

ICSD for WWW

Details of the selected entries

1 entry selected.

CC=Collection Code: [AB2X4]=ANX Form: [cF56]=Pearson: [e d a]=Wyckoff Symbol: [Al2MgO4]=Structure Type:
*****Click the ANX, Pearson or Wyckoff Symbol to find structures with that symbol***.**

CC=76268 CIF

Title	Lattice parameters, coefficients of thermal expansion and atomic weights of purest silicon and germanium.
Authors	Straumanis, M.E.;Aka, E.Z.
Reference	Journal of Applied Physics (1952) 23 , 330-334 Link Xref SCOPUS SCIRUS Google
Compound	Si1 - Silicon [N] [cF8] [a] []
Cell	5.43086(3), 5.43086, 5.43086, 90., 90., 90. FD3-MS (227) V=160.18
Remarks	PDF =27-1402 : TEM =283 : No R value given in the paper. At least one temperature factor missing in the paper. The coordinates are those given in the paper but the atomic distances do not agree with those calculated during testing.The coordinates are probably correct. Cell at 291 K: 5.43082, at 298 K: 5.43097 Linear expansion coefficient 4.15 * 10**-6

Atom (site)	Oxid.	x, y, z, B, Occupancy					
Si1	(8a)	0	0	0	0	0	1

Demo database (The **Full database** will be used if available after the first query is entered)
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CC=82080	Help <input type="text" value="CIF"/> <input type="button" value="Export"/> <input type="button" value="Bonds"/> <input type="button" value="Pattern"/> <input type="button" value="Structure"/> <input type="button" value="Jmol"/>
Title	Synthesis and characterization of sol-gel Pt/(Ti O2) catalyst.
Authors	Sanchez, E.;Lopez, T.;Gomez, R.;Bokhimi, X.;Morales, A.;Novaro, O.
Reference	Journal of Solid State Chemistry (1996) 122, 309-314 Link XRef SCOPUS SCIRUS Google
Compound	O2 Ti0.784 - [Anatase] Titanium oxide (0.78/2) [N308] [ti11] [e a] []
Cell	3.807(2), 3.807(2), 9.09(2), 90., 90., 90. I41/AMDZ (141) V=131.74
Remarks	DEF MIN =Anatase : RVP XDP No R value given in the paper. At least one temperature factor missing in the paper. Nanophase with 8 nm grain size, Pt favours the primary formation of rutile Minority phase (19%) in mixture with rutile

Atom (site) Oxid.	x, y, z, B, Occupancy					
Ti1 (4a) 0	0	0.75	0.125	0	0.784(8)	
O1 (8e) 0	0	0.25	0.0782	0	1	

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CC=33842 [Help](#) CIF

Title	The crystal structure of rutile as a function of temperature up to 1600 degrees C.
Authors	Sugiyama, K.;Takeuchi, Y.
Reference	Zeitschrift fuer Kristallographie (1991) 194 , 305-313 Link Xref SCOPUS SCIRUS Google
Compound	O2 Ti1 - [Rutile] Titanium oxide [AX2] [tP6] [f a] [TiO2(tP6)]
Cell	4.6344(3), 4.6344(3), 2.9919(2), 90., 90., 90. P42/MNM (136) V=64.26
Remarks	R=0.052500 : TEM =1333 : TYP =TiO2(tP6) : MIN =Rutile :

Atom (site) Oxid.	x, y, z, B, Occupancy					
Ti1 (2a) 4	0	0	0	0	0	1
O1 (4f) -2	0.3056(2)	0.3056(2)				1
Atom (site) Oxid.	Beta11, Beta22, Beta33, Beta12, Beta13, Beta23					
Ti1 (2a) 4	0.0260(2)	0.0260(2)	0.0401(5)	-0.0004(1)		0 0
O1 (4f) -2	0.0224(4)	0.0224(4)	0.038(1)	-0.0088(4)		0 0

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