

Electronic Supplementary Information

Photophysical Properties and NO photorelease 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)(NH₃)₄]²⁺ in S₀ electronic state (BP86/def2-TZVPP level of theory):

20			
BP86/DEF2-TZVPP S_0			
Ru	-0.0354901590	-0.0000255988	0.0000001650
N	0.1141957226	2.1537014636	-0.0000012944
N	0.1154228581	0.0000194251	2.1536464834
N	0.1172159963	-2.1535480762	-0.0000012193
N	0.1154221103	0.0000192740	-2.1536410027
N	-1.8069072663	-0.0010613112	-0.0000000338
O	-2.9557304564	-0.0015722845	-0.0000009786
Cl	2.2601114032	0.0015008470	0.0000013205
H	1.1150703030	2.3922673265	-0.0000028062
H	-0.3005094557	2.6189434741	-0.8156271339
H	-0.3005088042	2.6189480333	0.8156199441
H	1.1164123192	-0.0000536293	-2.3917100456
H	-0.2991585383	-0.8155415625	-2.6191141133
H	-0.2989443087	0.8157080245	-2.6190653550
H	1.1164128337	-0.0000534090	2.3917152569
H	-0.2991585722	-0.8155416743	2.6191199372
H	-0.2989432749	0.8157069828	2.6190704725
H	1.1184795945	-2.3904776539	-0.0000027897
H	-0.2966962877	-2.6194719279	0.8156357044
H	-0.2966970184	-2.6194677234	-0.8156425111

b) *trans*-[RuCl(NO)(NH₃)₄]²⁺ in T₁ electronic state (BP86/def2-TZVPP level of theory):

20			
BP86/DEF2-TZVPP T_1			
Ru	0.0578080345	-0.0125522875	0.0533565256
N	0.0101115631	2.1345876603	-0.1048087936
N	0.0609669871	-0.1193276015	2.2187838017
N	0.2059117717	-2.1643094274	-0.0123150864
N	0.1915554735	-0.0584177485	-2.0957389341
N	-1.8695127374	0.0451471403	0.1266738438
O	-2.7541606145	0.6360216622	-0.3523189783
Cl	2.3649748616	0.2192626050	0.2130057603
H	0.8374075311	2.4710091085	-0.6147812252
H	-0.8232220565	2.5197830742	-0.5676338998
H	0.0576026700	2.6014694739	0.8093933800
H	1.1812654800	-0.0248055106	-2.3746354045
H	-0.2098562976	-0.8949803796	-2.5368441293
H	-0.2713252201	0.7299418545	-2.5642442548
H	0.9859813077	-0.4153267191	2.5570178304
H	-0.6416752983	-0.7645094077	2.6006973868
H	-0.1281106855	0.7801028210	2.6770147266
H	1.0662141842	-2.4646295769	-0.4884157283
H	0.2604329527	-2.5790321826	0.9256793366
H	-0.5823699075	-2.6394365584	-0.4698841579

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

$$\sigma_{\text{NO}} = -0.71 (2p_z^{\text{O}}) + 0.61 (2p_z^{\text{N}}) + 0.41 (2s^{\text{O}})$$

$$\pi_{x,y} = 0.69 (2p_{x,y}^{\text{O}}) + 0.61 (2p_{x,y}^{\text{N}})$$

$$\text{Cl } p_z = 0.86 (3p_z^{\text{Cl}})$$

$$\text{Cl } p_{x,y} = 0.90 (3p_{x,y}^{\text{Cl}})$$

$$d_{xy} = 1.01 (3d_{xy}^{\text{Ru}})$$

$$d_{xz,yz} = 0.84 (3d_{xz,yz}^{\text{Ru}}) + 0.44 (2p_{x,y}^{\text{O}})$$

$$d_{xz,yz} - \pi_{x,y}^* = 0.54 (3d_{xz,yz}^{\text{Ru}}) - 0.68 (2p_{x,y}^{\text{O}}) + 0.81 (2p_{x,y}^{\text{N}})$$

$$d_{z^2} = 0.82 (3d_{z^2}^{\text{Ru}})$$

$$d_{x^2-y^2} = 0.85 (3d_{x^2-y^2}^{\text{Ru}})$$

$$\sigma_{\text{NO}}^* = 1.21 (2p_z^{\text{O}}) + 1.17 (2p_z^{\text{N}})$$

3- SA-CASSCF(18,14)-in-BP86 Energies:

S₀ = -908.69600765 HARTREE
S₁ = -908.56482410 HARTREE
S₂ = -908.56475482 HARTREE
S₃ = -908.55823252 HARTREE
S₄ = -908.55703180 HARTREE
S₅ = -908.55434476 HARTREE
S₆ = -908.52689246 HARTREE
S₇ = -908.50178800 HARTREE
S₈ = -908.50171230 HARTREE
S₉ = -908.49213272 HARTREE
S₁₀ = -908.47161806 HARTREE
S₁₁ = -908.47121374 HARTREE
T₁ = -908.57899301 HARTREE
T₂ = -908.56878741 HARTREE
T₃ = -908.56872527 HARTREE
T₄ = -908.56789007 HARTREE
T₅ = -908.56767316 HARTREE
T₆ = -908.56095640 HARTREE
T₇ = -908.55332921 HARTREE
T₈ = -908.53560140 HARTREE
T₉ = -908.51846934 HARTREE
T₁₀ = -908.51835248 HARTREE
T₁₁ = -908.49829973 HARTREE
T₁₂ = -908.49809014 HARTREE

4- Singlet electronic configurations
state 1, S_0

$$\begin{aligned}
|S_0\rangle = & +0.8876 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^2 \rangle \\
& -0.1083 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^2 (d_{yz} - \pi_y^*)^\alpha \rangle \\
& +0.1083 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^2 (d_{yz} - \pi_y^*)^\beta \rangle \\
& -0.1089 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\beta (d_{xz} - \pi_x^*)^\alpha \rangle \\
& +0.1089 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{xz} - \pi_x^*)^\beta \rangle \\
& -0.1459 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{yz} - \pi_y^*)^2 \rangle \\
& -0.1467 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{xz} - \pi_x^*)^2 \rangle \\
& +0.1149 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^\beta (d_{xz} - \pi_x^*)^\alpha (d_{yz} - \pi_y^*)^\beta \rangle \\
& +0.1149 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^\alpha (d_{xz} - \pi_x^*)^\beta (d_{yz} - \pi_y^*)^\alpha \rangle
\end{aligned}$$

State 2, S_1

$$\begin{aligned}
|S_1\rangle = & +0.6314 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^2 (d_{yz} - \pi_y^*)^\beta \rangle \\
& -0.6314 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{yz})^2 (d_{yz} - \pi_y^*)^\alpha \rangle \\
& +0.1553 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^\beta (d_{yz})^2 (d_{yz} - \pi_y^*)^2 \rangle \\
& -0.1553 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^\alpha (d_{yz})^2 (d_{yz} - \pi_y^*)^2 \rangle \\
& +0.1307 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^\beta (d_{xz} - \pi_x^*)^\alpha (d_{yz} - \pi_y^*)^\beta \rangle \\
& +0.1307 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{yz})^\alpha (d_{xz} - \pi_x^*)^\beta (d_{yz} - \pi_y^*)^\alpha \rangle \\
& -0.1085 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^\alpha (d_{xz} - \pi_x^*)^\beta (d_{yz} - \pi_y^*)^\beta \rangle \\
& -0.1085 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{yz})^\beta (d_{xz} - \pi_x^*)^\alpha (d_{yz} - \pi_y^*)^\alpha \rangle
\end{aligned}$$

State 3, S_2

$$\begin{aligned}
|S_2\rangle = & -0.6314 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^2 (d_{xz} - \pi_x^*)^\beta \rangle \\
& +0.6314 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{yz})^2 (d_{xz} - \pi_x^*)^\alpha \rangle \\
& -0.1557 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^\beta (d_{xz} - \pi_x^*)^2 \rangle \\
& +0.1557 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{yz})^\alpha (d_{xz} - \pi_x^*)^2 \rangle \\
& +0.1303 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^\beta (d_{yz})^2 (d_{xz} - \pi_x^*)^\beta (d_{yz} - \pi_y^*)^\alpha \rangle \\
& +0.1303 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^\alpha (d_{yz})^2 (d_{xz} - \pi_x^*)^\alpha (d_{yz} - \pi_y^*)^\beta \rangle \\
& -0.1081 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^\alpha (d_{yz})^2 (d_{xz} - \pi_x^*)^\beta (d_{yz} - \pi_y^*)^\beta \rangle \\
& -0.1081 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^\beta (d_{yz})^2 (d_{xz} - \pi_x^*)^\alpha (d_{yz} - \pi_y^*)^\alpha \rangle
\end{aligned}$$

State 4, S_3

$$\begin{aligned}
|S_3\rangle = & -0.1020 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^2 (d_{x^2-y^2})^\beta \rangle \\
& +0.1020 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{yz})^2 (d_{x^2-y^2})^\alpha \rangle \\
& +0.5362 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\beta (d_{yz} - \pi_y^*)^\alpha \rangle \\
& -0.5362 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{yz} - \pi_y^*)^\beta \rangle \\
& -0.3631 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^2 (d_{xz} - \pi_x^*)^\alpha \rangle \\
& +0.3631 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^2 (d_{xz} - \pi_x^*)^\beta \rangle
\end{aligned}$$

State 5, S_4

$$\begin{aligned}
|S_4\rangle = & +0.1567 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{yz})^2 (d_z)^2 \alpha \rangle \\
& -0.1567 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^2 (d_z)^2 \beta \rangle \\
& +0.3503 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\beta (d_{yz} - \pi_y^*)^\alpha \rangle \\
& -0.3503 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{yz} - \pi_y^*)^\beta \rangle \\
& +0.5269 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^2 (d_{xz} - \pi_x^*)^\alpha \rangle \\
& -0.5269 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^2 (d_{xz} - \pi_x^*)^\beta \rangle
\end{aligned}$$

State 6, S_5

$$\begin{aligned}
|S_5\rangle = & -0.4601 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{xz} - \pi_x^*)^\alpha \rangle \\
& +0.4601 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^2 (d_{yz} - \pi_y^*)^\beta \rangle \\
& +0.4595 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\beta (d_{xz} - \pi_x^*)^\alpha \rangle \\
& -0.4595 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{xz} - \pi_x^*)^\beta \rangle \\
& -0.1572 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^2 (d_{yz} - \pi_y^*)^2 \rangle \\
& +0.1570 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{xz} - \pi_x^*)^2 \rangle
\end{aligned}$$

State 7, S_6

$$\begin{aligned}
|S_6\rangle = & +0.6232 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^2 (d_{x^2-y^2})^\beta \rangle \\
& -0.6232 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{yz})^2 (d_{x^2-y^2})^\alpha \rangle \\
& -0.1002 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{xz} - \pi_x^*)^2 (d_{x^2-y^2})^\beta \rangle \\
& +0.1002 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{xz} - \pi_x^*)^2 (d_{x^2-y^2})^\alpha \rangle
\end{aligned}$$

State 8, S_7

$$\begin{aligned}
|S_7\rangle = & -0.5822 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\beta (d_z)^2 \alpha \rangle \\
& +0.5822 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_z)^2 \beta \rangle \\
& -0.1566 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\beta (d_{x^2-y^2})^\alpha \rangle \\
& +0.1566 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{x^2-y^2})^\beta \rangle \\
& -0.1546 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^\beta (d_{yz} - \pi_y^*)^\alpha (d_z)^2 \alpha \rangle \\
& -0.1546 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^\alpha (d_{yz} - \pi_y^*)^\beta (d_z)^2 \beta \rangle \\
& +0.1311 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^\beta (d_{yz} - \pi_y^*)^\beta (d_z)^2 \alpha \rangle \\
& +0.1311 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^\alpha (d_{yz} - \pi_y^*)^\alpha (d_z)^2 \beta \rangle \\
& +0.1175 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^\beta (d_{yz} - \pi_y^*)^2 (d_z)^2 \alpha \rangle \\
& -0.1175 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^\alpha (d_{yz} - \pi_y^*)^2 (d_z)^2 \beta \rangle
\end{aligned}$$

State 9, S_8

$$\begin{aligned}
|S_8\rangle = & -0.5818 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^2 (d_{z^2})^\beta \rangle \\
& +0.5818 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^2 (d_{z^2})^\alpha \rangle \\
& +0.1577 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^2 (d_{x^2-y^2})^\beta \rangle \\
& -0.1577 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^2 (d_{x^2-y^2})^\alpha \rangle \\
& -0.1544 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^\beta (d_{xz} - \pi_x^*)^\alpha (d_{z^2})^\alpha \rangle \\
& -0.1544 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^\alpha (d_{xz} - \pi_x^*)^\beta (d_{z^2})^\beta \rangle \\
& +0.1310 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^\alpha (d_{xz} - \pi_x^*)^\beta (d_{z^2})^\alpha \rangle \\
& +0.1310 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^\beta (d_{xz} - \pi_x^*)^\alpha (d_{z^2})^\beta \rangle \\
& +0.1178 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{xz} - \pi_x^*)^2 (d_{z^2})^\beta \rangle \\
& -0.1178 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{xz} - \pi_x^*)^2 (d_{z^2})^\alpha \rangle
\end{aligned}$$

State 10, S_9

$$\begin{aligned}
|S_9\rangle = & -0.6062 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\beta (d_{xz})^2 (d_{yz})^2 (d_{z^2})^\alpha \rangle \\
& +0.6062 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^2 (d_{z^2})^\beta \rangle \\
& +0.1116 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\beta (d_{yz} - \pi_y^*)^\alpha \rangle \\
& -0.1116 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{yz} - \pi_y^*)^\beta \rangle \\
& +0.1127 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^2 (d_{xz} - \pi_x^*)^\alpha \rangle \\
& -0.1127 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^2 (d_{xz} - \pi_x^*)^\beta \rangle
\end{aligned}$$

State 11, S_{10}

$$\begin{aligned}
|S_{10}\rangle = & +0.1459 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\beta (d_{z^2})^\alpha \rangle \\
& -0.1459 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{z^2})^\beta \rangle \\
& -0.5570 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\beta (d_{x^2-y^2})^\alpha \rangle \\
& +0.5570 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{x^2-y^2})^\beta \rangle \\
& +0.1464 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^\beta (d_{yz} - \pi_y^*)^\beta (d_{x^2-y^2})^\alpha \rangle \\
& +0.1464 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^\alpha (d_{yz} - \pi_y^*)^\alpha (d_{x^2-y^2})^\beta \rangle \\
& -0.1406 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{xz} - \pi_x^*)^\beta (d_{x^2-y^2})^\alpha \rangle \\
& +0.1406 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{xz} - \pi_x^*)^\alpha (d_{x^2-y^2})^\beta \rangle \\
& -0.1287 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\beta (d_{yz})^\beta (d_{yz} - \pi_y^*)^\alpha (d_{x^2-y^2})^\alpha \rangle \\
& -0.1287 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^\alpha (d_{yz} - \pi_y^*)^\beta (d_{x^2-y^2})^\beta \rangle \\
& +0.1069 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^\beta (d_{yz} - \pi_y^*)^2 (d_{x^2-y^2})^\alpha \rangle \\
& -0.1069 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{yz})^\alpha (d_{yz} - \pi_y^*)^2 (d_{x^2-y^2})^\beta \rangle
\end{aligned}$$

State 12, S_{11}

$$\begin{aligned}
|S_{11}\rangle = & +0.1472 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\alpha(d_{yz})^2(d_{z^2})^\beta\rangle \\
& -0.1472 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\beta(d_{yz})^2(d_{z^2})^\alpha\rangle \\
& +0.5566 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\alpha(d_{yz})^2(d_{x^2-y^2})^\beta\rangle \\
& -0.5566 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\beta(d_{yz})^2(d_{x^2-y^2})^\alpha\rangle \\
& -0.1459 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\beta(d_{yz})^\alpha(d_{xz} - \pi_x^*)^\beta(d_{x^2-y^2})^\alpha\rangle \\
& -0.1459 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\alpha(d_{yz})^\beta(d_{xz} - \pi_x^*)^\alpha(d_{x^2-y^2})^\beta\rangle \\
& -0.1398 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{yz})^2(d_{yz} - \pi_y^*)^\beta(d_{x^2-y^2})^\alpha\rangle \\
& +0.1398 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{yz})^2(d_{yz} - \pi_y^*)^\alpha(d_{x^2-y^2})^\beta\rangle \\
& +0.1289 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\beta(d_{yz})^\beta(d_{xz} - \pi_x^*)^\alpha(d_{x^2-y^2})^\alpha\rangle \\
& +0.1289 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\alpha(d_{yz})^\alpha(d_{xz} - \pi_x^*)^\beta(d_{x^2-y^2})^\beta\rangle \\
& -0.1072 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\alpha(d_{xz} - \pi_x^*)^2(d_{x^2-y^2})^\beta\rangle \\
& +0.1072 |(\text{Cl } p_x)^2(\text{Cl } p_y)^2(\text{Cl } p_z)^2(\sigma_{\text{NO}})^2(\pi_x)^2(\pi_y)^2(d_{xy})^2(d_{xz})^\beta(d_{xz} - \pi_x^*)^2(d_{x^2-y^2})^\alpha\rangle
\end{aligned}$$

5- Triplet electronic configurations

State 1, T_1

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

State 2, T_2

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

State 3, T_3

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

State 4, T_4

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

State 5, T_5

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

State 6, T_6

$$|T_6\rangle = -0.4539 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^2 (d_{x^2-y^2})^\alpha \\ -0.5447 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{yz} - \pi_y^*)^\alpha \\ +0.5848 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^2 (d_{xz} - \pi_x^*)^\alpha$$

State 7, T_7

$$|T_7\rangle = +0.7469 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^2 (d_{x^2-y^2})^\alpha \\ -0.3266 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^2 (d_{yz})^\alpha (d_{yz} - \pi_y^*)^\alpha \\ +0.3398 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^2 (d_{xz})^\alpha (d_{yz})^2 (d_{xz} - \pi_x^*)^\alpha \\ +0.1337 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^\alpha (d_{yz})^2 (d_{yz} - \pi_y^*)^\beta (d_{x^2-y^2})^\alpha \\ +0.1335 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{yz})^\alpha (d_{xz} - \pi_x^*)^\beta (d_{x^2-y^2})^\alpha \\ -0.1242 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{xz})^2 (d_{xz} - \pi_x^*)^2 (d_{x^2-y^2})^\alpha \\ -0.1239 |(Cl p_x)^2 (Cl p_y)^2 (Cl p_z)^2 (\sigma_{NO})^2 (\pi_x)^2 (\pi_y)^2 (d_{xy})^\alpha (d_{yz})^2 (d_{yz} - \pi_y^*)^2 (d_{x^2-y^2})^\alpha$$

