SADABS -ADVANCED FACE INDEX ABS CORRECTION

Notes and user input are in red and italicized.

SADABS-2006/1 - Bruker AXS area detector scaling and absorption correction

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Expert mode (Y or N) [N]: N

Enter listing filename [sad.abs]:

Laue group numbers:

[1] -1	[8] -3m (rhombohedral axes)
[2] 2/m (Y unique)	[9] -31m (Z unique)
[3] mmm	[10] -3m1 (Z unique)
[4] 4/m (Z unique)	[11] 6/m (Z unique)
[5] 4/mmm (Z unique)	[12] 6/mmm (Z unique)
[6] -3 (rhombohedral axes)	[13] m3
[7] -3 (Z unique)	[14] m3m

[0] to write list of equivalent indices for Laue/point groups to listing file

Enter Laue group number [2]: 2

	a	*b*	*c*	α	β	γ	Laue		
Triclinic							-1		
Monoclinic				90		90	2/m		
Orthorhombic				90	90	90	mmm		
Tetragonal	a=b	a=b		90	90	90	4/m	4/mmm	
Trigonal	a=b	a=b		90	90	120	-3	-3m1	-31m
Hexagonal	a=b	a=b		90	90	120	6/m	6/mmm	
Cubic	a=b=c	a=b=c	a=b=c	90	90	90	m-3	m-3m	

Read reflection files written by EVALCCD (with extension .sad specified) or by SAINT (extension .raw, default if no extension, or .ram for incommensurate structures). Either individual files for each scan or a single merged file may be read. It is important that all files are from the same crystal and that reflections have been indexed consistently, i.e. that the orientation matrices are similar (no rows with signs reversed)! Note that XPREP can re-index a .raw or .sad file transforming the direction cosines

Enter filename (/ if no more) [ ]: ch1.raw
Enter filename (/ if no more) [ch2.raw]:
Enter filename (/ if no more) [ch3.raw]:
Enter filename (/ if no more) [ch4.raw]:
Enter filename (/ if no more) [ch5.raw]: /

Mean and maximum errors in direction cosine check function = 0.001 0.004

The mean error should not exceed 0.005, and is usually caused by matrix changes during data processing.

Approximate wavelength, cell and maximum 2-theta (from cosines etc.):
0.71122 10.445 7.855 12.004 89.986 90.861 90.009 55.01

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PART 1 - Refinement of parameters to model systematic errors

Thresholds should now be specified for excluding reflections from the parameter refinement; these reflections may still be corrected and included in the final output .hkl file

9025 Reflections of which 2374 unique; 4.56 data per frame

Redundancy:	1	2	3	4	5	6	7	8	9+
Number of groups:	173	387	462	548	476	200	104	24	0

Mean(I/sigma):	-inf	0	1	2	3	5	10	15	20	+inf
Number of groups:	456	196	164	118	119	391	271	182	477	

The following restraint esd could be increased for strong absorbers.
Restraint esd for equal consecutive scale factors [0.005]: .005
Number of refinement cycles [15]: 15
Weak (W), moderate (M) or strong (S) empirical absorption correction or face-indexed numerical (N) absorption correction [M]: N

Enter N and then input the P4P file with the face commands. These can be input manually or determined with the SMART FACE routine.

Full name of .p4p or .spin file containing indexed crystal faces:
chg.p4p

Instructions in the P4P file

```
FACE     1.00 -1.00 -2.00     0.200
FACE    -1.00  1.00  2.00     0.200
FACE    -2.00 -2.00  1.00     0.400
FACE     2.00  2.00 -1.00     0.400
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```
FACE      0.00   0.00   1.00      0.030
FACE      0.00   0.00  -1.00      0.030
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Here the face is given in miller indices and the distance from the center of the crystal to that face is given in millimeters.

6 Faces + 8 Corners = 12 Edges + 2

Enter value of mu in mm-1 or <CR> to determine mu:

I choose to refine mu. If mu is known then input the value here.

Cycle 0 Mu 0.00 mm-1 Rint 0.1032
Cycle 1 Mu 1.00 mm-1 Rint 0.0665
Cycle 2 Mu 2.50 mm-1 Rint 0.0748
Cycle 3 Mu 1.58 mm-1 Rint 0.0572
Cycle 4 Mu 1.63 mm-1 Rint 0.0572
Cycle 5 Mu 1.61 mm-1 Rint 0.0572
Cycle 6 Mu 1.62 mm-1 Rint 0.0572

Refined linear absorption coefficient = 1.62 mm-1

Retain this value (CR) or input new value:

This value is consistent with the proposed empirical formula. If not then I would input the correct value. This is a good indicator for your face identification.

Calculating transmission and t-bar for all data

Linear absorption coefficient set to 1.62 mm-1, giving Rint = 0.0572

Minimum and maximum transmission coefficients = 0.36126 and 0.91129

Make a note of these values and record them in the CIF.

Minimum and maximum t-bar = 0.0573 and 0.5508 mm

All Rint values calculated using selected reflections only

6035 Reflections employed for parameter determination

Effective data to parameter ratio = 2.25

R(int) = 0.0678 (selected reflections only, before parameter refinement)
Cycle R(incid) R(diffr) Mean wt.
1 0.0468 0.0373 0.9233

2	0.0351	0.0345	0.9280
3	0.0342	0.0341	0.9284
4	0.0339	0.0340	0.9286
5	0.0338	0.0339	0.9287
6	0.0337	0.0338	0.9288
7	0.0337	0.0337	0.9293
8	0.0336	0.0337	0.9297
9	0.0336	0.0336	0.9297
10	0.0335	0.0336	0.9298
11	0.0335	0.0336	0.9298
12	0.0335	0.0335	0.9298
13	0.0335	0.0335	0.9298
14	0.0334	0.0335	0.9299
15	0.0334	0.0335	0.9299

R(int) = 0.0335 (selected reflections only, after parameter refinement)
Repeat parameter refinement (R) or accept (A) [A]: A
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PART 2 - Reject outliers and establish error model

Rejected reflections are ignored in the statistics and Postscript plots (except the detector diagnostics) and in the output .hkl file.

Before applying rejections there are:

9025 total and 2374 unique reflections assuming Friedel's law.
8398 total and 2339 unique reflections left after |I-<I>|/su test

g = 0.0754 gives best error model.

Enter new value for g or <CR> to accept:

Run	2-theta	R(int)	Incid. factors	Diffr. factors	K	Total	I>2sig(I)
1	-28.0	0.0375	0.632 - 0.722	0.913 - 1.245	0.808	2572	2107
2	-28.0	0.0322	0.909 - 1.084	0.828 - 1.079	0.777	2526	2073
3	-28.0	0.0378	1.211 - 1.396	0.863 - 1.098	0.851	1653	1162
4	-28.0	0.0299	1.179 - 1.302	0.838 - 1.140	0.751	1647	1378

su = K * Sqrt[sigma^2(I) + (g<I>)^2] where sigma(I) is estimated by SAINT

R(int) is good and all the Ks and I>sig(I) are about equal.

The above statistics are based on all non-rejected data, ignoring reflections without equivalents when estimating R(int) and K.

Repeat parameter refinement (P) or accept (A) [A]: A

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PART 3 - Output Postscript diagnostics and corrected data

Write Postscript diagnostic file (Y or N) [Y]: N
Repeat (R), write unmerged .hkl (W), merged .hkl (M), .sca (S), XD format (D), testxtl.dat (BioXhit) (T) or quit (Q) [W]: W
Reflection output file [sad.hkl]: ch.hkl
Lambda/2 correction factor (0 if no monochromator [0.0015]: .0015

8398 Corrected reflections written to file ch.hkl

Estimated minimum and maximum transmission: 0.2203 0.8544

These values should be close to the Tmax and Tmin reported after the face correction.

The ratio of these values is more reliable than their absolute values!

Repeat (R), write unmerged .hkl (W), merged .hkl (M), .sca (S), XD format (D), testxtl.dat (BioXhit) (T) or quit (Q) [Q]: Q

I have generated ch.hkl which contains the hkl file I will use in XPREP.

Note : If the SADABS face indexed correction is applied to the HKL file do not attempt the FACE correction again in XPREP.