

| | | | | | | | |
|-----|---------------------|-------------|-------------|---------------|---------------|---------------|---------------|
| | χ_{STO} | ϕ_{1s} | ϕ_{2s} | ϕ_{1p_x} | ϕ_{1p_y} | ϕ_{1p_z} | |
| | | ↓ | ↓ | ↓ | ↓ | ↓ | |
| | | 0 | 1 | 2 | 3 | 4 | |
| | | -0.91415 | 1.39733 | 1.98729 | 1.98729 | 1.98729 | ← orb. energ. |
| | | 2.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | ← population |
| 0He | 1s | -0.592633 | -1.149540 | 0.000000 | 0.000000 | -0.000000 | |
| 0He | 2s | -0.513015 | 1.187212 | -0.000000 | -0.000000 | 0.000000 | |
| 0He | 1p _z | -0.000000 | -0.000000 | -0.300180 | -0.953879 | -0.002418 | |
| 0He | 1p _x | 0.000000 | -0.000000 | -0.007525 | -0.000167 | 0.999972 | |
| 0He | 1p _y | 0.000000 | 0.000000 | -0.953853 | 0.300190 | -0.007128 | |
| | | | | C_i | | | |