## Name and formula

| | |
|---|---|
| Reference code: | 03-065-3362 |
| Compound name: | Titanium |
| Empirical formula: | Ti |
| Chemical formula: | Ti |

## Crystallographic parameters

| | |
|---|---|
| Crystal system: | Hexagonal |
| Space group: | P63/mmc |
| Space group number: | 194 |
| a (A): | 2.9504 |
| b (A): | 2.9504 |
| c (A): | 4.6833 |
| Alpha (°): | 90.0000 |
| Beta (°): | 90.0000 |
| Gamma (°): | 120.0000 |
| Volume of cell (10^6 pm^3): | 35.31 |
| Z: | 2.00 |
| RIR: | 6.77 |

## Subfiles and quality

| | |
|---|---|
| Subfiles: | Alloy, metal or intermetalic |
| | Common Phase |
| | Explosive |
| | Forensic |
| | Inorganic |
| | NIST Pattern |
| Quality: | Indexed (I) |

## Comments

| | |
|---|---|
| Creation Date: | 2/11/2005 |
| Modification Date: | 1/17/2013 |
| Additional Patterns: | See PDF 01-089-2762 |
| NIST M&A collection code: | N AL4838 7420 |
| Physical property: | Hydrogen storage materials |
| Temperature Factor: | IB=Ti |
| Minor Warning: | No e.s.d reported/abstracted on the cell dimension. No Rfactor reported/abstracted. |

## References

Primary reference: *Calculated from NIST using POWD-12++*
Structure: H.Clark, *J. Met*, **1**, 588, (1949)

## Peak list

| No. | h | k | l | d [A] | 2Theta[deg] | I [%] |
|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 0 | 2.55510 | 35.092 | 25.7 |
| 2 | 0 | 0 | 2 | 2.34160 | 38.412 | 25.8 |
| 3 | 1 | 0 | 1 | 2.24300 | 40.171 | 100.0 |
| 4 | 1 | 0 | 2 | 1.72630 | 53.002 | 12.4 |
| 5 | 1 | 1 | 0 | 1.47520 | 62.955 | 12.6 |
| 6 | 1 | 0 | 3 | 1.33210 | 70.656 | 12.1 |
| 7 | 2 | 0 | 0 | 1.27760 | 74.160 | 1.7 |
| 8 | 1 | 1 | 2 | 1.24820 | 76.214 | 12.1 |
| 9 | 2 | 0 | 1 | 1.23250 | 77.363 | 8.7 |
| 10 | 0 | 0 | 4 | 1.17080 | 82.284 | 1.6 |
| 11 | 2 | 0 | 2 | 1.12150 | 86.762 | 1.9 |
| 12 | 1 | 0 | 4 | 1.06440 | 92.721 | 1.6 |
| 13 | 2 | 0 | 3 | 0.98870 | 102.357 | 3.7 |
| 14 | 2 | 1 | 0 | 0.96570 | 105.814 | 1.2 |
| 15 | 2 | 1 | 1 | 0.94580 | 109.065 | 6.6 |
| 16 | 1 | 1 | 4 | 0.91710 | 114.266 | 4.2 |
| 17 | 2 | 1 | 2 | 0.89280 | 119.263 | 2.0 |
| 18 | 1 | 0 | 5 | 0.87940 | 122.312 | 2.9 |
| 19 | 2 | 0 | 4 | 0.86320 | 126.347 | 0.9 |
| 20 | 3 | 0 | 0 | 0.85170 | 129.492 | 1.9 |
| 21 | 2 | 1 | 3 | 0.82130 | 139.405 | 5.5 |
| 22 | 3 | 0 | 2 | 0.80040 | 148.474 | 3.7 |

## Stick Pattern

