, σ_{1u}, σ_{2g}, σ_{3u}	σ_{2u}, σ_{3g}, $\pi_u^\pm$, $\pi_g^\pm$
H, J_i	σ_{1g}, σ_{1u}, σ_{2u}, σ_{3u}	σ_{2g}, σ_{3g}, $\pi_u^\pm$, $\pi_g^\pm$
I_i	σ_{1g}, σ_{1u}, σ_{2g}, σ_{3g}	σ_{2u}, σ_{3u}, $\pi_u^\pm$, $\pi_g^\pm$
L_i, N_i	σ_{1g}, σ_{1u}, σ_{2u}, σ_{3g}	σ_{2g}, σ_{3u}, $\pi_u^\pm$, $\pi_g^\pm$
Q	σ_{1g}, σ_{1u}, $\pi_u^\pm$, $\pi_g^\pm$	σ_{2g}, σ_{2u}, σ_{3g}, σ_{3u}

$$\begin{aligned}
H_{AA} = {} & p - h(\pi_g^+) - h(\pi_u^-) - 2h(\sigma_{3u}) \\
& + s + t - t(\pi_g^+) - t(\pi_u^-) - 2t(\sigma_{3u}) \\
& + J(\pi_g^+, \pi_u^-) + 2J(\pi_g^+, \sigma_{3g}) + 2J(\pi_g^+, \pi_g^-) + 2J(\pi_g^+, \pi_u^+) \\
& \quad + 2J(\sigma_{3g}, \pi_u^-) + 2J(\pi_u^-, \pi_g^-) + 2J(\pi_u^-, \pi_u^+) \\
& \quad + J(\sigma_{3g}, \sigma_{3g}) + 4J(\sigma_{3g}, \pi_g^-) + 4J(\sigma_{3g}, \pi_u^+) \\
& \quad + J(\pi_g^-, \pi_g^-) + 4J(\pi_g^-, \pi_u^+) \\
& \quad + J(\pi_u^+, \pi_u^+) \\
& - \tfrac{1}{2}\{f + g - g(\pi_g^+) - g(\pi_u^-) - 2g(\sigma_{3u}) \\
& \quad + 2K(\pi_g^+, \pi_u^-) + 2K(\pi_g^+, \sigma_{3g}) + 2K(\pi_g^+, \pi_g^-) + 2K(\pi_g^+, \pi_u^+) \\
& \quad + 2K(\pi_u^-, \sigma_{3g}) + 2K(\pi_u^-, \pi_g^-) + 2K(\pi_u^-, \pi_u^+) \\
& \quad + 4K(\sigma_{3g}, \pi_g^-) + 4K(\sigma_{3g}, \pi_u^+) \\
& \quad + 4K(\pi_g^-, \pi_u^+)\} \\
& \pm \{(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+) - (\pi_g^+\pi_u^+|\pi_g^+\pi_u^+)\}
\end{aligned}$$

$$\begin{aligned}
H_{BB} = {} & p - h(\pi_g^+) - h(\pi_u^-) - 2h(\sigma_{3g}) \\
& + s + t - t(\pi_g^+) - t(\pi_u^-) - 2t(\sigma_{3g}) \\
& + J(\pi_g^+, \pi_u^-) + 2J(\pi_g^+, \sigma_{3u}) + 2J(\pi_g^+, \pi_g^-) + 2J(\pi_g^+, \pi_u^+) \\
& \quad + 2J(\pi_u^-, \sigma_{3u}) + 2J(\pi_u^-, \pi_g^-) + 2J(\pi_u^-, \pi_u^+) \\
& \quad + J(\sigma_{3u}, \sigma_{3u}) + 4J(\sigma_{3u}, \pi_g^-) + 4J(\sigma_{3u}, \pi_u^+) \\
& \quad + J(\pi_g^-, \pi_g^-) + 4J(\pi_g^-, \pi_u^+) \\
& \quad + J(\pi_u^+, \pi_u^+) \\
& - \tfrac{1}{2}\{f + g - g(\pi_g^+) - g(\pi_u^-) - 2g(\sigma_{3g}) \\
& \quad + 2K(\pi_g^+, \pi_u^-) + 2K(\pi_g^+, \sigma_{3u}) + 2K(\pi_g^+, \pi_g^-) + 2K(\pi_g^+, \pi_u^+) \\
& \quad + 2K(\pi_u^-, \sigma_{3u}) + 2K(\pi_u^-, \pi_g^-) + 2K(\pi_u^-, \pi_u^+) \\
& \quad + 4K(\sigma_{3u}, \pi_g^-) + 4K(\sigma_{3u}, \pi_u^+) \\
& \quad + 4K(\pi_g^-, \pi_u^+)\} \\
& \pm \{(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+) - (\pi_g^+\pi_u^+|\pi_g^+\pi_u^+)\}
\end{aligned}$$

$$\begin{aligned}
H_{CC} = {} & p - h(\pi_g^+) - h(\pi_u^+) - 2h(\pi_u^-) \\
& + s + t - t(\pi_g^+) - t(\pi_u^+) - 2t(\pi_u^-) \\
& + J(\pi_g^+, \pi_u^+) + 2J(\pi_g^+, \sigma_{3g}) + 2J(\pi_g^+, \pi_g^-) + 2J(\pi_g^+, \sigma_{3u}) \\
& \quad + 2J(\pi_u^+, \sigma_{3g}) + 2J(\pi_u^+, \pi_g^-) + 2J(\pi_u^+, \sigma_{3u}) \\
& \quad + J(\sigma_{3g}, \sigma_{3g}) + 4J(\sigma_{3g}, \pi_g^-) + 4J(\sigma_{3g}, \sigma_{3u}) \\
& \quad + J(\pi_g^-, \pi_g^-) + 4J(\pi_g^-, \sigma_{3u}) \\
& \quad + J(\sigma_{3u}, \sigma_{3u})
\end{aligned}$$

$$
\begin{aligned}
&-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_u{}^+)-2g(\pi_u{}^-)\\
&\quad+2K(\pi_g{}^+,\pi_u{}^+)+2K(\pi_g{}^+,\sigma_{3g})+2K(\pi_g{}^+,\pi_g{}^-)+2K(\pi_g{}^+,\sigma_{3u})\\
&\qquad+2K(\pi_u{}^+,\sigma_{3g})+2K(\pi_u{}^+,\pi_g{}^-)+2K(\pi_u{}^+,\sigma_{3u})\\
&\qquad\qquad+4K(\sigma_{3g},\pi_g{}^-)+4K(\sigma_{3g},\sigma_{3u})\\
&\qquad\qquad\qquad+4K(\pi_g{}^-,\sigma_{3u})\}\\
&\mp(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)
\end{aligned}
$$

$$
\begin{aligned}
H_{DD}=&\,p-h(\pi_g{}^+)-h(\pi_u{}^+)-2h(\pi_g{}^-)\\
&+s+t-t(\pi_g{}^+)-t(\pi_u{}^+)-2t(\pi_g{}^-)\\
&+J(\pi_g{}^+,\pi_u{}^+)+2J(\pi_g{}^+,\sigma_{3g})+2J(\pi_g{}^+,\pi_u{}^-)+2J(\pi_g{}^+,\sigma_{3u})\\
&\qquad+2J(\pi_u{}^+,\sigma_{3g})+2J(\pi_u{}^+,\pi_u{}^-)+2J(\pi_u{}^+,\sigma_{3u})\\
&\qquad+J(\sigma_{3g},\sigma_{3g})+4J(\sigma_{3g},\pi_u{}^-)+4J(\sigma_{3g},\sigma_{3u})\\
&\qquad\qquad+J(\pi_u{}^-,\pi_u{}^-)+4J(\pi_u{}^-,\sigma_{3u})\\
&\qquad\qquad\qquad+J(\sigma_{3u},\sigma_{3u})\\
&-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_u{}^+)-2g(\pi_g{}^-)\\
&\quad+2K(\pi_g{}^+,\pi_u{}^+)+2K(\pi_g{}^+,\sigma_{3g})+2K(\pi_g{}^+,\pi_u{}^-)+2K(\pi_g{}^+,\sigma_{3u})\\
&\qquad+2K(\pi_u{}^+,\sigma_{3g})+2K(\pi_u{}^+,\pi_u{}^-)+2K(\pi_u{}^+,\sigma_{3u})\\
&\qquad\qquad+4K(\sigma_{3g},\pi_u{}^-)+4K(\sigma_{3g},\sigma_{3u})\\
&\qquad\qquad\qquad+4K(\pi_u{}^-,\sigma_{3u})\}\\
&\mp(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)
\end{aligned}
$$

$$
\left.\begin{array}{l}
H_{E_1E_1}(^3\textstyle\sum u^-)\\
H_{E_2E_2}(^3\textstyle\sum u^+)\\
H_{E_3E_3}(^3\textstyle\sum u^-)
\end{array}\right\}
$$

$$
\begin{aligned}
&=p-h(\pi_g{}^+)-h(\pi_g{}^-)-h(\sigma_{3g})-h(\sigma_{3u})\\
&\quad+s+t-t(\pi_g{}^+)-t(\pi_g{}^-)-t(\sigma_{3g})-t(\sigma_{3u})\\
&\quad+J(\pi_g{}^+,\pi_g{}^-)+J(\pi_g{}^+,\sigma_{3g})+J(\pi_g{}^+,\sigma_{3u})+2J(\pi_g{}^+,\pi_u{}^+)+2J(\pi_g{}^+,\pi_u{}^-)\\
&\qquad+J(\pi_g{}^-,\sigma_{3g})+J(\pi_g{}^-,\sigma_{3u})+2J(\pi_g{}^-,\pi_u{}^+)+2J(\pi_g{}^-,\pi_u{}^-)\\
&\qquad\qquad+J(\sigma_{3g},\sigma_{3u})+2J(\sigma_{3g},\pi_u{}^+)+2J(\sigma_{3g},\pi_u{}^-)\\
&\qquad\qquad\qquad+2J(\sigma_{3u},\pi_u{}^+)+2J(\sigma_{3u},\pi_u{}^-)\\
&\qquad\qquad\qquad+J(\pi_u{}^+,\pi_u{}^+)+4J(\pi_u{}^+,\pi_u{}^-)\\
&\qquad\qquad\qquad\qquad+J(\pi_u{}^-,\pi_u{}^-)\\
&\quad-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_g{}^-)-g(\sigma_{3g})-g(\sigma_{3u})\\
&\qquad+2K(\pi_g{}^+,\pi_u{}^+)+2K(\pi_g{}^+,\pi_u{}^-)+2K(\pi_g{}^-,\pi_u{}^+)+2K(\pi_g{}^-,\pi_u{}^-)\\
&\qquad+2K(\sigma_{3g},\pi_u{}^+)+2K(\sigma_{3g},\pi_u{}^-)+2K(\sigma_{3u},\pi_u{}^+)+2K(\sigma_{3u},\pi_u{}^-)\\
&\qquad\qquad+4K(\pi_u{}^+,\pi_u{}^-)\}\\
&\quad+\left\{\begin{array}{ll}
-K(\pi_g{}^+,\pi_g{}^-)-K(\pi_g{}^+,\sigma_{3g})-K(\pi_g{}^+,\sigma_{3u}) & +K(\sigma_{3g},\sigma_{3u})\\
+K(\pi_g{}^+,\pi_g{}^-)-K(\pi_g{}^+,\sigma_{3g})-K(\pi_g{}^+,\sigma_{3u}) & -K(\sigma_{3g},\sigma_{3u})\\
-K(\pi_g{}^+,\pi_g{}^-) & -K(\sigma_{3g},\sigma_{3u})
\end{array}\right.
\end{aligned}
$$

$$
\left.\begin{array}{l}
H_{F_1F_1}(^3\textstyle\sum u^-)\\
H_{F_2F_2}(^3\textstyle\sum u^+)\\
H_{F_3F_3}(^3\textstyle\sum u^-)
\end{array}\right\}
$$

$$
\begin{aligned}
&=p-h(\pi_u{}^+)-h(\pi_u{}^-)-h(\sigma_{3g})-h(\sigma_{3u})\\
&\quad+s+t-t(\pi_u{}^+)-t(\pi_u{}^-)-t(\sigma_{3g})-t(\sigma_{3u})\\
&\quad+J(\pi_u{}^+,\pi_u{}^-)+J(\pi_u{}^+,\sigma_{3g})+J(\pi_u{}^+,\sigma_{3u})+2J(\pi_u{}^+,\pi_g{}^+)+2J(\pi_u{}^+,\pi_g{}^-)\\
&\qquad+J(\pi_u{}^-,\sigma_{3g})+J(\pi_u{}^-,\sigma_{3u})+2J(\pi_u{}^-,\pi_g{}^+)+2J(\pi_u{}^-,\pi_g{}^-)\\
&\qquad\qquad+J(\sigma_{3g},\sigma_{3u})+2J(\sigma_{3g},\pi_g{}^+)+2J(\sigma_{3g},\pi_g{}^-)\\
&\qquad\qquad\qquad+2J(\sigma_{3u},\pi_g{}^+)+2J(\sigma_{3u},\pi_g{}^-)\\
&\qquad\qquad\qquad+J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_g{}^-)\\
&\qquad\qquad\qquad\qquad+J(\pi_g{}^-,\pi_g{}^-)\\
&\quad-\tfrac{1}{2}\{f+g-g(\pi_u{}^+)-g(\pi_u{}^-)-g(\sigma_{3g})-g(\sigma_{3u})\\
&\qquad+2K(\pi_u{}^+,\pi_g{}^+)+2K(\pi_u{}^+,\pi_g{}^-)+2K(\pi_u{}^-,\pi_g{}^+)+2K(\pi_u{}^-,\pi_g{}^-)\\
&\qquad+2K(\sigma_{3g},\pi_g{}^+)+2K(\sigma_{3g},\pi_g{}^-)+2K(\sigma_{3u},\pi_g{}^+)+2K(\sigma_{3u},\pi_g{}^-)\\
&\qquad\qquad+4K(\pi_g{}^+,\pi_g{}^-)\}\\
&\quad+\left\{\begin{array}{ll}
-K(\pi_u{}^+,\pi_u{}^-)-K(\pi_u{}^+,\sigma_{3g})-K(\pi_u{}^+,\sigma_{3u}) & +K(\sigma_{3g},\sigma_{3u})\\
+K(\pi_u{}^+,\pi_u{}^-)-K(\pi_u{}^+,\sigma_{3g})-K(\pi_u{}^+,\sigma_{3u}) & -K(\sigma_{3g},\sigma_{3u})\\
-K(\pi_u{}^+,\pi_u{}^-) & -K(\sigma_{3g},\sigma_{3u})
\end{array}\right.
\end{aligned}
$$

$$
\begin{aligned}
H_{GG}=\;& p-h(\pi_g{}^+)-h(\pi_u{}^-)-2h(\sigma_{2u})\\
&+s+t-t(\pi_g{}^+)-t(\pi_u{}^-)-2t(\sigma_{2u})\\
&+J(\pi_g{}^+,\pi_u{}^-)+2J(\pi_g{}^+,\sigma_{3g})+2J(\pi_g{}^+,\pi_g{}^-)+2J(\pi_g{}^+,\pi_u{}^+)\\
&\qquad+2J(\pi_u{}^-,\sigma_{3g})+2J(\pi_u{}^-,\pi_g{}^-)+2J(\pi_u{}^-,\pi_u{}^+)\\
&\qquad+J(\sigma_{3g},\sigma_{3g})+4J(\sigma_{3g},\pi_g{}^-)+4J(\sigma_{3g},\pi_u{}^+)\\
&\qquad\qquad+J(\pi_g{}^-,\pi_g{}^-)+4J(\pi_g{}^-,\pi_u{}^+)\\
&\qquad\qquad\qquad+J(\pi_u{}^+,\pi_u{}^+)\\
&-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_u{}^-)-2g(\sigma_{2u})\\
&\quad+2K(\pi_g{}^+,\pi_u{}^-)+2K(\pi_g{}^+,\sigma_{3g})+2K(\pi_g{}^+,\pi_g{}^-)+2K(\pi_g{}^+,\pi_u{}^+)\\
&\qquad+2K(\pi_u{}^-,\sigma_{3g})+2K(\pi_u{}^-,\pi_g{}^-)+2K(\pi_u{}^-,\pi_u{}^+)\\
&\qquad\qquad+4K(\sigma_{3g},\pi_g{}^-)+4K(\sigma_{3g},\pi_u{}^+)\\
&\qquad\qquad\qquad+4K(\pi_g{}^-,\pi_u{}^+)\}\\
&\pm\{(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)-(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\}
\end{aligned}
$$

$$
\begin{aligned}
H_{HH}=\;& p-h(\pi_g{}^+)-h(\pi_u{}^-)-2h(\sigma_{2g})\\
&+s+t-t(\pi_g{}^+)-t(\pi_u{}^-)-2t(\sigma_{2g})\\
&+J(\pi_g{}^+,\pi_u{}^-)+2J(\pi_g{}^+,\sigma_{3g})+2J(\pi_g{}^+,\pi_g{}^-)+2J(\pi_g{}^+,\pi_u{}^+)\\
&\qquad+2J(\pi_u{}^-,\sigma_{3g})+2J(\pi_u{}^-,\pi_g{}^-)+2J(\pi_u{}^-,\pi_u{}^+)\\
&\qquad+J(\sigma_{3g},\sigma_{3g})+4J(\sigma_{3g},\pi_g{}^-)+4J(\sigma_{3g},\pi_u{}^+)\\
&\qquad\qquad+J(\pi_g{}^-,\pi_g{}^-)+4J(\pi_g{}^-,\pi_u{}^+)\\
&\qquad\qquad\qquad+J(\pi_u{}^+,\pi_u{}^+)\\
&-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_u{}^-)-2g(\sigma_{2g})\\
&\quad+2K(\pi_g{}^+,\pi_u{}^-)+2K(\pi_g{}^+,\sigma_{3g})+2K(\pi_g{}^+,\pi_g{}^-)+2K(\pi_g{}^+,\pi_u{}^+)\\
&\qquad+2K(\pi_u{}^-,\sigma_{3g})+2K(\pi_u{}^-,\pi_g{}^-)+2K(\pi_u{}^-,\pi_u{}^+)\\
&\qquad\qquad+4K(\sigma_{3g},\pi_g{}^-)+4K(\sigma_{3g},\pi_u{}^+)\\
&\qquad\qquad\qquad+4K(\pi_g{}^-,\pi_u{}^+)\}\\
&\pm\{(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)-(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\}
\end{aligned}
$$

$$
\left.\begin{matrix}H_{I_1I_1}\\H_{I_2I_2}\\H_{I_3I_3}\end{matrix}\right\}
\begin{aligned}
=\;& p-h(\pi_g{}^+)-h(\pi_u{}^-)-h(\sigma_{3u})-h(\sigma_{2u})\\
&+s+t-t(\pi_g{}^+)-t(\pi_u{}^-)-t(\sigma_{3u})-t(\sigma_{2u})\\
&+J(\pi_g{}^+,\pi_u{}^-)+J(\pi_g{}^+,\sigma_{3u})+J(\pi_g{}^+,\sigma_{2u})+2J(\pi_g{}^+,\pi_g{}^-)+2J(\pi_g{}^+,\pi_u{}^+)\\
&\qquad+J(\pi_u{}^-,\sigma_{3u})+J(\pi_u{}^-,\sigma_{2u})+2J(\pi_u{}^-,\pi_g{}^-)+2J(\pi_u{}^-,\pi_u{}^+)\\
&\qquad\qquad+J(\sigma_{3u},\sigma_{2u})+2J(\sigma_{3u},\pi_g{}^-)+2J(\sigma_{3u},\pi_u{}^+)\\
&\qquad\qquad\qquad+2J(\sigma_{2u},\pi_g{}^-)+2J(\sigma_{2u},\pi_u{}^+)\\
&\qquad\qquad\qquad+J(\pi_g{}^-,\pi_g{}^-)+4J(\pi_g{}^-,\pi_u{}^+)\\
&\qquad\qquad\qquad\qquad+J(\pi_u{}^+,\pi_u{}^+)\\
&-\tfrac{1}{2}\{f+g-g(\pi_g{}^+)-g(\pi_u{}^-)-g(\sigma_{3u})-g(\sigma_{2u})\\
&\quad+2K(\pi_g{}^+,\pi_g{}^-)+2K(\pi_g{}^+,\pi_u{}^+)+2K(\pi_u{}^-,\pi_g{}^-)+2K(\pi_u{}^-,\pi_u{}^+)\\
&\quad+2K(\sigma_{3u},\pi_g{}^-)+2K(\sigma_{3u},\pi_u{}^+)+2K(\sigma_{2u},\pi_g{}^-)+2K(\sigma_{2u},\pi_u{}^+)\\
&\qquad\qquad+4K(\pi_g{}^-,\pi_u{}^+)\}\\
&+\begin{cases}-K(\pi_g{}^+,\pi_u{}^-)-\tfrac{1}{2}K(\pi_g{}^+,\sigma_{3u})-\tfrac{1}{2}K(\pi_g{}^+,\sigma_{2u})-\tfrac{1}{2}K(\pi_u{}^-,\sigma_{3u})-\tfrac{1}{2}K(\pi_u{}^-,\sigma_{2u})\\ \qquad\qquad+K(\sigma_{2u},\sigma_{3u})\\ +K(\pi_g{}^+,\pi_u{}^-)-\tfrac{1}{2}K(\pi_g{}^+,\sigma_{3u})-\tfrac{1}{2}K(\pi_g{}^+,\sigma_{2u})-\tfrac{1}{2}K(\pi_u{}^-,\sigma_{3u})-\tfrac{1}{2}K(\pi_u{}^-,\sigma_{2u})\\ \qquad\qquad-K(\sigma_{2u},\sigma_{3u})\\ -K(\pi_g{}^+,\pi_u{}^-)\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad-K(\sigma_{2u},\sigma_{3u})\end{cases}\\
&\pm\begin{cases}(\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)-(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\\ (\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)+(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\\ (\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)-(\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+)\end{cases}
\end{aligned}
$$

$$
\left.\begin{matrix}H_{J_1J_1}\\H_{J_2J_2}\\H_{J_3J_3}\end{matrix}\right\}
\begin{aligned}
=\;& p-h(\pi_g{}^+)-h(\pi_u{}^-)-h(\sigma_{3g})-h(\sigma_{2g})\\
&+s+t-t(\pi_g{}^+)-t(\pi_u{}^-)-t(\sigma_{3g})-t(\sigma_{2g})
\end{aligned}
$$

$$
\begin{aligned}
&+J(\pi_g^+,\pi_u^-)+J(\pi_g^+,\sigma_{3g})+J(\pi_g^+,\sigma_{2g})+2J(\pi_g^+,\pi_g^-)+2J(\pi_g^+,\pi_u^+)\\
&\quad+J(\pi_u^-,\sigma_{3g})+J(\pi_u^-,\sigma_{2g})+2J(\pi_u^-,\pi_g^-)+2J(\pi_u^-,\pi_u^+)\\
&\quad+J(\sigma_{3g},\sigma_{2g})+2J(\sigma_{3g},\pi_g^-)+2J(\sigma_{3g},\pi_u^+)\\
&\quad+2J(\sigma_{2g},\pi_g^-)+2J(\sigma_{2g},\pi_u^+)\\
&\quad+J(\pi_g^-,\pi_g^-)+4J(\pi_g^-,\pi_u^+)\\
&\quad+J(\pi_u^+,\pi_u^+)\\
&-\tfrac{1}{2}\{f+g-g(\pi_g^+)-g(\pi_u^-)-g(\sigma_{3g})-g(\sigma_{2g})\\
&\quad+2K(\pi_g^+,\pi_g^-)+2K(\pi_g^+,\pi_u^+)+2K(\pi_u^-,\pi_g^-)+2K(\pi_u^-,\pi_u^+)\\
&\quad+2K(\sigma_{3g},\pi_g^-)+2K(\sigma_{3g},\pi_u^+)+2K(\sigma_{2g},\pi_g^-)+2K(\sigma_{2g},\pi_u^+)\\
&\quad+4K(\pi_g^-,\pi_u^+)\}\\
&+\begin{cases}
-K(\pi_g^+,\pi_u^-)-\tfrac{1}{2}K(\pi_g^+,\sigma_{3g})-\tfrac{1}{2}K(\pi_g^+,\sigma_{2g})-\tfrac{1}{2}K(\pi_u^-,\sigma_{3g})-\tfrac{1}{2}K(\pi_u^-,\sigma_{2g})\\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad+K(\sigma_{2g},\sigma_{3g})\\
+K(\pi_g^+,\pi_u^-)-\tfrac{1}{2}K(\pi_g^+,\sigma_{3g})-\tfrac{1}{2}K(\pi_g^+,\sigma_{2g})-\tfrac{1}{2}K(\pi_u^-,\sigma_{3g})-\tfrac{1}{2}K(\pi_u^-,\sigma_{2g})\\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad-K(\sigma_{2g},\sigma_{3g})\\
-K(\pi_g^+,\pi_u^-)\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad-K(\sigma_{2g},\sigma_{3g})
\end{cases}\\
&\pm\begin{cases}
(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+)-(\pi_g^+\pi_u^+|\pi_g^+\pi_u^+)\\
(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+)+(\pi_g^+\pi_u^+|\pi_g^+\pi_u^+)\\
(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+)-(\pi_g^+\pi_u^+|\pi_g^+\pi_u^+)
\end{cases}
\end{aligned}
$$

$$
\left.\begin{matrix}
H_{K_1K_1}(^3\textstyle\sum_u^-)\\
H_{K_2K_2}(^3\textstyle\sum_u^+)\\
H_{K_3K_3}(^3\textstyle\sum_u^-)
\end{matrix}\right\}=p-h(\pi_u^+)-h(\pi_u^-)-h(\sigma_{3g})-h(\sigma_{2u})
$$

$$
\begin{aligned}
&+s+t-t(\pi_u^+)-t(\pi_u^-)-t(\sigma_{3g})-t(\sigma_{2u})\\
&+J(\pi_u^+,\pi_u^-)+J(\pi_u^+,\sigma_{3g})+J(\pi_u^+,\sigma_{2u})+2J(\pi_u^+,\pi_g^+)+2J(\pi_u^+,\pi_g^-)\\
&\quad+J(\pi_u^-,\sigma_{3g})+J(\pi_u^-,\sigma_{2u})+2J(\pi_u^-,\pi_g^+)+2J(\pi_u^-,\pi_g^-)\\
&\quad+J(\sigma_{3g},\sigma_{2u})+2J(\sigma_{3g},\pi_g^+)+2J(\sigma_{3g},\pi_g^-)\\
&\quad+2J(\sigma_{2u},\pi_g^+)+2J(\sigma_{2u},\pi_g^-)\\
&\quad+J(\pi_g^+,\pi_g^+)+4J(\pi_g^+,\pi_g^-)\\
&\quad+J(\pi_g^-,\pi_g^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_u^+)-g(\pi_u^-)-g(\sigma_{3g})-g(\sigma_{2u})\\
&\quad+2K(\pi_u^+,\pi_g^+)+2K(\pi_u^+,\pi_g^-)+2K(\pi_u^-,\pi_g^+)+2K(\pi_u^-,\pi_g^-)\\
&\quad+2K(\sigma_{3g},\pi_g^+)+2K(\sigma_{3g},\pi_g^-)+2K(\sigma_{2u},\pi_g^+)+2K(\sigma_{2u},\pi_g^-)\\
&\quad+4K(\pi_g^+,\pi_g^-)\}\\
&+\begin{cases}
-K(\pi_u^+,\pi_u^-)-K(\pi_u^+,\sigma_{3g})-K(\pi_u^+,\sigma_{2u})+K(\sigma_{3g},\sigma_{2u})\\
+K(\pi_u^+,\pi_u^-)-K(\pi_u^+,\sigma_{3g})-K(\pi_u^+,\sigma_{2u})-K(\sigma_{3g},\sigma_{2u})\\
-K(\pi_u^+,\pi_u^-)\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad-K(\sigma_{3g},\sigma_{2u})
\end{cases}
\end{aligned}
$$

$$
\left.\begin{matrix}
H_{L_1L_1}(^3\textstyle\sum_u^-)\\
H_{L_2L_2}(^3\textstyle\sum_u^+)\\
H_{L_3L_3}(^3\textstyle\sum_u^-)
\end{matrix}\right\}=p-h(\pi_u^+)-h(\pi_u^-)-h(\sigma_{3u})-h(\sigma_{2g})
$$

$$
\begin{aligned}
&+s+t-t(\pi_u^+)-t(\pi_u^-)-t(\sigma_{3u})-t(\sigma_{2g})\\
&+J(\pi_u^+,\pi_u^-)+J(\pi_u^+,\sigma_{3u})+J(\pi_u^+,\sigma_{2g})+2J(\pi_u^+,\pi_g^+)+2J(\pi_u^+,\pi_g^-)\\
&\quad+J(\pi_u^-,\sigma_{3u})+J(\pi_u^-,\sigma_{2g})+2J(\pi_u^-,\pi_g^+)+2J(\pi_u^-,\pi_g^-)\\
&\quad+J(\sigma_{3u},\sigma_{2g})+2J(\sigma_{3u},\pi_g^+)+2J(\sigma_{3u},\pi_g^-)\\
&\quad+2J(\sigma_{2g},\pi_g^+)+2J(\sigma_{2g},\pi_g^-)\\
&\quad+J(\pi_g^+,\pi_g^+)+4J(\pi_g^+,\pi_g^-)\\
&\quad+J(\pi_g^-,\pi_g^-)\\
&-\tfrac{1}{2}\{f+g-g(\pi_u^+)-g(\pi_u^-)-g(\sigma_{3u})-g(\sigma_{2g})\\
&\quad+2K(\pi_u^+,\pi_g^+)+2K(\pi_u^+,\pi_g^-)+2K(\pi_u^-,\pi_g^+)+2K(\pi_u^-,\pi_g^-)\\
&\quad+2K(\sigma_{3u},\pi_g^+)+2K(\sigma_{3u},\pi_g^-)+2K(\sigma_{2g},\pi_g^+)+2K(\sigma_{2g},\pi_g^-)\\
&\quad+4K(\pi_g^+,\pi_g^-)\}\\
&+\begin{cases}
-K(\pi_u^+,\pi_u^-)-K(\pi_u^+,\sigma_{3u})-K(\pi_u^+,\sigma_{2g})+K(\sigma_{2g},\sigma_{3u})\\
+K(\pi_u^+,\pi_u^-)-K(\pi_u^+,\sigma_{3u})-K(\pi_u^+,\sigma_{2g})-K(\sigma_{2g},\sigma_{3u})\\
-K(\pi_u^+,\pi_u^-)\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad-K(\sigma_{2g},\sigma_{3u})
\end{cases}
\end{aligned}
$$

$$\left.\begin{array}{l} H_{M_1M_1}(^3\Sigma_u^-) \\ H_{M_2M_2}(^3\Sigma_u^+) \\ H_{M_3M_3}(^3\Sigma_u^-) \end{array}\right\} = p - h(\pi_g^+) - h(\pi_g^-) - h(\sigma_{3g}) - h(\sigma_{2u})$$

$$\begin{aligned}
&+s+t-t(\pi_g^+)-t(\pi_g^-)-t(\sigma_{3g})-t(\sigma_{2u}) \\
&+J(\pi_g^+,\pi_g^-)+J(\pi_g^+,\sigma_{3g})+J(\pi_g^+,\sigma_{2u})+2J(\pi_g^+,\pi_u^+)+2J(\pi_g^+,\pi_u^-) \\
&\qquad +J(\pi_g^-,\sigma_{3g})+J(\pi_g^-,\sigma_{2u})+2J(\pi_g^-,\pi_u^+)+2J(\pi_g^-,\pi_u^-) \\
&\qquad\qquad +J(\sigma_{3g},\sigma_{2u})+2J(\sigma_{3g},\pi_u^+)+2J(\sigma_{3g},\pi_u^-) \\
&\qquad\qquad\qquad +2J(\sigma_{2u},\pi_u^+)+2J(\sigma_{2u},\pi_u^-) \\
&\qquad\qquad\qquad +J(\pi_u^+,\pi_u^+)+4J(\pi_u^+,\pi_u^-) \\
&\qquad\qquad\qquad\qquad +J(\pi_u^-,\pi_u^-) \\
&-\tfrac{1}{2}\{f+g-g(\pi_g^+)-g(\pi_g^-)-g(\sigma_{3g})-g(\sigma_{2u}) \\
&\quad +2K(\pi_g^+,\pi_u^+)+2K(\pi_g^+,\pi_u^-)+2K(\pi_g^-,\pi_u^+)+2K(\pi_g^-,\pi_u^-) \\
&\quad +2K(\sigma_{3g},\pi_u^+)+2K(\sigma_{3g},\pi_u^-)+2K(\sigma_{2u},\pi_u^+)+2K(\sigma_{2u},\pi_u^-) \\
&\qquad\qquad +4K(\pi_u^+,\pi_u^-)\} \\
&+\left\{\begin{array}{ll} -K(\pi_g^+,\pi_g^-)-K(\pi_g^+,\sigma_{3g})-K(\pi_g^+,\sigma_{2u}) & +K(\sigma_{3g},\sigma_{2u}) \\ +K(\pi_g^+,\pi_g^-)-K(\pi_g^+,\sigma_{3g})-K(\pi_g^+,\sigma_{2u}) & -K(\sigma_{3g},\sigma_{2u}) \\ -K(\pi_g^+,\pi_g^-) & -K(\sigma_{3g},\sigma_{2u}) \end{array}\right.
\end{aligned}$$

$$\left.\begin{array}{l} H_{N_1N_1}(^3\Sigma_u^-) \\ H_{N_2N_2}(^3\Sigma_u^+) \\ H_{N_3N_3}(^3\Sigma_u^-) \end{array}\right\} = p - h(\pi_g^+) - h(\pi_g^-) - h(\sigma_{3u}) - h(\sigma_{2g})$$

$$\begin{aligned}
&+s+t-t(\pi_g^+)-t(\pi_g^-)-t(\sigma_{3u})-t(\sigma_{2g}) \\
&+J(\pi_g^+,\pi_g^-)+J(\pi_g^+,\sigma_{3u})+J(\pi_g^+,\sigma_{2g})+2J(\pi_g^+,\pi_u^+)+2J(\pi_g^+,\pi_u^-) \\
&\qquad +J(\pi_g^-,\sigma_{3u})+J(\pi_g^-,\sigma_{2g})+2J(\pi_g^-,\pi_u^+)+2J(\pi_g^-,\pi_u^-) \\
&\qquad\qquad +J(\sigma_{2g},\sigma_{3u})+2J(\sigma_{3u},\pi_u^+)+2J(\sigma_{3u},\pi_u^-) \\
&\qquad\qquad\qquad +2J(\sigma_{2g},\pi_u^+)+2J(\sigma_{2g},\pi_u^-) \\
&\qquad\qquad\qquad +J(\pi_u^+,\pi_u^+)+4J(\pi_u^+,\pi_u^-) \\
&\qquad\qquad\qquad\qquad +J(\pi_u^-,\pi_u^-) \\
&-\tfrac{1}{2}\{f+g-g(\pi_g^+)-g(\pi_g^-)-g(\sigma_{3u})-g(\sigma_{2g}) \\
&\quad +2K(\pi_g^+,\pi_u^+)+2K(\pi_g^+,\pi_u^-)+2K(\pi_g^-,\pi_u^+)+2K(\pi_g^-,\pi_u^-) \\
&\quad +2K(\sigma_{3u},\pi_u^+)+2K(\sigma_{3u},\pi_u^-)+2K(\sigma_{2g},\pi_u^+)+2K(\sigma_{2g},\pi_u^-) \\
&\qquad\qquad +4K(\pi_u^+,\pi_u^-)\} \\
&+\left\{\begin{array}{ll} -K(\pi_g^+,\pi_g^-)-K(\pi_g^+,\sigma_{3u})-K(\pi_g^+,\sigma_{2g}) & +K(\sigma_{3u},\sigma_{2g}) \\ +K(\pi_g^+,\pi_g^-)-K(\pi_g^+,\sigma_{3u})-K(\pi_g^+,\sigma_{2g}) & -K(\sigma_{3u},\sigma_{2g}) \\ -K(\pi_g^+,\pi_g^-) & -K(\sigma_{3u},\sigma_{2g}) \end{array}\right.
\end{aligned}$$

$$\begin{aligned}
H_{QQ}(^3\Sigma_u^+) = {} & p - h(\sigma_{2g}) - h(\sigma_{2u}) - 2h(\sigma_{3u}) \\
& +s+t(\sigma_{2g})+t(\sigma_{2u})+2t(\sigma_{3g}) \\
& +J(\sigma_{2g},\sigma_{2u})+2J(\sigma_{2g},\sigma_{3g})+2J(\sigma_{2u},\sigma_{3g})+J(\sigma_{3g},\sigma_{3g}) \\
& -\tfrac{1}{2}\{f+g(\sigma_{2g})+g(\sigma_{2u})+2g(\sigma_{3g}) \\
& \quad +2K(\sigma_{2g},\sigma_{2u})+2K(\sigma_{2g},\sigma_{3g})+2K(\sigma_{2u},\sigma_{3g})\}
\end{aligned}$$

$H_{AB} = (\sigma_{3g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})$ $\qquad H_{AD} = \mp(\sigma_{3u}\pi_g^+|\sigma_{3u}\pi_g^-)$

$H_{AC} = -(\sigma_{3u}\pi_u^+|\sigma_{3u}\pi_u^-)$

$H_{AE_1}(^3\Sigma_u^-) = -2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+) + (\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)$

$H_{AE_2}(^3\Sigma_u^+) = -(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)$ $\qquad H_{AE_3}(^3\Sigma_u^-) = -\sqrt{2}\,(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)$

$H_{AF_1}(^3\Sigma_u^-) = -2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+) + (\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)$

$H_{AF_2}(^3\Sigma_u^+) = (\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)$ $\qquad H_{AG} = (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{3u})$

$H_{AF_3}(^3\Sigma_u^-) = -\sqrt{2}\,(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)$ $\qquad H_{AH} = (\sigma_{2g}\sigma_{3u}|\sigma_{2g}\sigma_{3u})$

$$\begin{aligned}
H_{AI_1} = {} & \sqrt{2}\,[(\sigma_{2u}|h|\sigma_{3u}) + 3(\sigma_{2u}\sigma_{3u}|\pi_g^+\pi_g^+) + 3(\sigma_{2u}\sigma_{3u}|\pi_u^+\pi_u^+) + (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{2u}) \\
& +2(\sigma_{2u}\sigma_{3u}|\sigma_{3g}\sigma_{3g}) + 2(\sigma_{2u}\sigma_{3u}|\sigma_{2g}\sigma_{2g}) + 2(\sigma_{2u}\sigma_{3u}|\sigma_{1u}\sigma_{1u}) + 2(\sigma_{2u}\sigma_{3u}|\sigma_{1g}\sigma_{1g}) \\
& -\{\tfrac{2}{2}(\sigma_{2u}\pi_g^+|\sigma_{3u}\pi_g^-) + \tfrac{3}{2}(\sigma_{2u}\pi_u^+|\sigma_{3u}\pi_u^-) + (\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) \\
& +(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u}) + (\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u}) + (\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})\}]
\end{aligned}$$

$$H_{AI_2} = -\frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_g^+|\sigma_{3u}\pi_g^-) - (\sigma_{2u}\pi_u^+|\sigma_{3u}\pi_u^-)\}$$

$H_{AI_3}=(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)+(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-)$ $\quad H_{AJ_2}=0$

$H_{AJ_1}=-\sqrt{2}\,(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})$ $\quad H_{AJ_3}=0$

$H_{AK_1}(^3\sum u^-)=H_{AK_2}(^3\sum u^+)=H_{AK_3}(^3\sum u^-)=0$

$H_{AL_1}(^3\sum u^-)=-2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{AL_2}(^3\sum u^+)=-(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$ $\quad H_{AL_3}(^3\sum u^-)=\sqrt{2}\,(\sigma_{2g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{AM_1}(^3\sum u^-)=H_{AM_2}(^3\sum u^+)=H_{AM_3}(^3\sum u^-)=0$

$H_{AN_1}(^3\sum u^-)=-2(\sigma_{2g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{AN_2}(^3\sum u^+)=(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$ $\quad H_{AO}(^3\sum u^+)=0$

$H_{AN_3}(^3\sum u^-)=\sqrt{2}\,(\sigma_{2g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$ $\quad H_{AP}(^3\sum u^+)=0$

$H_{AQ}(^3\sum u^+)=\sqrt{2}\,\{-(\sigma_{2g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)+(\sigma_{2g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$

$H_{AR}(^3\sum u^+)=0$

$H_{BE_1}(^3\sum u^-)=-2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{BE_2}(^3\sum u^+)=(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$ $\quad H_{BE_3}(^3\sum u^-)=\sqrt{2}\,(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{BF_1}(^3\sum u^-)=-2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{BF_2}(^3\sum u^+)=-(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$ $\quad H_{BI_1}=-\sqrt{2}\,(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$

$H_{BF_3}(^3\sum u^-)=\sqrt{2}\,(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$ $\quad H_{BI_2}=0$

$H_{BG}=(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$ $\quad H_{BI_3}=0$

$H_{BK_1}(^3\sum u^-)=-2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{BK_2}(^3\sum u^+)=-(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$ $\quad H_{BK_3}(^3\sum u^-)=\sqrt{2}\,(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{BM_1}(^3\sum u^-)=-2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{BM_2}(^3\sum u^+)=(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$ $\quad H_{BM_3}(^3\sum u^-)=\sqrt{2}\,(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$H_{E_1E_3}(^3\sum u^-)=\sqrt{2}\,\{K(\pi_g{}^+,\ \sigma_{3g})-K(\pi_g{}^+,\ \sigma_{3u})\}$

$H_{E_1F_1}(^3\sum u^-)=(\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-)-(\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+)=H_{E_3F_3}(^3\sum u^-)$

$H_{E_1F_3}(^3\sum u^-)=0=H_{E_3F_1}(^3\sum u^-)$

$H_{E_2F_2}(^3\sum u^+)=(\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-)+(\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+)$

$H_{E_1G}(^3\sum u^-)=H_{E_3G}(^3\sum u^-)=H_{E_2G}(^3\sum u^+)=0$

$H_{E_1I_1}(^3\sum u^-)=\dfrac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)-(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$

$H_{E_1I_2}(^3\sum u^-)=-\dfrac{1}{\sqrt{2}}(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$ $\quad H_{E_2I_1}(^3\sum u^+)=\dfrac{1}{\sqrt{2}}(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{E_1I_3}(^3\sum u^-)=-(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{E_2I_2}(^3\sum u^+)=\dfrac{1}{\sqrt{2}}\{-2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)+(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)\}$

$H_{E_2I_3}(^3\sum u^+)=-(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$ $\quad H_{E_3I_2}(^3\sum u^-)=-(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$

$H_{E_3I_1}(^3\sum u^-)=(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$ $\quad H_{E_3I_3}(^3\sum u^-)=-\sqrt{2}\,(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)$

$H_{E_1K_1}(^3\sum u^-)=H_{E_1K_3}(^3\sum u^-)=H_{E_3K_1}(^3\sum u^-)=H_{E_3K_3}(^3\sum u^-)=H_{E_2K_2}(^3\sum u^+)=0$

$$\begin{aligned}H_{E_1M_1}(^3\sum u^-)=-[&(\sigma_{2u}|h|\sigma_{3u})+2(\sigma_{2u}\sigma_{3u}|\pi_g{}^+\pi_g{}^+)+4(\sigma_{2u}\sigma_{3u}|\pi_u{}^+\pi_u{}^+)+(\sigma_{2u}\sigma_{3u}|\sigma_{3g}\sigma_{3g})\\&+(\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{2u})+(\sigma_{2u}\sigma_{3u}|\sigma_{3u}\sigma_{3u})+2(\sigma_{2u}\sigma_{3u}|\sigma_{2g}\sigma_{2g})+2(\sigma_{2u}\sigma_{3u}|\sigma_{1u}\sigma_{1u})\\&+2(\sigma_{2u}\sigma_{3u}|\sigma_{1g}\sigma_{1g})\\&-\{2(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-)+(\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u})+(\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u})+(\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})\}\\&-\{(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)+2(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})\}]\end{aligned}$$

$H_{E_1M_3}(^3\sum u^-)=-\sqrt{2}\,(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{E_2M_2}(^3\sum u^+)=H_{E_1M_1}(^3\sum u^-)-2(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$

$H_{E_3M_1}(^3\sum u^-)=-\sqrt{2}\,(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{E_3M_3}(^3\sum u^-)=H_{E_1M_1}(^3\sum u^-)+(\sigma_{2u}\pi_g{}^+|\sigma_{3u}\pi_g{}^-)-2(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$

$H_{F_1F_3}(^3\sum u^-)=\sqrt{2}\,\{K(\sigma_{3g},\ \pi_u{}^+)-K(\sigma_{3u},\ \pi_u{}^+)\}$

$H_{F_1G}(^3\sum u^-)=H_{F_3G}(^3\sum u^-)=H_{F_2G}(^3\sum u^+)=0$

$H_{F_1I_1}(^3\sum u^-)=\dfrac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+)-(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)]$

$H_{F_1I_2}(^3\sum u^-)=\dfrac{1}{\sqrt{2}}(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$ $\quad H_{F_1I_3}(^3\sum u^-)=-(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$

$$H_{F_2I_1}(^3\Sigma_u^+) = -\frac{1}{\sqrt{2}}(\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-)$$

$$H_{F_2I_2}(^3\Sigma_u^+) = \frac{1}{\sqrt{2}}\{-2(\sigma_{3g}\sigma_{2u}|\pi_g^+\pi_u^+) + (\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-)\}$$

$$H_{F_2I_3}(^3\Sigma_u^+) = (\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-) \qquad H_{F_3I_2}(^3\Sigma_u^-) = (\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-)$$

$$H_{F_3I_1}(^3\Sigma_u^-) = (\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-) \qquad H_{F_3I_3}(^3\Sigma_u^-) = -\sqrt{2}\,(\sigma_{3g}\sigma_{2u}|\pi_g^+\pi_u^+)$$

$$\begin{aligned}H_{F_1K_1}(^3\Sigma_u^-) = -[&(\sigma_{2u}|h|\sigma_{3u}) + 2(\sigma_{2u}\sigma_{3u}|\pi_u^+\pi_u^+) + 4(\sigma_{2u}\sigma_{3u}|\pi_g^+\pi_g^+) + (\sigma_{2u}\sigma_{3u}|\sigma_{3g}\sigma_{3g})\\ &+ (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{2u}) + (\sigma_{2u}\sigma_{3u}|\sigma_{3u}\sigma_{3u}) + 2(\sigma_{2u}\sigma_{3u}|\sigma_{2g}\sigma_{2g}) + 2(\sigma_{2u}\sigma_{3u}|\sigma_{1u}\sigma_{1u})\\ &+ 2(\sigma_{2u}\sigma_{3u}|\sigma_{1g}\sigma_{1g})\\ &- \{2(\sigma_{2u}\pi_g^+|\sigma_{3u}\pi_g^-) + (\sigma_{2g}\sigma_{2u}|\sigma_{2g}\sigma_{3u}) + (\sigma_{1u}\sigma_{2u}|\sigma_{1u}\sigma_{3u}) + (\sigma_{1g}\sigma_{2u}|\sigma_{1g}\sigma_{3u})\}\\ &- \{(\sigma_{2u}\pi_u^+|\sigma_{3u}\pi_u^-) + 2(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})\}]\end{aligned}$$

$$H_{F_1K_3}(^3\Sigma_u^-) = -\sqrt{2}\,(\sigma_{2u}\pi_u^+|\sigma_{3u}\pi_u^-)$$

$$H_{F_2K_2}(^3\Sigma_u^+) = H_{F_1K_1}(^3\Sigma_u^-) - 2(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$$

$$H_{F_3K_1}(^3\Sigma_u^-) = -\sqrt{2}\,(\sigma_{2u}\pi_u^+|\sigma_{3u}\pi_u^-)$$

$$H_{F_3K_3}(^3\Sigma_u^-) = H_{F_1K_1}(^3\Sigma_u^-) + (\sigma_{2u}\pi_u^+|\sigma_{3u}\pi_u^-) - 2(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$$

$$H_{F_1M_1}(^3\Sigma_u^-) = H_{F_1M_3}(^3\Sigma_u^-) = H_{F_2M_2}(^3\Sigma_u^+) = H_{F_3M_1}(^3\Sigma_u^-) = H_{F_3M_3}(^3\Sigma_u^-) = 0$$

$$H_{GI_1} = H_{AI_1} + \sqrt{2}\,\{(\sigma_{2u}\sigma_{3u}|\sigma_{3u}\sigma_{3u}) - (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{2u})\}$$

$$H_{GI_2} = \frac{1}{\sqrt{2}}\{(\sigma_{2u}\pi_g^+|\sigma_{3u}\pi_g^-) - (\sigma_{2u}\pi_u^+|\sigma_{3u}\pi_u^-)\}$$

$$H_{GI_3} = -\{(\sigma_{2u}\pi_g^+|\sigma_{3u}\pi_g^-) + (\sigma_{2u}\pi_u^+|\sigma_{3u}\pi_u^-)\}$$

$$H_{GK_1}(^3\Sigma_u^-) = -2(\sigma_{3g}\sigma_{2u}|\pi_g^+\pi_u^+) + (\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-)$$

$$H_{GK_2}(^3\Sigma_u^+) = (\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-) \qquad H_{GK_3}(^3\Sigma_u^-) = -\sqrt{2}\,(\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-)$$

$$H_{GM_1}(^3\Sigma_u^-) = -2(\sigma_{3g}\sigma_{2u}|\pi_g^+\pi_u^+) + (\sigma_{3g}\pi_u^+|\sigma_{2u}\pi_g^-)$$

$$H_{GM_2}(^3\Sigma_u^+) = -(\sigma_{3g}\pi_u^+|\sigma_{2u}\pi_g^-) \qquad H_{GM_3}(^3\Sigma_u^-) = -\sqrt{2}\,(\sigma_{3g}\pi_u^+|\sigma_{2u}\pi_g^-)$$

$$H_{I_1I_2} = \tfrac{1}{2}\{-K(\pi_g^+, \sigma_{3u}) + K(\pi_g^+, \sigma_{2u}) + K(\pi_u^-, \sigma_{3u}) - K(\pi_u^-, \sigma_{2u})\}$$

$$H_{I_1I_3} = \frac{1}{\sqrt{2}}\{K(\pi_g^+, \sigma_{3u}) - K(\pi_g^+, \sigma_{2u}) + K(\pi_u^-, \sigma_{3u}) - K(\pi_u^-, \sigma_{2u})\}$$

$$H_{I_2I_3} = \frac{1}{\sqrt{2}}\{-K(\pi_g^+, \sigma_{3u}) - K(\pi_g^+, \sigma_{2u}) + K(\pi_u^-, \sigma_{3u}) + K(\pi_u^-, \sigma_{2u})\}$$

$$H_{I_1K_1}(^3\Sigma_u^-) = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+) - (\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)\}$$

$$H_{I_1K_2}(^3\Sigma_u^+) = -\frac{1}{\sqrt{2}}(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-) \qquad H_{I_1K_3}(^3\Sigma_u^-) = (\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)$$

$$H_{I_2K_1}(^3\Sigma_u^-) = -\frac{1}{\sqrt{2}}(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)$$

$$H_{I_2K_2}(^3\Sigma_u^+) = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+) - (\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)\}$$

$$H_{I_2K_3}(^3\Sigma_u^-) = -(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-) \qquad H_{I_3K_2}(^3\Sigma_u^+) = -(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)$$

$$H_{I_3K_1}(^3\Sigma_u^-) = (\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-) \qquad H_{I_3K_3}(^3\Sigma_u^-) = \sqrt{2}\,(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+)$$

$$H_{I_1M_1}(^3\Sigma_u^-) = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+) - (\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)\}$$

$$H_{I_1M_2}(^3\Sigma_u^+) = \frac{1}{\sqrt{2}}(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-) \qquad H_{I_2M_1}(^3\Sigma_u^-) = \frac{1}{\sqrt{2}}(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)$$

$$H_{I_1M_3}(^3\Sigma_u^-) = (\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)$$

$$H_{I_2M_2}(^3\Sigma_u^+) = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+) - (\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)\}$$

$$H_{I_2M_3}(^3\Sigma_u^-) = (\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-) \qquad H_{I_3M_2}(^3\Sigma_u^+) = (\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)$$

$$H_{I_3M_1}(^3\Sigma_u^-) = (\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-) \qquad H_{I_3M_3}(^3\Sigma_u^-) = \sqrt{2}\,(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+)$$

$$H_{K_1K_3}(^3\Sigma_u^-) = \sqrt{2}\,\{K(\pi_u^+, \sigma_{3g}) - K(\pi_u^+, \sigma_{2u})\}$$

$$H_{K_1M_1}(^3\Sigma_u^-) = (\pi_g^+\pi_u^+|\pi_g^-\pi_u^-) - (\pi_g^+\pi_u^-|\pi_g^-\pi_u^+)$$

$$H_{K_1M_3}(^3\Sigma_u^-) = 0$$

$$H_{K_2M_2}(^3\Sigma_u^+) = (\pi_g^+\pi_u^+|\pi_g^-\pi_u^-) + (\pi_g^+\pi_u^-|\pi_g^-\pi_u^+)$$

$H_{K_3M_1}(^3\Sigma_u^-)=0$
$H_{K_3M_3}(^3\Sigma_u^-)=(\pi_g^+\pi_u^+|\pi_g^-\pi_u^-)-(\pi_g^+\pi_u^-|\pi_g^-\pi_u^+)$
$H_{M_1M_3}(^3\Sigma_u^-)=\sqrt{2}\{K(\pi_g^+,\sigma_{3g})-K(\pi_g^+,\sigma_{2u})\}$

In the above formulae, the upper or the lower sign of a double sign corresponds to $^3\Sigma_u^+$ or $^3\Sigma_u^-$ state, respectively.

(vi) $^1\Sigma_u^+$ and $^1\Sigma_u^-$ (O_2)

$H_{AA}(^1\Sigma_u^+)=H_{AA}(^3\Sigma_u^-)+2(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+)+2K(\pi_g^+,\pi_u^-)$
$H_{AA}(^1\Sigma_u^-)=H_{AA}(^3\Sigma_u^+)-2(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+)+2K(\pi_g^+,\pi_u^-)$
$H_{BB}(^1\Sigma_u^+)=H_{BB}(^3\Sigma_u^-)+2(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+)+2K(\pi_g^+,\pi_u^-)$
$H_{BB}(^1\Sigma_u^-)=H_{BB}(^3\Sigma_u^+)-2(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+)+2K(\pi_g^+,\pi_u^-)$
$H_{E_1E_1}(^1\Sigma_u^+)=H_{E_2E_2}(^3\Sigma_u^+)+2K(\sigma_{3g},\sigma_{3u})$
$H_{E_2E_2}(^1\Sigma_u^-)=H_{E_1E_1}(^3\Sigma_u^-)+2K(\pi_g^+,\sigma_{3g})+2K(\pi_g^+,\sigma_{3u})-2K(\sigma_{3g},\sigma_{3u})$
$H_{F_1F_1}(^1\Sigma_u^+)=H_{F_2F_2}(^3\Sigma_u^+)+2K(\sigma_{3g},\sigma_{3u})$
$H_{F_2F_2}(^1\Sigma_u^-)=H_{F_1F_1}(^3\Sigma_u^-)+2K(\pi_u^+,\sigma_{3g})+2K(\pi_u^+,\sigma_{3u})-2K(\sigma_{3g},\sigma_{3u})$
$H_{GG}(^1\Sigma_u^+)=H_{GG}(^3\Sigma_u^-)+2(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+)+2K(\pi_g^+,\pi_u^-)$
$H_{GG}(^1\Sigma_u^-)=H_{GG}(^3\Sigma_u^+)-2(\pi_g^+\pi_g^-|\pi_u^-\pi_u^+)+2K(\pi_g^+,\pi_u^-)$
$H_{I_1I_1}(^1\Sigma_u^+)=H_{I_1I_1}(^3\Sigma_u^+)+2(\pi_g^+\pi_u^+|\pi_g^+\pi_u^+)+2K(\sigma_{3u},\sigma_{2u})$
$H_{I_1I_1}(^1\Sigma_u^-)=H_{I_1I_1}(^3\Sigma_u^-)+K(\pi_g^+,\sigma_{3u})+K(\pi_g^+,\sigma_{2u})+K(\pi_u^+,\sigma_{3u})+K(\pi_u^+,\sigma_{2u})$
$-2K(\sigma_{3u},\sigma_{2u})-2(\pi_g^+\pi_u^+|\pi_g^+\pi_u^+)$
$H_{K_1K_1}(^1\Sigma_u^+)=H_{K_2K_2}(^3\Sigma_u^+)+2K(\sigma_{3g},\sigma_{2u})$
$H_{K_2K_2}(^1\Sigma_u^-)=H_{K_1K_1}(^3\Sigma_u^-)+2K(\pi_u^+,\sigma_{3g})+2K(\pi_u^+,\sigma_{2u})-2K(\sigma_{3g},\sigma_{2u})$
$H_{M_1M_1}(^1\Sigma_u^+)=H_{M_2M_2}(^3\Sigma_u^+)+2K(\sigma_{3g},\sigma_{2u})$
$H_{M_2M_2}(^1\Sigma_u^-)=H_{M_1M_1}(^3\Sigma_u^-)+2K(\pi_g^+,\sigma_{3g})+2K(\pi_g^+,\sigma_{2u})-2K(\sigma_{3g},\sigma_{2u})$
$H_{AB}=(\sigma_{3g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})$ $\quad H_{AD}=\mp(\sigma_{3u}\pi_g^+|\sigma_{3u}\pi_g^-)$
$H_{AC}=-(\pi_u^+\sigma_{3u}|\pi_u^-\sigma_{3u})$
$H_{AE_1}(^1\Sigma_u^+)=-2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+)+(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)$
$H_{AE_2}(^1\Sigma_u^-)=\sqrt{2}(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)$
$H_{AF_1}(^1\Sigma_u^+)=-2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+)+(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)$
$H_{AF_2}(^1\Sigma_u^-)=-\sqrt{3}(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)$ $\quad H_{AH}=(\sigma_{2g}\sigma_{3u}|\sigma_{2g}\sigma_{3u})$
$H_{AG}=(\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{3u})$ $\quad H_{AI_1}=H_{AI_1}(^3\Sigma_u^\pm)$
$H_{AI_2}=\sqrt{\frac{3}{2}}\{(\sigma_{2u}\pi_g^+|\sigma_{3u}\pi_g^-)-(\sigma_{2u}\pi_u^+|\sigma_{3u}\pi_u^-)\}$
$H_{AJ_1}=-\sqrt{2}(\sigma_{2g}\sigma_{3u}|\sigma_{3g}\sigma_{3u})$ $\quad H_{AK_1}(^1\Sigma_u^+)=H_{AK_2}(^1\Sigma_u^-)=0$
$H_{AJ_2}=0$
$H_{AL_1}(^1\Sigma_u^+)=-2(\sigma_{2g}\sigma_{3u}|\pi_g^+\pi_u^+)+(\sigma_{2g}\pi_g^+|\sigma_{3u}\pi_u^-)$
$H_{AL_2}(^1\Sigma_u^-)=\sqrt{3}(\sigma_{2g}\pi_g^+|\sigma_{3u}\pi_u^-)$ $\quad H_{AM_1}(^1\Sigma_u^+)=H_{AM_2}(^1\Sigma_u^-)=0$
$H_{AN_1}(^1\Sigma_u^+)=-2(\sigma_{2g}\sigma_{3u}|\pi_g^+\pi_u^+)+(\sigma_{2g}\pi_u^+|\sigma_{3u}\pi_g^-)$
$H_{AN_2}(^1\Sigma_u^-)=-\sqrt{3}(\sigma_{2g}\pi_u^+|\sigma_{3u}\pi_g^-)$ $\quad H_{AP}(^1\Sigma_u^+)=0$
$H_{AO}(^1\Sigma_u^+)=0$
$H_{AQ}(^1\Sigma_u^+)=\sqrt{2}\{(\sigma_{2g}\pi_u^+|\sigma_{2u}\pi_g^-)+(\sigma_{2g}\pi_g^+|\sigma_{2u}\pi_u^-)\}$
$H_{AR}(^1\Sigma_u^+)=0$ $\quad H_{BM_2}(^1\Sigma_u^-)=-\sqrt{3}(\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-)$
$H_{BE_1}(^1\Sigma_u^+)=H_{BE_1}(^3\Sigma_u^-)$ $\quad H_{E_1F_1}(^1\Sigma_u^+)=H_{E_2F_2}(^3\Sigma_u^+)$
$H_{BE_2}(^1\Sigma_u^-)=-\sqrt{3}(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-)$ $\quad H_{E_2F_2}(^1\Sigma_u^-)=H_{E_1F_1}(^3\Sigma_u^-)$
$H_{BF_1}(^1\Sigma_u^+)=H_{BF_1}(^3\Sigma_u^-)$ $\quad H_{E_1G}(^1\Sigma_u^+)=H_{E_2G}(^1\Sigma_u^-)=0$
$H_{BF_2}(^1\Sigma_u^-)=\sqrt{3}(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-)$ $\quad H_{E_1I_1}(^1\Sigma_u^+)=H_{E_1I_1}(^3\Sigma_u^-)$
$H_{BG}=(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$ $\quad H_{E_2I_1}(^1\Sigma_u^-)=-\sqrt{\frac{3}{2}}(\sigma_{3g}\pi_u^+|\sigma_{2u}\pi_g^-)$
$H_{BI_1}=-\sqrt{2}(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$ $\quad H_{E_1K_1}(^1\Sigma_u^+)=H_{E_2K_2}(^1\Sigma_u^-)=0$
$H_{BK_1}(^1\Sigma_u^+)=H_{BK_1}(^3\Sigma_u^-)$ $\quad H_{E_1M_1}(^1\Sigma_u^+)=H_{E_1M_1}(^3\Sigma_u^-)$
$H_{BK_2}(^1\Sigma_u^-)=\sqrt{3}(\sigma_{3g}\pi_u^+\pi_g^-|\sigma_{2u})$ $\quad H_{E_2M_2}(^1\Sigma_u^-)=H_{E_2M_2}(^3\Sigma_u^+)+2(\sigma_{2u}\pi_g^+|\sigma_{3u}\pi_g^-)$
$H_{BM_1}(^1\Sigma_u^+)=H_{BM_1}(^3\Sigma_u^-)$ $\quad H_{F_1G}(^1\Sigma_u^+)=H_{F_2G}(^1\Sigma_u^-)=0$

$$H_{F_1I_1}(^1\Sigma_u{}^+)=H_{F_1I_1}(^3\Sigma_u{}^-) \qquad H_{GM_1}(^1\Sigma_u{}^+)=H_{GM_1}(^3\Sigma_u{}^-)$$

$$H_{F_2I_1}(^1\Sigma_u{}^-)=\sqrt{\frac{3}{2}}(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{GM_2}(^1\Sigma_u{}^-)=\sqrt{3}(\sigma_{3g}\pi_u{}^+|\sigma_{2u}\pi_g{}^-)$$

$$H_{F_1K_1}(^1\Sigma_u{}^+)=H_{F_1K_1}(^3\Sigma_u{}^-) \qquad H_{I_1K_1}(^1\Sigma_u{}^+)=H_{I_1K_1}(^3\Sigma_u{}^-)$$

$$H_{F_2K_2}(^1\Sigma_u{}^-)=H_{F_2K_2}(^3\Sigma_u{}^+)+2(\sigma_{2u}\pi_u{}^+|\sigma_{3u}\pi_u{}^-) \qquad H_{I_1K_2}(^1\Sigma_u{}^-)=\sqrt{\frac{3}{2}}(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$$

$$H_{F_1M_1}=(^1\Sigma_u{}^+)=H_{F_2M_2}(^1\Sigma_u{}^-)=0 \qquad H_{I_1M_1}(^1\Sigma_u{}^+)=H_{I_1M_1}(^3\Sigma_u{}^-)$$

$$H_{GI_1}=H_{GI_1}(^3\Sigma_u{}^\pm) \qquad H_{I_1M_2}(^1\Sigma_u{}^-)=-\sqrt{\frac{3}{2}}(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$$

$$H_{GK_1}(^1\Sigma_u{}^+)=H_{GK_1}(^3\Sigma_u{}^-) \qquad H_{K_1M_1}(^1\Sigma_u{}^+)=H_{K_2M_2}(^3\Sigma_u{}^+)$$

$$H_{GK_2}(^1\Sigma_u{}^-)=-\sqrt{3}(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-) \qquad H_{K_2M_2}(^1\Sigma_u{}^-)=H_{K_1M_1}(^3\Sigma_u{}^-)$$

In the above formulae, the upper or the lower sign of a double sign corresponds to $^1\Sigma_u{}^+$ or $^1\Sigma_u{}^-$ state, respectively.

(vii) $^1\Delta_g$ (O_2)

Configurations used	α, β	γ
A, B, C, D, G_i	σ_{1g}, σ_{1u}, σ_{2g}, σ_{2u}	σ_{3g}, σ_{3u}, $\pi_u{}^\pm$, $\pi_g{}^\pm$
H, J	σ_{1g}, σ_{1u}, σ_{2g}, σ_{3g}	σ_{2u}, σ_{3u}, $\pi_u{}^\pm$, $\pi_g{}^\pm$

$$\begin{aligned}
H_{AA} =\ & p-2h(\sigma_{3u})-2h(\pi_g{}^-)\\
& +s+t-2t(\sigma_{3u})-2t(\pi_g{}^-)\\
& +J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_u{}^+)+4J(\pi_g{}^+,\pi_u{}^-)+4J(\pi_g{}^+,\sigma_{3g})\\
& \qquad +J(\pi_u{}^+,\pi_u{}^+)+4J(\pi_u{}^+,\pi_u{}^-)+4J(\pi_u{}^+,\sigma_{3g})\\
& \qquad\qquad +J(\pi_u{}^-,\pi_u{}^-)+4J(\pi_u{}^-,\sigma_{3g})\\
& \qquad\qquad\qquad +J(\sigma_{3g},\sigma_{3g})\\
& -\tfrac{1}{2}\{f+q-2g(\sigma_{3u})-2g(\pi_g{}^-)\\
& \quad +4K(\pi_g{}^+,\pi_u{}^+)+4K(\pi_g{}^+,\pi_u{}^-)+4K(\pi_g{}^+,\sigma_{3g})\\
& \qquad +4K(\pi_u{}^+,\pi_u{}^-)+4K(\pi_u{}^+,\sigma_{3g})\\
& \qquad\qquad +4K(\pi_u{}^-,\sigma_{3g})\}
\end{aligned}$$

$$\begin{aligned}
H_{CC} =\ & p-2h(\pi_u{}^-)-2h(\sigma_{3u})\\
& +s+t-2t(\pi_u{}^-)-2t(\sigma_{3u})\\
& +J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_g{}^-)+4J(\pi_g{}^+,\pi_u{}^+)+4J(\pi_g{}^+,\sigma_{3g})\\
& \qquad +J(\pi_g{}^-,\pi_g{}^-)+4J(\pi_g{}^-,\pi_u{}^+)+4J(\pi_g{}^-,\sigma_{3g})\\
& \qquad\qquad +J(\pi_u{}^+,\pi_u{}^+)+4J(\pi_u{}^+,\sigma_{3g})\\
& \qquad\qquad\qquad +J(\sigma_{3g},\sigma_{3g})\\
& -\tfrac{1}{2}\{f+g-2g(\pi_u{}^-)-2g(\sigma_{3u})\\
& \quad +4K(\pi_g{}^+,\pi_g{}^-)+4K(\pi_g{}^+,\pi_u{}^+)+4K(\pi_g{}^+,\sigma_{3g})\\
& \qquad +4K(\pi_g{}^-,\pi_u{}^+)+4K(\pi_g{}^-,\sigma_{3g})\\
& \qquad\qquad +4K(\pi_u{}^+,\sigma_{3g})\}
\end{aligned}$$

$$\begin{aligned}
H_{DD} =\ & p-2h(\pi_g{}^-)-2h(\sigma_{3g})\\
& +s+t-2t(\pi_g{}^-)-2t(\sigma_{3g})\\
& +J(\pi_g{}^+,\pi_g{}^+)+4J(\pi_g{}^+,\pi_u{}^+)+4J(\pi_g{}^+,\pi_u{}^-)+4J(\pi_g{}^+,\sigma_{3u})\\
& \qquad +J(\pi_u{}^+,\pi_u{}^+)+4J(\pi_u{}^+,\pi_u{}^-)+4J(\pi_u{}^+,\sigma_{3u})\\
& \qquad\qquad +J(\pi_u{}^-,\pi_u{}^-)+4J(\pi_u{}^-,\sigma_{3u})\\
& \qquad\qquad\qquad +J(\sigma_{3u},\sigma_{3u})\\
& -\tfrac{1}{2}\{f+g-2g(\pi_g{}^-)-2g(\sigma_{3g})\\
& \quad +4K(\pi_g{}^+,\pi_u{}^+)+4K(\pi_g{}^+,\pi_u{}^-)+4K(\pi_g{}^+,\sigma_{3u})\\
& \qquad +4K(\pi_u{}^+,\pi_u{}^-)+4K(\pi_u{}^+,\sigma_{3u})\\
& \qquad\qquad +4K(\pi_u{}^-,\sigma_{3u})\}
\end{aligned}$$

$$
\left.\begin{matrix} H_{G_1G_1} \\ H_{G_2G_2} \end{matrix}\right\} = p - h(\pi_g^-) - h(\pi_u^-) - h(\sigma_{3u}) - h(\sigma_{3g})
$$

$$
\begin{aligned}
&+s+t-t(\pi_g^-)-t(\pi_u^-)-t(\sigma_{3u})-t(\sigma_{3g}) \\
&+J(\pi_g^-,\pi_u^-)+J(\pi_g^-,\sigma_{3u})+J(\pi_g^-,\sigma_{3g})+2J(\pi_g^-,\pi_g^+)+2J(\pi_g^-,\pi_u^+) \\
&\qquad +J(\pi_u^-,\sigma_{3u})+J(\pi_u^-,\sigma_{3g})+2J(\pi_u^-,\pi_g^+)+2J(\pi_u^-,\pi_u^+) \\
&\qquad\qquad +J(\sigma_{3u},\sigma_{3g})+2J(\sigma_{3u},\pi_g^+)+2J(\sigma_{3u},\pi_u^+) \\
&\qquad\qquad\qquad +2J(\sigma_{3g},\pi_g^+)+2J(\sigma_{3g},\pi_u^+) \\
&\qquad\qquad\qquad +J(\pi_g^+,\pi_g^+)+4J(\pi_g^+,\pi_u^+) \\
&\qquad\qquad\qquad\qquad +J(\pi_u^+,\pi_u^+) \\
&-\tfrac{1}{2}\{f+g-g(\pi_g^-)-g(\pi_u^-)-g(\sigma_{3u})-g(\sigma_{3g}) \\
&\quad +2K(\pi_g^-,\pi_g^+)+2K(\pi_g^-,\pi_u^+)+2K(\pi_u^-,\pi_g^+)+2K(\pi_u^-,\pi_u^+) \\
&\quad +2K(\sigma_{3u},\pi_g^+)+2K(\sigma_{3u},\pi_u^+)+2K(\sigma_{3g},\pi_g^+)+2K(\sigma_{3g},\pi_u^+) \\
&\qquad\qquad +4K(\pi_g^+,\pi_u^+)\}
\end{aligned}
$$

$$
+\begin{cases} K(\pi_g^-,\pi_u^-)-\tfrac{1}{2}K(\pi_g^-,\sigma_{3u})-\tfrac{1}{2}K(\pi_g^-,\sigma_{3g})-\tfrac{1}{2}K(\pi_u^-,\sigma_{3u})-\tfrac{1}{2}K(\pi_u^-,\sigma_{3g})+K(\sigma_{3u},\sigma_{3g}) \\ -K(\pi_g^-,\pi_u^-)+\tfrac{1}{2}K(\pi_g^-,\sigma_{3u})+\tfrac{1}{2}K(\pi_g^-,\sigma_{3g})+\tfrac{1}{2}K(\pi_u^-,\sigma_{3u})+\tfrac{1}{2}K(\pi_u^-,\sigma_{3g})-K(\sigma_{3u},\sigma_{3g}) \end{cases}
$$

$$
\begin{aligned}
H_{HH} &= p-2h(\pi_g^-)-2h(\sigma_{2u}) \\
&+s+t-2t(\pi_g^-)-2t(\sigma_{2u}) \\
&+J(\pi_g^+,\pi_g^+)+4J(\pi_g^+,\pi_u^+)+4J(\pi_g^+,\pi_u^-)+4J(\pi_g^+,\sigma_{3u}) \\
&\qquad +J(\pi_u^+,\pi_u^+)+4J(\pi_u^+,\pi_u^-)+4J(\pi_u^+,\sigma_{3u}) \\
&\qquad\qquad +J(\pi_u^-,\pi_u^-)+4J(\pi_u^-,\sigma_{3u}) \\
&\qquad\qquad\qquad +J(\sigma_{3u},\sigma_{3u}) \\
&-\tfrac{1}{2}\{f+g-2g(\pi_g^-)-2g(\sigma_{2u}) \\
&\quad +4K(\pi_g^+,\pi_u^+)+4K(\pi_g^+,\pi_u^-)+4K(\pi_g^+,\sigma_{3u}) \\
&\qquad +4K(\pi_u^+,\pi_u^-)+4K(\pi_u^+,\sigma_{3u}) \\
&\qquad\qquad +4K(\pi_u^-,\sigma_{3u})\}
\end{aligned}
$$

$$
\begin{aligned}
H_{JJ} &= p-h(\sigma_{3u})-h(\sigma_{2u})-2h(\pi_g^-) \\
&+s+t-t(\sigma_{3u})-t(\sigma_{2u})-2t(\pi_g^-) \\
&+J(\sigma_{3u},\sigma_{2u})+2J(\sigma_{3u},\pi_g^+)+2J(\sigma_{3u},\pi_u^+)+2J(\sigma_{3u},\pi_u^-) \\
&\qquad +2J(\sigma_{2u},\pi_g^+)+2J(\sigma_{2u},\pi_u^+)+2J(\sigma_{2u},\pi_u^-) \\
&\qquad +J(\pi_g^+,\pi_g^+)+4J(\pi_g^+,\pi_u^+)+4J(\pi_g^+,\pi_u^-) \\
&\qquad\qquad +J(\pi_u^+,\pi_u^+)+4J(\pi_u^+,\pi_u^-) \\
&\qquad\qquad\qquad +J(\pi_u^-,\pi_u^-) \\
&-\tfrac{1}{2}\{f+g-g(\sigma_{3u})-g(\sigma_{2u})-2g(\pi_g^-) \\
&\quad -2K(\sigma_{3u},\sigma_{2u})+2K(\sigma_{3u},\pi_g^+)+2K(\sigma_{3u},\pi_u^+)+2K(\sigma_{3u},\pi_u^-) \\
&\qquad +2K(\sigma_{2u},\pi_g^+)+2K(\sigma_{2u},\pi_u^+)+2K(\sigma_{2u},\pi_u^-) \\
&\qquad\qquad +4K(\pi_g^+,\pi_u^+)+4K(\pi_g^+,\pi_u^-) \\
&\qquad\qquad\qquad +4K(\pi_u^+,\pi_u^-)\}
\end{aligned}
$$

$$
\begin{aligned}
H_{AC} &= (\pi_g^+\pi_u^+|\pi_g^+\pi_u^+) & H_{CG_2} &= -\sqrt{3}\,(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-) \\
H_{AD} &= (\sigma_{3g}\sigma_{3u}|\sigma_{3g}\sigma_{3u}) & H_{CH} &= 0 \\
H_{AG_1} &= 2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+)-(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-) & H_{CJ} &= 0 \\
H_{AG_2} &= \sqrt{3}\,(\sigma_{3g}\pi_g^+|\sigma_{3u}\pi_u^-) & H_{DG_1} &= 2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+)-(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-) \\
H_{AH} &= (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{3u}) & H_{DG_2} &= -\sqrt{3}\,(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-) \\
H_{AJ} &= H_{AJ_1}({}^3\textstyle\sum_g^-) & H_{DH} &= (\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{2u}) \\
H_{CD} &= 0 & H_{DJ} &= -\sqrt{2}\,(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u}) \\
H_{CG_1} &= 2(\sigma_{3g}\sigma_{3u}|\pi_g^+\pi_u^+)-(\sigma_{3g}\pi_u^+|\sigma_{3u}\pi_g^-) & &
\end{aligned}
$$

$$
H_{G_1G_2} = \frac{\sqrt{3}}{2}\{K(\pi_g^-,\sigma_{3u})-K(\pi_g^-,\sigma_{3g})-K(\pi_u^-,\sigma_{3u})+K(\pi_u^-,\sigma_{3g})\}
$$

$$
H_{G_1H} = H_{G_2H} = 0
$$

$$
H_{G_1J} = \frac{1}{\sqrt{2}}\{-2(\sigma_{3g}\sigma_{2u}|\pi_g^+\pi_u^+)+(\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-)\}
$$

$$
H_{G_2J} = -\sqrt{\frac{3}{2}}(\sigma_{3g}\pi_g^+|\sigma_{2u}\pi_u^-) \qquad H_{HJ} = H_{HJ_1}({}^3\textstyle\sum_g^-)
$$

(viii) $^1\sum_g{}^+$ (O_2)

Configurations used	α, β	γ
$(A, B, E, F)\ J_i$	σ_{1g}, σ_{1u}, σ_{2g}, σ_{2u}	σ_{3g}, σ_{3u}, $\pi_u{}^\pm$, $\pi_g{}^\pm$
L, N_1	σ_{1g}, σ_{1u}, σ_{2g}, σ_{3g}	σ_{2u}, σ_{3u}, $\pi_u{}^\pm$, $\pi_g{}^\pm$

$$H_{AA} = H_{AA}(^3\textstyle\sum_g{}^-) + 2K(\pi_g{}^+, \pi_g{}^-) \qquad H_{EE} = H_{BB}(^3\textstyle\sum_g{}^-) + 2K(\pi_g{}^+, \pi_g{}^-)$$

$$H_{BB} = H_{CC}(^3\textstyle\sum_g{}^-) + 2K(\pi_u{}^+, \pi_u{}^-) \qquad H_{FF} = H_{DD}(^3\textstyle\sum_g{}^-) + 2K(\pi_u{}^+, \pi_u{}^-)$$

$$\left.\begin{matrix} H_{J_1J_1} \\ H_{J_2J_2} \end{matrix}\right\} = p - h(\pi_g{}^+) - h(\pi_u{}^-) - h(\sigma_{3u}) - h(\sigma_{3g})$$
$$+ s + t - t(\pi_g{}^+) - t(\pi_u{}^-) - t(\sigma_{3u}) - t(\sigma_{3g})$$
$$+ J(\pi_g{}^+, \pi_u{}^-) + J(\pi_g{}^+, \sigma_{3u}) + J(\pi_g{}^+, \sigma_{3g}) + 2J(\pi_g{}^+, \pi_g{}^-) + 2J(\pi_g{}^+, \pi_u{}^+)$$
$$+ J(\pi_u{}^-, \sigma_{3u}) + J(\pi_u{}^-, \sigma_{3g}) + 2J(\pi_u{}^-, \pi_g{}^-) + 2J(\pi_u{}^-, \pi_u{}^+)$$
$$+ J(\sigma_{3u}, \sigma_{3g}) + 2J(\sigma_{3u}, \pi_g{}^-) + 2J(\sigma_{3u}, \pi_u{}^+)$$
$$+ 2J(\sigma_{3g}, \pi_g{}^-) + 2J(\sigma_{3g}, \pi_u{}^+)$$
$$+ J(\pi_g{}^-, \pi_g{}^-) + 4J(\pi_g{}^-, \pi_u{}^+)$$
$$+ J(\pi_u{}^+, \pi_u{}^+)$$
$$- \tfrac{1}{2}\{f + g - g(\pi_g{}^+) - g(\pi_u{}^-) - g(\sigma_{3u}) - g(\sigma_{3g})$$
$$+ 2K(\pi_g{}^+, \pi_g{}^-) + 2K(\pi_g{}^+, \pi_u{}^+) + 2K(\pi_u{}^-, \pi_g{}^-) + 2K(\pi_u{}^-, \pi_u{}^+)$$
$$+ 2K(\sigma_{3u}, \pi_g{}^-) + 2K(\sigma_{3u}, \pi_u{}^+) + 2K(\sigma_{3g}, \pi_g{}^-) + 2K(\sigma_{3g}, \pi_u{}^+)$$
$$+ 4K(\pi_g{}^-, \pi_u{}^+)\}$$
$$+ \left\{\begin{matrix} K(\pi_g{}^+, \pi_u{}^-) - \tfrac{1}{2}K(\pi_g{}^+, \sigma_{3u}) - \tfrac{1}{2}K(\pi_g{}^+, \sigma_{3g}) - \tfrac{1}{2}K(\pi_u{}^-, \sigma_{3u}) - \tfrac{1}{2}K(\pi_u{}^-, \sigma_{3g}) + K(\sigma_{3u}, \sigma_{3g}) \\ + (\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+) + (\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+) \\ - K(\pi_g{}^+, \pi_u{}^-) + \tfrac{1}{2}K(\pi_g{}^+, \sigma_{3u}) + \tfrac{1}{2}K(\pi_g{}^+, \sigma_{3g}) + \tfrac{1}{2}K(\pi_u{}^-, \sigma_{3u}) + \tfrac{1}{2}K(\pi_u{}^-, \sigma_{3g}) - K(\sigma_{3u}, \sigma_{3g}) \\ + (\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+) - (\pi_g{}^+\pi_u{}^+|\pi_g{}^+\pi_u{}^+) \end{matrix}\right.$$

$$H_{LL} = p - h(\pi_g{}^+) - h(\pi_g{}^-) - 2h(\sigma_{2u})$$
$$+ s + t - t(\pi_g{}^+) - t(\pi_g{}^-) - 2t(\sigma_{2u})$$
$$+ J(\pi_g{}^+, \pi_g{}^-) + 2J(\pi_g{}^+, \sigma_{3u}) + 2J(\pi_g{}^+, \pi_u{}^+) + 2J(\pi_g{}^+, \pi_u{}^-)$$
$$+ 2J(\pi_g{}^-, \sigma_{3u}) + 2J(\pi_g{}^-, \pi_u{}^+) + 2J(\pi_g{}^-, \pi_u{}^-)$$
$$+ J(\sigma_{3u}, \sigma_{3u}) + 4J(\sigma_{3u}, \pi_u{}^+) + 4J(\sigma_{3u}, \pi_u{}^-)$$
$$+ J(\pi_u{}^+, \pi_u{}^+) + 4J(\pi_u{}^+, \pi_u{}^-)$$
$$+ J(\pi_u{}^-, \pi_u{}^-)$$
$$- \tfrac{1}{2}\{f + g - g(\pi_g{}^+) - g(\pi_g{}^-) - 2g(\sigma_{2u})$$
$$- 2K(\pi_g{}^+, \pi_g{}^-) + 2K(\pi_g{}^+, \sigma_{3u}) + 2K(\pi_g{}^+, \pi_u{}^+) + 2K(\pi_g{}^+, \pi_u{}^-)$$
$$+ 2K(\pi_g{}^-, \sigma_{3u}) + 2K(\pi_g{}^-, \pi_u{}^+) + 2K(\pi_g{}^-, \pi_u{}^-)$$
$$+ 4K(\sigma_{3u}, \pi_u{}^+) + 4K(\sigma_{3u}, \pi_u{}^-)$$
$$+ 4K(\pi_u{}^+, \pi_u{}^-)\}$$

$$H_{N_1N_1} = p - h(\pi_g{}^+) - h(\pi_g{}^-) - h(\sigma_{3u}) - h(\sigma_{2u})$$
$$+ s + t - t(\pi_g{}^+) - t(\pi_g{}^-) - t(\sigma_{3u}) - t(\sigma_{2u})$$
$$+ J(\pi_g{}^+, \pi_g{}^-) + J(\pi_g{}^+, \sigma_{3u}) + J(\pi_g{}^+, \sigma_{2u}) + 2J(\pi_g{}^+, \pi_u{}^+) + 2J(\pi_g{}^+, \pi_u{}^-)$$
$$+ J(\pi_g{}^-, \sigma_{3u}) + J(\pi_g{}^-, \sigma_{2u}) + 2J(\pi_g{}^-, \pi_u{}^+) + 2J(\pi_g{}^-, \pi_u{}^-)$$
$$+ J(\sigma_{3u}, \sigma_{2u}) + 2J(\sigma_{3u}, \pi_u{}^+) + 2J(\sigma_{3u}, \pi_u{}^-)$$
$$+ 2J(\sigma_{2u}, \pi_u{}^+) + 2J(\sigma_{2u}, \pi_u{}^-)$$
$$+ J(\pi_u{}^+, \pi_u{}^+) + 4J(\pi_u{}^+, \pi_u{}^-)$$
$$+ J(\pi_u{}^-, \pi_u{}^-)$$
$$- \tfrac{1}{2}\{f + g - g(\pi_g{}^+) - g(\pi_g{}^-) - g(\sigma_{3u}) - g(\sigma_{2u})$$
$$+ 2K(\pi_g{}^+, \pi_u{}^+) + 2K(\pi_g{}^+, \pi_u{}^-) + 2K(\pi_g{}^-, \pi_u{}^+) + 2K(\pi_g{}^-, \pi_u{}^-)$$
$$+ 2K(\sigma_{3u}, \pi_u{}^+) + 2K(\sigma_{3u}, \pi_u{}^-) + 2K(\sigma_{2u}, \pi_u{}^+) + 2K(\sigma_{2u}, \pi_u{}^-)$$
$$+ 4K(\pi_u{}^+, \pi_u{}^-)\}$$
$$+ K(\pi_g{}^+, \pi_g{}^-) - K(\pi_g{}^+, \sigma_{3u}) - K(\pi_g{}^+, \sigma_{2u}) + K(\sigma_{3u}, \sigma_{2u})$$

$$H_{AB} = (\pi_g{}^+\pi_u{}^+|\pi_g{}^-\pi_u{}^-) + (\pi_g{}^+\pi_u{}^-|\pi_g{}^-\pi_u{}^+)$$

$$H_{AE} = (\sigma_{3g}\sigma_{3u}|\sigma_{3g}\sigma_{3u}) \qquad H_{AF} = 0$$

$H_{AJ_1} = -2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$

$H_{AJ_2} = -\sqrt{3}\,(\sigma_{3g}\pi_g{}^+|\sigma_{3u}\pi_u{}^-)$ $\qquad H_{AN_1} = H_{AJ_1}(^3\Sigma_g{}^-)$

$H_{AL} = (\sigma_{2u}\sigma_{3u}|\sigma_{2u}\sigma_{3u})$ $\qquad H_{BE} = 0$

$H_{BJ_1} = -2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{BJ_2} = \sqrt{3}\,(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$ $\qquad H_{BN_1} = 0$

$H_{BL} = 0$

$H_{EJ_1} = -2(\sigma_{3g}\sigma_{3u}|\pi_g{}^+\pi_u{}^+) + (\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$

$H_{EJ_2} = \sqrt{3}\,(\sigma_{3g}\pi_u{}^+|\sigma_{3u}\pi_g{}^-)$ $\qquad H_{EN_1} = -\sqrt{2}\,(\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{3u})$

$H_{EL} = (\sigma_{3g}\sigma_{2u}|\sigma_{3g}\sigma_{2u})$

$H_{J_1J_2} = \frac{\sqrt{3}}{2}\{K(\pi_g{}^+, \sigma_{3u}) - K(\pi_g{}^+, \sigma_{3g}) - K(\pi_u{}^-, \sigma_{3u}) + K(\pi_u{}^-, \sigma_{3g})\}$

$H_{J_1L} = H_{J_2L} = 0$

$H_{J_1N_1} = \frac{1}{\sqrt{2}}\{2(\sigma_{3g}\sigma_{2u}|\pi_g{}^+\pi_u{}^+) - (\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)\}$

$H_{J_2N_1} = \sqrt{\frac{3}{2}}\,(\sigma_{3g}\pi_g{}^+|\sigma_{2u}\pi_u{}^-)$ $\qquad H_{LN_1} = H_{HJ_1}(^3\Sigma_g{}^-)$

(ix) $^3\Delta_u$ (O_2)

$H_{AA}(^3\Delta_u) = H_{AA}(^3\Sigma_u{}^+) + K(\pi_g{}^+, \pi_u{}^-) - (\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)$

(x) $^1\Delta_u$ (O_2)

$H_{AA}(^1\Delta_u) = H_{AA}(^3\Sigma_u{}^-) + K(\pi_g{}^+, \pi_u{}^-) + (\pi_g{}^+\pi_g{}^-|\pi_u{}^-\pi_u{}^+)$

Table XXXVIII Formulae for Evaluating F_{ij}

O_2: $F_{ij} = (\Phi_i|\sum_k f_k s_{kz}|\Phi_j)$

f_k and s_{kz} are one electron operators of orbit and spin z component, respectively. In our case f is $\frac{P_2}{r^3}$ or $\delta(r)$. Only the matrix elements non-vanising within approximations of 9 and 15 dimensional configurational interactions are listed here.

$F_{AA} = (\pi_g{}^+|f|\pi_g{}^+)$ $\qquad F_{F_1F_1} = \frac{1}{2}\{(\pi_g{}^-|f|\pi_g{}^-) + (\pi_u{}^+|f|\pi_u{}^+)\}$

$F_{AJ_3} = -\frac{1}{2}(\sigma_{2u}|f|\sigma_{3u})$ $\qquad F_{F_1F_3} = \frac{1}{2\sqrt{2}}\{(\sigma_{3u}|f|\sigma_{3u}) - (\sigma_{3g}|f|\sigma_{3g})\}$

$F_{BB} = F_{AA}$ $\qquad F_{F_1M_3} = \frac{1}{2\sqrt{2}}(\sigma_{2g}|f|\sigma_{3g})$

$F_{CC} = (\pi_u{}^+|f|\pi_u{}^+)$ $\qquad F_{F_2F_2} = \frac{1}{2}\{(\sigma_{3g}|f|\sigma_{3g}) + (\sigma_{3u}|f|\sigma_{3u})\}$

$F_{DD} = F_{E_1E_1} = F_{CC}$ $\qquad F_{F_2F_3} = \frac{1}{2\sqrt{2}}\{(\pi_u{}^+|f|\pi_u{}^+) - (\pi_g{}^-|f|\pi_g{}^-)\}$

$F_{E_2E_2} = F_{AA}$ $\qquad F_{F_2M_2} = -\frac{1}{2}(\sigma_{2g}|f|\sigma_{3g})$

$F_{F_3F_3} = \frac{1}{4}\{(\pi_u{}^+|f|\pi_u{}^+) + (\pi_g{}^-|f|\pi_g{}^-) + (\sigma_{3g}|f|\sigma_{3g}) + (\sigma_{3u}|f|\sigma_{3u})\}$

$F_{F_3M_1} = -\frac{1}{2\sqrt{2}}(\sigma_{2g}|f|\sigma_{3g})$ $\qquad F_{HJ_3} = \frac{1}{2}(\sigma_{3u}|f|\sigma_{2u})$

$F_{F_3M_3} = -\frac{1}{4}(\sigma_{2g}|f|\sigma_{3g})$ $\qquad F_{J_1J_1} = F_{AA}$

$F_{HH} = F_{AA}$ $\qquad F_{J_1J_3} = \frac{1}{2\sqrt{2}}\{(\sigma_{2u}|f|\sigma_{2u}) - (\sigma_{3u}|f|\sigma_{3u})\}$

$F_{J_3J_3} = \frac{1}{4}\{2(\pi_g{}^+|f|\pi_g{}^+) + (\sigma_{3u}|f|\sigma_{3u}) + (\sigma_{2u}|f|\sigma_{2u})\}$

$F_{LL} = F_{AA}$ $\qquad F_{M_2M_2} = \frac{1}{2}\{(\sigma_{3u}|f|\sigma_{3u}) + (\sigma_{2g}|f|\sigma_{2g})\}$

$F_{M_1M_1} = F_{F_1F_1}$ $\qquad F_{M_2M_3} = F_{F_2F_3}$

$F_{M_1M_3} = \frac{1}{2\sqrt{2}}\{(\sigma_{2g}|f|\sigma_{2g}) - (\sigma_{3u}|f|\sigma_{3u})\}$

$F_{M_3M_3} = \frac{1}{4}\{(\pi_u{}^+|f|\pi_u{}^+) + (\pi_g{}^-|f|\pi_g{}^-) + (\sigma_{3u}|f|\sigma_{3u}) + (\sigma_{2g}|f|\sigma_{2g})\}$

$F_{O_1O_1} = F_{AA}$

Table XXXIX. Formulae for evaluating the matrix elements in the dipole velocity method

(i) $^1\Sigma_g^+ - ^1\Sigma_u^+$ (Li_2)

i	j	$(\Phi_i(^1\Sigma_g^+)\|\sum_k \zeta_k\|\Phi_j(^1\Sigma_u^+))$
1	1	$\sqrt{2}\,(\sigma_{2g}\|\zeta\|\sigma_{2u})$
1	2	$\sqrt{2}\,(\sigma_{2g}\|\zeta\|\sigma_{3u})$
2	3	$\sqrt{2}\,(\sigma_{3g}\|\zeta\|\sigma_{2u})$
2	4	$\sqrt{2}\,(\sigma_{3g}\|\zeta\|\sigma_{3u})$
3	1	$\sqrt{2}\,(\sigma_{2u}\|\zeta\|\sigma_{2g})$
3	3	$\sqrt{2}\,(\sigma_{2u}\|\zeta\|\sigma_{3g})$
4	2	$\sqrt{2}\,(\sigma_{3u}\|\zeta\|\sigma_{2g})$
4	4	$\sqrt{2}\,(\sigma_{3u}\|\zeta\|\sigma_{3g})$
5	1	$(\sigma_{3g}\|\zeta\|\sigma_{2u})$
5	2	$(\sigma_{3g}\|\zeta\|\sigma_{3u})$
5	3	$(\sigma_{2g}\|\zeta\|\sigma_{2u})$
5	4	$(\sigma_{2g}\|\zeta\|\sigma_{3u})$
6	1	$(\sigma_{3u}\|\zeta\|\sigma_{2g})$
6	2	$(\sigma_{2u}\|\zeta\|\sigma_{2g})$
6	3	$(\sigma_{3u}\|\zeta\|\sigma_{3g})$
6	4	$(\sigma_{2u}\|\zeta\|\sigma_{3g})$
7	5	$\sqrt{2}\,(\pi_g^-\|\zeta\|\pi_u^-)$
8	5	$\sqrt{2}\,(\pi_u^-\|\zeta\|\pi_g^-)$

(ii) $^1\Sigma_g^+ - ^1\Pi_u$ (Li_2)

i	j	$(\Phi_i(^1\Sigma_g^+)\|\sum_k(\xi_k \pm i\eta_k)\|\Phi_j(^1\Pi_u))$
1	1	$\sqrt{2}\,(\sigma_{2g}\|\xi \pm i\eta\|\pi_u^\mp)$
2	2	$\sqrt{2}\,(\sigma_{3g}\|\xi \pm i\eta\|\pi_u^\mp)$
3	3	$\sqrt{2}\,(\sigma_{2u}\|\xi \pm i\eta\|\pi_g^\mp)$
4	4	$\sqrt{2}\,(\sigma_{3u}\|\xi \pm i\eta\|\pi_g^\mp)$
5	1	$(\sigma_{3g}\|\xi \pm i\eta\|\pi_u^\mp)$
5	2	$(\sigma_{2g}\|\xi \pm i\eta\|\pi_u^\mp)$
6	3	$(\sigma_{3u}\|\xi \pm i\eta\|\pi_g^\mp)$
6	4	$(\sigma_{2u}\|\xi \pm i\eta\|\pi_g^\mp)$
7	3	$(\pi_g^\pm\|\xi \pm i\eta\|\sigma_{2u})$
7	4	$(\pi_g^\pm\|\xi \pm i\eta\|\sigma_{3u})$
8	1	$(\pi_u^\pm\|\xi \pm i\eta\|\sigma_{2g})$
8	2	$(\pi_u^\pm\|\xi \pm i\eta\|\sigma_{3g})$

(iii) $^3\Sigma_g^- - ^3\Sigma_u^-$ (O_2)

i	j	$(\Phi_i(^3\Sigma_g^-)\|\sum_k \zeta_k\|\Phi_j(^3\Sigma_u^-))$
A	A	$-\sqrt{2}\,(\pi_u^-\|\zeta\|\pi_g^-)$
A	E_1	$\sqrt{2}\,(\sigma_{3g}\|\zeta\|\sigma_{3u})$
B	B	$-\sqrt{2}\,(\pi_u^-\|\zeta\|\pi_g^-)$
B	E_1	$\sqrt{2}\,(\sigma_{3u}\|\zeta\|\sigma_{3g})$
C	A	$-\sqrt{2}\,(\pi_g^+\|\zeta\|\pi_u^+)$
C	F_1	$\sqrt{2}\,(\sigma_{3g}\|\zeta\|\sigma_{3u})$
F_1	A	$\sqrt{2}\,(\sigma_{3u}\|\zeta\|\sigma_{3g})$
F_1	B	$\sqrt{2}\,(\sigma_{3g}\|\zeta\|\sigma_{3u})$
F_1	E_1	$-\sqrt{2}\,(\pi_g^+\|\zeta\|\pi_u^+)$
F_1	F_1	$-\sqrt{2}\,(\pi_u^-\|\zeta\|\pi_g^-)$
F_1	I_1	$-\,(\sigma_{2u}\|\zeta\|\sigma_{3g})$
J_1	E_1	$-\,(\sigma_{3g}\|\zeta\|\sigma_{2u})$
J_1	I_1	$-\sqrt{2}\,(\pi_u^-\|\zeta\|\pi_g^-)$

Errata

Unfortunately, in Part X of our series of papers,[1] we found some numerical errors in the seventh significant figures of the integrals for Set III and found also the following misprints and numerical errors.

Page	Line	Column	Table	
63	2			Molecular Integrals X
64	14			$R(\varphi_i(1)\varphi_j(1)\|\varphi_k(2)\varphi_l(2))=\cdots$
66	9–25			ψ should be replaced by Φ
	18			$\cdots,\ n)\sum_{k=1}^{n}\delta(r_{ak})S_{kz}\Phi_j(1, 2, \cdots$
	23–25			(R=4.5, $\cdots$ for Li_2 and 2.30 for O_2) *In the numerical values of H_{ij} of the O_2 molecule, however, the energy of the nuclear repulsion, $\frac{Z^2}{R}=\frac{64}{2.3}$, is included contrary to the Li_2 case.*
				In the above, $\cdots$
72–76			XXX (xi)	heading ; $R(\varphi_i(1)\varphi_j(1)\|\varphi_k(2)\varphi_l(2))$
77	23	11	XXXII (iv)	$\overline{\overline{1}}$
79	3	2	XXXIII (a)	$^1\Pi_u$ should be replaced by $^1\Sigma_u^+$
79	24	2	XXXIII (b)	$^1\Pi_u$ should be replaced by $^1\Sigma_u^+$
85	18–21	1–5	XXXIII (i)	4.5 −16.*13951* −16.*34025* −16.*07596*
				55 5.0 −16.*31351* −16.*31923* −16.*27021*
				5.5 −16.*16034* −16.*03542* −16.*13132*
86	21–213	1–5	XXXIII (j)	4.5 −16.*26276* −16.*47833* −16.*22966*
				55 5.0 −16.*42444* −16.*44350* −16.*40855*
				5.5 −16.*26119* −16.*14839* −16.*25708*
87	31–		XXXIII (1)	Following footnotes should be added. *Such matrix elements are omitted here that have the same numerical values as those given in Tables (h), (i), (j), and (k), where (1s) core electrons are taken into account explicitly.*
88	1	3	XXXIV (6)	$2R^3q_{ij}$ should be replaced by R^3q_{ij}
94	34–36		XXXV	4.5 −16.164*993*
				5.0 −16.341*226*
				5.5 −16.189*098*