SUPPLEMENTARY MATERIALS

SUPPLEMENTARY TABLE I. Comparison of zircon structural models from (a) the literature starting model from Finger (1974) and (b) the refinement of POWGEN data of sample CPD #4.

1. Finger (1974)

Zircon

*I*41*/amd*, a = 6.612(2), c = 5.994(2) Å

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | x | y | z | *B*iso |
| Zr | 0 | 0.75 | 0.125 | 0.4 |
| Si | 0 | 0.75 | 0.625 | 0.5 |
| O | 0 | 0.0660(5) | 0.1941(5) | 0.72 |

Zr – O 2.267(3) Å ×4, 2.130(3) Å ×4

Si – O 1.630(3) Å ×4

O – Zr – O 92.167°

O – Zr – O 157.575°

O – Si – O 96.581°

O – Si – O 116.276°

1. This work – 29.5(4) wt%

Zircon

*I*41*/amd*, a = 6.6081(2), c = 5.9940(2) Å

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | x | y | z | *B*iso |
| Zr | 0 | 0.75 | 0.125 | 0.44(3) |
| Si | 0 | 0.75 | 0.625 | 0.56(5) |
| O | 0 | 0.0655(2) | 0.1960(2) | 0.71(2) |

Zr – O 2.278(1) ×4, 2.128(2) ×4

Si – O 1.6241(8) ×4

O – Zr – O 92.30(2)°

O – Zr – O 156.91(8)°

O – Si – O 97.3(1)°

O – Si – O 115.87(6)°

SUPPLEMENTARY TABLE II. Comparison of corundum structural models from (a) the literature starting model from Cox *et al* (1980) and (b) the refinement of POWGEN data of sample CPD #4.

(a) Cox *et al* (1980)

Corundum (Al2O3)

*R-*3*c*, a = 4.7640(1), c = 13.0091(3) Å

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | x | y | z | *B*iso |
| Al | 0 | 0 | 0.3522 | 0.26 |
| O | 0.6937 | 0 | 0.25 | 0.24 |

Al – O 1.8577(3) Å ×3, 1.9721(5) Å ×3

O – Al – O 101.148° ×3, 90.830°, 86.375°, 164.219°

(b) This work – 51.1(4) wt%

Corundum

*R-*3*c*, a = 4.75944(3), c = 12.9927(1) Å

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | x | y | z | *B*iso |
| Al | 0 | 0 | 0.35216(5) | 0.239(7) |
| O | 0.69372(6) | 0 | 0.25 | 0.266(4) |

Al – O 1.8548(3) Å ×3, 1.9715(5) Å ×3

O – Al – O 101.17(2)° ×3, 90.783(9)°, 86.369(6)°, 164.22(3)°

SUPPLEMENTARY TABLE III. Comparison of magnetite structural models from (a) the literature starting model from Fleet (1981) and (b) the refinement of POWGEN data of sample CPD #4.

1. Fleet (1981)

Magnetite (Fe3O4)

*Fd-*3*m*, a = 8.3941(7)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | x | y | z | *B*iso |
| Fe1 | 0.125 | 0.125 | 0.125 | 0.35(1) |
| Fe2 | 0.5 | 0.5 | 0.5 | 0.46(1) |
| O | 0.2549(1) | 0.2549(1) | 0.2549(1) | 0.54(2) |

Fe1 – O 1.8872(8) Å ×4

Fe2 – O 2.0600(8) Å ×6

O – Fe1 – O 109.471°

O – Fe2 – O 180.00°, 92.24° ×3, 87.76° ×2

1. This work – 19.4(2) wt%

Magnetite (Fe3O4)

*Fd-*3*m*, a = 8.3961(1) Å

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | x | y | z | *B*iso |
| Fe1 | 0.125 | 0.125 | 0.125 | 0.46(2) |
| Fe2 | 0.5 | 0.5 | 0.5 | 0.63(3) |
| O | 0.2545(2) | 0.2545(2) | 0.2545(2) | 0.59(3) |

Fe1 – O 1.883(2) Å ×4

Fe2 – O 2.062(1) Å ×6

O – Fe1 – O 109.471°

O – Fe2 – O 180.00°, 92.10(8)° ×3, 87.90(8)° ×2