

Name and formula

Reference code: 01-089-2282

ICSD name: Titanium Aluminum Carbide

Empirical formula: AlTi_3

Chemical formula: Ti_3AlC

Crystallographic parameters

Crystal system: Cubic

Space group: $\text{Pm}\bar{3}\text{m}$

Space group number: 221

a (Å): 4.1560

b (Å): 4.1560

c (Å): 4.1560

Alpha (°): 90.0000

Beta (°): 90.0000

Gamma (°): 90.0000

Calculated density (g/cm^3): 4.22

Volume of cell (10^6 pm^3): 71.78

Z: 1.00

RIR: 5.20

Subfiles and Quality

Subfiles: Inorganic
Alloy, metal or intermetallic
Modelled additional pattern

Quality: Calculated (C)

Comments

ICSD collection code: 042925

Test from ICSD: No R value given.
At least one TF missing.

References

Primary reference: *Calculated from ICSD using POWD-12++*

Structure: Jeitschko, W., Nowotny, H., Benesovsky, F., *Monatsh. Chem.*, **95**, 319, (1964)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	1	0	0	4.15600	21.363	17.0
2	1	1	0	2.93874	30.392	1.1
3	1	1	1	2.39947	37.450	100.0
4	2	0	0	2.07800	43.517	56.5
5	2	1	0	1.85862	48.969	3.8
6	2	1	1	1.69668	54.002	0.4

7	2	2	0	1.46937	63.234	26.3
8	2	2	1	1.38533	67.565	1.1
9	3	1	0	1.31424	71.764	0.1
10	3	1	1	1.25308	75.864	20.7
11	2	2	2	1.19973	79.891	6.9
12	3	2	0	1.15267	83.868	0.4
13	3	2	1	1.11074	87.816	0.1

Stick Pattern

