|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *ortho* | x | y | z | *meta* | x | y | z | *para* | x | y | z |
| C | 0.929524 | 1.201798 | 0.004406 | C | 1.149333 | 0.000000 | 0.004406 | C | 0.219594 | 1.200621 | 0.004406 |
| C | -0.467155 | 1.218866 | 0.003076 | C | 0.467155 | 1.218866 | 0.003076 | C | 0.933394 | 0.000000 | 0.003076 |
| C | -1.149333 | 0.000000 | 0.004406 | C | -0.929524 | 1.201798 | 0.004406 | C | 0.219594 | -1.200621 | 0.004406 |
| C | -0.451384 | -1.196271 | 0.004406 | C | -1.617911 | 0.000000 | 0.004406 | C | -1.165385 | -1.195099 | 0.004406 |
| C | 0.936596 | -1.209325 | 0.004012 | C | -0.936596 | -1.209325 | 0.004012 | C | -1.871357 | 0.000000 | 0.004012 |
| C | 1.617911 | 0.000000 | 0.004406 | C | 0.451384 | -1.196271 | 0.004406 | C | -1.165385 | 1.195099 | 0.004406 |
| H | 1.473890 | 2.140139 | 0.010419 | H | 2.234139 | -0.003493 | 0.010419 | H | 0.759505 | 2.141532 | 0.010419 |
| H | -2.234139 | -0.003493 | 0.010419 | H | -1.473890 | 2.140139 | 0.010419 | H | 0.759505 | -2.141532 | 0.010419 |
| H | -1.001728 | -2.130086 | 0.004256 | H | -2.701780 | 0.010932 | 0.004256 | H | -1.698386 | -2.138921 | 0.004256 |
| H | 1.478404 | -2.146539 | 0.003507 | H | -1.478404 | -2.146539 | 0.003507 | H | -2.953912 | 0.000000 | 0.003507 |
| H | 2.701780 | 0.010932 | 0.004256 | H | 1.001728 | -2.130086 | 0.004256 | H | -1.698386 | 2.138921 | 0.004256 |
| N | -1.163275 | 2.423006 | 0.055678 | N | 1.163275 | 2.423006 | 0.055678 | N | 2.324270 | 0.000000 | 0.055678 |
| H | -0.660946 | 3.227706 | -0.285441 | H | 2.111292 | 2.389253 | -0.285441 | H | 2.769522 | 0.837632 | -0.285441 |
| H | -2.111292 | 2.389253 | -0.285441 | H | 0.660946 | 3.227706 | -0.285441 | H | 2.769522 | -0.837632 | -0.285441 |