|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *ortho* | x | y | z | *meta* | x | y | z | *para* | x | y | z |
| C | 1.264507 | 1.206166 | 0.000000 | C | 0.840747 | 0.000000 | 0.000000 | C | -0.426213 | 1.213150 | 0.000000 |
| C | -0.119004 | 1.180611 | 0.000000 | C | 0.119004 | 1.180611 | 0.000000 | C | 0.239386 | 0.000000 | 0.000000 |
| C | -0.840747 | 0.000000 | 0.000000 | C | -1.264507 | 1.206166 | 0.000000 | C | -0.426213 | -1.213150 | 0.000000 |
| C | -0.145057 | -1.198252 | 0.000000 | C | -1.946383 | 0.000000 | 0.000000 | C | -1.811756 | -1.205190 | 0.000000 |
| C | 1.243905 | -1.198224 | 0.000000 | C | -1.243905 | -1.198224 | 0.000000 | C | -2.502215 | 0.000000 | 0.000000 |
| C | 1.946383 | 0.000000 | 0.000000 | C | 0.145057 | -1.198252 | 0.000000 | C | -1.811756 | 1.205190 | 0.000000 |
| H | 1.777408 | 2.157049 | 0.000000 | H | 1.920455 | 0.038427 | 0.000000 | H | 0.143876 | 2.130889 | 0.000000 |
| H | -1.920455 | 0.038427 | 0.000000 | H | -1.777408 | 2.157049 | 0.000000 | H | 0.143876 | -2.130889 | 0.000000 |
| H | -0.689690 | -2.133869 | 0.000000 | H | -3.028970 | -0.003332 | 0.000000 | H | -2.352824 | -2.142873 | 0.000000 |
| H | 1.782362 | -2.138052 | 0.000000 | H | -1.782362 | -2.138052 | 0.000000 | H | -3.585364 | 0.000000 | 0.000000 |
| H | 3.028970 | -0.003332 | 0.000000 | H | 0.689690 | -2.133869 | 0.000000 | H | -2.352824 | 2.142873 | 0.000000 |
| N | -0.852588 | 2.461015 | 0.000000 | N | 0.852588 | 2.461015 | 0.000000 | N | 1.715049 | 0.000000 | 0.000000 |
| O | -0.197823 | 3.483690 | 0.000000 | O | 2.065976 | 2.413367 | 0.000000 | O | 2.276907 | 1.076521 | 0.000000 |
| O | -2.065976 | 2.413367 | 0.000000 | O | 0.197823 | 3.483690 | 0.000000 | O | 2.276907 | -1.076521 | 0.000000 |