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**Luminescence Emission in a Nanocrystal Doped by a Transition  
Metal Impurity**

George Chappell Jr.

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LUMINESCENCE EMISSION IN A NANOCRYSTAL DOPED BY A  
TRANSITION METAL IMPURITY

A thesis submitted to  
the Graduate College of  
Marshall University  
In partial fulfillment of  
the requirements for the degree of  
Master of Arts  
in  
Mathematics

by  
George Chappell, Jr.

Approved by  
Dr. Que Huong Nguyen, Committee Chairperson  
Dr. Carl Mummert  
Dr. Scott Sarra

MARSHALL UNIVERSITY  
May 2020

APPROVAL OF THESIS/DISSERTATION

We, the faculty supervising the work of George Chappell, Jr., affirm that the thesis, *Luminescence Emission in a Nanocrystal Doped by a Transition Metal Impurity*, meets the high academic standards for original scholarship and creative work established by the Department of Mathematics and the College of Science. This work also conforms to the formatting guidelines of Marshall University. With our signatures, we approve the manuscript for publication.

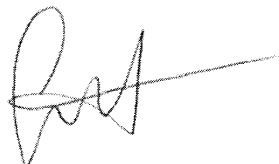


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## ACKNOWLEDGEMENTS

I had a hard time starting to write this section. There are a lot of thanks to go around and perhaps had I majored in English Composition instead of mathematics I could have properly expressed it all. In spite of this short coming, I'll try to do my best.

Starting with Dr. Que Huong Nguyen, my adviser, I was grateful from the moment she agreed to take me on as her grad student. I didn't expect that. Though I didn't know of any administrative hurdles at the time, I'm sure she did. For that matter, any matter of people did. However she was the first to say yes, and hasn't stopped with her consistent and adamant message of "Yes, you can." For these six years she has encouraged me, insisting that I can do this even though I never thought I could have finished. Then there is all the personal effort she had put into the project herself with mentoring and making my own work shine. While a thesis without an adviser can't succeed, I feel that Dr. Nguyen went well above what could have been expected of her.

On the subject of administrative hurdles, I clearly remember the emphasized words "There is a precedence," when discussing a cross discipline thesis. In addition to Dr. Nguyen's efforts the thesis wouldn't have gotten off the ground without the work of Dr. Alfred Akinsete and Dr. Carl Mummert. I enjoy mathematics, but it's applications in physics is like the universe's poetry. The way the laws of the universe seem to fall together, like they *must* be that way is beautiful and I am ever so grateful for those who put in the effort required to allow me to uncover some more of those mysteries.

Dr. Mummert has helped in more direct ways, including, but in no way limited to helping with the technical side of putting this document and my slides together, helping with the algorithm for finding the sign of a permutation, and general advice.

Much of this thesis relies heavily on programming, and it would have been impossible to write this without the programming skills I acquired while taking Dr. Scott Sarra's Numerical courses.

Lastly, though trite, it's also true that I couldn't have done this without the support of my family and friends. Be it financial or emotional support, my parents, brother, and my friends

got me through this. Though their names may not be cited nor appear anywhere in this work, like those mentioned before, their contributions will not be forgotten.

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## ABSTRACT

In this thesis we consider the structure of magnetic ion centers with  $3d$ -electrons in quantum dots under the effects of Coulomb and exchange interaction between the  $3d$ -electrons of the impurity centers and the confined electrons (or holes) existing inside the nanocrystals. In particular, we are interested how this interaction changes the photoluminescence properties of those materials. We will make use of representation theory and the symmetry of the crystal structure to find the orthonormal wave functions that make up the wave functions of the outer,  $3d$ -electrons inside our dot. The Coulomb and exchange interaction between the extra electron and the states of the impurity ions together with the confinement effect are expected to mix the wave functions, split the impurity energy levels, break the previous selection rules, and change the transition probabilities.

## CHAPTER 1

### INTRODUCTION

In Bulk II-VI semiconductor compounds, such as CdSe, CdS, ZnS, ZnSe, or GaAs, doping of transition metal or rare-earth elements is used to obtain efficient magnetic and optical properties. With recent developments in nanotechnology, magnetic ion-doped quantum dots have become a great interest and are studied intensively. Successful incorporation of magnetic ions into single colloidal nanocrystals in different labs has been reported [1–4], opening the door for many applications using doped dots in spintronics and quantum information technology. Optical spectra from single quantum dot doped by magnetic elements such as Mn, Fe, Cr, Co have been investigated [1, 5–7].

The impurity states in a doped nanocrystal are reported to play an important role in the electronic structure, transition probabilities, and the optical properties of the nanocrystal. The optical properties of the impurity centers in nanocrystals are very different from the bulk cases. One such example is  $\text{Mn}^{2+}$ . Well known as an activator for photoluminescence (PL) and electroluminescence, the  $\text{Mn}^{2+}$  ion has been among the first magnetic ions to be doped into a semiconductor nanocrystal [1]. It was claimed [1, 7] that the Mn-doped ZnS nanocrystal can yield both high luminescence efficiency and significant lifetime shortening. The yellow emission is reported slightly shifted toward a lower energy (in nanocrystal ZnS:Mn it peaks at 2.10 eV instead of around 2.12 eV in bulk). The reported line width of the yellow emissions in the PL spectrum for a nanocrystal is larger than in bulk and, more importantly, the luminescence lifetime of the  ${}^4T-{}^6A$  transition was reported to decrease by 5 orders of magnitude, from 1.8 ms in bulk to 3.7ns and 20.5ns in nanocrystals, while maintaining the high (18%) quantum efficiency. Considerable attention has been paid to optical properties of this kind of material afterward, and the increase in luminescence efficiency as well as the lifetime shortening of different quantum dots and quantum wells have been reported [8–12]. Different models have been proposed to explain the processes occurring with the impurity centers inside the confined nanocrystals [7, 13, 14], but the effects of the confinement on the energy structure and transitions of impurity center in the nanocrystals remain controversial and probably consist of several different mechanisms.

Some of these include strong hybridization of the  $s$ - $p$  electrons of the ZnS host and  $3d$ -electrons of the impurity due to confinement, and the modification of the crystal field near the surface of the nanocrystals [7]. In [15], Huong and Birman proposed that the Coulomb and exchange interaction of the  $3d$ -electrons of the impurity centers with the confined electrons (or holes) existing inside the nanocrystals could change the photoluminescence properties in general. This could explain the observed shortening of lifetime and enhancement of the quantum efficiency in the specific  $\text{Mn}^{2+}$  center case. In the strong confinement approximation, the boundary conditions enhance the coupling, and the effect on PL will be large.

Following the study of the effect of the confinement on the  $\text{Mn}^{2+}$  center in a semiconductor nanocrystal [15], in this thesis we consider the structure of magnetic ion centers with  $3d$ -electrons in quantum dots under the effects of Coulomb and exchange interaction between the  $3d$ -electrons of the impurity centers and the confined electrons (or holes) existing inside the nanocrystals could change the photoluminescence properties of the semiconductor dot. The impurity centers of interest are of magnetic elements with  $3d$ -electrons for instance,  $\text{Mn}^{2+}$ ,  $\text{Fe}^{2+}$ , and  $\text{Co}^{2+}$  in II-VI semiconductor nanocrystals. The Coulomb and exchange interaction between the extra electron and the states of the impurity ions, together with the confinement effect, are expected to mix the wave functions, split the impurity energy levels, break the previous selection rules, and change the transition probabilities.

## CHAPTER 2

### WAVE FUNCTIONS OF THE CONFINED ELECTRON AND THE IMPURITY CENTER

In our theory, the electrons of the quantum dot will strongly interact with the electron of the impurity center. Due to this interaction, the original energy level of the impurity center in the crystal field will be split, the wave function will be mixed, and the selection rules will be broken. Then the previously forbidden transition will become allowed and the photoluminescence of the nanocrystal will be changed.

#### 2.1 THE EXTRA ELECTRON CONFINED INSIDE THE DOPED DOT

In order to calculate the interaction between the impurity doping center and an electron which might exist inside the dot or be injected into the dot to control the emission in the nanocrystal, we will use the wave function of the electron confined in a spherical quantum dot.

For the electron confined in the dot and localized at some lattice point, we use the Wannier electron function

$$\psi_{1s}^{\text{dot}} = \sum_i R_{1s}^{\text{dot}} Y_0^0 \left| \frac{1}{2}, \sigma \right\rangle, \quad (2.1)$$

where  $Y_l^m$  are the spherical harmonics,  $|\frac{1}{2}, \sigma\rangle$  is the electron spin function, and  $R_{1s}^{\text{dot}}$  is the envelope function of the 1s electron confined in a sphere of radius  $R$ . Here

$$R_{nl}^{\text{dot}} = \sqrt{\frac{2}{R^3}} \frac{j_l(\chi_{nl} \frac{r}{R})}{j_{l+1}(\chi_{nl})}, \quad (2.2)$$

where  $j_l$  is the spherical Bessel function and  $\chi_{nl}$  is the  $n^{\text{th}}$  root of the spherical Bessel Functions. The envelope function is chosen to meet the boundary condition, which requires the wave function is zero at the boundary of the quantum dot.

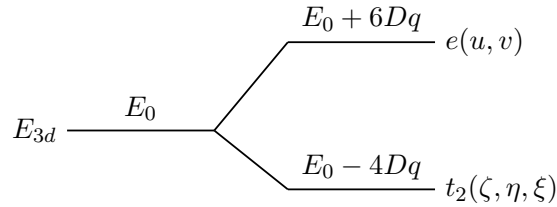
#### 2.2 A SINGLE 3d-ELECTRON IN THE CRYSTAL FIELD

Impurity centers are foreign ions replacing host ions or placed interstitially in the lattice. When such a center is placed in the crystal field of the host semiconductor lattice, the crystal

(due to the ions of the lattice) affects the energy structure of the ion from the crystal field state of the ion.

We are interested in doping the semiconductor lattice ZnS with transition metal ions, though the computational result should hold for any crystal lattice with  $O_h$  symmetry. Transition metals belong to the special class of elements which have  $n$ ,  $3d$ -electrons ( $3d^n$  shell) in the outer shell. In this section we will introduce the wave function of a single  $3d$ -electron in octahedral crystal field, then in the next section we will see how to obtain the states of the  $n$ ,  $3d$ -electrons.

The  $3d$ -electrons, where the  $d$  corresponds with  $l = 2$ , are five-fold degenerate energy level. In an octahedral crystal field, the fivefold degenerate  $3d$  level will split principally into two levels: the twofold degenerate level  $e$  with the additional energy  $+6Dq$  and the threefold degenerate level  $t_2$  with the additional energy  $-4Dq$  [16, 17], where  $D = \frac{1}{4\pi\epsilon_0} \frac{35ze^2}{4a^5}$  and  $q = \frac{2}{105} \langle r^4 \rangle_{3d}$ , with  $q$  being the distance between the lattice sites and  $-ze$  being the charge of the ion and  $-e$  the charge of an electron. The parameters  $D$  and  $q$  always appear together as a product  $Dq$ , which could be regarded as the strength of the octahedral field. The wave functions of  $3d$ -electron orbitals are  $u$  and  $v$  which belong to the  $E$  irreducible representation and  $\zeta$ ,  $\eta$ , and  $\xi$  which belong to the  $T_2$  reducible representation of the  $O_h$  symmetry group.



**Figure 1.** ENERGY SPLITTING OF A SINGLE  $3d$ -ELECTRON IN AN OCTOAHEDRAL CRYSTAL FIELD

Here the wave functions have the form

$$\begin{aligned}
|u\rangle &= R_{3d}Y_2^0 \\
|v\rangle &= 2^{-\frac{1}{2}}R_{3d}(Y_2^2 + Y_2^{-2}) \\
|\zeta\rangle &= i2^{-\frac{1}{2}}R_{3d}(Y_2^1 + Y_2^{-1}) \\
|\eta\rangle &= -2^{-\frac{1}{2}}R_{3d}(Y_2^1 - Y_2^{-1}) \\
|\xi\rangle &= i2^{-\frac{1}{2}}R_{3d}(Y_2^2 - Y_2^{-2}),
\end{aligned}$$

where  $Y_l^m$  are the spherical harmonics and the radial functions of the  $nd$ -electrons.

### 2.3 THE $3d^n$ ELECTRON IN AN OCTAHEDRAL CRYSTAL FIELD

The magnetic ions of interest have configurations with outer  $3d^n$  electrons. Mn has a  $3d^5$  configuration, Fe has a  $3d^6$  configuration, and  $\text{Co}^{2+}$  has a  $3d^7$  configuration. For  $\text{Mn}^{2+}$  in the crystal field of ZnS nanocrystal, the transition of our interest is  ${}^4T_1-{}^6A_1$ . The transition  ${}^2T_1-{}^4T_2$  for Co and the transition  ${}^3A_2-{}^5E$  for  $\text{Fe}^{2+}$  will be considered. Due to spin differences, the above transitions are spin forbidden. In the strong-crystal-field case, the wave functions of the multi- $3d$ -electron Hamiltonian will be the product of these one-electron orbitals. Let us start with the reduction process for the two  $3d$ -electron configurations.

### 2.4 FOR $3d^2$ CONFIGURATIONS

For two  $3d$ -electrons, the wave functions will belong to representations contained within the Kronecker products of the possible representations for the electrons. In particular we are interested in the products

$$\begin{aligned}
e \times e &= A_1 + A_2 + E \\
e \times t_2 &= T_1 + T_2 \\
t_2 \times t_2 &= A_1 + E + T_1 + T_2,
\end{aligned}$$

where  $A$  is one dimensional,  $E$  is two dimensional, and  $T$  is three dimensional. Here we use the notation found in [18] where lower case letters are used for the electrons and the systems use

capital letters. A subscript 1 indicates symmetric basis functions, and a 2 indicates anti-symmetric basis functions. Here symmetric and anti-symmetric refer only to the orbital wave functions. The total wave functions (including spin) of the system must be anti-symmetric.

From here we can find the wave function for the system in each of these configurations. In our notation, the wave functions are denoted as  $|a, B\rangle$  where  $a$  gives the electron configuration, and  $B$  is the representation the system belongs to. The order of induction should not matter since electrons in the same state are indistinguishable from one another. Also, here  $u$  and  $v$  are wave functions belonging to the  $E$  representation, while  $\xi$ ,  $\eta$ , and  $\zeta$  belong to  $T_2$ .

At this step we still do not include spin in the configuration. Another point of notation is that we use subscripts to indicate the order in which the electron with that wave function was introduced. For example, instead of  $|e^2, A_1\rangle = \frac{1}{\sqrt{2}}(u(r_1)v(r_2) + u(r_2)v(r_1))$ , we will write  $\frac{1}{\sqrt{2}}(u_1v_2 + u_2v_1)$ . Here, the multiplicative operation indicates a Slater determinant. For example,  $u_1v_2 = |u_1v_2| = \frac{1}{\sqrt{2}}(u_1v_2 - u_2v_1)$  where multiplication on the left is ordinary multiplication. More generally, for  $n$  functions,  $f_i$ , and  $n$  electrons located at  $r_1 \dots r_n$ ,

$$|f_1 \dots f_n| = \frac{1}{\sqrt{n!}} \begin{vmatrix} f_1(r_1) & f_2(r_1) & & f_n(r_1) \\ f_1(r_2) & f_2(r_2) & \cdots & f_n(r_2) \\ & \vdots & \ddots & \vdots \\ f_1(r_n) & f_2(r_n) & \cdots & f_n(r_n) \end{vmatrix}$$

For  $E$ , we have two functions  $Eu$  and  $Ev$ . For induction we use  $Eu$  for  $u$  and  $Ev$  for  $v$ . For  $e \times e$  the wave functions are

$$\begin{aligned} |e^2, {}^1A_1\rangle &= \frac{1}{\sqrt{2}}(u_1u_2 + v_1v_2) \\ |e^2, {}^3A_2\rangle &= \frac{1}{\sqrt{2}}(u_1v_2 - v_1u_2) \\ |e^2, {}^1Eu\rangle &= \frac{1}{\sqrt{2}}(u_1u_2 - v_1v_2) \\ |e^2, {}^1Ev\rangle &= \frac{1}{\sqrt{2}}(u_1v_2 + v_1u_2). \end{aligned}$$

For  $t_2 \times t_2 = A_1 + E + T_1 + T_2$ , we obtain

$$\begin{aligned}
|t^2, A_1\rangle &= \frac{1}{\sqrt{3}}(\xi_1\xi_2 + \eta_1\eta_2 + \zeta_1\zeta_2) \\
|t^2, E^1\rangle &= \frac{1}{\sqrt{3}}(\xi_1\xi_2 + \epsilon\eta_1\eta_2 + \epsilon^2\zeta_1\zeta_2) \\
|t^2, E^2\rangle &= \frac{1}{\sqrt{3}}(\xi_1\xi_2 + \epsilon^2\eta_1\eta_2 + \epsilon\zeta_1\zeta_2) \\
|t^2, T_1^1\rangle &= \frac{1}{\sqrt{3}}\eta_1\zeta_2 \\
|t^2, T_1^2\rangle &= \frac{1}{\sqrt{3}}\zeta_1\xi_2 \\
|t^2, T_1^3\rangle &= \frac{1}{\sqrt{3}}\xi_1\eta_2 \\
|t^2, T_2^1\rangle &= \frac{1}{\sqrt{3}}\zeta_1\eta_2 \\
|t^2, T_2^2\rangle &= \frac{1}{\sqrt{3}}\xi_1\zeta_2 \\
|t^2, T_2^3\rangle &= \frac{1}{\sqrt{3}}\eta_1\xi_2
\end{aligned}$$

Here,  $\epsilon$  is the first cube root of unity.

Continuing the reduction we can get all wave functions for  $t^m e^k$  configurations, for  $m, k \in \mathbb{Z}$  and  $m + k = n$ .

## 2.5 FOR $3d^3$ CONFIGURATIONS

Starting from  $e^2$ , we have systems with wave function which are basis functions for the  $A_1$ ,  $A_2$ , and  $E$  representations. Suppose we then introduce an electron with a wave function belonging to the  $e$  representation, then the resulting system's representation would be  $E$ , if it previously was  $A_1$  or  $A_2$ , or  $A_1$ ,  $A_2$ , and  $E$  if the system's representation was  $E$ . That is  $A_1 \times e = E$ ,  $A_2 \times e = E$  and  $E \times e = A_1 + A_2 + E$ . Now we compute the wave functions inductively, starting with a system in  $A_1$



$$|e^3, E^1\rangle = |e^2, A_1\rangle u_3 = \frac{1}{\sqrt{2}}(u_1v_2 + u_2v_1)u_3$$

$$|e^2, E^2\rangle = |e^2, A_1\rangle v_3 = \frac{1}{\sqrt{2}}(u_1v_2 + u_2v_1)v_3.$$

Here the subscript indicates at what point in the induction the electron with that wave function was added. Also, note how we did this for each basis function of  $E$ . We then do the same for  $A_2$ :

$$|e^3, E^3\rangle = |e^2, A_2\rangle u_3 = \frac{1}{\sqrt{2}}(u_1v_2 - u_2v_1)u_3$$

$$|e^2, E^4\rangle = |e^2, A_2\rangle v_3 = \frac{1}{\sqrt{2}}(u_1v_2 - u_2v_1)v_3.$$

Moving along, we come to the case of the system with the  $|e^2, E\rangle$  state. In this case we have

$$|e^3, A_1\rangle = \frac{1}{\sqrt{2}}(|e^2, E^1\rangle v_3 + |e^2, E^2\rangle u_3) = \frac{1}{\sqrt{2}}(u_1u_2v_3 + v_1v_2u_3)$$

$$|e^3, A_2\rangle = \frac{1}{\sqrt{2}}(|e^2, E^1\rangle v_3 - |e^2, E^2\rangle u_3) = \frac{1}{\sqrt{2}}(u_1u_2v_3 - v_1v_2u_3)$$

$$|e^3, E^5\rangle = |e^2, E^1\rangle u_3 = u_1u_2u_3$$

$$|e^3, E^6\rangle = |e^2, E^2\rangle v_3 = v_1v_2v_3$$

Continuing with the process, we will show some more results for  $A_1 \times t_2$  and  $T_2 \times t_2$ , for example. For  $A_1 \times t_2$ ,

$$|t^3, T_2^1\rangle = |t^2, A_1\rangle \xi_3 = \frac{1}{\sqrt{3}}(\xi_1\xi_2 + \eta_1\eta_2 + \zeta_1\zeta_2)\xi_3$$

$$|t^3, T_2^2\rangle = |t^2, A_1\rangle \eta_3 = \frac{1}{\sqrt{3}}(\xi_1\xi_2 + \eta_1\eta_2 + \zeta_1\zeta_2)\eta_3$$

$$|t^3, T_2^3\rangle = |t^2, A_1\rangle \zeta_3 = \frac{1}{\sqrt{3}}(\xi_1\xi_2 + \eta_1\eta_2 + \zeta_1\zeta_2)\zeta_3$$

and for  $T_2 \times t_2$ :

$$\begin{aligned}
|t^3, A_1\rangle &= \frac{1}{\sqrt{3}} (|t^3, T_2^1\rangle \xi_3 + |t^3, T_2^2\rangle \eta_3 + |t^3, T_2^3\rangle \zeta_3) \\
&= \frac{1}{3} (\zeta_1 \eta_2 \xi_3 + \xi_1 \zeta_2 \eta_3 + \eta_1 \xi_2 \zeta_3) \\
|t^3, E^1\rangle &= \frac{1}{\sqrt{3}} (|t^3, T_2^1\rangle \xi_3 + \epsilon |t^3, T_2^2\rangle \eta_3 + \epsilon^2 |t^3, T_2^3\rangle \zeta_3) \\
&= \frac{1}{3} (\zeta_1 \eta_2 \xi_3 + \epsilon \xi_1 \zeta_2 \eta_3 + \epsilon^2 \eta_1 \xi_2 \zeta_3) \\
|t^3, E^2\rangle &= \frac{1}{\sqrt{3}} (|t^3, T_2^1\rangle \xi_3 + \epsilon^2 |t^3, T_2^2\rangle \eta_3 + \epsilon |t^3, T_2^3\rangle \zeta_3) \\
&= \frac{1}{3} (\zeta_1 \eta_2 \xi_3 + \epsilon^2 \xi_1 \zeta_2 \eta_3 + \epsilon \eta_1 \xi_2 \zeta_3) \\
|t^3, T_1^1\rangle &= \frac{1}{\sqrt{3}} |t^2, T_2^3\rangle \zeta_3 = \frac{1}{3} \eta_1 \xi_2 \zeta_3 \\
|t^3, T_1^2\rangle &= \frac{1}{\sqrt{3}} |t^2, T_2^2\rangle \xi_3 = \frac{1}{3} \xi_1 \zeta_2 \xi_3 \\
|t^3, T_1^3\rangle &= \frac{1}{\sqrt{3}} |t^2, T_2^1\rangle \eta_3 = \frac{1}{3} \zeta_1 \eta_2 \eta_3 \\
|t^3, T_2^1\rangle &= \frac{1}{\sqrt{3}} |t^2, T_2^2\rangle \eta_3 = \frac{1}{3} \xi_1 \zeta_2 \eta_3 \\
|t^3, T_2^2\rangle &= \frac{1}{\sqrt{3}} |t^2, T_2^1\rangle \zeta_3 = \frac{1}{3} \zeta_1 \eta_2 \zeta_3 \\
|t^3, T_2^3\rangle &= \frac{1}{\sqrt{3}} |t^2, T_2^3\rangle \xi_3 = \frac{1}{3} \eta_1 \xi_2 \xi_3.
\end{aligned}$$

The process for finding the wave functions for  $e^2 \times t$  and  $e \times t^2$  is much the same. We start with a system wave function in the appropriate representation and then introduce an electron in the appropriate representation.

## 2.6 WAVE FUNCTIONS FOR $t^7$

We obtain all the reduction up to  $3d^7$  to cover a series of transition metals. The following is a representative result for  $t^7$  which also involves spin, which is indicated with a + for up, and a - for down:

$$\begin{aligned}
|t^7, {}^4T_1x\rangle &= |t^3, {}^4A_2\rangle |t^4, {}^1T_2\xi\rangle \\
&= -\frac{1}{\sqrt{2}} (\xi^+\eta^+\zeta^+) (\xi^2\eta^+\zeta^- - \xi^2\eta^-\zeta^+) \\
&= -\frac{1}{\sqrt{2}} (\xi^+\eta^+\zeta^+\xi^2\eta^+\zeta^- - \xi^+\eta^+\zeta^+\xi^2\eta^-\zeta^+) \\
|t^7, {}^4T_1y\rangle &= |t^3, {}^4A_2\rangle |t^4, {}^1T_2\eta\rangle \\
&= -\frac{1}{\sqrt{2}} (\xi^+\eta^+\zeta^+) (\xi^+\eta^2\zeta^- - \xi^-\eta^2\zeta^+) \\
&= -\frac{1}{\sqrt{2}} (\xi^+\eta^+\zeta^+\xi^+\eta^2\zeta^- - \xi^+\eta^+\zeta^+\xi^-\eta^2\zeta^+) \\
|t^7, {}^4T_1z\rangle &= |t^3, {}^4A_2\rangle |t^4, {}^1T_2\zeta\rangle \\
&= -\frac{1}{\sqrt{2}} (\xi^+\eta^+\zeta^+) (\xi^+\eta^-\zeta^2 - \xi^-\eta^+\zeta^2) \\
&= -\frac{1}{\sqrt{2}} (\xi^+\eta^+\zeta^+\xi^+\eta^-\zeta^2 - \xi^+\eta^+\zeta^+\xi^-\eta^+\zeta^2) \\
|t^7, {}^2Eu\rangle &= |t^4, {}^1A_1\rangle |t^3, {}^2Eu\rangle \\
&= \frac{1}{\sqrt{6}} (\xi^2\eta^2 + \eta^2\zeta^2 + \zeta^2\xi^2) (\xi^+\eta^-\zeta^+ - \xi^-\eta^+\zeta^+) \\
&= \frac{1}{\sqrt{6}} (\xi^2\eta^2\xi^+\eta^-\zeta^+ + \eta^2\zeta^2\xi^+\eta^-\zeta^+ + \zeta^2\xi^2\xi^+\eta^-\zeta^+ \\
&\quad - \xi^2\eta^2\xi^-\eta^+\zeta^+ - \eta^2\zeta^2\xi^-\eta^+\zeta^+ - \zeta^2\xi^2\xi^-\eta^+\zeta^+) \\
|t^7, {}^2Ev\rangle &= |t^4, {}^1A_1\rangle |t^3, {}^2Ev\rangle \\
&= \frac{1}{\sqrt{6}} (\xi^2\eta^2 + \eta^2\zeta^2 + \zeta^2\xi^2) (2\xi^+\eta^+\zeta^- - \xi^+\eta^-\zeta^+ - \xi^-\eta^+\zeta^+) \\
&= \frac{1}{\sqrt{6}} (2\xi^2\eta^2\xi^+\eta^+\zeta^- + 2\eta^2\zeta^2\xi^+\eta^+\zeta^- + 2\zeta^2\xi^2\xi^+\eta^+\zeta^- \\
&\quad - \xi^2\eta^2\xi^+\eta^-\zeta^+ + \eta^2\zeta^2\xi^+\eta^-\zeta^+ + \zeta^2\xi^2\xi^+\eta^-\zeta^+ \\
&\quad - \xi^2\eta^2\xi^-\eta^+\zeta^+ + \eta^2\zeta^2\xi^-\eta^+\zeta^+ + \zeta^2\xi^2\xi^-\eta^+\zeta^+).
\end{aligned}$$

## CHAPTER 3

### ELECTRON-IMPURITY CENTER EXCHANGE INTERACTION

In this chapter, we look at the exchange and Coulomb interactions, as well as programs to aid in computing the exchange operator.

#### 3.1 THE EXCHANGE INTERACTION

In this section, we look at how to calculate the exchange interaction of the extra electron in the dot with the  $3d$ -electrons of the impurity. The operator of the interaction is the Coulomb interaction

$$V(r_1, r_2) = \frac{q_1 q_2}{r_{12}} = \frac{q_1 q_2}{r_>} \sum_{k \geq 0} \frac{r_<^k}{r_>^k} P_k(\cos \theta),$$

where  $r_{12}$  is the magnitude of the distance between electrons at  $r_1$  and  $r_2$ ;  $r_<$  and  $r_>$  are the smaller and larger of  $r_1$  and  $r_2$ ; and  $P_k$  are the Legendre polynomials, which is defined as

$$P_k(\cos \theta) = \frac{4\pi}{2k+1} \sum_{m \in [-k, k]} Y_k^m(1) \overline{Y_k^m}(2).$$

Here, the overline atop the second  $Y$  indicates the complex conjugate and the arguments relate to the electron with that subscript.

Then  $V(r_1, r_2)$  can be written as

$$V(r_1, r_2) = \frac{q_1 q_2}{r_>} \sum_{k \geq 0} \frac{4\pi}{2k+1} \left( \frac{r_<}{r_>} \right)^k \sum_{-k \leq m \leq k} Y_k^m(\text{Co}) \overline{Y_k^m}(\text{dot}).$$

We will compute  $\langle \psi \varphi | V | \varphi \psi \rangle$ , where  $\varphi$  is the confined electron wave function, and  $\psi$  is the wave function of the  $3d^n$  impurity we calculated in Section 2. For example, for  $|t^7, {}^4T_1y\rangle$ ,

$\psi = -\frac{1}{\sqrt{2}} (\xi^+ \eta^+ \zeta^+ \xi^+ \eta^2 \zeta^- - \xi^+ \eta^+ \zeta^+ \xi^- \eta^2 \zeta^+)$  and so

$$\langle \psi \varphi | V | \varphi \psi \rangle = \frac{1}{2} \langle (\xi^+ \eta^+ \zeta^+ \xi^+ \eta^2 \zeta^- - \xi^+ \eta^+ \zeta^+ \xi^- \eta^2 \zeta^+) \varphi | V | \varphi (\xi^+ \eta^+ \zeta^+ \xi^+ \eta^2 \zeta^- - \xi^+ \eta^+ \zeta^+ \xi^- \eta^2 \zeta^+) \rangle.$$

To compute this we may write it as a sum. Since the exchange may be between the dot electron and any one of seven  $3d$  electrons, this becomes

$$\begin{aligned}
2 \langle \psi \varphi | V | \varphi \psi \rangle &= \langle (\xi^+ \eta^+ \zeta^+) (\xi^+ \eta^2 \zeta^- - \xi^- \eta^2 \zeta^+) \varphi | V | \varphi (\xi^+ \eta^+ \zeta^+) (\xi^+ \eta^2 \zeta^- - \xi^- \eta^2 \zeta^+) \rangle \\
&= \langle \xi^+ \eta^+ \zeta^+ \xi^+ \eta^2 \zeta^- \varphi | V | \varphi \xi^+ \eta^+ \zeta^+ \xi^+ \eta^2 \zeta^- \rangle \\
&\quad - \langle \xi^+ \eta^+ \zeta^+ \xi^+ \eta^2 \zeta^- \varphi | V | \varphi \xi^+ \eta^+ \zeta^+ \xi^- \eta^2 \zeta^+ \rangle \\
&\quad - \langle \xi^+ \eta^+ \zeta^+ \xi^- \eta^2 \zeta^+ \varphi | V | \varphi \xi^+ \eta^+ \zeta^+ \xi^+ \eta^2 \zeta^- \rangle \\
&\quad + \langle \xi^+ \eta^+ \zeta^+ \xi^- \eta^2 \zeta^+ \varphi | V | \varphi \xi^+ \eta^+ \zeta^+ \xi^- \eta^2 \zeta^+ \rangle \\
&= \langle \xi \varphi | V | \varphi \xi \rangle \langle \eta^+ \zeta^+ \xi^+ \eta^2 \zeta^- | \eta^+ \zeta^+ \xi^+ \eta^2 \zeta^- \rangle \\
&\quad + \langle \eta^+ \varphi | V | \varphi \eta^+ \rangle \langle \xi^+ \zeta^+ \xi^+ \eta^2 \zeta^- | \xi^+ \zeta^+ \xi^+ \eta^2 \zeta^- \rangle \\
&\quad + \langle \zeta^+ \varphi | V | \varphi \zeta^+ \rangle \langle \xi^+ \eta^+ \xi^+ \eta^2 \zeta^- | \xi^+ \eta^+ \xi^+ \eta^2 \zeta^- \rangle \\
&\quad + \langle \xi^+ \varphi | V | \varphi \xi^+ \rangle \langle \xi^+ \eta^+ \zeta^+ \eta^2 \zeta^- | \xi^+ \eta^+ \zeta^+ \eta^2 \zeta^- \rangle \\
&\quad + \langle \eta^+ \varphi | V | \varphi \eta^+ \rangle \langle \xi^+ \eta^+ \zeta^+ \xi^+ \eta^- \zeta^- | \xi^+ \eta^+ \zeta^+ \xi^+ \eta^- \zeta^- \rangle \\
&\quad + \langle \eta^- \varphi | V | \varphi \eta^- \rangle \langle \xi^+ \eta^+ \zeta^+ \xi^+ \eta^+ \zeta^- | \xi^+ \eta^+ \zeta^+ \xi^+ \eta^+ \zeta^- \rangle \\
&\quad + \langle \zeta^- \varphi | V | \varphi \zeta^- \rangle \langle \xi^+ \eta^+ \zeta^+ \xi^+ \eta^2 | \xi^+ \eta^+ \zeta^+ \xi^+ \eta^2 \rangle
\end{aligned}$$

where  $\theta^2 = \theta^+ \theta^-$  for  $\theta \in \{\xi, \eta, \zeta\}$ .

### 3.1.1 LOOKING FOR NORMALIZATION AND ELIMINATING ZERO TERMS

We want to compute the operator  $V$  of the exchange interaction matrix elements and seven  $3d$ -electrons of the impurity center for this wave function.

We would be working with something like

$$\langle \psi \varphi | V | \varphi \psi \rangle = \langle (\xi^+ \eta^+ \zeta^+ \xi^2 \eta^+ \zeta^- - \xi^+ \eta^+ \zeta^+ \xi^2 \eta^- \zeta^+) \varphi | V | \varphi (\xi^+ \eta^+ \zeta^+ \xi^2 \eta^+ \zeta^- - \xi^+ \eta^+ \zeta^+ \xi^2 \eta^- \zeta^+) \rangle$$

however it quickly turns into something much nicer. We first distribute to form four integrals over eight variables. However, because the operator  $V$  is the sum of the seven components ( $r_1$  through

$r_7$ ), each of these four integrals may be written as the sum of seven others. So, for instance

$$\begin{aligned} \langle \xi^+ \eta^+ \zeta^+ \xi^2 \eta^+ \zeta^- \varphi | V | \varphi \xi^+ \eta^+ \zeta^+ \xi^2 \eta^+ \zeta^- \rangle &= \langle \xi^+ \varphi | V | \varphi \xi^+ \rangle \langle \eta^+ | \eta^+ \rangle \dots \langle \zeta^- | \zeta^- \rangle + \dots \\ &+ \langle \xi^+ | \xi^+ \rangle \dots \langle \zeta^- \varphi | V | \varphi \zeta^- \rangle. \end{aligned}$$

In this case all of the bra-kets not containing  $V$  will be identically 1. We do the same for  $\langle \xi^+ \eta^+ \zeta^+ \xi^2 \eta^+ \zeta^- \varphi | V | \varphi \xi^+ \eta^+ \zeta^+ \xi^2 \eta^- \zeta^+ \rangle$ , however this time we find that every term would include either  $\langle \zeta^- | \zeta^+ \rangle$  or  $\langle \eta^+ | \eta^- \rangle$ . Due to orthonormality, these are identically 0 and therefore the whole thing is identically 0. Collecting terms, we end up with

$$\langle \psi \varphi | V | \varphi \psi \rangle = 6 \langle \xi \varphi | V | \varphi \xi \rangle + 4 \langle \eta \varphi | V | \varphi \eta \rangle + 4 \langle \zeta \varphi | V | \varphi \zeta \rangle.$$

To obtain the correct values for the actual wave function, halve the coefficients.

### 3.1.2 MATRIX ELEMENTS AS THE PRODUCT OF RADIAL AND ANGULAR PARTS

In spherical coördinates, each of  $V$ ,  $\varphi$ ,  $\xi$ ,  $\eta$ , and  $\zeta$  may be written in separation of coördinates as the product of a radial part and an angular part. As a specific example, using

$$\begin{aligned} \xi &= \frac{i}{\sqrt{2}} R_{3d} (Y_2^2 + Y_2^{-2}) \\ \eta &= \frac{1}{\sqrt{2}} R_{3d} (Y_2^1 - Y_2^{-1}) \\ \zeta &= \frac{-i}{\sqrt{2}} R_{3d} (Y_2^2 - Y_2^{-2}) \\ \varphi &= R_{1s}^{\text{dot}} Y_{00} \\ V(r_1, r_2) &= \frac{q_1 q_2}{r_>} \sum_{k \geq 0} \frac{4\pi}{2k+1} \left( \frac{r_{\leq}}{r_>} \right)^k \sum_{-k \leq m \leq k} Y_k^m(1) \bar{Y}_k^m(2), \end{aligned}$$

we can see that  $\langle \eta \varphi | V | \varphi \eta \rangle$  is equal to

$$\left\langle R_{3d} R_{1s}^{\text{dot}} \left| \frac{q_1 q_2}{r_>} \sum_{k \geq 0} \frac{4\pi}{2k+1} \left( \frac{r_{\leq}}{r_>} \right)^k \right| R^{\text{dot}} R_{3d} \right\rangle \left\langle (Y_{21} - Y_{2-1}) Y_{00} \left| \sum_{-k \leq m \leq k} Y_k^m(1) \bar{Y}_k^m(2) \right| Y_{00} (Y_{21} - Y_{2-1}) \right\rangle.$$

### 3.1.3 THE ANGULAR PART

The angular part of  $\langle \eta\varphi|V|\varphi\eta\rangle$  is

$$\left\langle (Y_{21} - Y_{2-1}) Y_{00} \left| \sum_{-k \leq m \leq k} Y_{km}(1) \bar{Y}_{km}(2) \right| Y_{00} (Y_{21} - Y_{2-1}) \right\rangle.$$

This may be expanded out as

$$\begin{aligned} & \sum_{-k \leq m \leq k} \langle (Y_{21} - Y_{2-1}) Y_{00} | Y_{km}(1) \bar{Y}_{km}(2) | Y_{00} (Y_{21} - Y_{2-1}) \rangle \\ &= \sum_{-k \leq m \leq k} \langle Y_{21} Y_{00} | Y_{km}(1) \bar{Y}_{km}(2) | Y_{00} Y_{21} \rangle \\ & \quad - \sum_{-k \leq m \leq k} \langle Y_{2-1} Y_{00} | Y_{km}(1) \bar{Y}_{km}(2) | Y_{00} Y_{21} \rangle \\ & \quad - \sum_{-k \leq m \leq k} \langle Y_{21} Y_{00} | Y_{km}(1) \bar{Y}_{km}(2) | Y_{00} Y_{2-1} \rangle \\ & \quad + \sum_{-k \leq m \leq k} \langle Y_{2-1} Y_{00} | Y_{km}(1) \bar{Y}_{km}(2) | Y_{00} Y_{2-1} \rangle \\ &= \sum_{-k \leq m \leq k} \langle Y_{21} | Y_{km} | Y_{00} \rangle \langle Y_{00} | Y_{km} | Y_{21} \rangle \\ & \quad - \sum_{-k \leq m \leq k} \langle Y_{2-1} | Y_{km} | Y_{00} \rangle \langle Y_{00} | Y_{km} | Y_{21} \rangle \\ & \quad - \sum_{-k \leq m \leq k} \langle Y_{21} | Y_{km} | Y_{00} \rangle \langle Y_{00} | Y_{km} | Y_{2-1} \rangle \\ & \quad + \sum_{-k \leq m \leq k} \langle Y_{2-1} | Y_{km} | Y_{00} \rangle \langle Y_{00} | Y_{km} | Y_{2-1} \rangle. \end{aligned}$$

From the normal-orthogonality of spherical harmonics, we know that most of this is identically zero. In particular, the only items we consider are those which satisfy  $p^i = p + p^t$ ,  $k + l^i + l^t$  is even, and  $l^i - l^t \leq l^i + l^t$ , where  $p, l, k$  come from  $\langle Y_{l^i}^{p^i} | Y_k^l | Y_{l^t}^{p^t} \rangle$ . Here the  $t$  and  $i$  are not exponents, but rather are used to distinguish the variable in the first position of one function from another.

Let us find our possible  $k$ , focusing on

$$\sum_{-k \leq m \leq k} \langle Y_{2-1} | Y_{km} | Y_{00} \rangle \langle Y_{00} | Y_{km} | Y_{2-1} \rangle,$$

and  $\langle Y_{2-1} | Y_{km} | Y_{00} \rangle$  in particular. Here  $l^i = 2$ ,  $p^i = -1$ ,  $p = m \in [-k, k]$ , and  $l^t = l^t = 0$ .

However, there is only one possible  $m$  and one physically possible  $k$ . It is convenient that the angular part of  $R_{1s}^{\text{dot}}$  is  $Y_{00}$  since this leads to a special case of the Clebsch-Gordon coefficients with

$$\begin{aligned} \langle Y_{j_1 m_1} | Y_{j_2 m_2} | Y_{00} \rangle &= \delta_{j_1 j_2} \delta_{m_1 - m_2} \frac{(-1)^{j_1 - m_1}}{\sqrt{2j_2 + 1}} \\ \langle Y_{j_1 m_1} | Y_{j_2 m_2} | Y_{00} \rangle &= \langle Y_{00} | Y_{j_2 m_2} | Y_{j_1 - m_1} \rangle. \end{aligned}$$

From this it is clear that  $k = 2$  and we can easily find the  $m$ . For  $\langle \xi \varphi | V | \varphi \xi \rangle$  we have

$$\begin{aligned} \sum_{-k \leq m \leq k} \langle Y_2^2 | Y_k^m | Y_{00} \rangle \langle Y_0^0 | Y_k^m | Y_2^2 \rangle &= 0 \\ \sum_{-k \leq m \leq k} \langle Y_2^{-2} | Y_k^m | Y_{00} \rangle \langle Y_0^0 | Y_k^m | Y_2^2 \rangle &= \langle Y_2^{-2} | Y_2^2 | Y_0^0 \rangle \langle Y_0^0 | Y_2^2 | Y_2^2 \rangle = \frac{1}{5} \\ \sum_{-k \leq m \leq k} \langle Y_2^2 | Y_k^m | Y_{00} \rangle \langle Y_0^0 | Y_k^m | Y_2^{-2} \rangle &= \langle Y_2^2 | Y_2^{-2} | Y_0^0 \rangle \langle Y_0^0 | Y_2^{-2} | Y_2^{-2} \rangle = \frac{1}{5} \\ \sum_{-k \leq m \leq k} \langle Y_2^{-2} | Y_k^m | Y_0^0 \rangle \langle Y_0^0 | Y_k^m | Y_2^{-2} \rangle &= 0. \end{aligned}$$

So  $\langle \xi \varphi | V | \varphi \xi \rangle = -\frac{1}{5}$  since we did not include the  $\frac{1}{\sqrt{2}}$  coefficient. This will be the same for all the wave functions, so these three only need to be computed once.

As for the others, they are computed to be  $\langle \eta \varphi | V | \varphi \eta \rangle = -\frac{1}{5}$  and  $\langle \zeta \varphi | V | \varphi \zeta \rangle = \frac{1}{5}$ . From this we can say that the angular part of  $\langle ({}^4T_1 x) \varphi | V | \varphi ({}^4T_1 x) \rangle$  is  $-\frac{3}{5}$ .



### 3.1.4 RADIAL PART

Lastly, before moving on to the splitting, we need to look at the radial part which fortunately is the same for all wave functions. What we are computing is then

$$\left\langle R_{3d}R_{1s}^{\text{dot}} \left| \frac{q_1q_2}{r_>} \sum_{k \geq 0} \frac{4\pi}{2k+1} \left( \frac{r_{<}}{r_>} \right)^k \right| R_{1s}^{\text{dot}} R_{3d} \right\rangle,$$

however we know  $k$  from the work above and so this works out to be

$$\left\langle R_{3d}R_{1s}^{\text{dot}} \left| \frac{q_1q_2}{r_>} \frac{4\pi}{5} \left( \frac{r_{<}}{r_>} \right)^2 \right| R_{1s}^{\text{dot}} R_{3d} \right\rangle.$$

Since we have two electrons, one at  $r$  and the other at  $r'$ , which are indistinguishable from one another, we must consider the case for both  $r \leq r'$  and  $r \geq r'$ . In so doing we must set up two integrals. Before we do that, however, we can simplify this a bit, by removing some constants. We then will parameterize the resulting integration.

First we can pull out the constants  $\frac{4e^2\pi}{5}$ , but also break up  $R_{1s}^{\text{dot}}$ . This function is [19]

$$R_{1s}^{\text{dot}}(r) = \frac{j_0\left(\pi \frac{r}{R}\right)}{j_1(\pi)2\sqrt{\pi}R^3}.$$

With this, we have

$$\left\langle R_{3d}R_{1s}^{\text{dot}} \left| \frac{q_1q_2}{r_>} \frac{4\pi}{5} \left( \frac{r_{<}}{r_>} \right)^2 \right| R_{1s}^{\text{dot}} R_{3d} \right\rangle = \frac{e^2}{5j_1(\pi)R^3} \left\langle R_{3d}j_0\left(\pi \frac{r'}{R}\right) \left| \frac{1}{r_>} \left( \frac{r_{<}}{r_>} \right)^2 \right| j_0\left(\pi \frac{r}{R}\right) R_{3d} \right\rangle.$$

Then with the parameterization this would be  $\frac{e^2}{5j_1(\pi)R^3}\rho$ , where

$$\begin{aligned} \rho = & \int_0^R \int_0^r \frac{r'^2}{r^3} j_0\left(\pi \frac{r}{R}\right) j_0\left(\pi \frac{r'}{R}\right) R_{3d}(r)R_{3d}(r') dr' dr \\ & + \int_0^R \int_0^{r'} \frac{r^2}{r'^3} j_0\left(\pi \frac{r}{R}\right) j_0\left(\pi \frac{r'}{R}\right) R_{3d}(r)R_{3d}(r') dr dr'. \end{aligned}$$

### 3.1.5 LOOKING FOR NON-ZERO INTEGRALS

Let us look at finding the zeros for  $\langle {}^4T_{1x}\varphi | rY_1^q | {}^2Eu\varphi \rangle$ . From before we have

$$\begin{aligned} |t^7, {}^4T_{1x}\rangle &= -\frac{1}{\sqrt{2}} (\xi^+\eta^+\zeta^+) (\xi^2\eta^+\zeta^- - \xi^2\eta^-\zeta^+) \\ |t^7, {}^2Eu\rangle &= \frac{1}{\sqrt{6}} (\xi^2\eta^2 + \eta^2\zeta^2 + \zeta^2\xi^2) (\xi^+\eta^-\zeta^+ - \xi^-\eta^+\zeta^+). \end{aligned}$$

Since the order itself is not important so long as we pay attention to the sign, we may rewrite these two as

$$\begin{aligned} &-\frac{1}{\sqrt{2}} (\xi^+\xi^+\eta^+\zeta^+\xi^-) (\eta^+\zeta^- - \eta^-\zeta^+) \\ &= -\xi^+\xi^+\eta^+\zeta^+\eta^+\zeta^-\xi^- - \xi^+\xi^+\eta^+\zeta^+\xi^-\xi^-\eta^- \\ &\frac{1}{\sqrt{6}} (\xi^2\eta^2 + \eta^2\zeta^2 + \zeta^2\xi^2) (\xi^+\eta^- - \xi^-\eta^+) \zeta^+ \\ &= \xi^2\eta^2 (\xi^+\eta^- - \xi^-\eta^+) \zeta^+ + \eta^2\zeta^2 (\xi^+\eta^- - \xi^-\eta^+) \zeta^+ + \zeta^2\xi^2 (\xi^+\eta^- - \xi^-\eta^+) \zeta^+ \\ &= \xi^2\eta^2\xi^+\eta^-\zeta^+ + \eta^2\zeta^2\xi^+\eta^-\zeta^+ + \zeta^2\xi^2\xi^+\eta^-\zeta^+ \\ &\quad - \xi^2\eta^2\xi^-\eta^+\zeta^+ - \eta^2\zeta^2\xi^-\eta^+\zeta^+ - \zeta^2\xi^2\xi^-\eta^+\zeta^+. \end{aligned}$$

## 3.2 A PROGRAM

Since there are approximately 121 billion combinations which need computing, it is impractical to do so by hand. Fortunately the computation is largely an if-then check which can be looped over.

To facilitate computing this with a computer, we represent these system wave functions as an integer array with each integer representing a simple electron wave function. By rearranging the elements of the array, or rather the indices, we effectively permute the function. We do this for two functions, comparing the  $i^{\text{th}}$  integer in one with that of the second. If they are equal, we either increment or decrement the coefficient on that product of three inner products. Whether it is incremented or decremented is determined by the sign of the permutation.

For this task we use Julia as our programming language. It is fast and easy to use and

read. Julia performs best when parts of a task are broken up so that the compiled code may be inlined easily. To this end we break the job of computing the matrix coefficients up into a collection of separate Julia function, each taking care of one part of the larger computation.

### 3.2.1 LIST OF PERMUTATIONS OF INDICES

The first function we need is the one that generates the list of partial permutations of the indices. Since what we are actually computing is the integer coefficient on some  $\langle \theta_1 \varphi | Y_1^q r | \varphi \theta_2 \rangle$ , two of the indexed wave functions will be tied up. Those wave functions are independent on the same variable as the functions that make up our operator. They can not be pulled out of the integral in the same way, and therefore do not play a part in this particular computation. The method chosen to accomplish this is a brute-force approach and we store all our the permutations we will need. This is very fast and takes a relatively little space. We have six loops iterating over the numbers 1 through 7 sans those numbers which are already in the temporary array P. If we were looking for all permutations of the numbers 1 through 7, we would need eight loops, however, that is not what we desire. At each step, the current value is set before moving to the next loop. In the innermost loop we set the  $N^{\text{th}}$  column to equal our constructed permutation and then decrement N.

```
function eightPerms()
    N = Int64(factorial(7)/2)
    PERMS = Array{Int8,2}(undef,6,N)
    P = Array{Int8,1}(undef,6)
    for a in (1:7)
        P[1] = a
        for b in setdiff(1:7,a)
            P[2] = b
            for c in setdiff(1:7,P[1:2])
                P[3] = c
                for d in setdiff(1:7,P[1:3])
                    P[4] = d
```

```

        for e in setdiff(1:7,P[1:4])
            P[5] = e
            for f in setdiff(1:7,P[1:5])
                P[6] = f
                PERMS[:,N] = P
                N -= 1
            end
        end
    end
end
end
end
return PERMS
end

```

The end result is a  $6 \times 2520$  array of 8 bit integers. Each column will serve as a list of indices which we can loop over later. It is significant that our indices are in columns since Julia is column major. This makes accessing them much faster.

### 3.2.2 DETERMINING THE SIGN FOR PERMUTATIONS OF $(0, 1, 2, 3, 4)$

The next function we will need gives us the sign of the coefficients which is that of the permutation. To find the sign of the permutation, we count number of inversions, when a larger index precedes a smaller one. In the case of this example, there were not any inversions. On the other hand, the permutation  $(0, 2, 1, 3, 4)$  has a single inversion with 2 coming before 1 and so we need to make the sign negative for any results with that permutation. Like before, this is handled by a computer.

Each time we exchange two adjacent numbers, the sign changes. An alternative, simpler method which produces the same result is to count the number of inversions. Also, it should be pointed out that although this is not a complete permutation, there exists a bijection between each of the partial permutations we are working with and a permutation of the same length.

```

function PermSign(perm::Array{Int8},pLen::Int)

counter = 0

Threads@threads for i in 1:pLen
    for j in i:pLen

        if perm[i] > perm[j]
            atomic_add!(counter,1)
        end

    end
end

return (-1)^counter

end

```

This function is very simple. We count the number of inversions by looking first over the elements of the permutation and then looping over those that come after it. We only check those that come after to both avoid double counting as well as simplify the process.

### 3.2.3 ENCODING THE FUNCTIONS

Now that we have our permuted indices and the signs of those permutations, the next thing we need is to give the program something to apply these indices to. While it is possible to feed a program the wave functions as a string, this would not be very efficient, and would present unnecessary challenges. So instead we define a bijection between each wave function and an array of integers. Before we do so, however, we rearrange the electron wave functions so that there are no negative signs. We may do this since we are working with Slater determinants, and the transposition of adjacent electron wave functions results in a sign change. This is done to avoid

having to keep track of which sections of the wave functions are additive and which are subtractive for reasons other than the permutations. In this way,  $\sqrt{2} |t^7, {}^4T_1x\rangle$  would be  $\xi^+\eta^+\zeta^+\xi^+\xi^-\eta^+\zeta^- + \xi^+\eta^+\zeta^+\xi^-\xi^+\eta^-\zeta^+$ .

Since the distributive property remains, we need to be able to select specific pieces of each of these wave functions. We also need to be able to compare the electron wave functions for a particular index. So, we have each column represent one of the subsystem wave functions and then the rows are for the indexed electrons.

$$\begin{pmatrix} \xi^+ & \xi^+ \\ \eta^+ & \eta^+ \\ \zeta^+ & \zeta^+ \\ \xi^+ & \xi^- \\ \xi^- & \xi^+ \\ \eta^+ & \eta^- \\ \zeta^- & \zeta^+ \end{pmatrix}.$$

However, while computers can compare and call strings, I assume that it is faster to work on integers. For this reason each wave function is represented as an integer. To be more specific, we map  $\xi$  to 0,  $\eta$  to 1, and  $\zeta$  to 2. If it is spin up, we leave it as is, but if it is spin down, we add 10. Now  $|{}^4T_1x\rangle$  as an array is

$$\begin{pmatrix} 00 & 00 \\ 01 & 01 \\ 02 & 02 \\ 00 & 10 \\ 10 & 00 \\ 01 & 11 \\ 12 & 02 \end{pmatrix}.$$

Here the first digit from the left indicates the spin (up or down) and the second whether it is  $\xi$ ,  $\eta$ , or  $\zeta$ . Note the change from  $\eta^-\zeta^+$  to  $\zeta^+\eta^-$ . This is to ensure that there are no negative signs. This is admissible because we are dealing with the Slater determinant. It is easier to do

small reorderings like this than it is to try and keep track of the signs. In the code, the functions are stored as

```
Tx = [0 0;1 1;2 2;1 1;10 10; 1 2;12 11]
```

in the code. Also,  $|^2Eu\rangle$  has the encoding

```
Eu = [0 1 2 0 1 2,10 11 12 10 11 12;1 2 0 1 2 0;11 12 10 11 12 10;
0 0 0 1 1 1;11 11 11 10 10 10;2 2 2 2 2 2].
```

### 3.2.4 DETERMINING ZERO

The last function we need is meant to determine whether or not we have a zero or not for a specific pair system wave functions and permutations. Since the spins and electron wave functions with the same variable must be equal (due to orthonormality) we check to see if the integers representing them are equal. Suppose we have an array of indices [3 2 1 4 5 6] for both the left and right. We test for zero with the following script.

```
X = [3 2 1 4 5 6]
Y = [3 2 1 4 5 6]
output = 0
for i in 1:6
    for j in 1:6
        suboutput = 1
        for k in 1:6
            if Tx[X[k],i] != Eu[Y[k],j]:
                suboutput = 0
            end
        end
        output += suboutput
    end
end
```

The outer-most loop, `i`, goes through the columns of  $\mathbf{T}\mathbf{x}$ , the middle loop goes through the columns of  $\mathbf{E}\mathbf{u}$ , and the inner-most loop picks out the appropriate sub-function, applying the permuted indices. Then, should any one of them equal zero, the `suboutput` is set to zero which gets added to the `output`.

That is the basic idea behind checking for zero. We do, however, want this to be more general.

```
function ZeroCheckPairJl(
    lwf::Array{Int,1},rwf::Array{Int,1},p::Array{Int,1},pLength::Int
)
    suboutput = 1
    Threads.@threads for k in 1:pLength
        if lwf[p[k]] != rwf[p[k]]
            suboutput = 0 # No worries over race conditions
        end
    end
    return suboutput
end
```

This function does not loop over columns of the wave functions. It takes as input a single column from each wave function and two columns from the array of permutations. It also takes the length of the permutation which should be the same length as all the other vectors being passed into the function. For our purposes this value is 6. For performance reasons, it is best to either hard code it, or compute it outside the function. It should be noted also that this loop executes over as many threads as allowed, and though each iteration is almost certainly accessing `suboutput`, each is doing so in the same way so there is no risk of corruption from race conditions.

Finally, the function which will compute  $\langle \theta_1 \varphi | Y_1^q r | \varphi \theta_2 \rangle$  is

```
function ZeroCheckJl(
    LWF::Array{Int,2},RWF::Array{Int,2},PERMS::Array{Int8,2}
)
```



```

output = 0
N      = size(PERMS,1)
pN     = size(PERMS,2)
rwN    = size(LWF,2)
lwN    = size(RWF,2)
for i in 1:pN
    Sign = PermSign(PERMS[:,i],N)
    for j in 1:pN
        Sign *= PermSign(PERMS[:,j],N)
        for k in 1:lwN
            for l in 1:rwN
                output += ZeroCheckPairPy(
                    PERMS[:,i],PERMS[:,j],LWF[k],RWF[l],N
                )*Sign
            end
        end
    end
end
return output
end

```

This function takes the full wave function and array of all permutations to be used as input. It then loops over the column indices of the permutation array twice, each time computing the sign of the permutation before doing the same for the wave functions provide. We check for zero and add either +1 or -1 to the output.

## CHAPTER 4

### RESULTS

Using the wave functions calculated in Chapter 2 and the interaction operators in Chapter 3, we are able to calculate matrix elements of exchange interaction between the electron confined in the dot and all 3d-electrons of the impurity center. These matrix elements play an important role in the splitting of impurity energy levels. As a result of the interaction, energy levels of the ground state and excited state will be split, and the transition between the two levels become allowable due to the change in selection rule. The exchange interaction between the extra electron on the impurity electrons splits the energy levels and makes the former spin-forbidden transition become allowable and decreases the lifetime of the transition.

This result leads to the fact that by injecting one extra electron into the dot, one can change the transition probability and the optical properties of the nanocrystal. In the future, we will apply this result to calculate for all important transition metals doping and predict the change in photoluminescence. The first step in the future study will be for Co and Fe doped ZnS and ZnSe nanocrystal, and the changes in luminescence transition and the shortening of the transition lifetime will be calculated to compare with the experimental results.

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## APPENDIX A

### APPROVAL LETTER



Office of Research Integrity

April 16, 2020

George Chappell  
2182 Timber Meadows  
Charlottesville, VA 22911

Dear Mr. Chappell:

This letter is in response to the submitted thesis abstract entitled "*Luminescence Emission in a Nanocrystal Doped by a Transition Metal Impurity*." After assessing the abstract, it has been deemed not to be human subject research and therefore exempt from oversight of the Marshall University Institutional Review Board (IRB). The Code of Federal Regulations (45CFR46) has set forth the criteria utilized in making this determination. Since the information in this study does not involve human subjects as defined in the above referenced instruction, it is not considered human subject research. If there are any changes to the abstract you provided then you would need to resubmit that information to the Office of Research Integrity for review and a determination.

I appreciate your willingness to submit the abstract for determination. Please feel free to contact the Office of Research Integrity if you have any questions regarding future protocols that may require IRB review.

Sincerely,

Bruce F. Day, ThD, CIP  
Director

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## APPENDIX B

### THE TREE OF WAVE FUNCTIONS

Here is the result of the induction process for identifying what wave functions we have. This is necessary to ensure that the desired wave functions exist.

#### B.1 $3d^2$

$$\begin{aligned} |e^1 t^0, {}^2E \times e\rangle &\rightarrow |e^2 t^0, {}^1A_1\rangle, |e^2 t^0, {}^3A_2\rangle, |e^2 t^0, {}^1E\rangle \\ |e^1 t^0, {}^2E \times t\rangle &\rightarrow |e^1 t^1, {}^1T_1\rangle, |e^1 t^1, {}^3T_2\rangle \\ |e^0 t^1, {}^2T_2 \times e\rangle &\rightarrow |e^1 t^1, {}^1T_1\rangle, |e^1 t^1, {}^3T_2\rangle \\ |e^0 t^1, {}^2T_2 \times t\rangle &\rightarrow |e^0 t^2, {}^1A_1\rangle, |e^0 t^2, {}^1E\rangle, |e^0 t^2, {}^1T_1\rangle, |e^0 t^2, {}^3T_2\rangle \end{aligned}$$

$$e^2 \rightarrow (A_1 E)_1 + (A_2)_3$$

$$et \rightarrow (T_1)_1 + (T_2)_3$$

$$t^2 \rightarrow (A_1 E T_1)_1 + (T_2)_3$$

## B.2 $3d^3$

$$|e^2t^0, {}^1A_1 \times e\rangle \rightarrow |e^3t^0, {}^2E\rangle$$

$$|e^2t^0, {}^3A_2 \times e\rangle \rightarrow |e^3t^0, {}^2E\rangle, |e^3t^0, {}^4E\rangle$$

$$|e^2t^0, {}^1E \times e\rangle \rightarrow |e^3t^0, {}^2A_1\rangle, |e^3t^0, {}^2A_2\rangle, |e^3t^0, {}^2E\rangle$$

$$|e^2t^0, {}^1A_1 \times t\rangle \rightarrow |e^2t^1, {}^2T_2\rangle$$

$$|e^2t^0, {}^3A_2 \times t\rangle \rightarrow |e^2t^1, {}^2T_1\rangle, |e^2t^1, {}^4T_1\rangle$$

$$|e^2t^0, {}^1E \times t\rangle \rightarrow |e^2t^1, {}^2T_1\rangle, |e^2t^1, {}^2T_2\rangle$$

$$|e^1t^1, {}^1T_1 \times e\rangle \rightarrow |e^2t^1, {}^2T_1\rangle, |e^2t^1, {}^2T_2\rangle$$

$$|e^1t^1, {}^3T_2 \times e\rangle \rightarrow |e^2t^1, {}^2T_1\rangle, |e^2t^1, {}^2T_2\rangle, |e^2t^1, {}^4T_1\rangle, |e^2t^1, {}^4T_2\rangle$$

$$|e^1t^1, {}^1T_1 \times t\rangle \rightarrow |e^1t^2, {}^2A_2\rangle, |e^1t^2, {}^2E\rangle, |e^1t^2, {}^2T_1\rangle, |e^1t^2, {}^2T_2\rangle$$

$$|e^1t^1, {}^3T_2 \times t\rangle \rightarrow |e^1t^2, {}^2A_1\rangle, |e^1t^2, {}^2E\rangle, |e^1t^2, {}^2T_1\rangle, |e^1t^2, {}^2T_2\rangle,$$

$$|e^1t^2, {}^4A_1\rangle, |e^1t^2, {}^4E\rangle, |e^1t^2, {}^4T_1\rangle, |e^1t^2, {}^4T_2\rangle$$

$$\begin{aligned}
|e^0t^2, {}^1A_1 \times e\rangle &\rightarrow |e^1t^2, {}^2E\rangle \\
|e^0t^2, {}^1E \times e\rangle &\rightarrow |e^1t^2, {}^2A_1\rangle, |e^1t^2, {}^2A_2\rangle, |e^1t^2, {}^2E\rangle \\
|e^0t^2, {}^1T_1 \times e\rangle &\rightarrow |e^1t^2, {}^2T_1\rangle, |e^1t^2, {}^2T_2\rangle \\
|e^0t^2, {}^3T_2 \times e\rangle &\rightarrow |e^1t^2, {}^2T_1\rangle, |e^1t^2, {}^2T_2\rangle, |e^1t^2, {}^4T_1\rangle, |e^1t^2, {}^4T_2\rangle \\
|e^0t^2, {}^1A_1 \times t\rangle &\rightarrow |e^0t^3, {}^2T_2\rangle \\
|e^0t^2, {}^1E \times t\rangle &\rightarrow |e^0t^3, {}^2T_1\rangle, |e^0t^3, {}^2T_2\rangle \\
|e^0t^2, {}^1T_1 \times t\rangle &\rightarrow |e^0t^3, {}^2A_2\rangle, |e^0t^3, {}^2E\rangle, |e^0t^3, {}^2T_1\rangle, |e^0t^3, {}^2T_2\rangle \\
|e^0t^2, {}^3T_2 \times t\rangle &\rightarrow |e^0t^3, {}^2A_1\rangle, |e^0t^3, {}^2E\rangle, |e^0t^3, {}^2T_1\rangle, |e^0t^3, {}^2T_2\rangle, \\
&|e^0t^3, {}^4A_1\rangle, |e^0t^3, {}^4E\rangle, |e^0t^3, {}^4T_1\rangle, |e^0t^3, {}^4T_2\rangle
\end{aligned}$$

$$e^3 \rightarrow (A_1A_2E)_2 + (E)_4$$

$$e^2t \rightarrow (T_1T_2)_2 + (T_1T_2)_4$$

$$et^2 \rightarrow (A_1A_2ET_1T_2)_2 + (A_1ET_1T_2)_4$$

$$t^3 \rightarrow (A_1A_2ET_1T_2)_2 + (A_1ET_1T_2)_4$$



### B.3 $3d^4$

$$|e^{3t^0}, {}^2A_1 \times e\rangle \rightarrow |e^{4t^0}, {}^1E\rangle, |e^{4t^0}, {}^3E\rangle$$

$$|e^{3t^0}, {}^2A_2 \times e\rangle \rightarrow |e^{4t^0}, {}^1E\rangle, |e^{4t^0}, {}^3E\rangle$$

$$|e^{3t^0}, {}^2E \times e\rangle \rightarrow |e^{4t^0}, {}^1A_1\rangle, |e^{4t^0}, {}^1A_2\rangle, |e^{4t^0}, {}^1E\rangle, |e^{4t^0}, {}^3A_1\rangle, |e^{4t^0}, {}^3A_2\rangle, |e^{4t^0}, {}^3E\rangle$$

$$|e^{3t^0}, {}^4E \times e\rangle \rightarrow |e^{4t^0}, {}^3A_1\rangle, |e^{4t^0}, {}^3A_2\rangle, |e^{4t^0}, {}^3E\rangle, |e^{4t^0}, {}^5A_1\rangle, |e^{4t^0}, {}^5A_2\rangle, |e^{4t^0}, {}^5E\rangle$$

$$|e^{3t^0}, {}^2A_1 \times t\rangle \rightarrow |e^{3t^1}, {}^1T_2\rangle, |e^{3t^1}, {}^3T_2\rangle$$

$$|e^{3t^0}, {}^2A_2 \times t\rangle \rightarrow |e^{3t^1}, {}^1T_1\rangle, |e^{3t^1}, {}^3T_1\rangle$$

$$|e^{3t^0}, {}^2E \times t\rangle \rightarrow |e^{3t^1}, {}^1T_1\rangle, |e^{3t^1}, {}^1T_2\rangle, |e^{3t^1}, {}^3T_1\rangle, |e^{3t^1}, {}^3T_2\rangle$$

$$|e^{3t^0}, {}^4E \times t\rangle \rightarrow |e^{3t^1}, {}^3T_1\rangle, |e^{3t^1}, {}^3T_2\rangle, |e^{3t^1}, {}^5T_1\rangle, |e^{3t^1}, {}^5T_2\rangle$$

$$\begin{aligned}
|e^2t^1, {}^2T_1 \times e\rangle &\rightarrow |e^3t^1, {}^1T_1\rangle, |e^3t^1, {}^1T_2\rangle, |e^3t^1, {}^3T_1\rangle, |e^3t^1, {}^3T_2\rangle \\
|e^2t^1, {}^4T_1 \times e\rangle &\rightarrow |e^3t^1, {}^3T_1\rangle, |e^3t^1, {}^3T_2\rangle, |e^3t^1, {}^5T_1\rangle, |e^3t^1, {}^5T_2\rangle \\
|e^2t^1, {}^2T_2 \times e\rangle &\rightarrow |e^3t^1, {}^1T_1\rangle, |e^3t^1, {}^1T_2\rangle, |e^3t^1, {}^3T_1\rangle, |e^3t^1, {}^3T_2\rangle \\
|e^2t^1, {}^4T_2 \times e\rangle &\rightarrow |e^3t^1, {}^3T_1\rangle, |e^3t^1, {}^3T_2\rangle, |e^3t^1, {}^5T_1\rangle, |e^3t^1, {}^5T_2\rangle \\
|e^2t^1, {}^2T_1 \times t\rangle &\rightarrow |e^2t^2, {}^1A_2\rangle, |e^2t^2, {}^1E\rangle, |e^2t^2, {}^1T_1\rangle, |e^2t^2, {}^1T_2\rangle, \\
&\quad |e^2t^2, {}^3A_2\rangle, |e^2t^2, {}^3E\rangle, |e^2t^2, {}^3T_1\rangle, |e^2t^2, {}^3T_2\rangle \\
|e^2t^1, {}^4T_1 \times t\rangle &\rightarrow |e^2t^2, {}^3A_2\rangle, |e^2t^2, {}^3E\rangle, |e^2t^2, {}^3T_1\rangle, |e^2t^2, {}^3T_2\rangle, \\
&\quad |e^2t^2, {}^5A_2\rangle, |e^2t^2, {}^5E\rangle, |e^2t^2, {}^5T_1\rangle, |e^2t^2, {}^5T_2\rangle \\
|e^2t^1, {}^2T_2 \times t\rangle &\rightarrow |e^2t^2, {}^1A_1\rangle, |e^2t^2, {}^1E\rangle, |e^2t^2, {}^1T_1\rangle, |e^2t^2, {}^1T_2\rangle, \\
&\quad |e^2t^2, {}^3A_1\rangle, |e^2t^2, {}^3E\rangle, |e^2t^2, {}^3T_1\rangle, |e^2t^2, {}^3T_2\rangle \\
|e^2t^1, {}^4T_2 \times t\rangle &\rightarrow |e^2t^2, {}^3A_1\rangle, |e^2t^2, {}^3E\rangle, |e^2t^2, {}^3T_1\rangle, |e^2t^2, {}^3T_2\rangle, \\
&\quad |e^2t^2, {}^5A_1\rangle, |e^2t^2, {}^5E\rangle, |e^2t^2, {}^5T_1\rangle, |e^2t^2, {}^5T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^1 t^2, {}^2 A_1 \times e\rangle &\rightarrow |e^2 t^2, {}^1 E\rangle, |e^2 t^2, {}^3 E\rangle \\
|e^1 t^2, {}^2 A_2 \times e\rangle &\rightarrow |e^2 t^2, {}^1 E\rangle, |e^2 t^2, {}^3 E\rangle \\
|e^1 t^2, {}^2 E \times e\rangle &\rightarrow |e^2 t^2, {}^1 A_1\rangle, |e^2 t^2, {}^1 A_2\rangle, |e^2 t^2, {}^1 E\rangle, |e^2 t^2, {}^3 A_1\rangle, |e^2 t^2, {}^3 A_2\rangle, |e^2 t^2, {}^3 E\rangle \\
|e^1 t^2, {}^2 T_1 \times e\rangle &\rightarrow |e^2 t^2, {}^1 T_1\rangle, |e^2 t^2, {}^1 T_2\rangle, |e^2 t^2, {}^3 T_1\rangle, |e^2 t^2, {}^3 T_2\rangle \\
|e^1 t^2, {}^2 T_2 \times e\rangle &\rightarrow |e^2 t^2, {}^1 T_1\rangle, |e^2 t^2, {}^1 T_2\rangle, |e^2 t^2, {}^3 T_1\rangle, |e^2 t^2, {}^3 T_2\rangle \\
|e^1 t^2, {}^4 A_1 \times e\rangle &\rightarrow |e^2 t^2, {}^3 E\rangle, |e^2 t^2, {}^5 E\rangle \\
|e^1 t^2, {}^4 E \times e\rangle &\rightarrow |e^2 t^2, {}^3 A_1\rangle, |e^2 t^2, {}^3 A_2\rangle, |e^2 t^2, {}^3 E\rangle, |e^2 t^2, {}^5 A_1\rangle, |e^2 t^2, {}^5 A_2\rangle, |e^2 t^2, {}^5 E\rangle \\
|e^1 t^2, {}^4 T_1 \times e\rangle &\rightarrow |e^2 t^2, {}^3 T_1\rangle, |e^2 t^2, {}^3 T_2\rangle, |e^2 t^2, {}^5 T_1\rangle, |e^2 t^2, {}^5 T_2\rangle \\
|e^1 t^2, {}^4 T_2 \times e\rangle &\rightarrow |e^2 t^2, {}^3 T_1\rangle, |e^2 t^2, {}^3 T_2\rangle, |e^2 t^2, {}^5 T_1\rangle, |e^2 t^2, {}^5 T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{1t^2}, {}^2A_1 \times t\rangle &\rightarrow |e^{1t^3}, {}^1T_2\rangle, |e^{1t^3}, {}^3T_2\rangle \\
|e^{1t^2}, {}^2A_2 \times t\rangle &\rightarrow |e^{1t^3}, {}^1T_1\rangle, |e^{1t^3}, {}^3T_1\rangle \\
|e^{1t^2}, {}^2E \times t\rangle &\rightarrow |e^{1t^3}, {}^1T_1\rangle, |e^{1t^3}, {}^1T_2\rangle, |e^{1t^3}, {}^3T_1\rangle, |e^{1t^3}, {}^3T_2\rangle \\
|e^{1t^2}, {}^2T_1 \times t\rangle &\rightarrow |e^{1t^3}, {}^1A_2\rangle, |e^{1t^3}, {}^1E\rangle, |e^{1t^3}, {}^1T_1\rangle, |e^{1t^3}, {}^1T_2\rangle, \\
&\quad |e^{1t^3}, {}^3A_2\rangle, |e^{1t^3}, {}^3E\rangle, |e^{1t^3}, {}^3T_1\rangle, |e^{1t^3}, {}^3T_2\rangle \\
|e^{1t^2}, {}^2T_2 \times t\rangle &\rightarrow |e^{1t^3}, {}^1A_1\rangle, |e^{1t^3}, {}^1E\rangle, |e^{1t^3}, {}^1T_1\rangle, |e^{1t^3}, {}^1T_2\rangle, \\
&\quad |e^{1t^3}, {}^3A_1\rangle, |e^{1t^3}, {}^3E\rangle, |e^{1t^3}, {}^3T_1\rangle, |e^{1t^3}, {}^3T_2\rangle \\
|e^{1t^2}, {}^4A_1 \times t\rangle &\rightarrow |e^{1t^3}, {}^3T_2\rangle, |e^{1t^3}, {}^5T_2\rangle \\
|e^{1t^2}, {}^4E \times t\rangle &\rightarrow |e^{1t^3}, {}^3T_1\rangle, |e^{1t^3}, {}^3T_2\rangle, |e^{1t^3}, {}^5T_1\rangle, |e^{1t^3}, {}^5T_2\rangle \\
|e^{1t^2}, {}^4T_1 \times t\rangle &\rightarrow |e^{1t^3}, {}^3A_2\rangle, |e^{1t^3}, {}^3E\rangle, |e^{1t^3}, {}^3T_1\rangle, |e^{1t^3}, {}^3T_2\rangle, \\
&\quad |e^{1t^3}, {}^5A_2\rangle, |e^{1t^3}, {}^5E\rangle, |e^{1t^3}, {}^5T_1\rangle, |e^{1t^3}, {}^5T_2\rangle \\
|e^{1t^2}, {}^4T_2 \times t\rangle &\rightarrow |e^{1t^3}, {}^3A_1\rangle, |e^{1t^3}, {}^3E\rangle, |e^{1t^3}, {}^3T_1\rangle, |e^{1t^3}, {}^3T_2\rangle, \\
&\quad |e^{1t^3}, {}^5A_1\rangle, |e^{1t^3}, {}^5E\rangle, |e^{1t^3}, {}^5T_1\rangle, |e^{1t^3}, {}^5T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^0 t^3, {}^2 A_1 \times e\rangle &\rightarrow |e^1 t^3, {}^1 E\rangle, |e^1 t^3, {}^3 E\rangle \\
|e^0 t^3, {}^2 A_2 \times e\rangle &\rightarrow |e^1 t^3, {}^1 E\rangle, |e^1 t^3, {}^3 E\rangle \\
|e^0 t^3, {}^2 E \times e\rangle &\rightarrow |e^1 t^3, {}^1 A_1\rangle, |e^1 t^3, {}^1 A_2\rangle, |e^1 t^3, {}^1 E\rangle, |e^1 t^3, {}^3 A_1\rangle, |e^1 t^3, {}^3 A_2\rangle, |e^1 t^3, {}^3 E\rangle \\
|e^0 t^3, {}^2 T_1 \times e\rangle &\rightarrow |e^1 t^3, {}^1 T_1\rangle, |e^1 t^3, {}^1 T_2\rangle, |e^1 t^3, {}^3 T_1\rangle, |e^1 t^3, {}^3 T_2\rangle \\
|e^0 t^3, {}^2 T_2 \times e\rangle &\rightarrow |e^1 t^3, {}^1 T_1\rangle, |e^1 t^3, {}^1 T_2\rangle, |e^1 t^3, {}^3 T_1\rangle, |e^1 t^3, {}^3 T_2\rangle \\
|e^0 t^3, {}^4 A_1 \times e\rangle &\rightarrow |e^1 t^3, {}^3 E\rangle, |e^1 t^3, {}^5 E\rangle \\
|e^0 t^3, {}^4 E \times e\rangle &\rightarrow |e^1 t^3, {}^3 A_1\rangle, |e^1 t^3, {}^3 A_2\rangle, |e^1 t^3, {}^3 E\rangle, |e^1 t^3, {}^5 A_1\rangle, |e^1 t^3, {}^5 A_2\rangle, |e^1 t^3, {}^5 E\rangle \\
|e^0 t^3, {}^4 T_1 \times e\rangle &\rightarrow |e^1 t^3, {}^3 T_1\rangle, |e^1 t^3, {}^3 T_2\rangle, |e^1 t^3, {}^5 T_1\rangle, |e^1 t^3, {}^5 T_2\rangle \\
|e^0 t^3, {}^4 T_2 \times e\rangle &\rightarrow |e^1 t^3, {}^3 T_1\rangle, |e^1 t^3, {}^3 T_2\rangle, |e^1 t^3, {}^5 T_1\rangle, |e^1 t^3, {}^5 T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^0 t^3, {}^2 A_1 \times t\rangle &\rightarrow |e^0 t^4, {}^1 T_2\rangle, |e^0 t^4, {}^3 T_2\rangle \\
|e^0 t^3, {}^2 A_2 \times t\rangle &\rightarrow |e^0 t^4, {}^1 T_1\rangle, |e^0 t^4, {}^3 T_1\rangle \\
|e^0 t^3, {}^2 E \times t\rangle &\rightarrow |e^0 t^4, {}^1 T_1\rangle, |e^0 t^4, {}^1 T_2\rangle, |e^0 t^4, {}^3 T_1\rangle, |e^0 t^4, {}^3 T_2\rangle \\
|e^0 t^3, {}^2 T_1 \times t\rangle &\rightarrow |e^0 t^4, {}^1 A_2\rangle, |e^0 t^4, {}^1 E\rangle, |e^0 t^4, {}^1 T_1\rangle, |e^0 t^4, {}^1 T_2\rangle, \\
&\quad |e^0 t^4, {}^3 A_2\rangle, |e^0 t^4, {}^3 E\rangle, |e^0 t^4, {}^3 T_1\rangle, |e^0 t^4, {}^3 T_2\rangle \\
|e^0 t^3, {}^2 T_2 \times t\rangle &\rightarrow |e^0 t^4, {}^1 A_1\rangle, |e^0 t^4, {}^1 E\rangle, |e^0 t^4, {}^1 T_1\rangle, |e^0 t^4, {}^1 T_2\rangle, \\
&\quad |e^0 t^4, {}^3 A_1\rangle, |e^0 t^4, {}^3 E\rangle, |e^0 t^4, {}^3 T_1\rangle, |e^0 t^4, {}^3 T_2\rangle \\
|e^0 t^3, {}^4 A_1 \times t\rangle &\rightarrow |e^0 t^4, {}^3 T_2\rangle, |e^0 t^4, {}^5 T_2\rangle \\
|e^0 t^3, {}^4 E \times t\rangle &\rightarrow |e^0 t^4, {}^3 T_1\rangle, |e^0 t^4, {}^3 T_2\rangle, |e^0 t^4, {}^5 T_1\rangle, |e^0 t^4, {}^5 T_2\rangle \\
|e^0 t^3, {}^4 T_1 \times t\rangle &\rightarrow |e^0 t^4, {}^3 A_2\rangle, |e^0 t^4, {}^3 E\rangle, |e^0 t^4, {}^3 T_1\rangle, |e^0 t^4, {}^3 T_2\rangle, \\
&\quad |e^0 t^4, {}^5 A_2\rangle, |e^0 t^4, {}^5 E\rangle, |e^0 t^4, {}^5 T_1\rangle, |e^0 t^4, {}^5 T_2\rangle \\
|e^0 t^3, {}^4 T_2 \times t\rangle &\rightarrow |e^0 t^4, {}^3 A_1\rangle, |e^0 t^4, {}^3 E\rangle, |e^0 t^4, {}^3 T_1\rangle, |e^0 t^4, {}^3 T_2\rangle, \\
&\quad |e^0 t^4, {}^5 A_1\rangle, |e^0 t^4, {}^5 E\rangle, |e^0 t^4, {}^5 T_1\rangle, |e^0 t^4, {}^5 T_2\rangle
\end{aligned}$$

$$e^4 \rightarrow (A_1 A_2 E)_1 + (A_1 A_2 E)_3 + (A_1 A_2 E)_5$$

$$e^3 t \rightarrow (T_1 T_2)_1 + (T_1 T_2)_3 + (T_1 T_2)_5$$

$$e^2 t^2 \rightarrow (A_1 A_2 E T_1 T_2)_1 + (A_1 A_2 E T_1 T_2)_3 + (A_1 A_2 E T_1 T_2)_5$$

$$e t^3 \rightarrow (A_1 A_2 E T_1 T_2)_1 + (A_1 A_2 E T_1 T_2)_3 + (A_1 A_2 E T_1 T_2)_5$$

$$t^4 \rightarrow (A_1 A_2 E T_1 T_2)_1 + (A_1 A_2 E T_1 T_2)_3 + (A_1 A_2 E T_1 T_2)_5$$

#### B.4 $3d^5$

$$\begin{aligned}
|e^{4t^0}, {}^1A_1 \times e\rangle &\rightarrow |e^{5t^0}, {}^2E\rangle \\
|e^{4t^0}, {}^1A_2 \times e\rangle &\rightarrow |e^{5t^0}, {}^2E\rangle \\
|e^{4t^0}, {}^1E \times e\rangle &\rightarrow |e^{5t^0}, {}^2A_1\rangle, |e^{5t^0}, {}^2A_2\rangle, |e^{5t^0}, {}^2E\rangle \\
|e^{4t^0}, {}^3A_1 \times e\rangle &\rightarrow |e^{5t^0}, {}^2E\rangle, |e^{5t^0}, {}^4E\rangle \\
|e^{4t^0}, {}^3A_2 \times e\rangle &\rightarrow |e^{5t^0}, {}^2E\rangle, |e^{5t^0}, {}^4E\rangle \\
|e^{4t^0}, {}^3E \times e\rangle &\rightarrow |e^{5t^0}, {}^2A_1\rangle, |e^{5t^0}, {}^2A_2\rangle, |e^{5t^0}, {}^2E\rangle, |e^{5t^0}, {}^4A_1\rangle, |e^{5t^0}, {}^4A_2\rangle, |e^{5t^0}, {}^4E\rangle \\
|e^{4t^0}, {}^5A_1 \times e\rangle &\rightarrow |e^{5t^0}, {}^4E\rangle, |e^{5t^0}, {}^6E\rangle \\
|e^{4t^0}, {}^5A_2 \times e\rangle &\rightarrow |e^{5t^0}, {}^4E\rangle, |e^{5t^0}, {}^6E\rangle \\
|e^{4t^0}, {}^5E \times e\rangle &\rightarrow |e^{5t^0}, {}^4A_1\rangle, |e^{5t^0}, {}^4A_2\rangle, |e^{5t^0}, {}^4E\rangle, |e^{5t^0}, {}^6A_1\rangle, |e^{5t^0}, {}^6A_2\rangle, |e^{5t^0}, {}^6E\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{4t^0}, {}^1A_1 \times t\rangle &\rightarrow |e^{4t^1}, {}^2T_2\rangle \\
|e^{4t^0}, {}^1A_2 \times t\rangle &\rightarrow |e^{4t^1}, {}^2T_1\rangle \\
|e^{4t^0}, {}^1E \times t\rangle &\rightarrow |e^{4t^1}, {}^2T_1\rangle, |e^{4t^1}, {}^2T_2\rangle \\
|e^{4t^0}, {}^3A_1 \times t\rangle &\rightarrow |e^{4t^1}, {}^2T_2\rangle, |e^{4t^1}, {}^4T_2\rangle \\
|e^{4t^0}, {}^3A_2 \times t\rangle &\rightarrow |e^{4t^1}, {}^2T_1\rangle, |e^{4t^1}, {}^4T_1\rangle \\
|e^{4t^0}, {}^3E \times t\rangle &\rightarrow |e^{4t^1}, {}^2T_1\rangle, |e^{4t^1}, {}^2T_2\rangle, |e^{4t^1}, {}^4T_1\rangle, |e^{4t^1}, {}^4T_2\rangle \\
|e^{4t^0}, {}^5A_1 \times t\rangle &\rightarrow |e^{4t^1}, {}^4T_2\rangle, |e^{4t^1}, {}^6T_2\rangle \\
|e^{4t^0}, {}^5A_2 \times t\rangle &\rightarrow |e^{4t^1}, {}^4T_1\rangle, |e^{4t^1}, {}^6T_1\rangle \\
|e^{4t^0}, {}^5E \times t\rangle &\rightarrow |e^{4t^1}, {}^4T_1\rangle, |e^{4t^1}, {}^4T_2\rangle, |e^{4t^1}, {}^6T_1\rangle, |e^{4t^1}, {}^6T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{3t^1, 1T_1} \times e\rangle &\rightarrow |e^{4t^1, 2T_1}\rangle, |e^{4t^1, 2T_2}\rangle \\
|e^{3t^1, 1T_2} \times e\rangle &\rightarrow |e^{4t^1, 2T_1}\rangle, |e^{4t^1, 2T_2}\rangle \\
|e^{3t^1, 3T_1} \times e\rangle &\rightarrow |e^{4t^1, 2T_1}\rangle, |e^{4t^1, 2T_2}\rangle, |e^{4t^1, 4T_1}\rangle, |e^{4t^1, 4T_2}\rangle \\
|e^{3t^1, 3T_2} \times e\rangle &\rightarrow |e^{4t^1, 2T_1}\rangle, |e^{4t^1, 2T_2}\rangle, |e^{4t^1, 4T_1}\rangle, |e^{4t^1, 4T_2}\rangle \\
|e^{3t^1, 5T_1} \times e\rangle &\rightarrow |e^{4t^1, 4T_1}\rangle, |e^{4t^1, 4T_2}\rangle, |e^{4t^1, 6T_1}\rangle, |e^{4t^1, 6T_2}\rangle \\
|e^{3t^1, 5T_2} \times e\rangle &\rightarrow |e^{4t^1, 4T_1}\rangle, |e^{4t^1, 4T_2}\rangle, |e^{4t^1, 6T_1}\rangle, |e^{4t^1, 6T_2}\rangle \\
|e^{3t^1, 1T_1} \times t\rangle &\rightarrow |e^{3t^2, 2A_2}\rangle, |e^{3t^2, 2E}\rangle, |e^{3t^2, 2T_1}\rangle, |e^{3t^2, 2T_2}\rangle \\
|e^{3t^1, 1T_2} \times t\rangle &\rightarrow |e^{3t^2, 2A_1}\rangle, |e^{3t^2, 2E}\rangle, |e^{3t^2, 2T_1}\rangle, |e^{3t^2, 2T_2}\rangle \\
|e^{3t^1, 3T_1} \times t\rangle &\rightarrow |e^{3t^2, 2A_2}\rangle, |e^{3t^2, 2E}\rangle, |e^{3t^2, 2T_1}\rangle, |e^{3t^2, 2T_2}\rangle, \\
&\quad |e^{3t^2, 4A_2}\rangle, |e^{3t^2, 4E}\rangle, |e^{3t^2, 4T_1}\rangle, |e^{3t^2, 4T_2}\rangle \\
|e^{3t^1, 3T_2} \times t\rangle &\rightarrow |e^{3t^2, 2A_1}\rangle, |e^{3t^2, 2E}\rangle, |e^{3t^2, 2T_1}\rangle, |e^{3t^2, 2T_2}\rangle, \\
&\quad |e^{3t^2, 4A_1}\rangle, |e^{3t^2, 4E}\rangle, |e^{3t^2, 4T_1}\rangle, |e^{3t^2, 4T_2}\rangle \\
|e^{3t^1, 5T_1} \times t\rangle &\rightarrow |e^{3t^2, 4A_2}\rangle, |e^{3t^2, 4E}\rangle, |e^{3t^2, 4T_1}\rangle, |e^{3t^2, 4T_2}\rangle, \\
&\quad |e^{3t^2, 6A_2}\rangle, |e^{3t^2, 6E}\rangle, |e^{3t^2, 6T_1}\rangle, |e^{3t^2, 6T_2}\rangle \\
|e^{3t^1, 5T_2} \times t\rangle &\rightarrow |e^{3t^2, 4A_1}\rangle, |e^{3t^2, 4E}\rangle, |e^{3t^2, 4T_1}\rangle, |e^{3t^2, 4T_2}\rangle, \\
&\quad |e^{3t^2, 6A_1}\rangle, |e^{3t^2, 6E}\rangle, |e^{3t^2, 6T_1}\rangle, |e^{3t^2, 6T_2}\rangle
\end{aligned}$$



$$\begin{aligned}
|e^2t^2, {}^1A_1 \times e\rangle &\rightarrow |e^3t^2, {}^2E\rangle \\
|e^2t^2, {}^1A_2 \times e\rangle &\rightarrow |e^3t^2, {}^2E\rangle \\
|e^2t^2, {}^1E \times e\rangle &\rightarrow |e^3t^2, {}^2A_1\rangle, |e^3t^2, {}^2A_2\rangle, |e^3t^2, {}^2E\rangle \\
|e^2t^2, {}^1T_1 \times e\rangle &\rightarrow |e^3t^2, {}^2T_1\rangle, |e^3t^2, {}^2T_2\rangle \\
|e^2t^2, {}^1T_2 \times e\rangle &\rightarrow |e^3t^2, {}^2T_1\rangle, |e^3t^2, {}^2T_2\rangle \\
|e^2t^2, {}^3A_1 \times e\rangle &\rightarrow |e^3t^2, {}^2E\rangle, |e^3t^2, {}^4E\rangle \\
|e^2t^2, {}^3A_2 \times e\rangle &\rightarrow |e^3t^2, {}^2E\rangle, |e^3t^2, {}^4E\rangle \\
|e^2t^2, {}^3E \times e\rangle &\rightarrow |e^3t^2, {}^2A_1\rangle, |e^3t^2, {}^2A_2\rangle, |e^3t^2, {}^2E\rangle, |e^3t^2, {}^4A_1\rangle, |e^3t^2, {}^4A_2\rangle, |e^3t^2, {}^4E\rangle \\
|e^2t^2, {}^3T_1 \times e\rangle &\rightarrow |e^3t^2, {}^2T_1\rangle, |e^3t^2, {}^2T_2\rangle, |e^3t^2, {}^4T_1\rangle, |e^3t^2, {}^4T_2\rangle \\
|e^2t^2, {}^3T_2 \times e\rangle &\rightarrow |e^3t^2, {}^2T_1\rangle, |e^3t^2, {}^2T_2\rangle, |e^3t^2, {}^4T_1\rangle, |e^3t^2, {}^4T_2\rangle \\
|e^2t^2, {}^5A_1 \times e\rangle &\rightarrow |e^3t^2, {}^4E\rangle, |e^3t^2, {}^6E\rangle \\
|e^2t^2, {}^5A_2 \times e\rangle &\rightarrow |e^3t^2, {}^4E\rangle, |e^3t^2, {}^6E\rangle \\
|e^2t^2, {}^5E \times e\rangle &\rightarrow |e^3t^2, {}^4A_1\rangle, |e^3t^2, {}^4A_2\rangle, |e^3t^2, {}^4E\rangle, |e^3t^2, {}^6A_1\rangle, |e^3t^2, {}^6A_2\rangle, |e^3t^2, {}^6E\rangle \\
|e^2t^2, {}^5T_1 \times e\rangle &\rightarrow |e^3t^2, {}^4T_1\rangle, |e^3t^2, {}^4T_2\rangle, |e^3t^2, {}^6T_1\rangle, |e^3t^2, {}^6T_2\rangle \\
|e^2t^2, {}^5T_2 \times e\rangle &\rightarrow |e^3t^2, {}^4T_1\rangle, |e^3t^2, {}^4T_2\rangle, |e^3t^2, {}^6T_1\rangle, |e^3t^2, {}^6T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^2t^2, {}^1A_1 \times t\rangle &\rightarrow |e^2t^3, {}^2T_2\rangle \\
|e^2t^2, {}^1A_2 \times t\rangle &\rightarrow |e^2t^3, {}^2T_1\rangle \\
|e^2t^2, {}^1E \times t\rangle &\rightarrow |e^2t^3, {}^2T_1\rangle, |e^2t^3, {}^2T_2\rangle \\
|e^2t^2, {}^1T_1 \times t\rangle &\rightarrow |e^2t^3, {}^2A_2\rangle, |e^2t^3, {}^2E\rangle, |e^2t^3, {}^2T_1\rangle, |e^2t^3, {}^2T_2\rangle \\
|e^2t^2, {}^1T_2 \times t\rangle &\rightarrow |e^2t^3, {}^2A_1\rangle, |e^2t^3, {}^2E\rangle, |e^2t^3, {}^2T_1\rangle, |e^2t^3, {}^2T_2\rangle \\
|e^2t^2, {}^3A_1 \times t\rangle &\rightarrow |e^2t^3, {}^2T_2\rangle, |e^2t^3, {}^4T_2\rangle \\
|e^2t^2, {}^3A_2 \times t\rangle &\rightarrow |e^2t^3, {}^2T_1\rangle, |e^2t^3, {}^4T_1\rangle \\
|e^2t^2, {}^3E \times t\rangle &\rightarrow |e^2t^3, {}^2T_1\rangle, |e^2t^3, {}^2T_2\rangle, |e^2t^3, {}^4T_1\rangle, |e^2t^3, {}^4T_2\rangle \\
|e^2t^2, {}^3T_1 \times t\rangle &\rightarrow |e^2t^3, {}^2A_2\rangle, |e^2t^3, {}^2E\rangle, |e^2t^3, {}^2T_1\rangle, |e^2t^3, {}^2T_2\rangle, \\
&\quad |e^2t^3, {}^4A_2\rangle, |e^2t^3, {}^4E\rangle, |e^2t^3, {}^4T_1\rangle, |e^2t^3, {}^4T_2\rangle \\
|e^2t^2, {}^3T_2 \times t\rangle &\rightarrow |e^2t^3, {}^2A_1\rangle, |e^2t^3, {}^2E\rangle, |e^2t^3, {}^2T_1\rangle, |e^2t^3, {}^2T_2\rangle, \\
&\quad |e^2t^3, {}^4A_1\rangle, |e^2t^3, {}^4E\rangle, |e^2t^3, {}^4T_1\rangle, |e^2t^3, {}^4T_2\rangle \\
|e^2t^2, {}^5A_1 \times t\rangle &\rightarrow |e^2t^3, {}^4T_2\rangle, |e^2t^3, {}^6T_2\rangle \\
|e^2t^2, {}^5A_2 \times t\rangle &\rightarrow |e^2t^3, {}^4T_1\rangle, |e^2t^3, {}^6T_1\rangle \\
|e^2t^2, {}^5E \times t\rangle &\rightarrow |e^2t^3, {}^4T_1\rangle, |e^2t^3, {}^4T_2\rangle, |e^2t^3, {}^6T_1\rangle, |e^2t^3, {}^6T_2\rangle \\
|e^2t^2, {}^5T_1 \times t\rangle &\rightarrow |e^2t^3, {}^4A_2\rangle, |e^2t^3, {}^4E\rangle, |e^2t^3, {}^4T_1\rangle, |e^2t^3, {}^4T_2\rangle, \\
&\quad |e^2t^3, {}^6A_2\rangle, |e^2t^3, {}^6E\rangle, |e^2t^3, {}^6T_1\rangle, |e^2t^3, {}^6T_2\rangle \\
|e^2t^2, {}^5T_2 \times t\rangle &\rightarrow |e^2t^3, {}^4A_1\rangle, |e^2t^3, {}^4E\rangle, |e^2t^3, {}^4T_1\rangle, |e^2t^3, {}^4T_2\rangle, \\
&\quad |e^2t^3, {}^6A_1\rangle, |e^2t^3, {}^6E\rangle, |e^2t^3, {}^6T_1\rangle, |e^2t^3, {}^6T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{1t^3}, {}^1A_1 \times e\rangle &\rightarrow |e^{2t^3}, {}^2E\rangle \\
|e^{1t^3}, {}^1A_2 \times e\rangle &\rightarrow |e^{2t^3}, {}^2E\rangle \\
|e^{1t^3}, {}^1E \times e\rangle &\rightarrow |e^{2t^3}, {}^2A_1\rangle, |e^{2t^3}, {}^2A_2\rangle, |e^{2t^3}, {}^2E\rangle \\
|e^{1t^3}, {}^1T_1 \times e\rangle &\rightarrow |e^{2t^3}, {}^2T_1\rangle, |e^{2t^3}, {}^2T_2\rangle \\
|e^{1t^3}, {}^1T_2 \times e\rangle &\rightarrow |e^{2t^3}, {}^2T_1\rangle, |e^{2t^3}, {}^2T_2\rangle \\
|e^{1t^3}, {}^3A_1 \times e\rangle &\rightarrow |e^{2t^3}, {}^2E\rangle, |e^{2t^3}, {}^4E\rangle \\
|e^{1t^3}, {}^3A_2 \times e\rangle &\rightarrow |e^{2t^3}, {}^2E\rangle, |e^{2t^3}, {}^4E\rangle \\
|e^{1t^3}, {}^3E \times e\rangle &\rightarrow |e^{2t^3}, {}^2A_1\rangle, |e^{2t^3}, {}^2A_2\rangle, |e^{2t^3}, {}^2E\rangle, |e^{2t^3}, {}^4A_1\rangle, |e^{2t^3}, {}^4A_2\rangle, |e^{2t^3}, {}^4E\rangle \\
|e^{1t^3}, {}^3T_1 \times e\rangle &\rightarrow |e^{2t^3}, {}^2T_1\rangle, |e^{2t^3}, {}^2T_2\rangle, |e^{2t^3}, {}^4T_1\rangle, |e^{2t^3}, {}^4T_2\rangle \\
|e^{1t^3}, {}^3T_2 \times e\rangle &\rightarrow |e^{2t^3}, {}^2T_1\rangle, |e^{2t^3}, {}^2T_2\rangle, |e^{2t^3}, {}^4T_1\rangle, |e^{2t^3}, {}^4T_2\rangle \\
|e^{1t^3}, {}^5A_1 \times e\rangle &\rightarrow |e^{2t^3}, {}^4E\rangle, |e^{2t^3}, {}^6E\rangle \\
|e^{1t^3}, {}^5A_2 \times e\rangle &\rightarrow |e^{2t^3}, {}^4E\rangle, |e^{2t^3}, {}^6E\rangle \\
|e^{1t^3}, {}^5E \times e\rangle &\rightarrow |e^{2t^3}, {}^4A_1\rangle, |e^{2t^3}, {}^4A_2\rangle, |e^{2t^3}, {}^4E\rangle, |e^{2t^3}, {}^6A_1\rangle, |e^{2t^3}, {}^6A_2\rangle, |e^{2t^3}, {}^6E\rangle \\
|e^{1t^3}, {}^5T_1 \times e\rangle &\rightarrow |e^{2t^3}, {}^4T_1\rangle, |e^{2t^3}, {}^4T_2\rangle, |e^{2t^3}, {}^6T_1\rangle, |e^{2t^3}, {}^6T_2\rangle \\
|e^{1t^3}, {}^5T_2 \times e\rangle &\rightarrow |e^{2t^3}, {}^4T_1\rangle, |e^{2t^3}, {}^4T_2\rangle, |e^{2t^3}, {}^6T_1\rangle, |e^{2t^3}, {}^6T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{1t^3}, {}^1A_1 \times t\rangle &\rightarrow |e^{1t^4}, {}^2T_2\rangle \\
|e^{1t^3}, {}^1A_2 \times t\rangle &\rightarrow |e^{1t^4}, {}^2T_1\rangle \\
|e^{1t^3}, {}^1E \times t\rangle &\rightarrow |e^{1t^4}, {}^2T_1\rangle, |e^{1t^4}, {}^2T_2\rangle \\
|e^{1t^3}, {}^1T_1 \times t\rangle &\rightarrow |e^{1t^4}, {}^2A_2\rangle, |e^{1t^4}, {}^2E\rangle, |e^{1t^4}, {}^2T_1\rangle, |e^{1t^4}, {}^2T_2\rangle \\
|e^{1t^3}, {}^1T_2 \times t\rangle &\rightarrow |e^{1t^4}, {}^2A_1\rangle, |e^{1t^4}, {}^2E\rangle, |e^{1t^4}, {}^2T_1\rangle, |e^{1t^4}, {}^2T_2\rangle \\
|e^{1t^3}, {}^3A_1 \times t\rangle &\rightarrow |e^{1t^4}, {}^2T_2\rangle, |e^{1t^4}, {}^4T_2\rangle \\
|e^{1t^3}, {}^3A_2 \times t\rangle &\rightarrow |e^{1t^4}, {}^2T_1\rangle, |e^{1t^4}, {}^4T_1\rangle \\
|e^{1t^3}, {}^3E \times t\rangle &\rightarrow |e^{1t^4}, {}^2T_1\rangle, |e^{1t^4}, {}^2T_2\rangle, |e^{1t^4}, {}^4T_1\rangle, |e^{1t^4}, {}^4T_2\rangle \\
|e^{1t^3}, {}^3T_1 \times t\rangle &\rightarrow |e^{1t^4}, {}^2A_2\rangle, |e^{1t^4}, {}^2E\rangle, |e^{1t^4}, {}^2T_1\rangle, |e^{1t^4}, {}^2T_2\rangle, \\
&\quad |e^{1t^4}, {}^4A_2\rangle, |e^{1t^4}, {}^4E\rangle, |e^{1t^4}, {}^4T_1\rangle, |e^{1t^4}, {}^4T_2\rangle \\
|e^{1t^3}, {}^3T_2 \times t\rangle &\rightarrow |e^{1t^4}, {}^2A_1\rangle, |e^{1t^4}, {}^2E\rangle, |e^{1t^4}, {}^2T_1\rangle, |e^{1t^4}, {}^2T_2\rangle, \\
&\quad |e^{1t^4}, {}^4A_1\rangle, |e^{1t^4}, {}^4E\rangle, |e^{1t^4}, {}^4T_1\rangle, |e^{1t^4}, {}^4T_2\rangle \\
|e^{1t^3}, {}^5A_1 \times t\rangle &\rightarrow |e^{1t^4}, {}^4T_2\rangle, |e^{1t^4}, {}^6T_2\rangle \\
|e^{1t^3}, {}^5A_2 \times t\rangle &\rightarrow |e^{1t^4}, {}^4T_1\rangle, |e^{1t^4}, {}^6T_1\rangle \\
|e^{1t^3}, {}^5E \times t\rangle &\rightarrow |e^{1t^4}, {}^4T_1\rangle, |e^{1t^4}, {}^4T_2\rangle, |e^{1t^4}, {}^6T_1\rangle, |e^{1t^4}, {}^6T_2\rangle \\
|e^{1t^3}, {}^5T_1 \times t\rangle &\rightarrow |e^{1t^4}, {}^4A_2\rangle, |e^{1t^4}, {}^4E\rangle, |e^{1t^4}, {}^4T_1\rangle, |e^{1t^4}, {}^4T_2\rangle, \\
&\quad |e^{1t^4}, {}^6A_2\rangle, |e^{1t^4}, {}^6E\rangle, |e^{1t^4}, {}^6T_1\rangle, |e^{1t^4}, {}^6T_2\rangle \\
|e^{1t^3}, {}^5T_2 \times t\rangle &\rightarrow |e^{1t^4}, {}^4A_1\rangle, |e^{1t^4}, {}^4E\rangle, |e^{1t^4}, {}^4T_1\rangle, |e^{1t^4}, {}^4T_2\rangle, \\
&\quad |e^{1t^4}, {}^6A_1\rangle, |e^{1t^4}, {}^6E\rangle, |e^{1t^4}, {}^6T_1\rangle, |e^{1t^4}, {}^6T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^0 t^4, {}^1 A_1 \times e\rangle &\rightarrow |e^1 t^4, {}^2 E\rangle \\
|e^0 t^4, {}^1 A_2 \times e\rangle &\rightarrow |e^1 t^4, {}^2 E\rangle \\
|e^0 t^4, {}^1 E \times e\rangle &\rightarrow |e^1 t^4, {}^2 A_1\rangle, |e^1 t^4, {}^2 A_2\rangle, |e^1 t^4, {}^2 E\rangle \\
|e^0 t^4, {}^1 T_1 \times e\rangle &\rightarrow |e^1 t^4, {}^2 T_1\rangle, |e^1 t^4, {}^2 T_2\rangle \\
|e^0 t^4, {}^1 T_2 \times e\rangle &\rightarrow |e^1 t^4, {}^2 T_1\rangle, |e^1 t^4, {}^2 T_2\rangle \\
|e^0 t^4, {}^3 A_1 \times e\rangle &\rightarrow |e^1 t^4, {}^2 E\rangle, |e^1 t^4, {}^4 E\rangle \\
|e^0 t^4, {}^3 A_2 \times e\rangle &\rightarrow |e^1 t^4, {}^2 E\rangle, |e^1 t^4, {}^4 E\rangle \\
|e^0 t^4, {}^3 E \times e\rangle &\rightarrow |e^1 t^4, {}^2 A_1\rangle, |e^1 t^4, {}^2 A_2\rangle, |e^1 t^4, {}^2 E\rangle, |e^1 t^4, {}^4 A_1\rangle, |e^1 t^4, {}^4 A_2\rangle, |e^1 t^4, {}^4 E\rangle \\
|e^0 t^4, {}^3 T_1 \times e\rangle &\rightarrow |e^1 t^4, {}^2 T_1\rangle, |e^1 t^4, {}^2 T_2\rangle, |e^1 t^4, {}^4 T_1\rangle, |e^1 t^4, {}^4 T_2\rangle \\
|e^0 t^4, {}^3 T_2 \times e\rangle &\rightarrow |e^1 t^4, {}^2 T_1\rangle, |e^1 t^4, {}^2 T_2\rangle, |e^1 t^4, {}^4 T_1\rangle, |e^1 t^4, {}^4 T_2\rangle \\
|e^0 t^4, {}^5 A_1 \times e\rangle &\rightarrow |e^1 t^4, {}^4 E\rangle, |e^1 t^4, {}^6 E\rangle \\
|e^0 t^4, {}^5 A_2 \times e\rangle &\rightarrow |e^1 t^4, {}^4 E\rangle, |e^1 t^4, {}^6 E\rangle \\
|e^0 t^4, {}^5 E \times e\rangle &\rightarrow |e^1 t^4, {}^4 A_1\rangle, |e^1 t^4, {}^4 A_2\rangle, |e^1 t^4, {}^4 E\rangle, |e^1 t^4, {}^6 A_1\rangle, |e^1 t^4, {}^6 A_2\rangle, |e^1 t^4, {}^6 E\rangle \\
|e^0 t^4, {}^5 T_1 \times e\rangle &\rightarrow |e^1 t^4, {}^4 T_1\rangle, |e^1 t^4, {}^4 T_2\rangle, |e^1 t^4, {}^6 T_1\rangle, |e^1 t^4, {}^6 T_2\rangle \\
|e^0 t^4, {}^5 T_2 \times e\rangle &\rightarrow |e^1 t^4, {}^4 T_1\rangle, |e^1 t^4, {}^4 T_2\rangle, |e^1 t^4, {}^6 T_1\rangle, |e^1 t^4, {}^6 T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^0 t^4, {}^1 A_1 \times t\rangle &\rightarrow |e^0 t^5, {}^2 T_2\rangle \\
|e^0 t^4, {}^1 A_2 \times t\rangle &\rightarrow |e^0 t^5, {}^2 T_1\rangle \\
|e^0 t^4, {}^1 E \times t\rangle &\rightarrow |e^0 t^5, {}^2 T_1\rangle, |e^0 t^5, {}^2 T_2\rangle \\
|e^0 t^4, {}^1 T_1 \times t\rangle &\rightarrow |e^0 t^5, {}^2 A_2\rangle, |e^0 t^5, {}^2 E\rangle, |e^0 t^5, {}^2 T_1\rangle, |e^0 t^5, {}^2 T_2\rangle \\
|e^0 t^4, {}^1 T_2 \times t\rangle &\rightarrow |e^0 t^5, {}^2 A_1\rangle, |e^0 t^5, {}^2 E\rangle, |e^0 t^5, {}^2 T_1\rangle, |e^0 t^5, {}^2 T_2\rangle \\
|e^0 t^4, {}^3 A_1 \times t\rangle &\rightarrow |e^0 t^5, {}^2 T_2\rangle, |e^0 t^5, {}^4 T_2\rangle \\
|e^0 t^4, {}^3 A_2 \times t\rangle &\rightarrow |e^0 t^5, {}^2 T_1\rangle, |e^0 t^5, {}^4 T_1\rangle \\
|e^0 t^4, {}^3 E \times t\rangle &\rightarrow |e^0 t^5, {}^2 T_1\rangle, |e^0 t^5, {}^2 T_2\rangle, |e^0 t^5, {}^4 T_1\rangle, |e^0 t^5, {}^4 T_2\rangle \\
|e^0 t^4, {}^3 T_1 \times t\rangle &\rightarrow |e^0 t^5, {}^2 A_2\rangle, |e^0 t^5, {}^2 E\rangle, |e^0 t^5, {}^2 T_1\rangle, |e^0 t^5, {}^2 T_2\rangle, \\
&\quad |e^0 t^5, {}^4 A_2\rangle, |e^0 t^5, {}^4 E\rangle, |e^0 t^5, {}^4 T_1\rangle, |e^0 t^5, {}^4 T_2\rangle \\
|e^0 t^4, {}^3 T_2 \times t\rangle &\rightarrow |e^0 t^5, {}^2 A_1\rangle, |e^0 t^5, {}^2 E\rangle, |e^0 t^5, {}^2 T_1\rangle, |e^0 t^5, {}^2 T_2\rangle, \\
&\quad |e^0 t^5, {}^4 A_1\rangle, |e^0 t^5, {}^4 E\rangle, |e^0 t^5, {}^4 T_1\rangle, |e^0 t^5, {}^4 T_2\rangle \\
|e^0 t^4, {}^5 A_1 \times t\rangle &\rightarrow |e^0 t^5, {}^4 T_2\rangle, |e^0 t^5, {}^6 T_2\rangle \\
|e^0 t^4, {}^5 A_2 \times t\rangle &\rightarrow |e^0 t^5, {}^4 T_1\rangle, |e^0 t^5, {}^6 T_1\rangle \\
|e^0 t^4, {}^5 E \times t\rangle &\rightarrow |e^0 t^5, {}^4 T_1\rangle, |e^0 t^5, {}^4 T_2\rangle, |e^0 t^5, {}^6 T_1\rangle, |e^0 t^5, {}^6 T_2\rangle \\
|e^0 t^4, {}^5 T_1 \times t\rangle &\rightarrow |e^0 t^5, {}^4 A_2\rangle, |e^0 t^5, {}^4 E\rangle, |e^0 t^5, {}^4 T_1\rangle, |e^0 t^5, {}^4 T_2\rangle, \\
&\quad |e^0 t^5, {}^6 A_2\rangle, |e^0 t^5, {}^6 E\rangle, |e^0 t^5, {}^6 T_1\rangle, |e^0 t^5, {}^6 T_2\rangle \\
|e^0 t^4, {}^5 T_2 \times t\rangle &\rightarrow |e^0 t^5, {}^4 A_1\rangle, |e^0 t^5, {}^4 E\rangle, |e^0 t^5, {}^4 T_1\rangle, |e^0 t^5, {}^4 T_2\rangle, \\
&\quad |e^0 t^5, {}^6 A_1\rangle, |e^0 t^5, {}^6 E\rangle, |e^0 t^5, {}^6 T_1\rangle, |e^0 t^5, {}^6 T_2\rangle
\end{aligned}$$

$$\begin{aligned}
e^5 &\rightarrow (A_1 A_2 E)_2 + (A_1 A_2 E)_4 + (A_1 A_2 E)_6 \\
e^4 t &\rightarrow (T_1 T_2)_2 + (T_1 T_2)_4 + (T_1 T_2)_6 \\
e^3 t^2 &\rightarrow (A_1 A_2 E T_1 T_2)_2 + (A_1 A_2 E T_1 T_2)_4 + (A_1 A_2 E T_1 T_2)_6 \\
e^2 t^3 &\rightarrow (A_1 A_2 E T_1 T_2)_2 + (A_1 A_2 E T_1 T_2)_4 + (A_1 A_2 E T_1 T_2)_6 \\
e t^4 &\rightarrow (A_1 A_2 E T_1 T_2)_6 + (A_1 A_2 E T_1 T_2)_6 + (A_1 A_2 E T_1 T_2)_6 \\
t^5 &\rightarrow (A_1 A_2 E T_1 T_2)_6 + (A_1 A_2 E T_1 T_2)_6 + (A_1 A_2 E T_1 T_2)_6
\end{aligned}$$

### B.5 $3d^6$

$$\begin{aligned}
|e^{5t^0, 2A_1} \times e\rangle &\rightarrow |e^{6t^0, 1E}\rangle, |e^{6t^0, 3E}\rangle \\
|e^{5t^0, 2A_2} \times e\rangle &\rightarrow |e^{6t^0, 1E}\rangle, |e^{6t^0, 3E}\rangle \\
|e^{5t^0, 2E} \times e\rangle &\rightarrow |e^{6t^0, 1A_1}\rangle, |e^{6t^0, 1A_2}\rangle, |e^{6t^0, 1E}\rangle, |e^{6t^0, 3A_1}\rangle, |e^{6t^0, 3A_2}\rangle, |e^{6t^0, 3E}\rangle \\
|e^{5t^0, 4A_1} \times e\rangle &\rightarrow |e^{6t^0, 3E}\rangle, |e^{6t^0, 5E}\rangle \\
|e^{5t^0, 4A_2} \times e\rangle &\rightarrow |e^{6t^0, 3E}\rangle, |e^{6t^0, 5E}\rangle \\
|e^{5t^0, 4E} \times e\rangle &\rightarrow |e^{6t^0, 3A_1}\rangle, |e^{6t^0, 3A_2}\rangle, |e^{6t^0, 3E}\rangle, |e^{6t^0, 5A_1}\rangle, |e^{6t^0, 5A_2}\rangle, |e^{6t^0, 5E}\rangle \\
|e^{5t^0, 6A_1} \times e\rangle &\rightarrow |e^{6t^0, 5E}\rangle, |e^{6t^0, 7E}\rangle \\
|e^{5t^0, 6A_2} \times e\rangle &\rightarrow |e^{6t^0, 5E}\rangle, |e^{6t^0, 7E}\rangle \\
|e^{5t^0, 6E} \times e\rangle &\rightarrow |e^{6t^0, 5A_1}\rangle, |e^{6t^0, 5A_2}\rangle, |e^{6t^0, 5E}\rangle, |e^{6t^0, 7A_1}\rangle, |e^{6t^0, 7A_2}\rangle, |e^{6t^0, 7E}\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{5t^0}, {}^2A_1 \times t\rangle &\rightarrow |e^{5t^1}, {}^1T_2\rangle, |e^{5t^1}, {}^3T_2\rangle \\
|e^{5t^0}, {}^2A_2 \times t\rangle &\rightarrow |e^{5t^1}, {}^1T_1\rangle, |e^{5t^1}, {}^3T_1\rangle \\
|e^{5t^0}, {}^2E \times t\rangle &\rightarrow |e^{5t^1}, {}^1T_1\rangle, |e^{5t^1}, {}^1T_2\rangle, |e^{5t^1}, {}^3T_1\rangle, |e^{5t^1}, {}^3T_2\rangle \\
|e^{5t^0}, {}^4A_1 \times t\rangle &\rightarrow |e^{5t^1}, {}^3T_2\rangle, |e^{5t^1}, {}^5T_2\rangle \\
|e^{5t^0}, {}^4A_2 \times t\rangle &\rightarrow |e^{5t^1}, {}^3T_1\rangle, |e^{5t^1}, {}^5T_1\rangle \\
|e^{5t^0}, {}^4E \times t\rangle &\rightarrow |e^{5t^1}, {}^3T_1\rangle, |e^{5t^1}, {}^3T_2\rangle, |e^{5t^1}, {}^5T_1\rangle, |e^{5t^1}, {}^5T_2\rangle \\
|e^{5t^0}, {}^6A_1 \times t\rangle &\rightarrow |e^{5t^1}, {}^5T_2\rangle, |e^{5t^1}, {}^7T_2\rangle \\
|e^{5t^0}, {}^6A_2 \times t\rangle &\rightarrow |e^{5t^1}, {}^5T_1\rangle, |e^{5t^1}, {}^7T_1\rangle \\
|e^{5t^0}, {}^6E \times t\rangle &\rightarrow |e^{5t^1}, {}^5T_1\rangle, |e^{5t^1}, {}^5T_2\rangle, |e^{5t^1}, {}^7T_1\rangle, |e^{5t^1}, {}^7T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{4t^1}, {}^2T_1 \times e\rangle &\rightarrow |e^{5t^1}, {}^1T_1\rangle, |e^{5t^1}, {}^1T_2\rangle, |e^{5t^1}, {}^3T_1\rangle, |e^{5t^1}, {}^3T_2\rangle \\
|e^{4t^1}, {}^2T_2 \times e\rangle &\rightarrow |e^{5t^1}, {}^1T_1\rangle, |e^{5t^1}, {}^1T_2\rangle, |e^{5t^1}, {}^3T_1\rangle, |e^{5t^1}, {}^3T_2\rangle \\
|e^{4t^1}, {}^4T_1 \times e\rangle &\rightarrow |e^{5t^1}, {}^3T_1\rangle, |e^{5t^1}, {}^3T_2\rangle, |e^{5t^1}, {}^5T_1\rangle, |e^{5t^1}, {}^5T_2\rangle \\
|e^{4t^1}, {}^4T_2 \times e\rangle &\rightarrow |e^{5t^1}, {}^3T_1\rangle, |e^{5t^1}, {}^3T_2\rangle, |e^{5t^1}, {}^5T_1\rangle, |e^{5t^1}, {}^5T_2\rangle \\
|e^{4t^1}, {}^6T_1 \times e\rangle &\rightarrow |e^{5t^1}, {}^5T_1\rangle, |e^{5t^1}, {}^5T_2\rangle, |e^{5t^1}, {}^7T_1\rangle, |e^{5t^1}, {}^7T_2\rangle \\
|e^{4t^1}, {}^6T_2 \times e\rangle &\rightarrow |e^{5t^1}, {}^5T_1\rangle, |e^{5t^1}, {}^5T_2\rangle, |e^{5t^1}, {}^7T_1\rangle, |e^{5t^1}, {}^7T_2\rangle
\end{aligned}$$



$$\begin{aligned}
|e^{4t^1, 2T_1} \times t\rangle &\rightarrow |e^{4t^2, 1A_2}\rangle, |e^{4t^2, 1E}\rangle, |e^{4t^2, 1T_1}\rangle, |e^{4t^2, 1T_2}\rangle, \\
&\quad |e^{4t^2, 3A_2}\rangle, |e^{4t^2, 3E}\rangle, |e^{4t^2, 3T_1}\rangle, |e^{4t^2, 3T_2}\rangle \\
|e^{4t^1, 2T_2} \times t\rangle &\rightarrow |e^{4t^2, 1A_1}\rangle, |e^{4t^2, 1E}\rangle, |e^{4t^2, 1T_1}\rangle, |e^{4t^2, 1T_2}\rangle, \\
&\quad |e^{4t^2, 3A_1}\rangle, |e^{4t^2, 3E}\rangle, |e^{4t^2, 3T_1}\rangle, |e^{4t^2, 3T_2}\rangle \\
|e^{4t^1, 4T_1} \times t\rangle &\rightarrow |e^{4t^2, 3A_2}\rangle, |e^{4t^2, 3E}\rangle, |e^{4t^2, 3T_1}\rangle, |e^{4t^2, 3T_2}\rangle, \\
&\quad |e^{4t^2, 5A_2}\rangle, |e^{4t^2, 5E}\rangle, |e^{4t^2, 5T_1}\rangle, |e^{4t^2, 5T_2}\rangle \\
|e^{4t^1, 4T_2} \times t\rangle &\rightarrow |e^{4t^2, 3A_1}\rangle, |e^{4t^2, 3E}\rangle, |e^{4t^2, 3T_1}\rangle, |e^{4t^2, 3T_2}\rangle, \\
&\quad |e^{4t^2, 5A_1}\rangle, |e^{4t^2, 5E}\rangle, |e^{4t^2, 5T_1}\rangle, |e^{4t^2, 5T_2}\rangle \\
|e^{4t^1, 6T_1} \times t\rangle &\rightarrow |e^{4t^2, 5A_2}\rangle, |e^{4t^2, 5E}\rangle, |e^{4t^2, 5T_1}\rangle, |e^{4t^2, 5T_2}\rangle, \\
&\quad |e^{4t^2, 7A_2}\rangle, |e^{4t^2, 7E}\rangle, |e^{4t^2, 7T_1}\rangle, |e^{4t^2, 7T_2}\rangle \\
|e^{4t^1, 6T_2} \times t\rangle &\rightarrow |e^{4t^2, 5A_1}\rangle, |e^{4t^2, 5E}\rangle, |e^{4t^2, 5T_1}\rangle, |e^{4t^2, 5T_2}\rangle, \\
&\quad |e^{4t^2, 7A_1}\rangle, |e^{4t^2, 7E}\rangle, |e^{4t^2, 7T_1}\rangle, |e^{4t^2, 7T_2}\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{3t^2, 2A_1} \times e\rangle &\rightarrow |e^{4t^2, 1E}\rangle, |e^{4t^2, 3E}\rangle \\
|e^{3t^2, 2A_2} \times e\rangle &\rightarrow |e^{4t^2, 1E}\rangle, |e^{4t^2, 3E}\rangle \\
|e^{3t^2, 2E} \times e\rangle &\rightarrow |e^{4t^2, 1A_1}\rangle, |e^{4t^2, 1A_2}\rangle, |e^{4t^2, 1E}\rangle, |e^{4t^2, 3A_1}\rangle, |e^{4t^2, 3A_2}\rangle, |e^{4t^2, 3E}\rangle \\
|e^{3t^2, 2T_1} \times e\rangle &\rightarrow |e^{4t^2, 1T_1}\rangle, |e^{4t^2, 1T_2}\rangle, |e^{4t^2, 3T_1}\rangle, |e^{4t^2, 3T_2}\rangle \\
|e^{3t^2, 2T_2} \times e\rangle &\rightarrow |e^{4t^2, 1T_1}\rangle, |e^{4t^2, 1T_2}\rangle, |e^{4t^2, 3T_1}\rangle, |e^{4t^2, 3T_2}\rangle \\
|e^{3t^2, 4A_1} \times e\rangle &\rightarrow |e^{4t^2, 3E}\rangle, |e^{4t^2, 5E}\rangle \\
|e^{3t^2, 4A_2} \times e\rangle &\rightarrow |e^{4t^2, 3E}\rangle, |e^{4t^2, 5E}\rangle \\
|e^{3t^2, 4E} \times e\rangle &\rightarrow |e^{4t^2, 3A_1}\rangle, |e^{4t^2, 3A_2}\rangle, |e^{4t^2, 3E}\rangle, |e^{4t^2, 5A_1}\rangle, |e^{4t^2, 5A_2}\rangle, |e^{4t^2, 5E}\rangle \\
|e^{3t^2, 4T_1} \times e\rangle &\rightarrow |e^{4t^2, 3T_1}\rangle, |e^{4t^2, 3T_2}\rangle, |e^{4t^2, 5T_1}\rangle, |e^{4t^2, 5T_2}\rangle \\
|e^{3t^2, 4T_2} \times e\rangle &\rightarrow |e^{4t^2, 3T_1}\rangle, |e^{4t^2, 3T_2}\rangle, |e^{4t^2, 5T_1}\rangle, |e^{4t^2, 5T_2}\rangle \\
|e^{3t^2, 6A_1} \times e\rangle &\rightarrow |e^{4t^2, 5E}\rangle, |e^{4t^2, 7E}\rangle \\
|e^{3t^2, 6A_2} \times e\rangle &\rightarrow |e^{4t^2, 5E}\rangle, |e^{4t^2, 7E}\rangle \\
|e^{3t^2, 6E} \times e\rangle &\rightarrow |e^{4t^2, 5A_1}\rangle, |e^{4t^2, 5A_2}\rangle, |e^{4t^2, 5E}\rangle, |e^{4t^2, 7A_1}\rangle, |e^{4t^2, 7A_2}\rangle, |e^{4t^2, 7E}\rangle \\
|e^{3t^2, 6T_1} \times e\rangle &\rightarrow |e^{4t^2, 5T_1}\rangle, |e^{4t^2, 5T_2}\rangle, |e^{4t^2, 7T_1}\rangle, |e^{4t^2, 7T_2}\rangle \\
|e^{3t^2, 6T_2} \times e\rangle &\rightarrow |e^{4t^2, 5T_1}\rangle, |e^{4t^2, 5T_2}\rangle, |e^{4t^2, 7T_1}\rangle, |e^{4t^2, 7T_2}\rangle
\end{aligned}$$

$$\begin{aligned}
|e^3t^2, {}^2A_1 \times t\rangle &\rightarrow |e^3t^3, {}^1T_2\rangle, |e^3t^3, {}^3T_2\rangle \\
|e^3t^2, {}^2A_2 \times t\rangle &\rightarrow |e^3t^3, {}^1T_1\rangle, |e^3t^3, {}^3T_1\rangle \\
|e^3t^2, {}^2E \times t\rangle &\rightarrow |e^3t^3, {}^1T_1\rangle, |e^3t^3, {}^1T_2\rangle, |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle \\
|e^3t^2, {}^2T_1 \times t\rangle &\rightarrow |e^3t^3, {}^1A_2\rangle, |e^3t^3, {}^1E\rangle, |e^3t^3, {}^1T_1\rangle, |e^3t^3, {}^1T_2\rangle, \\
&\quad |e^3t^3, {}^3A_2\rangle, |e^3t^3, {}^3E\rangle, |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle \\
|e^3t^2, {}^2T_2 \times t\rangle &\rightarrow |e^3t^3, {}^1A_1\rangle, |e^3t^3, {}^1E\rangle, |e^3t^3, {}^1T_1\rangle, |e^3t^3, {}^1T_2\rangle, \\
&\quad |e^3t^3, {}^3A_1\rangle, |e^3t^3, {}^3E\rangle, |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle \\
|e^3t^2, {}^4A_1 \times t\rangle &\rightarrow |e^3t^3, {}^3T_2\rangle, |e^3t^3, {}^5T_2\rangle \\
|e^3t^2, {}^4A_2 \times t\rangle &\rightarrow |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^5T_1\rangle \\
|e^3t^2, {}^4E \times t\rangle &\rightarrow |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle, |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle \\
|e^3t^2, {}^4T_1 \times t\rangle &\rightarrow |e^3t^3, {}^3A_2\rangle, |e^3t^3, {}^3E\rangle, |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle, \\
&\quad |e^3t^3, {}^5A_2\rangle, |e^3t^3, {}^5E\rangle, |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle \\
|e^3t^2, {}^4T_2 \times t\rangle &\rightarrow |e^3t^3, {}^3A_1\rangle, |e^3t^3, {}^3E\rangle, |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle, \\
&\quad |e^3t^3, {}^5A_1\rangle, |e^3t^3, {}^5E\rangle, |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle \\
|e^3t^2, {}^6A_1 \times t\rangle &\rightarrow |e^3t^3, {}^5T_2\rangle, |e^3t^3, {}^7T_2\rangle \\
|e^3t^2, {}^6A_2 \times t\rangle &\rightarrow |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^7T_1\rangle \\
|e^3t^2, {}^6E \times t\rangle &\rightarrow |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle, |e^3t^3, {}^7T_1\rangle, |e^3t^3, {}^7T_2\rangle \\
|e^3t^2, {}^6T_1 \times t\rangle &\rightarrow |e^3t^3, {}^5A_2\rangle, |e^3t^3, {}^5E\rangle, |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle, \\
&\quad |e^3t^3, {}^7A_2\rangle, |e^3t^3, {}^7E\rangle, |e^3t^3, {}^7T_1\rangle, |e^3t^3, {}^7T_2\rangle \\
|e^3t^2, {}^6T_2 \times t\rangle &\rightarrow |e^3t^3, {}^5A_1\rangle, |e^3t^3, {}^5E\rangle, |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle, \\
&\quad |e^3t^3, {}^7A_1\rangle, |e^3t^3, {}^7E\rangle, |e^3t^3, {}^7T_1\rangle, |e^3t^3, {}^7T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^2t^3, {}^2A_1 \times e\rangle &\rightarrow |e^3t^3, {}^1E\rangle, |e^3t^3, {}^3E\rangle \\
|e^2t^3, {}^2A_2 \times e\rangle &\rightarrow |e^3t^3, {}^1E\rangle, |e^3t^3, {}^3E\rangle \\
|e^2t^3, {}^2E \times e\rangle &\rightarrow |e^3t^3, {}^1A_1\rangle, |e^3t^3, {}^1A_2\rangle, |e^3t^3, {}^1E\rangle, |e^3t^3, {}^3A_1\rangle, |e^3t^3, {}^3A_2\rangle, |e^3t^3, {}^3E\rangle \\
|e^2t^3, {}^2T_1 \times e\rangle &\rightarrow |e^3t^3, {}^1T_1\rangle, |e^3t^3, {}^1T_2\rangle, |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle \\
|e^2t^3, {}^2T_2 \times e\rangle &\rightarrow |e^3t^3, {}^1T_1\rangle, |e^3t^3, {}^1T_2\rangle, |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle \\
|e^2t^3, {}^4A_1 \times e\rangle &\rightarrow |e^3t^3, {}^3E\rangle, |e^3t^3, {}^5E\rangle \\
|e^2t^3, {}^4A_2 \times e\rangle &\rightarrow |e^3t^3, {}^3E\rangle, |e^3t^3, {}^5E\rangle \\
|e^2t^3, {}^4E \times e\rangle &\rightarrow |e^3t^3, {}^3A_1\rangle, |e^3t^3, {}^3A_2\rangle, |e^3t^3, {}^3E\rangle, |e^3t^3, {}^5A_1\rangle, |e^3t^3, {}^5A_2\rangle, |e^3t^3, {}^5E\rangle \\
|e^2t^3, {}^4T_1 \times e\rangle &\rightarrow |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle, |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle \\
|e^2t^3, {}^4T_2 \times e\rangle &\rightarrow |e^3t^3, {}^3T_1\rangle, |e^3t^3, {}^3T_2\rangle, |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle \\
|e^2t^3, {}^6A_1 \times e\rangle &\rightarrow |e^3t^3, {}^5E\rangle, |e^3t^3, {}^7E\rangle \\
|e^2t^3, {}^6A_2 \times e\rangle &\rightarrow |e^3t^3, {}^5E\rangle, |e^3t^3, {}^7E\rangle \\
|e^2t^3, {}^6E \times e\rangle &\rightarrow |e^3t^3, {}^5A_1\rangle, |e^3t^3, {}^5A_2\rangle, |e^3t^3, {}^5E\rangle, |e^3t^3, {}^7A_1\rangle, |e^3t^3, {}^7A_2\rangle, |e^3t^3, {}^7E\rangle \\
|e^2t^3, {}^6T_1 \times e\rangle &\rightarrow |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle, |e^3t^3, {}^7T_1\rangle, |e^3t^3, {}^7T_2\rangle \\
|e^2t^3, {}^6T_2 \times e\rangle &\rightarrow |e^3t^3, {}^5T_1\rangle, |e^3t^3, {}^5T_2\rangle, |e^3t^3, {}^7T_1\rangle, |e^3t^3, {}^7T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^2t^3, {}^2A_1 \times t\rangle &\rightarrow |e^2t^4, {}^1T_2\rangle, |e^2t^4, {}^3T_2\rangle \\
|e^2t^3, {}^2A_2 \times t\rangle &\rightarrow |e^2t^4, {}^1T_1\rangle, |e^2t^4, {}^3T_1\rangle \\
|e^2t^3, {}^2E \times t\rangle &\rightarrow |e^2t^4, {}^1T_1\rangle, |e^2t^4, {}^1T_2\rangle, |e^2t^4, {}^3T_1\rangle, |e^2t^4, {}^3T_2\rangle \\
|e^2t^3, {}^2T_1 \times t\rangle &\rightarrow |e^2t^4, {}^1A_2\rangle, |e^2t^4, {}^1E\rangle, |e^2t^4, {}^1T_1\rangle, |e^2t^4, {}^1T_2\rangle, \\
&\quad |e^2t^4, {}^3A_2\rangle, |e^2t^4, {}^3E\rangle, |e^2t^4, {}^3T_1\rangle, |e^2t^4, {}^3T_2\rangle \\
|e^2t^3, {}^2T_2 \times t\rangle &\rightarrow |e^2t^4, {}^1A_1\rangle, |e^2t^4, {}^1E\rangle, |e^2t^4, {}^1T_1\rangle, |e^2t^4, {}^1T_2\rangle, \\
&\quad |e^2t^4, {}^3A_1\rangle, |e^2t^4, {}^3E\rangle, |e^2t^4, {}^3T_1\rangle, |e^2t^4, {}^3T_2\rangle \\
|e^2t^3, {}^4A_1 \times t\rangle &\rightarrow |e^2t^4, {}^3T_2\rangle, |e^2t^4, {}^5T_2\rangle \\
|e^2t^3, {}^4A_2 \times t\rangle &\rightarrow |e^2t^4, {}^3T_1\rangle, |e^2t^4, {}^5T_1\rangle \\
|e^2t^3, {}^4E \times t\rangle &\rightarrow |e^2t^4, {}^3T_1\rangle, |e^2t^4, {}^3T_2\rangle, |e^2t^4, {}^5T_1\rangle, |e^2t^4, {}^5T_2\rangle \\
|e^2t^3, {}^4T_1 \times t\rangle &\rightarrow |e^2t^4, {}^3A_2\rangle, |e^2t^4, {}^3E\rangle, |e^2t^4, {}^3T_1\rangle, |e^2t^4, {}^3T_2\rangle, \\
&\quad |e^2t^4, {}^5A_2\rangle, |e^2t^4, {}^5E\rangle, |e^2t^4, {}^5T_1\rangle, |e^2t^4, {}^5T_2\rangle \\
|e^2t^3, {}^4T_2 \times t\rangle &\rightarrow |e^2t^4, {}^3A_1\rangle, |e^2t^4, {}^3E\rangle, |e^2t^4, {}^3T_1\rangle, |e^2t^4, {}^3T_2\rangle, \\
&\quad |e^2t^4, {}^5A_1\rangle, |e^2t^4, {}^5E\rangle, |e^2t^4, {}^5T_1\rangle, |e^2t^4, {}^5T_2\rangle \\
|e^2t^3, {}^6A_1 \times t\rangle &\rightarrow |e^2t^4, {}^5T_2\rangle, |e^2t^4, {}^7T_2\rangle \\
|e^2t^3, {}^6A_2 \times t\rangle &\rightarrow |e^2t^4, {}^5T_1\rangle, |e^2t^4, {}^7T_1\rangle \\
|e^2t^3, {}^6E \times t\rangle &\rightarrow |e^2t^4, {}^5T_1\rangle, |e^2t^4, {}^5T_2\rangle, |e^2t^4, {}^7T_1\rangle, |e^2t^4, {}^7T_2\rangle \\
|e^2t^3, {}^6T_1 \times t\rangle &\rightarrow |e^2t^4, {}^5A_2\rangle, |e^2t^4, {}^5E\rangle, |e^2t^4, {}^5T_1\rangle, |e^2t^4, {}^5T_2\rangle, \\
&\quad |e^2t^4, {}^7A_2\rangle, |e^2t^4, {}^7E\rangle, |e^2t^4, {}^7T_1\rangle, |e^2t^4, {}^7T_2\rangle \\
|e^2t^3, {}^6T_2 \times t\rangle &\rightarrow |e^2t^4, {}^5A_1\rangle, |e^2t^4, {}^5E\rangle, |e^2t^4, {}^5T_1\rangle, |e^2t^4, {}^5T_2\rangle, \\
&\quad |e^2t^4, {}^7A_1\rangle, |e^2t^4, {}^7E\rangle, |e^2t^4, {}^7T_1\rangle, |e^2t^4, {}^7T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{1t^4, 2A_1} \times e\rangle &\rightarrow |e^{2t^4, 1E}\rangle, |e^{2t^4, 3E}\rangle \\
|e^{1t^4, 2A_2} \times e\rangle &\rightarrow |e^{2t^4, 1E}\rangle, |e^{2t^4, 3E}\rangle \\
|e^{1t^4, 2E} \times e\rangle &\rightarrow |e^{2t^4, 1A_1}\rangle, |e^{2t^4, 1A_2}\rangle, |e^{2t^4, 1E}\rangle, |e^{2t^4, 3A_1}\rangle, |e^{2t^4, 3A_2}\rangle, |e^{2t^4, 3E}\rangle \\
|e^{1t^4, 2T_1} \times e\rangle &\rightarrow |e^{2t^4, 1T_1}\rangle, |e^{2t^4, 1T_2}\rangle, |e^{2t^4, 3T_1}\rangle, |e^{2t^4, 3T_2}\rangle \\
|e^{1t^4, 2T_2} \times e\rangle &\rightarrow |e^{2t^4, 1T_1}\rangle, |e^{2t^4, 1T_2}\rangle, |e^{2t^4, 3T_1}\rangle, |e^{2t^4, 3T_2}\rangle \\
|e^{1t^4, 4A_1} \times e\rangle &\rightarrow |e^{2t^4, 3E}\rangle, |e^{2t^4, 5E}\rangle \\
|e^{1t^4, 4A_2} \times e\rangle &\rightarrow |e^{2t^4, 3E}\rangle, |e^{2t^4, 5E}\rangle \\
|e^{1t^4, 4E} \times e\rangle &\rightarrow |e^{2t^4, 3A_1}\rangle, |e^{2t^4, 3A_2}\rangle, |e^{2t^4, 3E}\rangle, |e^{2t^4, 5A_1}\rangle, |e^{2t^4, 5A_2}\rangle, |e^{2t^4, 5E}\rangle \\
|e^{1t^4, 4T_1} \times e\rangle &\rightarrow |e^{2t^4, 3T_1}\rangle, |e^{2t^4, 3T_2}\rangle, |e^{2t^4, 5T_1}\rangle, |e^{2t^4, 5T_2}\rangle \\
|e^{1t^4, 4T_2} \times e\rangle &\rightarrow |e^{2t^4, 3T_1}\rangle, |e^{2t^4, 3T_2}\rangle, |e^{2t^4, 5T_1}\rangle, |e^{2t^4, 5T_2}\rangle \\
|e^{1t^4, 6A_1} \times e\rangle &\rightarrow |e^{2t^4, 5E}\rangle, |e^{2t^4, 7E}\rangle \\
|e^{1t^4, 6A_2} \times e\rangle &\rightarrow |e^{2t^4, 5E}\rangle, |e^{2t^4, 7E}\rangle \\
|e^{1t^4, 6E} \times e\rangle &\rightarrow |e^{2t^4, 5A_1}\rangle, |e^{2t^4, 5A_2}\rangle, |e^{2t^4, 5E}\rangle, |e^{2t^4, 7A_1}\rangle, |e^{2t^4, 7A_2}\rangle, |e^{2t^4, 7E}\rangle \\
|e^{1t^4, 6T_1} \times e\rangle &\rightarrow |e^{2t^4, 5T_1}\rangle, |e^{2t^4, 5T_2}\rangle, |e^{2t^4, 7T_1}\rangle, |e^{2t^4, 7T_2}\rangle \\
|e^{1t^4, 6T_2} \times e\rangle &\rightarrow |e^{2t^4, 5T_1}\rangle, |e^{2t^4, 5T_2}\rangle, |e^{2t^4, 7T_1}\rangle, |e^{2t^4, 7T_2}\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{1t^4}, {}^2A_1 \times t\rangle &\rightarrow |e^{1t^5}, {}^1T_2\rangle, |e^{1t^5}, {}^3T_2\rangle \\
|e^{1t^4}, {}^2A_2 \times t\rangle &\rightarrow |e^{1t^5}, {}^1T_1\rangle, |e^{1t^5}, {}^3T_1\rangle \\
|e^{1t^4}, {}^2E \times t\rangle &\rightarrow |e^{1t^5}, {}^1T_1\rangle, |e^{1t^5}, {}^1T_2\rangle, |e^{1t^5}, {}^3T_1\rangle, |e^{1t^5}, {}^3T_2\rangle \\
|e^{1t^4}, {}^2T_1 \times t\rangle &\rightarrow |e^{1t^5}, {}^1A_2\rangle, |e^{1t^5}, {}^1E\rangle, |e^{1t^5}, {}^1T_1\rangle, |e^{1t^5}, {}^1T_2\rangle, \\
&\quad |e^{1t^5}, {}^3A_2\rangle, |e^{1t^5}, {}^3E\rangle, |e^{1t^5}, {}^3T_1\rangle, |e^{1t^5}, {}^3T_2\rangle \\
|e^{1t^4}, {}^2T_2 \times t\rangle &\rightarrow |e^{1t^5}, {}^1A_1\rangle, |e^{1t^5}, {}^1E\rangle, |e^{1t^5}, {}^1T_1\rangle, |e^{1t^5}, {}^1T_2\rangle, \\
&\quad |e^{1t^5}, {}^3A_1\rangle, |e^{1t^5}, {}^3E\rangle, |e^{1t^5}, {}^3T_1\rangle, |e^{1t^5}, {}^3T_2\rangle \\
|e^{1t^4}, {}^4A_1 \times t\rangle &\rightarrow |e^{1t^5}, {}^3T_2\rangle, |e^{1t^5}, {}^5T_2\rangle \\
|e^{1t^4}, {}^4A_2 \times t\rangle &\rightarrow |e^{1t^5}, {}^3T_1\rangle, |e^{1t^5}, {}^5T_1\rangle \\
|e^{1t^4}, {}^4E \times t\rangle &\rightarrow |e^{1t^5}, {}^3T_1\rangle, |e^{1t^5}, {}^3T_2\rangle, |e^{1t^5}, {}^5T_1\rangle, |e^{1t^5}, {}^5T_2\rangle \\
|e^{1t^4}, {}^4T_1 \times t\rangle &\rightarrow |e^{1t^5}, {}^3A_2\rangle, |e^{1t^5}, {}^3E\rangle, |e^{1t^5}, {}^3T_1\rangle, |e^{1t^5}, {}^3T_2\rangle, \\
&\quad |e^{1t^5}, {}^5A_2\rangle, |e^{1t^5}, {}^5E\rangle, |e^{1t^5}, {}^5T_1\rangle, |e^{1t^5}, {}^5T_2\rangle \\
|e^{1t^4}, {}^4T_2 \times t\rangle &\rightarrow |e^{1t^5}, {}^3A_1\rangle, |e^{1t^5}, {}^3E\rangle, |e^{1t^5}, {}^3T_1\rangle, |e^{1t^5}, {}^3T_2\rangle, \\
&\quad |e^{1t^5}, {}^5A_1\rangle, |e^{1t^5}, {}^5E\rangle, |e^{1t^5}, {}^5T_1\rangle, |e^{1t^5}, {}^5T_2\rangle \\
|e^{1t^4}, {}^6A_1 \times t\rangle &\rightarrow |e^{1t^5}, {}^5T_2\rangle, |e^{1t^5}, {}^7T_2\rangle \\
|e^{1t^4}, {}^6A_2 \times t\rangle &\rightarrow |e^{1t^5}, {}^5T_1\rangle, |e^{1t^5}, {}^7T_1\rangle \\
|e^{1t^4}, {}^6E \times t\rangle &\rightarrow |e^{1t^5}, {}^5T_1\rangle, |e^{1t^5}, {}^5T_2\rangle, |e^{1t^5}, {}^7T_1\rangle, |e^{1t^5}, {}^7T_2\rangle \\
|e^{1t^4}, {}^6T_1 \times t\rangle &\rightarrow |e^{1t^5}, {}^5A_2\rangle, |e^{1t^5}, {}^5E\rangle, |e^{1t^5}, {}^5T_1\rangle, |e^{1t^5}, {}^5T_2\rangle, \\
&\quad |e^{1t^5}, {}^7A_2\rangle, |e^{1t^5}, {}^7E\rangle, |e^{1t^5}, {}^7T_1\rangle, |e^{1t^5}, {}^7T_2\rangle \\
|e^{1t^4}, {}^6T_2 \times t\rangle &\rightarrow |e^{1t^5}, {}^5A_1\rangle, |e^{1t^5}, {}^5E\rangle, |e^{1t^5}, {}^5T_1\rangle, |e^{1t^5}, {}^5T_2\rangle, \\
&\quad |e^{1t^5}, {}^7A_1\rangle, |e^{1t^5}, {}^7E\rangle, |e^{1t^5}, {}^7T_1\rangle, |e^{1t^5}, {}^7T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{0t^5, 2A_1} \times e\rangle &\rightarrow |e^{1t^5, 1E}\rangle, |e^{1t^5, 3E}\rangle \\
|e^{0t^5, 2A_2} \times e\rangle &\rightarrow |e^{1t^5, 1E}\rangle, |e^{1t^5, 3E}\rangle \\
|e^{0t^5, 2E} \times e\rangle &\rightarrow |e^{1t^5, 1A_1}\rangle, |e^{1t^5, 1A_2}\rangle, |e^{1t^5, 1E}\rangle, |e^{1t^5, 3A_1}\rangle, |e^{1t^5, 3A_2}\rangle, |e^{1t^5, 3E}\rangle \\
|e^{0t^5, 2T_1} \times e\rangle &\rightarrow |e^{1t^5, 1T_1}\rangle, |e^{1t^5, 1T_2}\rangle, |e^{1t^5, 3T_1}\rangle, |e^{1t^5, 3T_2}\rangle \\
|e^{0t^5, 2T_2} \times e\rangle &\rightarrow |e^{1t^5, 1T_1}\rangle, |e^{1t^5, 1T_2}\rangle, |e^{1t^5, 3T_1}\rangle, |e^{1t^5, 3T_2}\rangle \\
|e^{0t^5, 4A_1} \times e\rangle &\rightarrow |e^{1t^5, 3E}\rangle, |e^{1t^5, 5E}\rangle \\
|e^{0t^5, 4A_2} \times e\rangle &\rightarrow |e^{1t^5, 3E}\rangle, |e^{1t^5, 5E}\rangle \\
|e^{0t^5, 4E} \times e\rangle &\rightarrow |e^{1t^5, 3A_1}\rangle, |e^{1t^5, 3A_2}\rangle, |e^{1t^5, 3E}\rangle, |e^{1t^5, 5A_1}\rangle, |e^{1t^5, 5A_2}\rangle, |e^{1t^5, 5E}\rangle \\
|e^{0t^5, 4T_1} \times e\rangle &\rightarrow |e^{1t^5, 3T_1}\rangle, |e^{1t^5, 3T_2}\rangle, |e^{1t^5, 5T_1}\rangle, |e^{1t^5, 5T_2}\rangle \\
|e^{0t^5, 4T_2} \times e\rangle &\rightarrow |e^{1t^5, 3T_1}\rangle, |e^{1t^5, 3T_2}\rangle, |e^{1t^5, 5T_1}\rangle, |e^{1t^5, 5T_2}\rangle \\
|e^{0t^5, 6A_1} \times e\rangle &\rightarrow |e^{1t^5, 5E}\rangle, |e^{1t^5, 7E}\rangle \\
|e^{0t^5, 6A_2} \times e\rangle &\rightarrow |e^{1t^5, 5E}\rangle, |e^{1t^5, 7E}\rangle \\
|e^{0t^5, 6E} \times e\rangle &\rightarrow |e^{1t^5, 5A_1}\rangle, |e^{1t^5, 5A_2}\rangle, |e^{1t^5, 5E}\rangle, |e^{1t^5, 7A_1}\rangle, |e^{1t^5, 7A_2}\rangle, |e^{1t^5, 7E}\rangle \\
|e^{0t^5, 6T_1} \times e\rangle &\rightarrow |e^{1t^5, 5T_1}\rangle, |e^{1t^5, 5T_2}\rangle, |e^{1t^5, 7T_1}\rangle, |e^{1t^5, 7T_2}\rangle \\
|e^{0t^5, 6T_2} \times e\rangle &\rightarrow |e^{1t^5, 5T_1}\rangle, |e^{1t^5, 5T_2}\rangle, |e^{1t^5, 7T_1}\rangle, |e^{1t^5, 7T_2}\rangle
\end{aligned}$$



$$\begin{aligned}
|e^0 t^5, {}^2 A_1 \times t\rangle &\rightarrow |e^0 t^6, {}^1 T_2\rangle, |e^0 t^6, {}^3 T_2\rangle \\
|e^0 t^5, {}^2 A_2 \times t\rangle &\rightarrow |e^0 t^6, {}^1 T_1\rangle, |e^0 t^6, {}^3 T_1\rangle \\
|e^0 t^5, {}^2 E \times t\rangle &\rightarrow |e^0 t^6, {}^1 T_1\rangle, |e^0 t^6, {}^1 T_2\rangle, |e^0 t^6, {}^3 T_1\rangle, |e^0 t^6, {}^3 T_2\rangle \\
|e^0 t^5, {}^2 T_1 \times t\rangle &\rightarrow |e^0 t^6, {}^1 A_2\rangle, |e^0 t^6, {}^1 E\rangle, |e^0 t^6, {}^1 T_1\rangle, |e^0 t^6, {}^1 T_2\rangle, \\
&\quad |e^0 t^6, {}^3 A_2\rangle, |e^0 t^6, {}^3 E\rangle, |e^0 t^6, {}^3 T_1\rangle, |e^0 t^6, {}^3 T_2\rangle \\
|e^0 t^5, {}^2 T_2 \times t\rangle &\rightarrow |e^0 t^6, {}^1 A_1\rangle, |e^0 t^6, {}^1 E\rangle, |e^0 t^6, {}^1 T_1\rangle, |e^0 t^6, {}^1 T_2\rangle, \\
&\quad |e^0 t^6, {}^3 A_1\rangle, |e^0 t^6, {}^3 E\rangle, |e^0 t^6, {}^3 T_1\rangle, |e^0 t^6, {}^3 T_2\rangle \\
|e^0 t^5, {}^4 A_1 \times t\rangle &\rightarrow |e^0 t^6, {}^3 T_2\rangle, |e^0 t^6, {}^5 T_2\rangle \\
|e^0 t^5, {}^4 A_2 \times t\rangle &\rightarrow |e^0 t^6, {}^3 T_1\rangle, |e^0 t^6, {}^5 T_1\rangle \\
|e^0 t^5, {}^4 E \times t\rangle &\rightarrow |e^0 t^6, {}^3 T_1\rangle, |e^0 t^6, {}^3 T_2\rangle, |e^0 t^6, {}^5 T_1\rangle, |e^0 t^6, {}^5 T_2\rangle \\
|e^0 t^5, {}^4 T_1 \times t\rangle &\rightarrow |e^0 t^6, {}^3 A_2\rangle, |e^0 t^6, {}^3 E\rangle, |e^0 t^6, {}^3 T_1\rangle, |e^0 t^6, {}^3 T_2\rangle, \\
&\quad |e^0 t^6, {}^5 A_2\rangle, |e^0 t^6, {}^5 E\rangle, |e^0 t^6, {}^5 T_1\rangle, |e^0 t^6, {}^5 T_2\rangle \\
|e^0 t^5, {}^4 T_2 \times t\rangle &\rightarrow |e^0 t^6, {}^3 A_1\rangle, |e^0 t^6, {}^3 E\rangle, |e^0 t^6, {}^3 T_1\rangle, |e^0 t^6, {}^3 T_2\rangle, \\
&\quad |e^0 t^6, {}^5 A_1\rangle, |e^0 t^6, {}^5 E\rangle, |e^0 t^6, {}^5 T_1\rangle, |e^0 t^6, {}^5 T_2\rangle \\
|e^0 t^5, {}^6 A_1 \times t\rangle &\rightarrow |e^0 t^6, {}^5 T_2\rangle, |e^0 t^6, {}^7 T_2\rangle \\
|e^0 t^5, {}^6 A_2 \times t\rangle &\rightarrow |e^0 t^6, {}^5 T_1\rangle, |e^0 t^6, {}^7 T_1\rangle \\
|e^0 t^5, {}^6 E \times t\rangle &\rightarrow |e^0 t^6, {}^5 T_1\rangle, |e^0 t^6, {}^5 T_2\rangle, |e^0 t^6, {}^7 T_1\rangle, |e^0 t^6, {}^7 T_2\rangle \\
|e^0 t^5, {}^6 T_1 \times t\rangle &\rightarrow |e^0 t^6, {}^5 A_2\rangle, |e^0 t^6, {}^5 E\rangle, |e^0 t^6, {}^5 T_1\rangle, |e^0 t^6, {}^5 T_2\rangle, \\
&\quad |e^0 t^6, {}^7 A_2\rangle, |e^0 t^6, {}^7 E\rangle, |e^0 t^6, {}^7 T_1\rangle, |e^0 t^6, {}^7 T_2\rangle \\
|e^0 t^5, {}^6 T_2 \times t\rangle &\rightarrow |e^0 t^6, {}^5 A_1\rangle, |e^0 t^6, {}^5 E\rangle, |e^0 t^6, {}^5 T_1\rangle, |e^0 t^6, {}^5 T_2\rangle, \\
&\quad |e^0 t^6, {}^7 A_1\rangle, |e^0 t^6, {}^7 E\rangle, |e^0 t^6, {}^7 T_1\rangle, |e^0 t^6, {}^7 T_2\rangle
\end{aligned}$$

$$\begin{aligned}
e^6 &\rightarrow (A_1A_2E)_1 + (A_1A_2E)_3 + (A_1A_2E)_5 + (A_1A_2E)_7 \\
e^5t &\rightarrow (T_1T_2)_1 + (T_1T_2)_3 + (T_1T_2)_5 + (T_1T_2)_7 \\
e^4t^2 &\rightarrow (A_1A_2ET_1T_2)_1 + (A_1A_2ET_1T_2)_3 + (A_1A_2ET_1T_2)_5 + (A_1A_2ET_1T_2)_7 \\
e^3t^3 &\rightarrow (A_1A_2ET_1T_2)_1 + (A_1A_2ET_1T_2)_3 + (A_1A_2ET_1T_2)_5 + (A_1A_2ET_1T_2)_7 \\
e^2t^4 &\rightarrow (A_1A_2ET_1T_2)_1 + (A_1A_2ET_1T_2)_3 + (A_1A_2ET_1T_2)_5 + (A_1A_2ET_1T_2)_7 \\
et^5 &\rightarrow (A_1A_2ET_1T_2)_1 + (A_1A_2ET_1T_2)_3 + (A_1A_2ET_1T_2)_5 + (A_1A_2ET_1T_2)_7 \\
t^6 &\rightarrow (A_1A_2ET_1T_2)_1 + (A_1A_2ET_1T_2)_3 + (A_1A_2ET_1T_2)_5 + (A_1A_2ET_1T_2)_7
\end{aligned}$$

## B.6 $3d^7$

$$|e^{6t^0}, {}^1A_1 \times e\rangle \rightarrow |e^{7t^0}, {}^2E\rangle$$

$$|e^{6t^0}, {}^1A_2 \times e\rangle \rightarrow |e^{7t^0}, {}^2E\rangle$$

$$|e^{6t^0}, {}^1E \times e\rangle \rightarrow |e^{7t^0}, {}^2A_1\rangle, |e^{7t^0}, {}^2A_2\rangle, |e^{7t^0}, {}^2E\rangle$$

$$|e^{6t^0}, {}^3A_1 \times e\rangle \rightarrow |e^{7t^0}, {}^2E\rangle, |e^{7t^0}, {}^4E\rangle$$

$$|e^{6t^0}, {}^3A_2 \times e\rangle \rightarrow |e^{7t^0}, {}^2E\rangle, |e^{7t^0}, {}^4E\rangle$$

$$|e^{6t^0}, {}^3E \times e\rangle \rightarrow |e^{7t^0}, {}^2A_1\rangle, |e^{7t^0}, {}^2A_2\rangle, |e^{7t^0}, {}^2E\rangle, |e^{7t^0}, {}^4A_1\rangle, |e^{7t^0}, {}^4A_2\rangle, |e^{7t^0}, {}^4E\rangle$$

$$|e^{6t^0}, {}^5A_1 \times e\rangle \rightarrow |e^{7t^0}, {}^4E\rangle, |e^{7t^0}, {}^6E\rangle$$

$$|e^{6t^0}, {}^5A_2 \times e\rangle \rightarrow |e^{7t^0}, {}^4E\rangle, |e^{7t^0}, {}^6E\rangle$$

$$|e^{6t^0}, {}^5E \times e\rangle \rightarrow |e^{7t^0}, {}^4A_1\rangle, |e^{7t^0}, {}^4A_2\rangle, |e^{7t^0}, {}^4E\rangle, |e^{7t^0}, {}^6A_1\rangle, |e^{7t^0}, {}^6A_2\rangle, |e^{7t^0}, {}^6E\rangle$$

$$|e^{6t^0}, {}^7A_1 \times e\rangle \rightarrow |e^{7t^0}, {}^6E\rangle, |e^{7t^0}, {}^8E\rangle$$

$$|e^{6t^0}, {}^7A_2 \times e\rangle \rightarrow |e^{7t^0}, {}^6E\rangle, |e^{7t^0}, {}^8E\rangle$$

$$|e^{6t^0}, {}^7E \times e\rangle \rightarrow |e^{7t^0}, {}^6A_1\rangle, |e^{7t^0}, {}^6A_2\rangle, |e^{7t^0}, {}^6E\rangle, |e^{7t^0}, {}^8A_1\rangle, |e^{7t^0}, {}^8A_2\rangle, |e^{7t^0}, {}^8E\rangle$$

$$\begin{aligned}
|e^{6t^0}, {}^1A_1 \times t\rangle &\rightarrow |e^{6t^1}, {}^2T_2\rangle \\
|e^{6t^0}, {}^1A_2 \times t\rangle &\rightarrow |e^{6t^1}, {}^2T_1\rangle \\
|e^{6t^0}, {}^1E \times t\rangle &\rightarrow |e^{6t^1}, {}^2T_1\rangle, |e^{6t^1}, {}^2T_2\rangle \\
|e^{6t^0}, {}^3A_1 \times t\rangle &\rightarrow |e^{6t^1}, {}^2T_2\rangle, |e^{6t^1}, {}^4T_2\rangle \\
|e^{6t^0}, {}^3A_2 \times t\rangle &\rightarrow |e^{6t^1}, {}^2T_1\rangle, |e^{6t^1}, {}^4T_1\rangle \\
|e^{6t^0}, {}^3E \times t\rangle &\rightarrow |e^{6t^1}, {}^2T_1\rangle, |e^{6t^1}, {}^2T_2\rangle, |e^{6t^1}, {}^4T_1\rangle, |e^{6t^1}, {}^4T_2\rangle \\
|e^{6t^0}, {}^5A_1 \times t\rangle &\rightarrow |e^{6t^1}, {}^4T_2\rangle, |e^{6t^1}, {}^6T_2\rangle \\
|e^{6t^0}, {}^5A_2 \times t\rangle &\rightarrow |e^{6t^1}, {}^4T_1\rangle, |e^{6t^1}, {}^6T_1\rangle \\
|e^{6t^0}, {}^5E \times t\rangle &\rightarrow |e^{6t^1}, {}^4T_1\rangle, |e^{6t^1}, {}^4T_2\rangle, |e^{6t^1}, {}^6T_1\rangle, |e^{6t^1}, {}^6T_2\rangle \\
|e^{6t^0}, {}^7A_1 \times t\rangle &\rightarrow |e^{6t^1}, {}^6T_2\rangle, |e^{6t^1}, {}^8T_2\rangle \\
|e^{6t^0}, {}^7A_2 \times t\rangle &\rightarrow |e^{6t^1}, {}^6T_1\rangle, |e^{6t^1}, {}^8T_1\rangle \\
|e^{6t^0}, {}^7E \times t\rangle &\rightarrow |e^{6t^1}, {}^6T_1\rangle, |e^{6t^1}, {}^6T_2\rangle, |e^{6t^1}, {}^8T_1\rangle, |e^{6t^1}, {}^8T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{5t^1, 1T_1} \times e\rangle &\rightarrow |e^{6t^1, 2T_1}\rangle, |e^{6t^1, 2T_2}\rangle \\
|e^{5t^1, 1T_2} \times e\rangle &\rightarrow |e^{6t^1, 2T_1}\rangle, |e^{6t^1, 2T_2}\rangle \\
|e^{5t^1, 3T_1} \times e\rangle &\rightarrow |e^{6t^1, 2T_1}\rangle, |e^{6t^1, 2T_2}\rangle, |e^{6t^1, 4T_1}\rangle, |e^{6t^1, 4T_2}\rangle \\
|e^{5t^1, 3T_2} \times e\rangle &\rightarrow |e^{6t^1, 2T_1}\rangle, |e^{6t^1, 2T_2}\rangle, |e^{6t^1, 4T_1}\rangle, |e^{6t^1, 4T_2}\rangle \\
|e^{5t^1, 5T_1} \times e\rangle &\rightarrow |e^{6t^1, 4T_1}\rangle, |e^{6t^1, 4T_2}\rangle, |e^{6t^1, 6T_1}\rangle, |e^{6t^1, 6T_2}\rangle \\
|e^{5t^1, 5T_2} \times e\rangle &\rightarrow |e^{6t^1, 4T_1}\rangle, |e^{6t^1, 4T_2}\rangle, |e^{6t^1, 6T_1}\rangle, |e^{6t^1, 6T_2}\rangle \\
|e^{5t^1, 7T_1} \times e\rangle &\rightarrow |e^{6t^1, 6T_1}\rangle, |e^{6t^1, 6T_2}\rangle, |e^{6t^1, 8T_1}\rangle, |e^{6t^1, 8T_2}\rangle \\
|e^{5t^1, 7T_2} \times e\rangle &\rightarrow |e^{6t^1, 6T_1}\rangle, |e^{6t^1, 6T_2}\rangle, |e^{6t^1, 8T_1}\rangle, |e^{6t^1, 8T_2}\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{5t^1}, {}^1T_1 \times t\rangle &\rightarrow |e^{5t^2}, {}^2A_2\rangle, |e^{5t^2}, {}^2E\rangle, |e^{5t^2}, {}^2T_1\rangle, |e^{5t^2}, {}^2T_2\rangle \\
|e^{5t^1}, {}^1T_2 \times t\rangle &\rightarrow |e^{5t^2}, {}^2A_1\rangle, |e^{5t^2}, {}^2E\rangle, |e^{5t^2}, {}^2T_1\rangle, |e^{5t^2}, {}^2T_2\rangle \\
|e^{5t^1}, {}^3T_1 \times t\rangle &\rightarrow |e^{5t^2}, {}^2A_2\rangle, |e^{5t^2}, {}^2E\rangle, |e^{5t^2}, {}^2T_1\rangle, |e^{5t^2}, {}^2T_2\rangle, \\
&\quad |e^{5t^2}, {}^4A_2\rangle, |e^{5t^2}, {}^4E\rangle, |e^{5t^2}, {}^4T_1\rangle, |e^{5t^2}, {}^4T_2\rangle \\
|e^{5t^1}, {}^3T_2 \times t\rangle &\rightarrow |e^{5t^2}, {}^2A_1\rangle, |e^{5t^2}, {}^2E\rangle, |e^{5t^2}, {}^2T_1\rangle, |e^{5t^2}, {}^2T_2\rangle, \\
&\quad |e^{5t^2}, {}^4A_1\rangle, |e^{5t^2}, {}^4E\rangle, |e^{5t^2}, {}^4T_1\rangle, |e^{5t^2}, {}^4T_2\rangle \\
|e^{5t^1}, {}^5T_1 \times t\rangle &\rightarrow |e^{5t^2}, {}^4A_2\rangle, |e^{5t^2}, {}^4E\rangle, |e^{5t^2}, {}^4T_1\rangle, |e^{5t^2}, {}^4T_2\rangle, \\
&\quad |e^{5t^2}, {}^6A_2\rangle, |e^{5t^2}, {}^6E\rangle, |e^{5t^2}, {}^6T_1\rangle, |e^{5t^2}, {}^6T_2\rangle \\
|e^{5t^1}, {}^5T_2 \times t\rangle &\rightarrow |e^{5t^2}, {}^4A_1\rangle, |e^{5t^2}, {}^4E\rangle, |e^{5t^2}, {}^4T_1\rangle, |e^{5t^2}, {}^4T_2\rangle, \\
&\quad |e^{5t^2}, {}^6A_1\rangle, |e^{5t^2}, {}^6E\rangle, |e^{5t^2}, {}^6T_1\rangle, |e^{5t^2}, {}^6T_2\rangle \\
|e^{5t^1}, {}^7T_1 \times t\rangle &\rightarrow |e^{5t^2}, {}^6A_2\rangle, |e^{5t^2}, {}^6E\rangle, |e^{5t^2}, {}^6T_1\rangle, |e^{5t^2}, {}^6T_2\rangle, \\
&\quad |e^{5t^2}, {}^8A_2\rangle, |e^{5t^2}, {}^8E\rangle, |e^{5t^2}, {}^8T_1\rangle, |e^{5t^2}, {}^8T_2\rangle \\
|e^{5t^1}, {}^7T_2 \times t\rangle &\rightarrow |e^{5t^2}, {}^6A_1\rangle, |e^{5t^2}, {}^6E\rangle, |e^{5t^2}, {}^6T_1\rangle, |e^{5t^2}, {}^6T_2\rangle, \\
&\quad |e^{5t^2}, {}^8A_1\rangle, |e^{5t^2}, {}^8E\rangle, |e^{5t^2}, {}^8T_1\rangle, |e^{5t^2}, {}^8T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{4t^2}, {}^1A_1 \times e\rangle &\rightarrow |e^{5t^2}, {}^2E\rangle \\
|e^{4t^2}, {}^1A_2 \times e\rangle &\rightarrow |e^{5t^2}, {}^2E\rangle \\
|e^{4t^2}, {}^1E \times e\rangle &\rightarrow |e^{5t^2}, {}^2A_1\rangle, |e^{5t^2}, {}^2A_2\rangle, |e^{5t^2}, {}^2E\rangle \\
|e^{4t^2}, {}^1T_1 \times e\rangle &\rightarrow |e^{5t^2}, {}^2T_1\rangle, |e^{5t^2}, {}^2T_2\rangle \\
|e^{4t^2}, {}^1T_2 \times e\rangle &\rightarrow |e^{5t^2}, {}^2T_1\rangle, |e^{5t^2}, {}^2T_2\rangle \\
|e^{4t^2}, {}^3A_1 \times e\rangle &\rightarrow |e^{5t^2}, {}^2E\rangle, |e^{5t^2}, {}^4E\rangle \\
|e^{4t^2}, {}^3A_2 \times e\rangle &\rightarrow |e^{5t^2}, {}^2E\rangle, |e^{5t^2}, {}^4E\rangle \\
|e^{4t^2}, {}^3E \times e\rangle &\rightarrow |e^{5t^2}, {}^2A_1\rangle, |e^{5t^2}, {}^2A_2\rangle, |e^{5t^2}, {}^2E\rangle, |e^{5t^2}, {}^4A_1\rangle, |e^{5t^2}, {}^4A_2\rangle, |e^{5t^2}, {}^4E\rangle \\
|e^{4t^2}, {}^3T_1 \times e\rangle &\rightarrow |e^{5t^2}, {}^2T_1\rangle, |e^{5t^2}, {}^2T_2\rangle, |e^{5t^2}, {}^4T_1\rangle, |e^{5t^2}, {}^4T_2\rangle \\
|e^{4t^2}, {}^3T_2 \times e\rangle &\rightarrow |e^{5t^2}, {}^2T_1\rangle, |e^{5t^2}, {}^2T_2\rangle, |e^{5t^2}, {}^4T_1\rangle, |e^{5t^2}, {}^4T_2\rangle \\
|e^{4t^2}, {}^5A_1 \times e\rangle &\rightarrow |e^{5t^2}, {}^4E\rangle, |e^{5t^2}, {}^6E\rangle \\
|e^{4t^2}, {}^5A_2 \times e\rangle &\rightarrow |e^{5t^2}, {}^4E\rangle, |e^{5t^2}, {}^6E\rangle \\
|e^{4t^2}, {}^5E \times e\rangle &\rightarrow |e^{5t^2}, {}^4A_1\rangle, |e^{5t^2}, {}^4A_2\rangle, |e^{5t^2}, {}^4E\rangle, |e^{5t^2}, {}^6A_1\rangle, |e^{5t^2}, {}^6A_2\rangle, |e^{5t^2}, {}^6E\rangle \\
|e^{4t^2}, {}^5T_1 \times e\rangle &\rightarrow |e^{5t^2}, {}^4T_1\rangle, |e^{5t^2}, {}^4T_2\rangle, |e^{5t^2}, {}^6T_1\rangle, |e^{5t^2}, {}^6T_2\rangle \\
|e^{4t^2}, {}^5T_2 \times e\rangle &\rightarrow |e^{5t^2}, {}^4T_1\rangle, |e^{5t^2}, {}^4T_2\rangle, |e^{5t^2}, {}^6T_1\rangle, |e^{5t^2}, {}^6T_2\rangle \\
|e^{4t^2}, {}^7A_1 \times e\rangle &\rightarrow |e^{5t^2}, {}^6E\rangle, |e^{5t^2}, {}^8E\rangle \\
|e^{4t^2}, {}^7A_2 \times e\rangle &\rightarrow |e^{5t^2}, {}^6E\rangle, |e^{5t^2}, {}^8E\rangle \\
|e^{4t^2}, {}^7E \times e\rangle &\rightarrow |e^{5t^2}, {}^6A_1\rangle, |e^{5t^2}, {}^6A_2\rangle, |e^{5t^2}, {}^6E\rangle, |e^{5t^2}, {}^8A_1\rangle, |e^{5t^2}, {}^8A_2\rangle, |e^{5t^2}, {}^8E\rangle \\
|e^{4t^2}, {}^7T_1 \times e\rangle &\rightarrow |e^{5t^2}, {}^6T_1\rangle, |e^{5t^2}, {}^6T_2\rangle, |e^{5t^2}, {}^8T_1\rangle, |e^{5t^2}, {}^8T_2\rangle \\
|e^{4t^2}, {}^7T_2 \times e\rangle &\rightarrow |e^{5t^2}, {}^6T_1\rangle, |e^{5t^2}, {}^6T_2\rangle, |e^{5t^2}, {}^8T_1\rangle, |e^{5t^2}, {}^8T_2\rangle
\end{aligned}$$





$$\begin{aligned}
|e^{3t^3}, {}^1A_1 \times e\rangle &\rightarrow |e^{4t^3}, {}^2E\rangle \\
|e^{3t^3}, {}^1A_2 \times e\rangle &\rightarrow |e^{4t^3}, {}^2E\rangle \\
|e^{3t^3}, {}^1E \times e\rangle &\rightarrow |e^{4t^3}, {}^2A_1\rangle, |e^{4t^3}, {}^2A_2\rangle, |e^{4t^3}, {}^2E\rangle \\
|e^{3t^3}, {}^1T_1 \times e\rangle &\rightarrow |e^{4t^3}, {}^2T_1\rangle, |e^{4t^3}, {}^2T_2\rangle \\
|e^{3t^3}, {}^1T_2 \times e\rangle &\rightarrow |e^{4t^3}, {}^2T_1\rangle, |e^{4t^3}, {}^2T_2\rangle \\
|e^{3t^3}, {}^3A_1 \times e\rangle &\rightarrow |e^{4t^3}, {}^2E\rangle, |e^{4t^3}, {}^4E\rangle \\
|e^{3t^3}, {}^3A_2 \times e\rangle &\rightarrow |e^{4t^3}, {}^2E\rangle, |e^{4t^3}, {}^4E\rangle \\
|e^{3t^3}, {}^3E \times e\rangle &\rightarrow |e^{4t^3}, {}^2A_1\rangle, |e^{4t^3}, {}^2A_2\rangle, |e^{4t^3}, {}^2E\rangle, |e^{4t^3}, {}^4A_1\rangle, |e^{4t^3}, {}^4A_2\rangle, |e^{4t^3}, {}^4E\rangle \\
|e^{3t^3}, {}^3T_1 \times e\rangle &\rightarrow |e^{4t^3}, {}^2T_1\rangle, |e^{4t^3}, {}^2T_2\rangle, |e^{4t^3}, {}^4T_1\rangle, |e^{4t^3}, {}^4T_2\rangle \\
|e^{3t^3}, {}^3T_2 \times e\rangle &\rightarrow |e^{4t^3}, {}^2T_1\rangle, |e^{4t^3}, {}^2T_2\rangle, |e^{4t^3}, {}^4T_1\rangle, |e^{4t^3}, {}^4T_2\rangle \\
|e^{3t^3}, {}^5A_1 \times e\rangle &\rightarrow |e^{4t^3}, {}^4E\rangle, |e^{4t^3}, {}^6E\rangle \\
|e^{3t^3}, {}^5A_2 \times e\rangle &\rightarrow |e^{4t^3}, {}^4E\rangle, |e^{4t^3}, {}^6E\rangle \\
|e^{3t^3}, {}^5E \times e\rangle &\rightarrow |e^{4t^3}, {}^4A_1\rangle, |e^{4t^3}, {}^4A_2\rangle, |e^{4t^3}, {}^4E\rangle, |e^{4t^3}, {}^6A_1\rangle, |e^{4t^3}, {}^6A_2\rangle, |e^{4t^3}, {}^6E\rangle \\
|e^{3t^3}, {}^5T_1 \times e\rangle &\rightarrow |e^{4t^3}, {}^4T_1\rangle, |e^{4t^3}, {}^4T_2\rangle, |e^{4t^3}, {}^6T_1\rangle, |e^{4t^3}, {}^6T_2\rangle \\
|e^{3t^3}, {}^5T_2 \times e\rangle &\rightarrow |e^{4t^3}, {}^4T_1\rangle, |e^{4t^3}, {}^4T_2\rangle, |e^{4t^3}, {}^6T_1\rangle, |e^{4t^3}, {}^6T_2\rangle \\
|e^{3t^3}, {}^7A_1 \times e\rangle &\rightarrow |e^{4t^3}, {}^6E\rangle, |e^{4t^3}, {}^8E\rangle \\
|e^{3t^3}, {}^7A_2 \times e\rangle &\rightarrow |e^{4t^3}, {}^6E\rangle, |e^{4t^3}, {}^8E\rangle \\
|e^{3t^3}, {}^7E \times e\rangle &\rightarrow |e^{4t^3}, {}^6A_1\rangle, |e^{4t^3}, {}^6A_2\rangle, |e^{4t^3}, {}^6E\rangle, |e^{4t^3}, {}^8A_1\rangle, |e^{4t^3}, {}^8A_2\rangle, |e^{4t^3}, {}^8E\rangle \\
|e^{3t^3}, {}^7T_1 \times e\rangle &\rightarrow |e^{4t^3}, {}^6T_1\rangle, |e^{4t^3}, {}^6T_2\rangle, |e^{4t^3}, {}^8T_1\rangle, |e^{4t^3}, {}^8T_2\rangle \\
|e^{3t^3}, {}^7T_2 \times e\rangle &\rightarrow |e^{4t^3}, {}^6T_1\rangle, |e^{4t^3}, {}^6T_2\rangle, |e^{4t^3}, {}^8T_1\rangle, |e^{4t^3}, {}^8T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^3t^3, {}^1A_1 \times t\rangle &\rightarrow |e^3t^4, {}^2T_2\rangle \\
|e^3t^3, {}^1A_2 \times t\rangle &\rightarrow |e^3t^4, {}^2T_1\rangle \\
|e^3t^3, {}^1E \times t\rangle &\rightarrow |e^3t^4, {}^2T_1\rangle, |e^3t^4, {}^2T_2\rangle \\
|e^3t^3, {}^1T_1 \times t\rangle &\rightarrow |e^3t^4, {}^2A_2\rangle, |e^3t^4, {}^2E\rangle, |e^3t^4, {}^2T_1\rangle, |e^3t^4, {}^2T_2\rangle \\
|e^3t^3, {}^1T_2 \times t\rangle &\rightarrow |e^3t^4, {}^2A_1\rangle, |e^3t^4, {}^2E\rangle, |e^3t^4, {}^2T_1\rangle, |e^3t^4, {}^2T_2\rangle \\
|e^3t^3, {}^3A_1 \times t\rangle &\rightarrow |e^3t^4, {}^2T_2\rangle, |e^3t^4, {}^4T_2\rangle \\
|e^3t^3, {}^3A_2 \times t\rangle &\rightarrow |e^3t^4, {}^2T_1\rangle, |e^3t^4, {}^4T_1\rangle \\
|e^3t^3, {}^3E \times t\rangle &\rightarrow |e^3t^4, {}^2T_1\rangle, |e^3t^4, {}^2T_2\rangle, |e^3t^4, {}^4T_1\rangle, |e^3t^4, {}^4T_2\rangle \\
|e^3t^3, {}^3T_1 \times t\rangle &\rightarrow |e^3t^4, {}^2A_2\rangle, |e^3t^4, {}^2E\rangle, |e^3t^4, {}^2T_1\rangle, |e^3t^4, {}^2T_2\rangle, \\
&\quad |e^3t^4, {}^4A_2\rangle, |e^3t^4, {}^4E\rangle, |e^3t^4, {}^4T_1\rangle, |e^3t^4, {}^4T_2\rangle \\
|e^3t^3, {}^3T_2 \times t\rangle &\rightarrow |e^3t^4, {}^2A_1\rangle, |e^3t^4, {}^2E\rangle, |e^3t^4, {}^2T_1\rangle, |e^3t^4, {}^2T_2\rangle, \\
&\quad |e^3t^4, {}^4A_1\rangle, |e^3t^4, {}^4E\rangle, |e^3t^4, {}^4T_1\rangle, |e^3t^4, {}^4T_2\rangle \\
|e^3t^3, {}^5A_1 \times t\rangle &\rightarrow |e^3t^4, {}^4T_2\rangle, |e^3t^4, {}^6T_2\rangle \\
|e^3t^3, {}^5A_2 \times t\rangle &\rightarrow |e^3t^4, {}^4T_1\rangle, |e^3t^4, {}^6T_1\rangle \\
|e^3t^3, {}^5E \times t\rangle &\rightarrow |e^3t^4, {}^4T_1\rangle, |e^3t^4, {}^4T_2\rangle, |e^3t^4, {}^6T_1\rangle, |e^3t^4, {}^6T_2\rangle \\
|e^3t^3, {}^5T_1 \times t\rangle &\rightarrow |e^3t^4, {}^4A_2\rangle, |e^3t^4, {}^4E\rangle, |e^3t^4, {}^4T_1\rangle, |e^3t^4, {}^4T_2\rangle, \\
&\quad |e^3t^4, {}^6A_2\rangle, |e^3t^4, {}^6E\rangle, |e^3t^4, {}^6T_1\rangle, |e^3t^4, {}^6T_2\rangle \\
|e^3t^3, {}^5T_2 \times t\rangle &\rightarrow |e^3t^4, {}^4A_1\rangle, |e^3t^4, {}^4E\rangle, |e^3t^4, {}^4T_1\rangle, |e^3t^4, {}^4T_2\rangle, \\
&\quad |e^3t^4, {}^6A_1\rangle, |e^3t^4, {}^6E\rangle, |e^3t^4, {}^6T_1\rangle, |e^3t^4, {}^6T_2\rangle \\
|e^3t^3, {}^7A_1 \times t\rangle &\rightarrow |e^3t^4, {}^6T_2\rangle, |e^3t^4, {}^8T_2\rangle \\
|e^3t^3, {}^7A_2 \times t\rangle &\rightarrow |e^3t^4, {}^6T_1\rangle, |e^3t^4, {}^8T_1\rangle \\
|e^3t^3, {}^7E \times t\rangle &\rightarrow |e^3t^4, {}^6T_1\rangle, |e^3t^4, {}^6T_2\rangle, |e^3t^4, {}^8T_1\rangle, |e^3t^4, {}^8T_2\rangle \\
|e^3t^3, {}^7T_1 \times t\rangle &\rightarrow |e^3t^4, {}^6A_2\rangle, |e^3t^4, {}^6E\rangle, |e^3t^4, {}^6T_1\rangle, |e^3t^4, {}^6T_2\rangle, \\
&\quad |e^3t^4, {}^8A_2\rangle, |e^3t^4, {}^8E\rangle, |e^3t^4, {}^8T_1\rangle, |e^3t^4, {}^8T_2\rangle \\
|e^3t^3, {}^7T_2 \times t\rangle &\rightarrow |e^3t^4, {}^6A_1\rangle, |e^3t^4, {}^6E\rangle, |e^3t^4, {}^6T_1\rangle, |e^3t^4, {}^6T_2\rangle, \\
&\quad |e^3t^4, {}^8A_1\rangle, |e^3t^4, {}^8E\rangle, |e^3t^4, {}^8T_1\rangle, |e^3t^4, {}^8T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{2t^4}, {}^1A_1 \times e\rangle &\rightarrow |e^{3t^4}, {}^2E\rangle \\
|e^{2t^4}, {}^1A_2 \times e\rangle &\rightarrow |e^{3t^4}, {}^2E\rangle \\
|e^{2t^4}, {}^1E \times e\rangle &\rightarrow |e^{3t^4}, {}^2A_1\rangle, |e^{3t^4}, {}^2A_2\rangle, |e^{3t^4}, {}^2E\rangle \\
|e^{2t^4}, {}^1T_1 \times e\rangle &\rightarrow |e^{3t^4}, {}^2T_1\rangle, |e^{3t^4}, {}^2T_2\rangle \\
|e^{2t^4}, {}^1T_2 \times e\rangle &\rightarrow |e^{3t^4}, {}^2T_1\rangle, |e^{3t^4}, {}^2T_2\rangle \\
|e^{2t^4}, {}^3A_1 \times e\rangle &\rightarrow |e^{3t^4}, {}^2E\rangle, |e^{3t^4}, {}^4E\rangle \\
|e^{2t^4}, {}^3A_2 \times e\rangle &\rightarrow |e^{3t^4}, {}^2E\rangle, |e^{3t^4}, {}^4E\rangle \\
|e^{2t^4}, {}^3E \times e\rangle &\rightarrow |e^{3t^4}, {}^2A_1\rangle, |e^{3t^4}, {}^2A_2\rangle, |e^{3t^4}, {}^2E\rangle, |e^{3t^4}, {}^4A_1\rangle, |e^{3t^4}, {}^4A_2\rangle, |e^{3t^4}, {}^4E\rangle \\
|e^{2t^4}, {}^3T_1 \times e\rangle &\rightarrow |e^{3t^4}, {}^2T_1\rangle, |e^{3t^4}, {}^2T_2\rangle, |e^{3t^4}, {}^4T_1\rangle, |e^{3t^4}, {}^4T_2\rangle \\
|e^{2t^4}, {}^3T_2 \times e\rangle &\rightarrow |e^{3t^4}, {}^2T_1\rangle, |e^{3t^4}, {}^2T_2\rangle, |e^{3t^4}, {}^4T_1\rangle, |e^{3t^4}, {}^4T_2\rangle \\
|e^{2t^4}, {}^5A_1 \times e\rangle &\rightarrow |e^{3t^4}, {}^4E\rangle, |e^{3t^4}, {}^6E\rangle \\
|e^{2t^4}, {}^5A_2 \times e\rangle &\rightarrow |e^{3t^4}, {}^4E\rangle, |e^{3t^4}, {}^6E\rangle \\
|e^{2t^4}, {}^5E \times e\rangle &\rightarrow |e^{3t^4}, {}^4A_1\rangle, |e^{3t^4}, {}^4A_2\rangle, |e^{3t^4}, {}^4E\rangle, |e^{3t^4}, {}^6A_1\rangle, |e^{3t^4}, {}^6A_2\rangle, |e^{3t^4}, {}^6E\rangle \\
|e^{2t^4}, {}^5T_1 \times e\rangle &\rightarrow |e^{3t^4}, {}^4T_1\rangle, |e^{3t^4}, {}^4T_2\rangle, |e^{3t^4}, {}^6T_1\rangle, |e^{3t^4}, {}^6T_2\rangle \\
|e^{2t^4}, {}^5T_2 \times e\rangle &\rightarrow |e^{3t^4}, {}^4T_1\rangle, |e^{3t^4}, {}^4T_2\rangle, |e^{3t^4}, {}^6T_1\rangle, |e^{3t^4}, {}^6T_2\rangle \\
|e^{2t^4}, {}^7A_1 \times e\rangle &\rightarrow |e^{3t^4}, {}^6E\rangle, |e^{3t^4}, {}^8E\rangle \\
|e^{2t^4}, {}^7A_2 \times e\rangle &\rightarrow |e^{3t^4}, {}^6E\rangle, |e^{3t^4}, {}^8E\rangle \\
|e^{2t^4}, {}^7E \times e\rangle &\rightarrow |e^{3t^4}, {}^6A_1\rangle, |e^{3t^4}, {}^6A_2\rangle, |e^{3t^4}, {}^6E\rangle, |e^{3t^4}, {}^8A_1\rangle, |e^{3t^4}, {}^8A_2\rangle, |e^{3t^4}, {}^8E\rangle \\
|e^{2t^4}, {}^7T_1 \times e\rangle &\rightarrow |e^{3t^4}, {}^6T_1\rangle, |e^{3t^4}, {}^6T_2\rangle, |e^{3t^4}, {}^8T_1\rangle, |e^{3t^4}, {}^8T_2\rangle \\
|e^{2t^4}, {}^7T_2 \times e\rangle &\rightarrow |e^{3t^4}, {}^6T_1\rangle, |e^{3t^4}, {}^6T_2\rangle, |e^{3t^4}, {}^8T_1\rangle, |e^{3t^4}, {}^8T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^2t^4, {}^1A_1 \times t\rangle &\rightarrow |e^2t^5, {}^2T_2\rangle \\
|e^2t^4, {}^1A_2 \times t\rangle &\rightarrow |e^2t^5, {}^2T_1\rangle \\
|e^2t^4, {}^1E \times t\rangle &\rightarrow |e^2t^5, {}^2T_1\rangle, |e^2t^5, {}^2T_2\rangle \\
|e^2t^4, {}^1T_1 \times t\rangle &\rightarrow |e^2t^5, {}^2A_2\rangle, |e^2t^5, {}^2E\rangle, |e^2t^5, {}^2T_1\rangle, |e^2t^5, {}^2T_2\rangle \\
|e^2t^4, {}^1T_2 \times t\rangle &\rightarrow |e^2t^5, {}^2A_1\rangle, |e^2t^5, {}^2E\rangle, |e^2t^5, {}^2T_1\rangle, |e^2t^5, {}^2T_2\rangle \\
|e^2t^4, {}^3A_1 \times t\rangle &\rightarrow |e^2t^5, {}^2T_2\rangle, |e^2t^5, {}^4T_2\rangle \\
|e^2t^4, {}^3A_2 \times t\rangle &\rightarrow |e^2t^5, {}^2T_1\rangle, |e^2t^5, {}^4T_1\rangle \\
|e^2t^4, {}^3E \times t\rangle &\rightarrow |e^2t^5, {}^2T_1\rangle, |e^2t^5, {}^2T_2\rangle, |e^2t^5, {}^4T_1\rangle, |e^2t^5, {}^4T_2\rangle \\
|e^2t^4, {}^3T_1 \times t\rangle &\rightarrow |e^2t^5, {}^2A_2\rangle, |e^2t^5, {}^2E\rangle, |e^2t^5, {}^2T_1\rangle, |e^2t^5, {}^2T_2\rangle, \\
&\quad |e^2t^5, {}^4A_2\rangle, |e^2t^5, {}^4E\rangle, |e^2t^5, {}^4T_1\rangle, |e^2t^5, {}^4T_2\rangle \\
|e^2t^4, {}^3T_2 \times t\rangle &\rightarrow |e^2t^5, {}^2A_1\rangle, |e^2t^5, {}^2E\rangle, |e^2t^5, {}^2T_1\rangle, |e^2t^5, {}^2T_2\rangle, \\
&\quad |e^2t^5, {}^4A_1\rangle, |e^2t^5, {}^4E\rangle, |e^2t^5, {}^4T_1\rangle, |e^2t^5, {}^4T_2\rangle \\
|e^2t^4, {}^5A_1 \times t\rangle &\rightarrow |e^2t^5, {}^4T_2\rangle, |e^2t^5, {}^6T_2\rangle \\
|e^2t^4, {}^5A_2 \times t\rangle &\rightarrow |e^2t^5, {}^4T_1\rangle, |e^2t^5, {}^6T_1\rangle \\
|e^2t^4, {}^5E \times t\rangle &\rightarrow |e^2t^5, {}^4T_1\rangle, |e^2t^5, {}^4T_2\rangle, |e^2t^5, {}^6T_1\rangle, |e^2t^5, {}^6T_2\rangle \\
|e^2t^4, {}^5T_1 \times t\rangle &\rightarrow |e^2t^5, {}^4A_2\rangle, |e^2t^5, {}^4E\rangle, |e^2t^5, {}^4T_1\rangle, |e^2t^5, {}^4T_2\rangle, \\
&\quad |e^2t^5, {}^6A_2\rangle, |e^2t^5, {}^6E\rangle, |e^2t^5, {}^6T_1\rangle, |e^2t^5, {}^6T_2\rangle \\
|e^2t^4, {}^5T_2 \times t\rangle &\rightarrow |e^2t^5, {}^4A_1\rangle, |e^2t^5, {}^4E\rangle, |e^2t^5, {}^4T_1\rangle, |e^2t^5, {}^4T_2\rangle, \\
&\quad |e^2t^5, {}^6A_1\rangle, |e^2t^5, {}^6E\rangle, |e^2t^5, {}^6T_1\rangle, |e^2t^5, {}^6T_2\rangle \\
|e^2t^4, {}^7A_1 \times t\rangle &\rightarrow |e^2t^5, {}^6T_2\rangle, |e^2t^5, {}^8T_2\rangle \\
|e^2t^4, {}^7A_2 \times t\rangle &\rightarrow |e^2t^5, {}^6T_1\rangle, |e^2t^5, {}^8T_1\rangle \\
|e^2t^4, {}^7E \times t\rangle &\rightarrow |e^2t^5, {}^6T_1\rangle, |e^2t^5, {}^6T_2\rangle, |e^2t^5, {}^8T_1\rangle, |e^2t^5, {}^8T_2\rangle \\
|e^2t^4, {}^7T_1 \times t\rangle &\rightarrow |e^2t^5, {}^6A_2\rangle, |e^2t^5, {}^6E\rangle, |e^2t^5, {}^6T_1\rangle, |e^2t^5, {}^6T_2\rangle, \\
&\quad |e^2t^5, {}^8A_2\rangle, |e^2t^5, {}^8E\rangle, |e^2t^5, {}^8T_1\rangle, |e^2t^5, {}^8T_2\rangle \\
|e^2t^4, {}^7T_2 \times t\rangle &\rightarrow |e^2t^5, {}^6A_1\rangle, |e^2t^5, {}^6E\rangle, |e^2t^5, {}^6T_1\rangle, |e^2t^5, {}^6T_2\rangle, \\
&\quad |e^2t^5, {}^8A_1\rangle, |e^2t^5, {}^8E\rangle, |e^2t^5, {}^8T_1\rangle, |e^2t^5, {}^8T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^{1t^5}, {}^1A_1 \times e\rangle &\rightarrow |e^{2t^5}, {}^2E\rangle \\
|e^{1t^5}, {}^1A_2 \times e\rangle &\rightarrow |e^{2t^5}, {}^2E\rangle \\
|e^{1t^5}, {}^1E \times e\rangle &\rightarrow |e^{2t^5}, {}^2A_1\rangle, |e^{2t^5}, {}^2A_2\rangle, |e^{2t^5}, {}^2E\rangle \\
|e^{1t^5}, {}^1T_1 \times e\rangle &\rightarrow |e^{2t^5}, {}^2T_1\rangle, |e^{2t^5}, {}^2T_2\rangle \\
|e^{1t^5}, {}^1T_2 \times e\rangle &\rightarrow |e^{2t^5}, {}^2T_1\rangle, |e^{2t^5}, {}^2T_2\rangle \\
|e^{1t^5}, {}^3A_1 \times e\rangle &\rightarrow |e^{2t^5}, {}^2E\rangle, |e^{2t^5}, {}^4E\rangle \\
|e^{1t^5}, {}^3A_2 \times e\rangle &\rightarrow |e^{2t^5}, {}^2E\rangle, |e^{2t^5}, {}^4E\rangle \\
|e^{1t^5}, {}^3E \times e\rangle &\rightarrow |e^{2t^5}, {}^2A_1\rangle, |e^{2t^5}, {}^2A_2\rangle, |e^{2t^5}, {}^2E\rangle, |e^{2t^5}, {}^4A_1\rangle, |e^{2t^5}, {}^4A_2\rangle, |e^{2t^5}, {}^4E\rangle \\
|e^{1t^5}, {}^3T_1 \times e\rangle &\rightarrow |e^{2t^5}, {}^2T_1\rangle, |e^{2t^5}, {}^2T_2\rangle, |e^{2t^5}, {}^4T_1\rangle, |e^{2t^5}, {}^4T_2\rangle \\
|e^{1t^5}, {}^3T_2 \times e\rangle &\rightarrow |e^{2t^5}, {}^2T_1\rangle, |e^{2t^5}, {}^2T_2\rangle, |e^{2t^5}, {}^4T_1\rangle, |e^{2t^5}, {}^4T_2\rangle \\
|e^{1t^5}, {}^5A_1 \times e\rangle &\rightarrow |e^{2t^5}, {}^4E\rangle, |e^{2t^5}, {}^6E\rangle \\
|e^{1t^5}, {}^5A_2 \times e\rangle &\rightarrow |e^{2t^5}, {}^4E\rangle, |e^{2t^5}, {}^6E\rangle \\
|e^{1t^5}, {}^5E \times e\rangle &\rightarrow |e^{2t^5}, {}^4A_1\rangle, |e^{2t^5}, {}^4A_2\rangle, |e^{2t^5}, {}^4E\rangle, |e^{2t^5}, {}^6A_1\rangle, |e^{2t^5}, {}^6A_2\rangle, |e^{2t^5}, {}^6E\rangle \\
|e^{1t^5}, {}^5T_1 \times e\rangle &\rightarrow |e^{2t^5}, {}^4T_1\rangle, |e^{2t^5}, {}^4T_2\rangle, |e^{2t^5}, {}^6T_1\rangle, |e^{2t^5}, {}^6T_2\rangle \\
|e^{1t^5}, {}^5T_2 \times e\rangle &\rightarrow |e^{2t^5}, {}^4T_1\rangle, |e^{2t^5}, {}^4T_2\rangle, |e^{2t^5}, {}^6T_1\rangle, |e^{2t^5}, {}^6T_2\rangle \\
|e^{1t^5}, {}^7A_1 \times e\rangle &\rightarrow |e^{2t^5}, {}^6E\rangle, |e^{2t^5}, {}^8E\rangle \\
|e^{1t^5}, {}^7A_2 \times e\rangle &\rightarrow |e^{2t^5}, {}^6E\rangle, |e^{2t^5}, {}^8E\rangle \\
|e^{1t^5}, {}^7E \times e\rangle &\rightarrow |e^{2t^5}, {}^6A_1\rangle, |e^{2t^5}, {}^6A_2\rangle, |e^{2t^5}, {}^6E\rangle, |e^{2t^5}, {}^8A_1\rangle, |e^{2t^5}, {}^8A_2\rangle, |e^{2t^5}, {}^8E\rangle \\
|e^{1t^5}, {}^7T_1 \times e\rangle &\rightarrow |e^{2t^5}, {}^6T_1\rangle, |e^{2t^5}, {}^6T_2\rangle, |e^{2t^5}, {}^8T_1\rangle, |e^{2t^5}, {}^8T_2\rangle \\
|e^{1t^5}, {}^7T_2 \times e\rangle &\rightarrow |e^{2t^5}, {}^6T_1\rangle, |e^{2t^5}, {}^6T_2\rangle, |e^{2t^5}, {}^8T_1\rangle, |e^{2t^5}, {}^8T_2\rangle
\end{aligned}$$



$$\begin{aligned}
|e^{0t^6}, {}^1A_1 \times e\rangle &\rightarrow |e^{1t^6}, {}^2E\rangle \\
|e^{0t^6}, {}^1A_2 \times e\rangle &\rightarrow |e^{1t^6}, {}^2E\rangle \\
|e^{0t^6}, {}^1E \times e\rangle &\rightarrow |e^{1t^6}, {}^2A_1\rangle, |e^{1t^6}, {}^2A_2\rangle, |e^{1t^6}, {}^2E\rangle \\
|e^{0t^6}, {}^1T_1 \times e\rangle &\rightarrow |e^{1t^6}, {}^2T_1\rangle, |e^{1t^6}, {}^2T_2\rangle \\
|e^{0t^6}, {}^1T_2 \times e\rangle &\rightarrow |e^{1t^6}, {}^2T_1\rangle, |e^{1t^6}, {}^2T_2\rangle \\
|e^{0t^6}, {}^3A_1 \times e\rangle &\rightarrow |e^{1t^6}, {}^2E\rangle, |e^{1t^6}, {}^4E\rangle \\
|e^{0t^6}, {}^3A_2 \times e\rangle &\rightarrow |e^{1t^6}, {}^2E\rangle, |e^{1t^6}, {}^4E\rangle \\
|e^{0t^6}, {}^3E \times e\rangle &\rightarrow |e^{1t^6}, {}^2A_1\rangle, |e^{1t^6}, {}^2A_2\rangle, |e^{1t^6}, {}^2E\rangle, |e^{1t^6}, {}^4A_1\rangle, |e^{1t^6}, {}^4A_2\rangle, |e^{1t^6}, {}^4E\rangle \\
|e^{0t^6}, {}^3T_1 \times e\rangle &\rightarrow |e^{1t^6}, {}^2T_1\rangle, |e^{1t^6}, {}^2T_2\rangle, |e^{1t^6}, {}^4T_1\rangle, |e^{1t^6}, {}^4T_2\rangle \\
|e^{0t^6}, {}^3T_2 \times e\rangle &\rightarrow |e^{1t^6}, {}^2T_1\rangle, |e^{1t^6}, {}^2T_2\rangle, |e^{1t^6}, {}^4T_1\rangle, |e^{1t^6}, {}^4T_2\rangle \\
|e^{0t^6}, {}^5A_1 \times e\rangle &\rightarrow |e^{1t^6}, {}^4E\rangle, |e^{1t^6}, {}^6E\rangle \\
|e^{0t^6}, {}^5A_2 \times e\rangle &\rightarrow |e^{1t^6}, {}^4E\rangle, |e^{1t^6}, {}^6E\rangle \\
|e^{0t^6}, {}^5E \times e\rangle &\rightarrow |e^{1t^6}, {}^4A_1\rangle, |e^{1t^6}, {}^4A_2\rangle, |e^{1t^6}, {}^4E\rangle, |e^{1t^6}, {}^6A_1\rangle, |e^{1t^6}, {}^6A_2\rangle, |e^{1t^6}, {}^6E\rangle \\
|e^{0t^6}, {}^5T_1 \times e\rangle &\rightarrow |e^{1t^6}, {}^4T_1\rangle, |e^{1t^6}, {}^4T_2\rangle, |e^{1t^6}, {}^6T_1\rangle, |e^{1t^6}, {}^6T_2\rangle \\
|e^{0t^6}, {}^5T_2 \times e\rangle &\rightarrow |e^{1t^6}, {}^4T_1\rangle, |e^{1t^6}, {}^4T_2\rangle, |e^{1t^6}, {}^6T_1\rangle, |e^{1t^6}, {}^6T_2\rangle \\
|e^{0t^6}, {}^7A_1 \times e\rangle &\rightarrow |e^{1t^6}, {}^6E\rangle, |e^{1t^6}, {}^8E\rangle \\
|e^{0t^6}, {}^7A_2 \times e\rangle &\rightarrow |e^{1t^6}, {}^6E\rangle, |e^{1t^6}, {}^8E\rangle \\
|e^{0t^6}, {}^7E \times e\rangle &\rightarrow |e^{1t^6}, {}^6A_1\rangle, |e^{1t^6}, {}^6A_2\rangle, |e^{1t^6}, {}^6E\rangle, |e^{1t^6}, {}^8A_1\rangle, |e^{1t^6}, {}^8A_2\rangle, |e^{1t^6}, {}^8E\rangle \\
|e^{0t^6}, {}^7T_1 \times e\rangle &\rightarrow |e^{1t^6}, {}^6T_1\rangle, |e^{1t^6}, {}^6T_2\rangle, |e^{1t^6}, {}^8T_1\rangle, |e^{1t^6}, {}^8T_2\rangle \\
|e^{0t^6}, {}^7T_2 \times e\rangle &\rightarrow |e^{1t^6}, {}^6T_1\rangle, |e^{1t^6}, {}^6T_2\rangle, |e^{1t^6}, {}^8T_1\rangle, |e^{1t^6}, {}^8T_2\rangle
\end{aligned}$$

$$\begin{aligned}
|e^0t^6, {}^1E \times t\rangle &\rightarrow |e^0t^7, {}^2T_1\rangle, |e^0t^7, {}^2T_2\rangle \\
|e^0t^6, {}^1T_1 \times t\rangle &\rightarrow |e^0t^7, {}^2A_2\rangle, |e^0t^7, {}^2E\rangle, |e^0t^7, {}^2T_1\rangle, |e^0t^7, {}^2T_2\rangle \\
|e^0t^6, {}^1T_2 \times t\rangle &\rightarrow |e^0t^7, {}^2A_1\rangle, |e^0t^7, {}^2E\rangle, |e^0t^7, {}^2T_1\rangle, |e^0t^7, {}^2T_2\rangle \\
|e^0t^6, {}^3A_1 \times t\rangle &\rightarrow |e^0t^7, {}^2T_2\rangle, |e^0t^7, {}^4T_2\rangle \\
|e^0t^6, {}^3A_2 \times t\rangle &\rightarrow |e^0t^7, {}^2T_1\rangle, |e^0t^7, {}^4T_1\rangle \\
|e^0t^6, {}^3E \times t\rangle &\rightarrow |e^0t^7, {}^2T_1\rangle, |e^0t^7, {}^2T_2\rangle, |e^0t^7, {}^4T_1\rangle, |e^0t^7, {}^4T_2\rangle \\
|e^0t^6, {}^3T_1 \times t\rangle &\rightarrow |e^0t^7, {}^2A_2\rangle, |e^0t^7, {}^2E\rangle, |e^0t^7, {}^2T_1\rangle, |e^0t^7, {}^2T_2\rangle, \\
&\quad |e^0t^7, {}^4A_2\rangle, |e^0t^7, {}^4E\rangle, |e^0t^7, {}^4T_1\rangle, |e^0t^7, {}^4T_2\rangle \\
|e^0t^6, {}^3T_2 \times t\rangle &\rightarrow |e^0t^7, {}^2A_1\rangle, |e^0t^7, {}^2E\rangle, |e^0t^7, {}^2T_1\rangle, |e^0t^7, {}^2T_2\rangle, \\
&\quad |e^0t^7, {}^4A_1\rangle, |e^0t^7, {}^4E\rangle, |e^0t^7, {}^4T_1\rangle, |e^0t^7, {}^4T_2\rangle \\
|e^0t^6, {}^5A_1 \times t\rangle &\rightarrow |e^0t^7, {}^4T_2\rangle, |e^0t^7, {}^6T_2\rangle \\
|e^0t^6, {}^5A_2 \times t\rangle &\rightarrow |e^0t^7, {}^4T_1\rangle, |e^0t^7, {}^6T_1\rangle \\
|e^0t^6, {}^5E \times t\rangle &\rightarrow |e^0t^7, {}^4T_1\rangle, |e^0t^7, {}^4T_2\rangle, |e^0t^7, {}^6T_1\rangle, |e^0t^7, {}^6T_2\rangle \\
|e^0t^6, {}^5T_1 \times t\rangle &\rightarrow |e^0t^7, {}^4A_2\rangle, |e^0t^7, {}^4E\rangle, |e^0t^7, {}^4T_1\rangle, |e^0t^7, {}^4T_2\rangle, \\
&\quad |e^0t^7, {}^6A_2\rangle, |e^0t^7, {}^6E\rangle, |e^0t^7, {}^6T_1\rangle, |e^0t^7, {}^6T_2\rangle \\
|e^0t^6, {}^5T_2 \times t\rangle &\rightarrow |e^0t^7, {}^4A_1\rangle, |e^0t^7, {}^4E\rangle, |e^0t^7, {}^4T_1\rangle, |e^0t^7, {}^4T_2\rangle, \\
&\quad |e^0t^7, {}^6A_1\rangle, |e^0t^7, {}^6E\rangle, |e^0t^7, {}^6T_1\rangle, |e^0t^7, {}^6T_2\rangle \\
|e^0t^6, {}^7A_1 \times t\rangle &\rightarrow |e^0t^7, {}^6T_2\rangle, |e^0t^7, {}^8T_2\rangle \\
|e^0t^6, {}^7A_2 \times t\rangle &\rightarrow |e^0t^7, {}^6T_1\rangle, |e^0t^7, {}^8T_1\rangle \\
|e^0t^6, {}^7E \times t\rangle &\rightarrow |e^0t^7, {}^6T_1\rangle, |e^0t^7, {}^6T_2\rangle, |e^0t^7, {}^8T_1\rangle, |e^0t^7, {}^8T_2\rangle \\
|e^0t^6, {}^7T_1 \times t\rangle &\rightarrow |e^0t^7, {}^6A_2\rangle, |e^0t^7, {}^6E\rangle, |e^0t^7, {}^6T_1\rangle, |e^0t^7, {}^6T_2\rangle, \\
&\quad |e^0t^7, {}^8A_2\rangle, |e^0t^7, {}^8E\rangle, |e^0t^7, {}^8T_1\rangle, |e^0t^7, {}^8T_2\rangle \\
|e^0t^6, {}^7T_2 \times t\rangle &\rightarrow |e^0t^7, {}^6A_1\rangle, |e^0t^7, {}^6E\rangle, |e^0t^7, {}^6T_1\rangle, |e^0t^7, {}^6T_2\rangle, \\
&\quad |e^0t^7, {}^8A_1\rangle, |e^0t^7, {}^8E\rangle, |e^0t^7, {}^8T_1\rangle, |e^0t^7, {}^8T_2\rangle
\end{aligned}$$