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 |
| *D2h* | ag | b3u | b2u | b1g | b1u | b2g | b3g | au |
| *D2* | a | b2 | b1 | b3 |  |  |  |  |
| *C2h* | ag | bu | au | bg |  |  |  |  |
| *C2v* | a1 | b1 | b2 | a2 |  |  |  |  |
| *Ci* | ag | au |  |  |  |  |  |  |
| *Cs* | a´ | a´´ |  |  |  |  |  |  |
| *C2* | a | b |  |  |  |  |  |  |
| *C1* | a |  |  |  |  |  |  |  |