|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Fdata-hc | | Fdata-hcnos-ext | | | | | Fdata-hc-provided | | Fdata-hcno | | | |
|  | H | C | H | C | N | O | S | H | C | H | C | N | O |
| Number of shells/pseudo | 2/1 | 4/2 | 2/1 | 2/2 | 3/2 | 3/2 | 3/2 | 2/1 | 2/2 | 2/1 | 4/2 | 4/2 | 4/2 |
| Shell 1 e occupation/cutoff | 1/3.80 | 2/4.00 | 1/4.65 | 2/5.95 | 2/5.42 | 2/5.32 | 2/7.00 | 1/4.50 | 1/4.50 | 1/3.80 | 2/4.00 | 2/3.60 | 2/3.30 |
| Shell 2 e occupation/cutoff | - | 2/4.50 | - | 2/5.95 | 3/5.42 | 4/5.32 | 4/7.00 | - | 3/4.50 | - | 2/4.50 | 3/4.10 | 4/3.80 |
| Shell 3 e occupation/cutoff | - | - | - | - | 0/4.62 | 0/5.32 | 0/5.50 | - | - | - | - | - | - |
| Exited Shell 1 e- occupation/cutoff | 0/3.80 | 0/4.00 | 0/4.65 | - | - | - | - | 0/4.50 | - | 0/3.80 | 0/4.00 | 0/3.60 | 0/3.30 |
| Exited Shell 2 e- occupation/cutoff | - | 0/4.50 | - | - | - | - | - | - | - | - | 0/4.50 | 0/4.10 | 0/3.80 |
| Atomic energy | -10.798 | -141.518 | 0 | 0 | 0 | 0 | 0 | -11.723 | 0 | -10.798 | -141.518 | -257.095 | -423.004 |