
Indexing data for examples appearing in paper

Indexing of Powder Diffraction Patterns by Iterative use
of Singular Value Decomposition

by

A. A. Coelho

Bruker AXS GmbH

Östliche Rheinbrückenstraße 49, D-76187 Karlsruhe,
Federal Republic of Germany

All units are in Angstroms for lattice parameter lengths and wavelength.
Units for Volume is Angstroms³

Example 1

Distributed with TREOR90

NBS Monograph 25 Sect.17 P.77 SR2CR2O7

A = 11.189680 ALFA = 90.000000

B = 11.189680 BETA = 90.000000

C = 9.482903 GAMMA = 90.000000

Tetragonal

Wavelength 1.540596

d

7.91

7.238

5.601

4.739

4.423

4.070

3.538

3.474

3.443

3.315

3.040

2.950

2.931

2.836

2.796

2.751

2.673

2.636

2.609

2.596

2.503

2.420

2.413

2.357
2.305

Example 2

Von Dreele, R. B. Stephens, P. W. Smith G. D. and Blessing, R. H. (2000).
Acta Cryst.. D56, 1549-1553.

Hexagonal/Trigonal

Vol = 418214.274

a = 81.3000

c = 73.0612

Wavelength 1.4011

d	I
3.082606	286.9333
3.140559	513.2841
3.156408	422.5167
3.188435	147.2428
3.210724	338.8536
3.239774	52.11361
3.282557	178.345
3.342452	281.8095
3.367994	518.055
3.483363	31.64179
3.519515	90.22909
3.531307	132.2404
3.617017	502.7378
3.661182	1464.545
3.845609	1202.408
3.909591	33.41721
3.96697	196.5019
4.149113	190.4147
4.170104	1147.535
4.324004	558.9846
4.368193	31.74863
4.71961	358.835
4.948572	212.0697
5.024163	554.7953
5.090083	210.1158
5.174718	101.9956
5.219193	1930.866
5.238378	778.2052
5.481424	691.0251
5.699556	415.4552
5.746338	267.452
6.003093	16.92363
6.235661	285.2046
6.563517	915.7387
7.689332	80.32933
7.930671	24.27313
8.448891	441.0228
10.9585	937.0932

Example 3

Distributed with TREOR90

NBS Monograph 25 Sect.17 P.7 $\text{NH}_4\text{B}_5\text{O}_8 \cdot 4\text{H}_2\text{O}$ Orthorhombic

A = 11.333113

B = 11.031460

C = 9.236147

UNIT CELL VOLUME = 1154.71 \AA^3

Wavelength 1.540596

d

6.00

5.67

5.52

4.951

4.617

4.427

3.544

3.383

3.334

3.271

3.003

2.926

2.868

2.834

2.760

2.680

2.627

2.586

2.533

2.479

2.414

2.367

2.332

2.317

2.312

Example 4

NBS Monograph 25 Sect.17 P.9 $(\text{NH}_4)_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ Monoclinic

A = 9.188087 ALFA = 90.000000

B = 12.472351 BETA = 106.917381

C = 6.241651 GAMMA = 90.000000

UNIT CELL VOLUME = 684.32

Wavelength 1.540596

d

7.19

6.24

5.98

5.388

5.248

5.090

4.397

4.316

4.243

4.166

4.147
3.952
3.757
3.586
3.466
3.410
3.376
3.119
3.037
3.027
2.943
2.913
2.903
2.892
2.853

Example 5

NBS.25 SEC.17 P.11 (NH₄)₂S₂O₃

A = 10.222344 ALFA = 90.000000

B = 6.497315 BETA = 94.669502

C = 8.807463 GAMMA = 90.000000

UNIT CELL VOLUME = 583.03 A**3

Wavelength 1.540596

d

5.480
5.093
4.741
4.553
4.386
4.257
3.501
3.469
3.353
3.248
3.199
3.046
3.010
2.925
2.915
2.785
2.739
2.629
2.612
2.582
2.569
2.547
2.536
2.500
2.453

Example 6

CdWO₄ NBS Monograph 25 Sect.2 p.9 1963

DIRECT PARAMETERS : A= 5.0702 B= 5.8574 C= 5.0309 BETA= 91.495

Wavelength 1.540596

d
5.8700
5.0400
3.8180
3.0770
3.0200
2.9280
2.5300
2.5140
2.3110
2.2870
2.2530
2.1310
2.0920
1.9530
1.9160
1.9070
1.8200
1.8090
1.7970
1.7740

=====
Example 7

Toraya, H. & Yamazaki, S. (2002). Acta Cryst. B58, 613-621

_cell_length_a 8.2127(5)
_cell_length_b 9.7930(4)
_cell_length_c 9.7954(5)
_cell_angle_alpha 90.0
_cell_angle_beta 94.848(5)
_cell_angle_gamma 90.0
_cell_volume 785.00(7)

Wavelength 1.540596

d	I
12.82524	3.538902
14.1355	243.0301
15.80112	13.53306
17.29824	17.06188
18.14356	387.2506
18.23888	151.2192
20.3266	51.67215
20.46554	65.51365
20.57436	48.18014
21.15915	49.95946
21.75385	448.5923
22.40305	270.983
23.31059	48.19589
23.43173	78.1321
23.60121	212.5369
25.80371	1133.913
25.98164	61.45789
27.13598	376.9806

27.30363 1239.714
27.44015 688.4894
28.45105 337.6683
28.85652 221.4901
29.46837 2812.193
29.64739 367.1465
30.46766 1224.841

Example 8

NBS.25 SEC.17 P.64 K2S2O8</P>
A = 5.117541 ALFA = 73.732178
B = 5.511826 BETA = 73.916046
C = 7.034377 GAMMA = 90.202797
UNIT CELL VOLUME = 182.31 A**3
Wavelength 1.540596

d

5.27
4.892
4.847
4.602
3.750
3.699
3.603
3.443
3.268
3.232
3.153
3.025
2.736
2.634
2.548
2.466
2.419
2.397
2.358
2.315
2.297
2.273
2.239
2.154
2.098

Example 9

NBS Monograph 25.16 P.92 280889
A = 7.085807 ALFA = 63.013237
B = 8.787556 BETA = 86.963554
C = 17.870726 GAMMA = 94.134857
UNIT CELL VOLUME = 984.40 A**3
Wavelength 1.540596

d

15.83
8.75

7.91
7.78
7.56
7.03
6.67
6.21
5.77
5.53
5.29
5.02
4.96
4.85
4.52
4.454
4.410
4.312
4.263
4.184
4.081
4.044
3.962
3.890
3.844

Example 10

Dinnebier, R. E., Bernatowicz, P. , Helluy, X. , Sebald, A. ,
Wunschel, M. , Fitch A. , & van Smaalen, S. (2002). *Acta Cryst.* B58, 52-61

_cell_length_a 9.92009(7)
_cell_length_b 14.51030(10)
_cell_length_c 9.13585(7)
_cell_angle_alpha 90.4769(4)
_cell_angle_beta 111.6724(4)
_cell_angle_gamma 89.9877(6)
_cell_volume 1222.04(2)
Wavelength 0.491213

d	I
4.53676	2.000375
4.608022	6.391603
4.620865	17.94653
4.834793	68.51934
4.874924	191.8681
4.994966	20.77921
5.021898	185.5379
5.338543	13.81484
5.390968	7.529976
5.489526	138.5839
5.537647	12.56903
5.690419	22.5604
6.889664	38.5248
6.923075	9.352411
7.250949	258.4238
7.294163	282.212
7.351469	287.6255

7.766485 261.2772
7.789209 254.7278
7.851037 262.4052
8.418365 18.38103
8.479813 14.50284
9.076779 8.796416
9.210652 7.838031
14.4883 4.450874

Example 11

van Langevelde, A., Peschar, R. & Schenk, H. (2001). Acta Cryst. B57, 372-377

_cell_length_a 12.0626(6)
_cell_length_b 41.7140(10)
_cell_length_c 5.4588(3)
_cell_angle_alpha 73.388(4)
_cell_angle_beta 100.408(5)
_cell_angle_gamma 118.274(4)
_cell_volume 2314.7(2)
Wavelength .699716

2Th I

2.237138 83.54735
3.358393 373.4113
3.423128 22.62696
3.775259 42.80713
4.378967 13.49232
4.481369 33.55852
5.183543 6.214883
5.600297 5.065171
6.066553 16.08208
6.726312 67.87632
6.849981 4.981914
7.022042 5.721908
7.112166 17.43463
7.483016 947.3223
7.543477 15.18942
7.630643 454.6099
7.677774 476.3506
7.714163 254.1279
7.94412 557.5694
8.005839 74.49574
8.100239 48.66022
8.28903 54.94569
8.368912 91.18119
8.394422 150.8924
8.47872 73.81423
8.736426 3329.254

Example 12

van Langevelde, A., Peschar, R. & Schenk, H. (2001). Acta Cryst. B57, 372-377

_cell_length_a 12.0053(7)
_cell_length_b 51.902(2)
_cell_length_c 5.4450(3)
_cell_angle_alpha 73.752(5)

_cell_angle_beta 100.256(6)
_cell_angle_gamma 117.691(5)
_cell_volume 2879.6(3)
Wavelength .650515

d	I
4.121799	637.9198
4.228878	1064.344
4.25249	323.641
4.318998	208.1025
4.337445	401.1985
4.366647	404.7261
4.390572	268.8189
4.479994	3060.441
4.55473	15327.89
4.581423	13899.51
4.704245	46.24569
4.791354	290.1386
4.818118	848.084
4.843434	491.0786
4.907142	68.71451
4.982293	135.6902
5.030066	662.6854
5.053859	223.0072
5.07659	310.0317
5.131312	607.6667
5.200391	1736.694
5.217864	1074.933
5.240796	572.5371
5.316574	1315.162
5.355795	1519.181
5.417448	65.6584
5.53077	35.15236
5.59437	331.9515
5.651844	26.98467
5.716024	52.30497
7.268071	30.73424
7.458782	352.4417
7.964829	59.16835
8.280228	37.6522
8.949042	339.9407
10.61297	109.5668
11.52145	38.93581
11.80009	48.09089
14.91353	4867.617
22.34175	1329.933
