

program PKS T. Higashi, 2001 Aug

----- Last update: T Higashi, 2004 Feb

date: Wed Dec 28 18:34:37 2011

Control Parameters

frame range: 1-6

spot size in pixels: 9 x 9

threshold of peak height: $av + 0.50 * sigav$

sigmacut of spot rejection: 3.00

diagnostic level: 0

Filename: C:/B2/suzuki111228_05/suzuki111228_05001.img

Scan axis: omega scan range: 0.00 - 1.00

Goniometer angles: 0.00 0.00 0.00

Camera distance: 127.40

Checking intensities ...

average intensity: 48 sigma intensity: 45

threshold of peak height: 70

intensity: maximum: 16383 (1.56% saturation) minimum: 7

Searching peaks ...

594 spots are picked

estimated spot radii: 13 11

estimated spotsize: 27 23

Checking intensities ...

average intensity: 48 sigma intensity: 45

threshold of peak height: 70

intensity: maximum: 16383 (1.56% saturation) minimum: 7

Searching peaks ...

688 spots are picked

Filename: C:/B2/suzuki111228_05/suzuki111228_05002. img

Scan axis: omega scan range: 1.00 – 2.00

Goniometer angles: 0.00 0.00 1.00

Camera distance: 127.40

Checking intensities ...

average intensity: 48 sigma intensity: 66

threshold of peak height: 81

intensity: maximum: 34016 (3.24% saturation) minimum: 7

Searching peaks ...

564 spots are picked

Filename: C:/B2/suzuki111228_05/suzuki111228_05003. img

Scan axis: omega scan range: 45.00 – 46.00

Goniometer angles: 0.00 0.00 45.00

Camera distance: 127.40

Checking intensities ...

average intensity: 50 sigma intensity: 37

threshold of peak height: 68

intensity: maximum: 2722 (0.26% saturation) minimum: 7

Searching peaks ...

610 spots are picked

Filename: C:/B2/suzuki111228_05/suzuki111228_05004. img

Scan axis: omega scan range: 46.00 – 47.00

Goniometer angles: 0.00 0.00 46.00

Camera distance: 127.40

Checking intensities ...

average intensity: 50 sigma intensity: 47

threshold of peak height: 73

intensity: maximum: 10098 (0.96% saturation) minimum: 7

Searching peaks ...

611 spots are picked

Filename: C:/B2/suzuki111228_05/suzuki111228_05005. img

Scan axis: omega scan range: 90.00 – 91.00

Goniometer angles: 0.00 0.00 90.00

Camera distance: 127.40

Checking intensities ...

average intensity: 40 sigma intensity: 45

threshold of peak height: 63

intensity: maximum: 7852 (0.75% saturation) minimum: 7

Searching peaks ...

775 spots are picked

Filename: C:/B2/suzuki111228_05/suzuki111228_05006. img

Scan axis: omega scan range: 91.00 – 92.00

Goniometer angles: 0.00 0.00 91.00

Camera distance: 127.40

Checking intensities ...

average intensity: 40 sigma intensity: 65

threshold of peak height: 73

intensity: maximum: 16480 (1.57% saturation) minimum: 7

Searching peaks ...

648 spots are picked

3896 total spots picked

fftindex T. Higashi 1999/Jun/15
----- Last update: 2004/Dec TH

date: Wed Dec 28 18:34:40 2011

peak file: peaks.dat

number of peaks to be used: 1000

cell length range: dmin = 3.0 Å, dmax = 200.0 Å

LSQ model: tight

tolerance for integral indices = 0.3

angle tolerance in LSQ = 1.0 deg

distance tolerance in LSQ = 2.0 mm

LS cycles = 5

eigenvalue filtering factor = 1.000000e-006

fft parameters	power	step	terms	grid size	range
first pass:	10	3.00 deg	1024	0.391 Å	–
second pass:	11	0.20 deg	2048	0.195 Å	3.00 deg

where terms = 2^{power} and grid size = $d_{\text{max}} / (2-1)^{\text{power}}$

2theta max: 180.00

powder treshold: 0

pseudo translation test: off

twin domain ID: 0

cell reduction tolerances:

accepted deviation of cell lengths = 0.60 Å

accepted deviation of cell angles = 1.20 deg

accepted deviation of metric tensor coeffs. = 0.80

local bin parameters:

local bin size = 30.00 deg
primary bins = 6
total bins = 28

Peak file: peaks.dat

frame template: C:/B2/suzuki111228_05/suzuki111228_05###.img

number frames: 6

peak selection:

2-theta limit = 180.0 deg; rejected: 0

powder peak threshold = 0; rejected: 0

peaks read = 3896

peaks to be used = 1000

FIRST PASS

SECOND PASS

Selected Real-Space Vectors

No	d (Å)	x	y	z	FOM
1	38.09	-0.7888	0.4915	0.3690	95.90
2	88.09	-0.6234	-0.5441	0.5615	83.68
3	88.09	0.8161	0.0010	0.5779	81.49
4	110.16	-0.7726	-0.2653	0.5768	75.27
5	118.75	0.3963	-0.5615	0.7264	69.78
6	118.75	-0.1120	-0.2454	0.9629	69.71
7	160.35	-0.4581	0.0512	0.8874	51.63
8	163.48	0.3270	0.3464	0.8793	50.67
9	171.88	-0.8454	0.0475	0.5320	46.84
10	171.88	0.9445	-0.3244	0.0514	46.47
11	181.84	0.1562	-0.0569	0.9861	44.77
12	5.47	0.9990	-0.0064	0.0440	29.82

13	5.08	0.0497	0.9957	0.0784	24.42
14	145.90	0.4723	0.5583	0.6821	22.93
15	2.73	0.0680	-0.9922	0.1043	22.78
16	2.73	-0.3013	0.5605	0.7714	17.21
17	116.41	0.1772	-0.4936	0.8515	15.45

REFINEMENT

key integers: 111111111110000000

number of parameters: 18

number of variables: 11

Cell Candidates

No		a	b	c	alpha	beta	gamma	volume	acc(%)
1	P	79.448	79.481	38.088	90.03	90.01	90.04	240506	95.8 45
2	C	76.183	158.931	79.459	90.04	90.05	90.00	962079	94.3 21
3	C	135.772	112.419	118.615	90.02	127.14	89.97	1443298	94.0 14
4	P	88.145	79.466	110.030	90.02	110.58	89.97	721539	95.6 9
5	P	88.126	110.084	110.127	118.61	107.44	110.60	721594	95.4 8
6	P	88.125	110.128	135.751	88.03	73.39	72.56	1202586	94.8 2
9	P	110.097	118.670	135.775	79.63	88.08	74.82	1683924	93.6 3
12	C	38.062	79.467	79.454	90.06	90.09	89.99	240319	93.3 2
13	P	118.667	135.707	139.242	97.27	96.85	100.35	2164825	94.0 1
14	P	110.071	79.494	139.125	90.05	98.99	90.00	1202400	93.6 1
16	P	110.125	135.750	160.217	113.56	97.82	91.97	2164702	91.9 2
17	P	118.669	135.706	171.909	103.11	91.47	100.35	2646058	92.2 1
18	C	324.783	112.415	118.594	90.04	91.55	89.98	4328365	90.4 2
19	C	189.469	112.339	118.680	90.00	107.73	90.02	2406095	89.9 1

cell: 79.448 79.481 38.088 90.03 90.01 90.04

lattice type: P, rotation and x-ray axes: +a* -c

phixyz: -28.604876 21.558185 -31.803130

Check Pseudo Translation

pseudo translation axis: $0.50a^* + 0.00b^* + 0.17c^*$

is implied by 2 peaks of 5 unindexed peaks