

System:

Point Group:

N. Electrons:

Multiplicity:

Level:

| | | IRREP | | | | | | | |
|-------|------|-------|--|--|--|--|--|--|--|
| | | | | | | | | | |
| SCF | DOCC | | | | | | | | |
| | OPSH | | | | | | | | |
| MCSCF | DOCC | | | | | | | | |
| | RAS | | | | | | | | |
| | CAS | | | | | | | | |
| | AUX | | | | | | | | |
| MRCI | FC | | | | | | | | |
| | FV | | | | | | | | |
| | | DOCC | | | | | | | |
| | | ACT | | | | | | | |
| | | AUX | | | | | | | |
| | | INT | | | | | | | |

| State | Multiplicity | N. electrons | Symmetry |
|-------|--------------|--------------|----------|
|-------|--------------|--------------|----------|

Number of distinct rows (DRTs):

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|----------|-------|----------|----------|----------|----------|----------|----------|-------|
| D_{2h} | a_g | b_{3u} | b_{2u} | b_{1g} | b_{1u} | b_{2g} | b_{3g} | a_u |
| D_2 | a | b_2 | b_1 | b_3 | | | | |
| C_{2h} | a_g | b_u | a_u | b_g | | | | |
| C_{2v} | a_1 | b_1 | b_2 | a_2 | | | | |
| C_i | a_g | a_u | | | | | | |
| C_s | a' | a'' | | | | | | |
| C_2 | a | b | | | | | | |
| C_1 | a | | | | | | | |