

Standard Reference Material[®] 640g
Line Position and Line Shape Standard for Powder
Diffraction (Silicon Powder)
CERTIFICATE

Purpose: The certified values delivered by this Standard Reference Material (SRM) are intended for the calibration of powder diffraction equipment with respect to line position and profile breadth as a function of 2θ angle.

Description: A unit of SRM 640g consists of approximately 7.5 g of silicon powder bottled under argon.

Certified Values: The certified value for the lattice parameter is shown in Table 1. Metrological traceability is to the International System of Units (SI). Units for lattice parameter dimension is length (expressed as nanometers). The certified values and uncertainties were calculated according to the method described in the ISO/JCGM Guide [1,2]. The certification procedure can be found in reference 3.

Table 1. Certified Lattice Parameter for SRM 640g

	Lattice Parameter (nm)	Expanded Uncertainty ($k = 2$)
a	0.543 110 9	$\pm 0.000\ 008\ 0$

Non-Certified Values: Non-certified values are provided in Appendix A.

Period of Validity: The certified value delivered by **SRM 640g** is valid indefinitely, within the measurement uncertainty specified. The certified values are nullified if the material is stored or used improperly, damaged, contaminated, or otherwise modified. Periodic recertification of this SRM is not required.

Maintenance of Certified Values: NIST will monitor this SRM over the period of its validity. If substantive technical changes occur that affect the certification, NIST will issue an amended certificate through the NIST SRM website (<https://www.nist.gov/srm>) and notify registered users. SRM users can register online from a link available on the NIST SRM website or fill out the user registration form that is supplied with the SRM. Registration will facilitate notification. Before making use of any of the values delivered by this material, users should verify they have the most recent version of this documentation, available through the NIST SRM website (<https://www.nist.gov/srm>).

Storage: SRM 640g was bottled under argon to protect against humidity. When not in use, store the unused portion of this powder tightly capped in the original bottle or in a manner with similar or greater protection against humidity.

Use: The loading of samples for Bragg-Brentano diffractometers should be performed so as to achieve a powder bed of a high packing density and a flat surface.

REFERENCES

- [1] Beauchamp, C.R.; Camara, J.E.; Carney, J.; Choquette, S.J.; Cole, K.D.; DeRose, P.C.; Duewer, D.L.; Epstein, M.S.; Kline, M.C.; Lippa, K.A.; Lucon, E.; Molloy, J.; Nelson, M.A.; Phinney, K.W.; Polakoski, M.; Possolo, A.; Sander, L.C.; Schiel, J.E.; Sharpless, K.E.; Toman, B.; Winchester, M.R.; Windover, D.; *Metrological Tools for the Reference Materials and Reference Instruments of the NIST Material Measurement Laboratory*; NIST Special Publication (NIST SP) 260-136, 2021 edition; National Institute of Standards and Technology, Gaithersburg, MD (2021); available at <https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.260-136-2021.pdf> (accessed Feb 2024).
- [2] JCGM 100:2008; *Evaluation of Measurement Data — Guide to the Expression of Uncertainty in Measurement* (GUM 1995 with Minor Corrections); Joint Committee for Guides in Metrology (2008); available at <https://www.bipm.org/en/committees/jc/jcgm/publications> (accessed Feb 2024); see also Taylor, B.N.; Kuyatt, C.E.; *Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results*; NIST Technical Note 1297; U.S. Government Printing Office: Washington, DC (1994); available at <https://www.nist.gov/pml/nist-technical-note-1297> (accessed Feb 2024).
- [3] Cline, J.P.; Mendenhall, M.H.; Black, D.; Henins, A.; Prothero, J.B.; *Certification of Standard Reference Material 640g Line Position and Line Shape Standard for Powder Diffraction (Silicon Powder)*; NIST Special Publication 260-245; National Institute of Standards and Technology, Gaithersburg, MD (2024); available at <https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.260-245.pdf> (accessed Feb 2024).

If you use this SRM in published work, please reference:

Cline JP, Mendenhall MH, Black D, Henins A, Prothero JB (2024) Certification of Standard Reference Material 640g Line Position and Line Shape Standard for Powder Diffraction (Silicon Powder). (National Institute of Standards and Technology, Gaithersburg, MD), NIST Special Publication (SP) 260-245. <https://doi.org/10.6028/NIST.SP.260-245>

Certain commercial equipment, instruments, or materials may be identified in this Certificate of Analysis to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

Users of this SRM should ensure that the Certificate in their possession is current. This can be accomplished by contacting the Office of Reference Materials 100 Bureau Drive, Stop 2300, Gaithersburg, Maryland 20899-2300; telephone (301) 975-2200; e-mail srminfo@nist.gov; or the Internet at <https://www.nist.gov/srm>.

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APPENDIX A

Non-Certified Values: Non-certified values are suitable for use in method development, method harmonization, and process control but do not provide metrological traceability to the SI or other higher-order reference system. The analyses associated with certification of SRM 640g included the computation of the diffraction line positions shown in Table A1.

Table A1. Non-Certified Peak Position Values for SRM 640g,
Computed Using Cu K α Radiation, $\lambda = 0.154\ 059\ 29\ \text{nm}$

<i>h</i>	<i>k</i>	<i>l</i>	2θ (degrees)
1	1	1	28.441
2	2	0	47.301
3	1	1	56.120
4	0	0	69.127
3	3	1	76.373
4	2	2	88.026
5	1	1	94.948
4	4	0	106.703
5	3	1	114.086
6	2	0	127.537
5	3	3	136.883

Period of Validity: These non-certified values are valid indefinitely within the measurement uncertainty specified. The value assignments are nullified if this material is stored or used improperly, damaged, contaminated, or otherwise modified.

Maintenance of Non-Certified Value: NIST will monitor this material to the end of its period of validity. If substantive technical changes occur that affect the non-certified values during this period, NIST will update this Appendix and notify registered users. SRM users can register online from a link available on the NIST SRM website or fill out the user registration form that is supplied with the SRM. Registration will facilitate notification. Before making use of any of the values delivered by this material, users should verify they have the most recent version of this documentation, available through the NIST SRM website (<https://www.nist.gov/srm>).

***** End of Appendix A *****