NIST Reference Standard on the Alpha-1. Primary peak position and relative intensity match against the NIST reference data, and the lattice cell refinement for the a and c cells also match. The instrument is operating correctly.

## Measurement Conditions:

Dataset Name NIST\_Reference\_05\_02\_2019a

File name C:\Users\atavakoli6\Desktop\NIST\_Reference\_05\_02\_2019a.xrdml

Comment Configuration=Sample Spinner, Owner=User-1, Creation date=11/1/2006 2:23:59 PM

 Goniometer=PW3050/60 (Theta/2Theta); Minimum step size 2Theta:0.001; Minimum step size Omega:0.001

 Sample stage=Spinner PW3064

 Diffractometer system=XPERT-PRO

 Measurement program=C:\PANalytical\Data Collector\Programs\NIST\_Reference.xrdmp, Identifier={937D76BB-8184-4FFD-B032-2B4C339E7253}

 PHD Lower Level = 6.28 (keV), PHD Upper Level = 12.80 (keV)

Measurement Start Date/Time 5/2/2019 1:54:25 PM

Operator User-1

Raw Data Origin XRD measurement (\*.XRDML)

Scan Axis Gonio

Start Position [°2θ] 20.0042

End Position [°2θ] 139.9962

Step Size [°2θ] 0.0080

Scan Step Time [s] 10.1600

Scan Type Continuous

PSD Mode Scanning

PSD Length [°2θ] 2.12

Offset [°2θ] 0.0000

Divergence Slit Type Fixed

Divergence Slit Size [°] 0.2500

Specimen Length [mm] 10.00

Measurement Temperature [°C] 25.00

Anode Material Cu

K-Alpha1 [Å] 1.54060

Generator Settings 40 mA, 45 kV

Diffractometer Type 0000000067011063

Diffractometer Number 0

Goniometer Radius [mm] 240.00

Dist. Focus-Diverg. Slit [mm] 100.00

Incident Beam Monochromator Yes

Spinning No

## Main Graphics, Analyze View:



## Peak List:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Pos. [°2θ] | Height [cts] | FWHM Left [°2θ] | d-spacing [Å] | Rel. Int. [%] |
| 25.6277 | 586.46 | 0.0602 | 3.47319 | 63.67 |
| 35.2003 | 918.83 | 0.0602 | 2.54752 | 99.76 |
| 37.8279 | 429.92 | 0.0602 | 2.37638 | 46.68 |
| 41.7257 | 4.02 | 0.0602 | 2.16296 | 0.44 |
| 43.4038 | 917.36 | 0.0602 | 2.08314 | 99.60 |
| 46.2284 | 13.96 | 0.0602 | 1.96222 | 1.52 |
| 52.6000 | 465.68 | 0.0602 | 1.73854 | 50.56 |
| 57.5466 | 921.06 | 0.0602 | 1.60031 | 100.00 |
| 59.7894 | 23.67 | 0.0602 | 1.54552 | 2.57 |
| 61.1784 | 30.63 | 0.0602 | 1.51372 | 3.32 |
| 61.3477 | 70.03 | 0.0602 | 1.50994 | 7.60 |
| 66.5651 | 363.83 | 0.0602 | 1.40369 | 39.50 |
| 68.2568 | 556.86 | 0.0602 | 1.37296 | 60.46 |
| 70.4621 | 11.76 | 0.0602 | 1.33530 | 1.28 |
| 74.3439 | 13.89 | 0.0602 | 1.27489 | 1.51 |
| 76.9155 | 160.24 | 0.0602 | 1.23855 | 17.40 |
| 77.2780 | 85.08 | 0.0602 | 1.23364 | 9.24 |
| 80.4613 | 6.96 | 0.0602 | 1.19266 | 0.76 |
| 80.7442 | 62.17 | 0.0602 | 1.18919 | 6.75 |
| 83.2595 | 3.64 | 0.0602 | 1.15954 | 0.39 |
| 83.2595 | 3.64 | 0.0602 | 1.15954 | 0.39 |
| 84.4001 | 50.53 | 0.0602 | 1.14675 | 5.49 |
| 85.1840 | 2.72 | 0.0602 | 1.13819 | 0.30 |
| 86.3954 | 37.26 | 0.0602 | 1.12532 | 4.04 |
| 86.5441 | 26.75 | 0.0602 | 1.12376 | 2.90 |
| 89.0366 | 74.21 | 0.0602 | 1.09864 | 8.06 |
| 90.7464 | 17.92 | 0.0602 | 1.08234 | 1.95 |
| 91.2303 | 87.99 | 0.0602 | 1.07786 | 9.55 |
| 94.8600 | 2.00 | 0.0602 | 1.04596 | 0.22 |
| 95.2891 | 176.57 | 0.0602 | 1.04238 | 19.17 |
| 98.4343 | 23.46 | 0.0602 | 1.01731 | 2.55 |
| 101.1118 | 132.70 | 0.0602 | 0.99748 | 14.41 |
| 102.8594 | 2.97 | 0.0602 | 0.98523 | 0.32 |
| 103.3561 | 23.97 | 0.0602 | 0.98185 | 2.60 |
| 104.6775 | 1.68 | 0.0602 | 0.97305 | 0.18 |
| 109.5792 | 4.95 | 0.0602 | 0.94279 | 0.54 |
| 109.8945 | 3.36 | 0.0602 | 0.94097 | 0.36 |
| 110.8664 | 1.62 | 0.0602 | 0.93544 | 0.18 |
| 111.0253 | 41.06 | 0.0602 | 0.93454 | 4.46 |
| 114.1041 | 28.44 | 0.0602 | 0.91794 | 3.09 |
| 116.1361 | 139.52 | 0.0602 | 0.90765 | 15.15 |
| 116.6330 | 48.34 | 0.0602 | 0.90521 | 5.25 |
| 117.8881 | 79.75 | 0.0602 | 0.89918 | 8.66 |
| 120.2477 | 4.92 | 0.0602 | 0.88836 | 0.53 |
| 122.0717 | 24.94 | 0.0602 | 0.88042 | 2.71 |
| 122.0717 | 24.94 | 0.0602 | 0.88042 | 2.71 |
| 124.6294 | 31.94 | 0.0602 | 0.86989 | 3.47 |
| 127.7135 | 183.09 | 0.0602 | 0.85809 | 19.88 |
| 129.9069 | 36.34 | 0.0602 | 0.85025 | 3.95 |
| 129.9069 | 36.34 | 0.0602 | 0.85025 | 3.95 |
| 131.1285 | 76.23 | 0.0602 | 0.84609 | 8.28 |
| 132.2489 | 5.51 | 0.0602 | 0.84238 | 0.60 |
| 132.6511 | 3.77 | 0.0602 | 0.84108 | 0.41 |
| 136.1095 | 158.11 | 0.0602 | 0.83047 | 17.17 |
| 136.1095 | 158.11 | 0.0602 | 0.83047 | 17.17 |
| 139.3975 | 2.02 | 0.0602 | 0.82132 | 0.22 |

## Pattern List: (Bookmark 4)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Visible | Ref. Code | Score | Compound Name | Displacement [°2Th.] | Scale Factor | Chemical Formula |
| \* | 04-007-9906 | 58 | Aluminum Oxide | 0.000 | 0.328 | Al2 O3 |