## Name and formula

| | |
|---|---|
| Reference code: | 98-004-4692 |
| Compound name: | Lanthanum Oxide - Ht (x-form) |
| Common name: | Lanthanum Oxide - Ht (x-form) |
| Chemical formula: | $La_2O_3$ |

## Crystallographic parameters

| | |
|---|---|
| Crystal system: | Cubic |
| Space group: | I m -3 m |
| Space group number: | 229 |
| a (Å): | 4.5100 |
| b (Å): | 4.5100 |
| c (Å): | 4.5100 |
| Alpha (°): | 90.0000 |
| Beta (°): | 90.0000 |
| Gamma (°): | 90.0000 |
| Calculated density (g/cm^3): | 5.90 |
| Volume of cell (10^6 pm^3): | 91.73 |
| Z: | 1.00 |
| RIR: | 11.39 |

## Subfiles and quality

| | |
|---|---|
| Subfiles: | User Inorganic |
| Quality: | User From Structure (=) |

## Comments

| | |
|---|---|
| Creation Date: | 12/16/2000 |
| Modification Date: | 8/1/2010 |
| Original ICSD space group: | IM3-M |
| AE: | La: 6o O6/2; O: 2l La2. Stable above 2373 K (2nd ref., Tomaszewski), 2303-2373 K: P63/mmc. Cell of Nd2 O3 at 2498 K: 4.41. At least one temperature factor is implausible or meaningless but agrees with the value given in the paper.. Structure type : La2O3(cI5). Temperature factors available. Temperature in Kelvin: 2473. Structure type prototype : La2O3(cI5). The structure has been assigned a PDF number (experimental powder diffraction data): 40-1284. The structure has been assigned a PDF number (calculated powder diffraction data): 01-089-4016. Neutron diffraction (powder). Structure type: La2O3(cI5). Recording date: 12/16/2000. Modification date: 8/1/2010. ANX formula: A2X3. Z: 1. Calculated density: 5.9. R value: 0.041. Pearson code: cI5. Wyckoff code: b a. PDF code: 00-040-1284 |

Publication title: Etude par diffraction neutronique des structures de haute temperature de La3 O3 et Nd2 O3
ICSD collection code: 44692
Structure: La2O3(cI5)
Chemical Name: Lanthanum Oxide - Ht (x-form)
Second Chemical Formula: La2 O3

## References

Structure: Traversse, J.P.;Aldebert, P., *Golden Book of Phase Transitions, Wroclaw*, **1**, 1 - 123, (2002)

## Peak list

| No. | h | k | l | d [A] | 2Theta[deg] | I [%] |
|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 1 | 3.18905 | 27.956 | 100.0 |
| 2 | 0 | 0 | 2 | 2.25500 | 39.948 | 22.2 |
| 3 | 1 | 1 | 2 | 1.84120 | 49.463 | 14.8 |
| 4 | 0 | 2 | 2 | 1.59453 | 57.775 | 6.1 |
| 5 | 0 | 1 | 3 | 1.42619 | 65.382 | 2.3 |
| 6 | 2 | 2 | 2 | 1.30192 | 72.550 | 0.9 |
| 7 | 1 | 2 | 3 | 1.20535 | 79.445 | 0.9 |
| 8 | 0 | 0 | 4 | 1.12750 | 86.187 | 0.2 |

## Structure

| No. | Name | Elem. | X | Y | Z | Biso | sof | Wyck. |
|---|---|---|---|---|---|---|---|---|
| 1 | O1 | O | 0.00000 | 0.50000 | 0.50000 | 2.3000 | 0.5000 | 6b |
| 2 | LA1 | La | 0.00000 | 0.00000 | 0.00000 | 10.0000 | 1.0000 | 2a |

## Stick Pattern