

## 5. DETERMINATION OF LATTICE PARAMETERS

Table 5.2.10.3. Silicon standard reflection angles ( $^{\circ}$ ) (NIST SRM 640c,  $a_0 = 5.431195 \text{ \AA}$ ,  $T = 295.6 \text{ K}$ )

$h$ $k$ $l$	$d$ ( $\text{\AA}$ )	$I$	Mo $K\alpha_1$ 0.709317 $\text{\AA}$	1.000000 $\text{\AA}$	1.250000 $\text{\AA}$	1.500000 $\text{\AA}$	1.750000 $\text{\AA}$	Cr $K\alpha_1$ 2.289746 $\text{\AA}$
1 1 1	3.13570	100.0	12.988	18.350	22.994	27.676	32.406	42.829
2 2 0	1.92022	71.1	21.287	30.186	37.990	45.981	54.217	73.202
3 1 1	1.63757	43.5	25.016	35.556	44.873	54.516	64.597	88.714
4 0 0	1.35780	11.8	30.283	43.215	54.813	67.059	80.245	114.955
3 3 1	1.24600	17.4	33.074	47.317	60.213	74.016	89.215	133.514
4 2 2	1.10864	22.3	37.314	53.616	68.635	85.142	104.232	
5 1 1 ]	1.04523	8.7	39.670	57.157	73.447	91.704	113.678	
3 3 3 ]	1.04523	2.9	39.670	57.157	73.447	91.704	113.678	
4 4 0	0.96011	6.0	43.356	62.768	81.229	102.734	131.386	
5 3 1	0.91804	9.8	45.452	66.000	85.812	109.563	144.772	
6 2 0	0.85871	7.1	48.789	71.221	93.411	121.713		
5 3 3	0.82825	2.9	50.707	74.268	97.981	129.788		
4 4 4	0.78393	1.5	53.797	79.258	105.739	146.162		
7 1 1 ]	0.76052	1.9	55.594	82.211	110.532	160.918		
5 5 1 ]	0.76052	1.9	55.594	82.211	110.532	160.918		
6 4 2	0.72577	5.7	58.506	87.090	118.893			
7 3 1 ]	0.70708	2.4	60.209	90.004	124.237			
5 5 3 ]	0.70708	1.2	60.209	90.004	124.237			
8 0 0	0.67890	0.5	62.987	94.866	134.030			
7 3 3	0.66353	0.8	64.620	97.797	140.757			
6 6 0 ]	0.64007	0.7	67.297	102.735	155.085			
8 2 2 ]	0.64007	1.3	67.297	102.735	155.085			
7 5 1 ]	0.62714	1.7	68.876	105.740	170.531			
5 5 5 ]	0.62714	0.2	68.876	105.740	170.531			
8 4 0	0.60723	0.9	71.473	110.855				
9 1 1 ]	0.59615	0.4	73.013	114.009				
7 5 3 ]	0.59615	0.8	73.013	114.009				
6 6 4	0.57897	0.7	75.551	119.447				
9 3 1	0.56934	0.6	77.061	122.854				
8 4 4	0.55432	0.5	79.555	128.846				
9 3 3 ]	0.54586	0.2	81.042	132.692				
7 7 1 ]	0.54586	0.2	81.042	132.692				
7 5 5 ]	0.54586	0.2	81.042	132.692				
10 2 0 ]	0.53257	0.4	83.509	139.717				
8 6 2 ]	0.53257	0.8	83.509	139.717				
9 5 1 ]	0.52505	0.4	84.982	144.460				
7 7 3 ]	0.52505	0.2	84.982	144.460				
9 5 3	0.50646	0.3	88.897	161.678				
10 4 2	0.49580	0.5	91.340					
11 1 1 ]	0.48971	0.1	92.808					
7 7 5 ]	0.48971	0.1	92.808					
8 8 0	0.48005	0.1	95.258					
11 3 1 ]	0.47453	0.2	96.729					
9 7 1 ]	0.47453	0.2	96.729					
9 5 5 ]	0.47453	0.1	96.729					

## 5.2.11. Intensity standards

The measurement of intensity falls within the scope of Parts 6 and 7. However, powder methods are much used in quantitative analysis, and the National Institute of Standards and Technology provides five standards for use as internal standards for this purpose and for checking the accuracy of diffractometer and camera intensity measurements. The five materials, certified as SRM 674, are  $\alpha$ - $\text{Al}_2\text{O}_3$  (corundum),  $\text{ZnO}$ ,  $\text{TiO}_2$  (rutile),  $\text{Cr}_2\text{O}_3$ , and  $\text{CeO}_2$ . Table 5.2.11.1, taken from the NIST certificate, is a

partial list of pertinent data. The lattice parameters have an uncertainty of 3 parts in  $10^5$ , which must be increased by a factor of 2 or 3 because of uncertainty in internal standards and thermal expansion. The five materials have a wide range of absorption coefficient and the crystallite size (about  $2 \mu\text{m}$ ) causes a small profile broadening. The table gives the intensities of the second- and third-strongest lines relative to the strongest = 100, and the final column gives the ratio of the strongest peak to the strongest peak of  $\text{Al}_2\text{O}_3$ .