Status Primary **Quality Mark:** Star **Environment:** Ambient **Temp:** 298.0 K **Chemical Formula:** Si
Empirical Formula: Si **Weight %:** Si100.00 **Atomic %:** Si100.00 **Compound Name:** Silicon
Mineral Name: Silicon, syn **CAS Number:** 7440-21-3 **Entry Date:** 09/01/1977 **Modification Date:** 09/01/2008
Modifications: Lambda

Radiation: CuKα1 (1.5406 Å) **Internal Standard:** W **d-Spacing:** Diffractometer **Intensity:** Diffractometer - Peak

Crystal System: Cubic **SPGR:** Fd-3m (227)
Author's Unit Cell [a: 5.43088(4) Å **Volume:** 160.18 Å³ **Z:** 8.00 **MolVol:** 20.02 **]**
Calculated Density: 2.329 g/cm³ **Color:** Gray **SS/FOM:** F(11) = 408.8(0.0021, 13) **I/Ic:** 4.7

Space Group: Fd-3m (227) **Molecular Wt:** 28.09 g/mol
Crystal Data [a: 5.431 Å **b:** 5.431 Å **c:** 5.431 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **XtlCell Vol:** 160.18 Å³
XtlCell Z: 8.00 **a/b:** 1.000 **c/b:** 1.000 **]**
Reduced Cell [a: 3.840 Å **b:** 3.840 Å **c:** 3.840 Å **α:** 60.00° **β:** 60.00° **γ:** 60.00° **RedCell Vol:** 40.05 Å³ **]**

Crystal (Symmetry Allowed): Centrosymmetric

Subfiles: Ceramic (Semiconductor), Common Phase, Educational Pattern, Forensic, Inorganic, Metal & Alloy, Mineral Related (Mineral, Synthetic)

Mineral Classification: Diamond (supergroup), 2C-diamond (group) **Pearson Symbol:** cF8.00
Prototype Structure (Formula Order): C **Prototype Structure (Alpha Order):** C
LPF Prototype Structure (Formula Order): C,cF8,227 **LPF Prototype Structure (Alpha Order):** C,cF8,227

Cross-Ref PDF #'s: 00-005-0565 (Alternate), 00-026-1481 (Alternate), 04-001-7247 (Experimental <-> LPF), 04-002-0118 (Experimental <-> LPF), 04-002-0891 (Experimental <-> LPF), 04-003-1456 (Experimental <-> LPF), 04-003-3352 (Experimental <-> LPF), 04-003-3353 (Experimental <-> LPF), 04-003-4734 (Experimental <-> LPF), 04-004-5099 (Experimental <-> LPF), 04-004-6896 (Experimental <-> LPF), 04-005-9699 (Experimental <-> LPF), 04-006-2527 (Experimental <-> LPF), 04-006-2591 (Experimental <-> LPF), 04-006-4528 (Experimental <-> LPF), 04-006-6436 (Experimental <-> LPF), 04-007-5232 (Experimental <-> LPF), 04-007-8736 (Experimental <-> LPF), 04-012-7888 (Experimental <-> LPF)

References:

Type	DOI	Reference
Primary Reference		Natl. Bur. Stand. (U. S.) Monogr. 25 1976, 13, 35.

Database Comments: Additional Patterns: To replace 00-005-0565 and 00-026-1481. General Comments: Reflections calculated from precision measurement of a0. a0 uncorrected for refraction. Sample Source or Locality: This sample is NBS Standard Reference Material No. 640. Temperature of Data Collection: 298(1) K. Unit Cell Data Source: Powder Diffraction.

d-spacings (11) - Si - 00-027-1402 (Stick, Fixed Slit Intensity) - X-ray (Cu Kα1 1.54056 Å)

2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*
28.442	**3.1355**	100	1	1	1		76.377	1.2459	11	3	3	1		114.087	0.9180	7	5	3	1	
47.302	**1.9201**	55	2	2	0		88.026	1.1086	12	4	2	2		127.541	0.8587	8	6	2	0	
56.121	**1.6375**	30	3	1	1		94.948	1.0452	6	5	1	1		136.890	0.8282	3	5	3	3	
69.130	1.3577	6	4	0	0		106.715	0.9600	3	4	4	0								