|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Space Group: Pnma (62 - Antipolar)** | | |  | Hubbard U Applied: | 4.622 eV |
| a (Å) | b (Å) | c (Å) |  | Magnetic Ordering: | Antiferromagnetic |
| 10.263 | 6.989 | 5.718 |  |  |  |
|  |  |  |  |  |  |
| alpha | beta | gamma |  |  |  |
| 90° | 90° | 90° |  |  |  |
|  |  |  |  |  |  |
| **Reduced Coordinates** | | |  |  |  |
| 0.668150910912 | 0.139786788500 | 0.261600737925 | K |  |  |
| 0.668150910912 | 0.860213211500 | 0.761600737925 | K |  |  |
| 0.331849089088 | 0.860213211500 | 0.761600737925 | K |  |  |
| 0.331849089088 | 0.139786788500 | 0.261600737925 | K |  |  |
| 0.168150910912 | 0.639786788500 | 0.238399262075 | K |  |  |
| 0.168150910912 | 0.360213211500 | 0.738399262075 | K |  |  |
| 0.831849089088 | 0.360213211500 | 0.738399262075 | K |  |  |
| 0.831849089088 | 0.639786788500 | 0.238399262075 | K |  |  |
| 0.000000000000 | 0.098493663541 | 0.271840359938 | Nb |  |  |
| 0.000000000000 | 0.901506336459 | 0.771840359938 | Nb |  |  |
| 0.500000000000 | 0.598493663541 | 0.228159640062 | Nb |  |  |
| 0.500000000000 | 0.401506336459 | 0.728159640062 | Nb |  |  |
| 0.871076847109 | 0.029378869763 | 0.503327812143 | O |  |  |
| 0.871076847109 | 0.029378869763 | 0.003327812143 | O |  |  |
| 0.128923152891 | 0.029378869763 | 0.503327812143 | O |  |  |
| 0.128923152891 | 0.029378869763 | 0.003327812143 | O |  |  |
| 0.371076847109 | 0.529378869763 | 0.496672187857 | O |  |  |
| 0.371076847109 | 0.470621130237 | 0.003327812143 | O |  |  |
| 0.628923152891 | 0.529378869763 | 0.496672187857 | O |  |  |
| 0.628923152891 | 0.470621130237 | 0.003327812143 | O |  |  |
| 0.000000000000 | 0.358730223584 | 0.337813523771 | O |  |  |
| 0.000000000000 | 0.641269776416 | 0.837813523771 | O |  |  |
| 0.500000000000 | 0.858730223584 | 0.162186476229 | O |  |  |
| 0.500000000000 | 0.141269776416 | 0.662186476229 | O |  |  |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Space Group: Cmcm (63 - Nonpolar)** | | |  | Hubbard U Applied: | 9.528 eV |
| a (Å) | b (Å) | c (Å) |  | Magnetic Ordering: | Ferromagnetic |
| 9.949 | 6.903 | 5.413 |  |  |  |
|  |  |  |  |  |  |
| alpha | beta | gamma |  |  |  |
| 90° | 90° | 90° |  |  |  |
|  |  |  |  |  |  |
| **Reduced Coordinates** | | |  |  |  |
| 0.664935717249 | 0.150458682156 | 0.250000000000 | K |  |  |
| 0.664935717249 | 0.849541317844 | 0.750000000000 | K |  |  |
| 0.335064282751 | 0.849541317844 | 0.750000000000 | K |  |  |
| 0.335064282751 | 0.150458682156 | 0.250000000000 | K |  |  |
| 0.164935717249 | 0.650458682156 | 0.250000000000 | K |  |  |
| 0.164935717249 | 0.349541317844 | 0.750000000000 | K |  |  |
| 0.835064282751 | 0.349541317844 | 0.750000000000 | K |  |  |
| 0.835064282751 | 0.650458682156 | 0.250000000000 | K |  |  |
| 0.000000000000 | 0.089728759116 | 0.250000000000 | V |  |  |
| 0.000000000000 | 0.910271240884 | 0.750000000000 | V |  |  |
| 0.500000000000 | 0.589728759116 | 0.250000000000 | V |  |  |
| 0.500000000000 | 0.410271240884 | 0.750000000000 | V |  |  |
| 0.874928761906 | 0.000000000000 | 0.500000000000 | O |  |  |
| 0.874928761906 | 0.000000000000 | 0.000000000000 | O |  |  |
| 0.125071238094 | 0.000000000000 | 0.500000000000 | O |  |  |
| 0.125071238094 | 0.000000000000 | 0.000000000000 | O |  |  |
| 0.374928761906 | 0.500000000000 | 0.500000000000 | O |  |  |
| 0.374928761906 | 0.500000000000 | 0.000000000000 | O |  |  |
| 0.625071238094 | 0.500000000000 | 0.500000000000 | O |  |  |
| 0.625071238094 | 0.500000000000 | 0.000000000000 | O |  |  |
| 0.000000000000 | 0.340065915362 | 0.250000000000 | O |  |  |
| 0.000000000000 | 0.659934084638 | 0.750000000000 | O |  |  |
| 0.500000000000 | 0.840065915362 | 0.250000000000 | O |  |  |
| 0.500000000000 | 0.159934084638 | 0.750000000000 | O |  |  |