Electronic Supplementary Information

Photophysical Properties and NO photorealese Mechanism of a Ruthenium Nitrosyl Model Complex by the CASSCF-in-DFT Embedding Approach

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1- Optimized Geometries:

a) trans-[RuCl(NO)(NH$_3$)$_4$]$^{2+}$ in S$_0$ electronic state (BP86/def2-TZVPP level of theory):

<table>
<thead>
<tr>
<th>Element</th>
<th>BP86/DEF2-TZVPP  S$_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ru</td>
<td>-0.0354901590 -0.0000255988 0.0000001650</td>
</tr>
<tr>
<td>N</td>
<td>0.1314957226 2.1537041636 -0.0000012944</td>
</tr>
<tr>
<td>Cl</td>
<td>-2.2214904763 -0.0000129740 -2.1536410027</td>
</tr>
</tbody>
</table>

b) trans-[RuCl(NO)(NH$_3$)$_4$]$^{2+}$ in T$_1$ electronic state (BP86/def2-TZVPP level of theory):

<table>
<thead>
<tr>
<th>Element</th>
<th>BP86/DEF2-TZVPP  T$_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ru</td>
<td>0.0578080345 -0.0125522875 0.0533565256</td>
</tr>
<tr>
<td>N</td>
<td>0.0101115631 2.1345876603 -0.1048087936</td>
</tr>
<tr>
<td>Cl</td>
<td>2.3649748616 0.2192626050 0.2130057603</td>
</tr>
</tbody>
</table>

2- Composition of molecular orbitals in terms of atomic orbitals:

\[ \sigma_{NO} = \alpha (2p_O^O) + \beta (2p_N^N) + \gamma (2s^O) \]

\[ \rho_{xy} = \alpha (2p_{xy}^O) + \beta (2p_{xy}^N) + \gamma (2s_{xy}) \]

\[ \sigma_{NO} = \alpha (3p_{z}) + \beta (3p_{Cl}^Cl) \]

\[ d_{xy} = 1.01 (3d_{xy}^Ru) \]

\[ d_{xz,yz} = 0.84 (3d_{xz,yz}^Ru) + 0.44 (2p_{xy}^O) \]

\[ d_{xz,yz} - \sigma_{xz,yz} = 0.54 (3d_{xz,yz}^Ru) - 0.68 (2p_{xy}^O) + 0.81 (2p_{xy}^N) \]

\[ d_{z^2} = 0.82 (3d_{z^2}^Ru) \]

\[ d_{xy}^2 = 0.85 (3d_{xy}^Ru) \]

\[ \sigma_{NO}^N = 1.21 (2p_O^O) + 1.17 (2p_N^N) \]
3- SA-CASSCF(18,14)-in-BP86 Energies:

\[ S_0 = -908.69600765 \text{ HARTREE} \]
\[ S_1 = -908.56482410 \text{ HARTREE} \]
\[ S_2 = -908.56475482 \text{ HARTREE} \]
\[ S_3 = -908.55823252 \text{ HARTREE} \]
\[ S_4 = -908.55703180 \text{ HARTREE} \]
\[ S_5 = -908.55434476 \text{ HARTREE} \]
\[ S_6 = -908.52689246 \text{ HARTREE} \]
\[ S_7 = -908.50178800 \text{ HARTREE} \]
\[ S_8 = -908.50171230 \text{ HARTREE} \]
\[ S_9 = -908.49213272 \text{ HARTREE} \]
\[ S_{10} = -908.47161806 \text{ HARTREE} \]
\[ S_{11} = -908.47121374 \text{ HARTREE} \]
\[ T_1 = -908.57899301 \text{ HARTREE} \]
\[ T_2 = -908.56878741 \text{ HARTREE} \]
\[ T_3 = -908.56872527 \text{ HARTREE} \]
\[ T_4 = -908.56789007 \text{ HARTREE} \]
\[ T_5 = -908.56767316 \text{ HARTREE} \]
\[ T_6 = -908.56095640 \text{ HARTREE} \]
\[ T_7 = -908.55332921 \text{ HARTREE} \]
\[ T_8 = -908.53560140 \text{ HARTREE} \]
\[ T_9 = -908.51846934 \text{ HARTREE} \]
\[ T_{10} = -908.51835248 \text{ HARTREE} \]
\[ T_{11} = -908.49829973 \text{ HARTREE} \]
\[ T_{12} = -908.49809014 \text{ HARTREE} \]
4. Singlet electronic configurations

state 1, \( S_0 \)

\[ |S_0 \rangle = +0.8876 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 \right| 
- 0.1083 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz} - \pi_y)^2 \right| 
+ 0.1083 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right| 
- 0.1089 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz} - \pi_y)^2 \right| 
- 0.1089 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right| 
- 0.1459 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz} - \pi_y)^2 \right| 
- 0.1457 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz} - \pi_y)^2 \right| 
+ 0.1149 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz} - \pi_y)^2 \right| 
+ 0.1149 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right|

State 2, \( S_1 \)

\[ |S_1 \rangle = +0.6314 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz} - \pi_y)^2 \right| 
- 0.6314 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right| 
+ 0.1553 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz} - \pi_y)^2 \right| 
- 0.1553 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right| 
+ 1.307 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right| 
+ 1.307 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 \frac{1}{\pi_y} \right| 
- 1.085 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 \frac{1}{\pi_y} \right| 
- 1.085 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 \frac{1}{\pi_y} \right|

State 3, \( S_2 \)

\[ |S_2 \rangle = -0.6314 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz} - \pi_y)^2 \right| 
+ 0.6314 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right| 
- 0.1553 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz} - \pi_y)^2 \right| 
+ 0.1553 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right| 
+ 1.303 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right| 
+ 1.303 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 \frac{1}{\pi_y} \right| 
- 1.081 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 \frac{1}{\pi_y} \right| 
- 1.081 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 \frac{1}{\pi_y} \right|

State 4, \( S_3 \)

\[ |S_3 \rangle = -0.1020 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz} - \pi_y)^2 \right| 
+ 0.1020 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz} - \pi_y)^2 \right| 
+ 0.5362 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz} - \pi_y)^2 \right| 
- 0.5362 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 \frac{1}{\pi_y} \right| 
- 0.3631 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz} - \pi_y)^2 \right| 
+ 0.3631 \left| (Cl_p_x)^2 (Cl_p_y)^2 (Cl_p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz} - \pi_y)^2 \right|
State 5, $S_5$

$$|S_5| = -0.4601 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$+ 0.4601 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$+ 0.4595 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$- 0.4595 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$- 0.1572 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz} - \pi_y)^2 \right|$$

$$+ 0.1570 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz} - \pi_x)^2 \right|$$

State 6, $S_6$

$$|S_6| = +0.6232 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz} - \pi_x)^2 (d_{xy})^2 (d_{xz}^2 - \pi_x)^2 \right|$$

$$- 0.6232 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz} - \pi_x)^2 (d_{xy})^2 (d_{xz}^2 - \pi_x)^2 \right|$$

$$- 0.1002 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz} - \pi_x)^2 (d_{xz}^2 - \pi_x)^2 \right|$$

$$+ 0.1002 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz} - \pi_x)^2 (d_{xz}^2 - \pi_x)^2 \right|$$

State 7, $S_7$

$$|S_7| = -0.5822 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xy})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$+ 0.5822 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xy})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$- 0.1566 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$+ 0.1566 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$- 0.1546 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$+ 0.1546 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$+ 0.1311 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$+ 0.1311 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$+ 0.1175 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$+ 0.1175 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$

$$- 0.1175 \left| (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (Cl_p)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{xz})^2 (d_{xz} - \pi_x)^2 \right|$$
State 9, $S_9$

$$|S_9\rangle = -0.5818 |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{yz})^2(d_{zy})^\beta\rangle$$
$$+0.5818 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{yz})^2(d_{zy})^\alpha\rangle$$
$$+0.1577 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{yz})^2(d_{x-z-y})^\beta\rangle$$
$$-0.1577 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{yz})^2(d_{zy})^\alpha\rangle$$
$$-0.1544 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{yz})^\alpha(d_{x-z-y})^\beta\rangle$$
$$-0.1544 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{yz})^\alpha(d_{x-z-y})^\alpha\rangle$$
$$+0.1310 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{yz})^\alpha(d_{x-z-y})^\beta\rangle$$
$$+0.1310 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{yz})^\alpha(d_{x-z-y})^\alpha\rangle$$
$$+0.1178 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{yz})^2(d_{x-z-y})^\beta\rangle$$
$$-0.1178 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{yz})^2(d_{x-z-y})^\alpha\rangle$$

State 10, $S_9$

$$|S_9\rangle = -0.6062 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{yz})^2(d_{zy})^\alpha\rangle$$
$$+0.6062 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{yz})^2(d_{zy})^\beta\rangle$$
$$+0.1116 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{yz})^\beta(d_{x-z-y})^\alpha\rangle$$
$$-0.1116 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{yz})^\beta(d_{x-z-y})^\beta\rangle$$
$$+0.1127 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{yz})^\alpha(d_{x-z-y})^\beta\rangle$$
$$-0.1127 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{yz})^\beta(d_{x-z-y})^\alpha\rangle$$

State 11, $S_{10}$

$$|S_{10}\rangle = +0.1459 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^2(d_{yz})^\beta(d_{zy})^\alpha\rangle$$
$$-0.1459 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{yz})^2(d_{zy})^\beta\rangle$$
$$-0.5570 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{xz-y})^\alpha\rangle$$
$$+0.5570 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{xz-y})^\beta\rangle$$
$$+0.1464 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{y-z-y})^\beta(d_{xz-y})^\beta\rangle$$
$$+0.1464 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{y-z-y})^\alpha(d_{xz-y})^\alpha\rangle$$
$$-0.1406 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{xz-y})^\alpha(d_{y-z-y})^\alpha\rangle$$
$$+0.1406 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{y-z-y})^\beta(d_{xz-y})^\beta\rangle$$
$$-0.1287 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\beta(d_{y-z-y})^\beta(d_{xz-y})^\alpha\rangle$$
$$-0.1287 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{xz})^\alpha(d_{y-z-y})^\alpha(d_{xz-y})^\beta\rangle$$
$$+0.1069 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{yz})^\beta(d_{y-z-y})^\alpha\rangle$$
$$-0.1069 \ |(\text{Cl}_p z)^2(\text{Cl}_p y)^2(\text{Cl}_p z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{\text{xy}})^2(d_{yz})^\alpha(d_{y-z-y})^\beta\rangle$$
\[ |S_{11} \rangle = +0.1472 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 \right\rangle \\
-0.1459 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \\
+0.5566 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \\
-0.5566 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \\
-0.1459 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \\
-0.1398 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \\
+0.1398 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \\
+0.1289 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \\
+0.1289 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \\
-0.1072 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \\
+0.1072 \left| (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\text{Cl}_p)_2 (\sigma_{\text{NO}})_2 (\pi_x)_2 (\pi_y)_2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 (d_{zy})^2 (d_{y^2 - y^2})^2 \right\rangle \]
5- Triplet electronic configurations

State 1, $T_1$

$$|T_1\rangle = +0.6796 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{xz}-\pi_z^z)^o} + 0.6586 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{yz}-\pi_y)^o}$$

State 2, $T_2$

$$|T_2\rangle = -0.9039 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{yz}-\pi_y)^o} - 0.1860 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{xz}-\pi_z^z)^o} - 0.1850 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^o(d_{yz}-\pi_y^o)^o} + 0.1701 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2(d_{yz}-\pi_y^o)^o} + 0.1323 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2(d_{yz}-\pi_y)^o}$$

State 3, $T_3$

$$|T_3\rangle = +0.9041 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^o} + 0.1864 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2} - 0.1844 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2(d_{yz}-\pi_y^o)^o} + 0.1695 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2(d_{yz}-\pi_y^o)^o} - 0.1324 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2(d_{yz}-\pi_y^o)^o}$$

State 4, $T_4$

$$|T_4\rangle = -0.6522 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^o} + 0.6731 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{yz}-\pi_y^o)^o}$$

State 5, $T_5$

$$|T_5\rangle = -0.1116 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2} - 0.6787 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{yz}-\pi_y^o)^o} - 0.6375 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2}$$

State 6, $T_6$

$$|T_6\rangle = -0.4539 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2(d_{zx}-\pi_y^o)^o} - 0.5447 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{yz}-\pi_y^o)^o} + 0.5848 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2}$$

State 7, $T_7$

$$|T_7\rangle = +0.7469 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{zw}-\pi_z^z)^2(d_{zx}-\pi_y^o)^o} - 0.3266 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{yz}-\pi_y^o)^o} + 0.3398 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{yz}-\pi_y^o)^o} + 0.1337 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{yz}-\pi_y^o)^o} + 0.1353 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^2(d_{yz}-\pi_y^o)^o} - 0.1242 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2(d_{zx}-\pi_y^o)^o} - 0.1239 \psi_{(Cl \ p_x^2)(Cl \ p_y^2)(Cl \ p_z^2)(\sigma_{NO})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{xz}-\pi_z^z)^2(d_{zx}-\pi_y^o)^o}$$
State 8, $T_8$
\[ |T_8\rangle = +0.8848 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^\alpha(d_{xz})^2(d_{yz})^2(d_{z^2})^\alpha \right\rangle \\
-0.1394 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^\alpha(d_{xz})^2(d_{yz})^2(d_{z^2})^\alpha \right\rangle \\
-0.1384 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^\alpha(d_{xz})^2(d_{yz})^2(d_{z^2})^\alpha \right\rangle \\
+0.1152 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^\alpha(d_{xz})^2(d_{yz})^2(d_{z^2})^\alpha \right\rangle \\
+0.1151 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^\alpha(d_{xz})^2(d_{yz})^2(d_{z^2})^\alpha \right\rangle \\
-0.1102 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^\alpha(d_{xz})^2(d_{yz})^2(d_{z^2})^\alpha \right\rangle \\
+0.1096 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^\alpha(d_{xz})^2(d_{yz})^2(d_{z^2})^\alpha \right\rangle \\
+0.1085 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^\alpha(d_{xz})^2(d_{yz})^2(d_{z^2})^\alpha \right\rangle \\

State 9, $T_9$
\[ |T_9\rangle = +0.8380 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.1503 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.2559 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1742 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.1707 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.1350 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1073 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\

State 10, $T_{10}$
\[ |T_{10}\rangle = +0.8370 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1556 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.2555 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1746 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1700 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1346 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.1068 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\

State 11, $T_{11}$
\[ |T_{11}\rangle = -0.1394 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.8129 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.3082 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1714 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.1713 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.1319 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\

State 12, $T_{12}$
\[ |T_{12}\rangle = +0.1454 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.8120 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
+0.3079 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1718 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1716 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\
-0.1314 \left| (Cl_p)^2(Cl_p_g)^2(Cl_p_z)^2(\sigma_{NO})^2(\pi_z)^2(\pi_y)^2(d_{xy})^2(d_{xz})^2(d_{yz})^\alpha \right\rangle \\

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