DAjust with AJUST & SGAid

Jordi Rius, Oriol Vallcorba, Inma Peral, Carlos Frontera, Carles Miravitlles

DAjust software

Pattern matching, space group determination and intensity extraction from powder diffraction data

Oriol Vallcorba
ovallcorba@icmab.com

CSIC
Consejo Superior de Investigaciones Científicas

ICMAB
Institut de Ciència de Materials de Barcelona
www.icmab.es
Campus de la UAB
08193-Bellaterra (Spain)

ALBA
CELLS - ALBA Synchrotron Light Facility

DAjust: introduction

AJUST: whole-pattern matching

Cell parameters refinement
Profile fitting
Intensity extraction

SGAID: ranked list of most probable space groups

DAjust: introduction

Iterative intensity refinement

Based on Le Bail *et al.* (1988) method

$$M = \sum_i w_i \left[y_{\mathrm{obs},i} - \left(y_{\mathrm{bkg},i} + \sum_k j_k I_k \Omega_{k,i} \right) \right]^2$$

$$I_{k,\mathrm{new}} = I_{k,\mathrm{old}} + c_k \sum_i w_i \Omega_{k,i} \left(y_{\mathrm{obs},i} - y_{\mathrm{calc},i} \right)$$

$$y_{\mathrm{calc},i} = y_{\mathrm{bkg},i} + \sum_k j_k I_k \Omega_{k,i}$$

$$c_k = \frac{1}{\sum_i w_i \Omega_{k,i}^2}$$

Profile parameters

pseudo-Voigt (TCH, 1987)
Pearson-VII

Criterion of fit

$$\chi = R_{\mathrm{wp}} / R_{\mathrm{exp}}$$

$$R_{\mathrm{wp}} = \left[\frac{\sum_i w_i \left(y_{\mathrm{obs},i} - y_{\mathrm{calc},i} \right)^2}{\sum_i w_i \left(y_{\mathrm{obs},i} - y_{\mathrm{bkg},i} \right)^2} \right]^{1/2}$$

$$R_{\mathrm{exp}} = \left[\frac{N - P}{\sum_i w_i \left(y_{\mathrm{obs},i} - y_{\mathrm{bkg},i} \right)^2} \right]^{1/2}$$

$$w_i = \frac{1}{\sum_i \left(y_{\mathrm{obs},i} - y_{\mathrm{bkg},i} \right)}$$

Options

Automated background, asymmetry correction, absorption, variable divergence,...

Vallcorba, O., Rius, J., Frontera, C., Peral, I. & Miravitlles, C. (**2012**). *J. Appl. Cryst.*, 45, 844–848
Le Bail, A., Duroy, H. & Fourquet, J. (**1988**). *Mater. Res. Bull.* 23, 447–452.
Thompson, P., Cox, D. E. & Hastings, J. B. (**1987**). *J. Appl. Cryst.* 20, 79–83

Overall procedure

Data acquisition

↓

indexing — *ab initio* calculations, known phases, ...

Metric and aprox. cell parameters

↓

DAJUST software

↓

Full pattern matching

- cell parameters refinement
- intensity extraction

→ **.QCK** **.POW**

TALP **XLENS**

overlapped ref., clusters, profile information,...

Space group determination

↓

Structure solution, refinement, ...

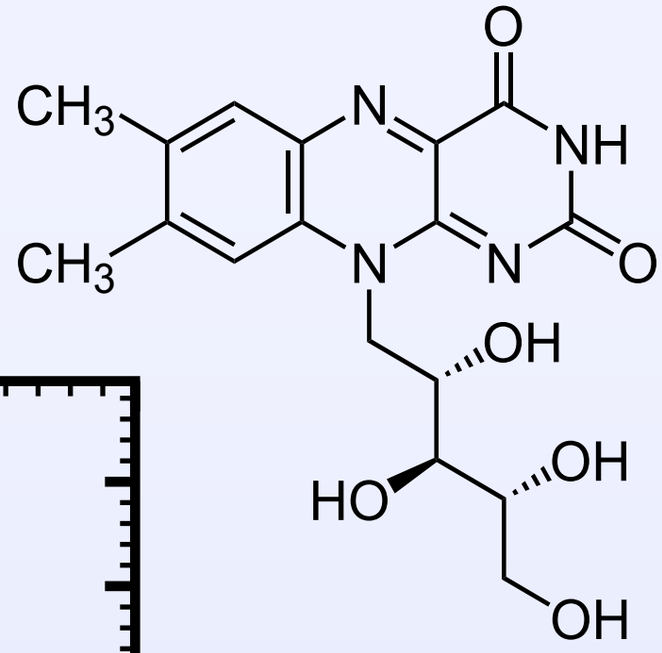
DAjust/SGAid example

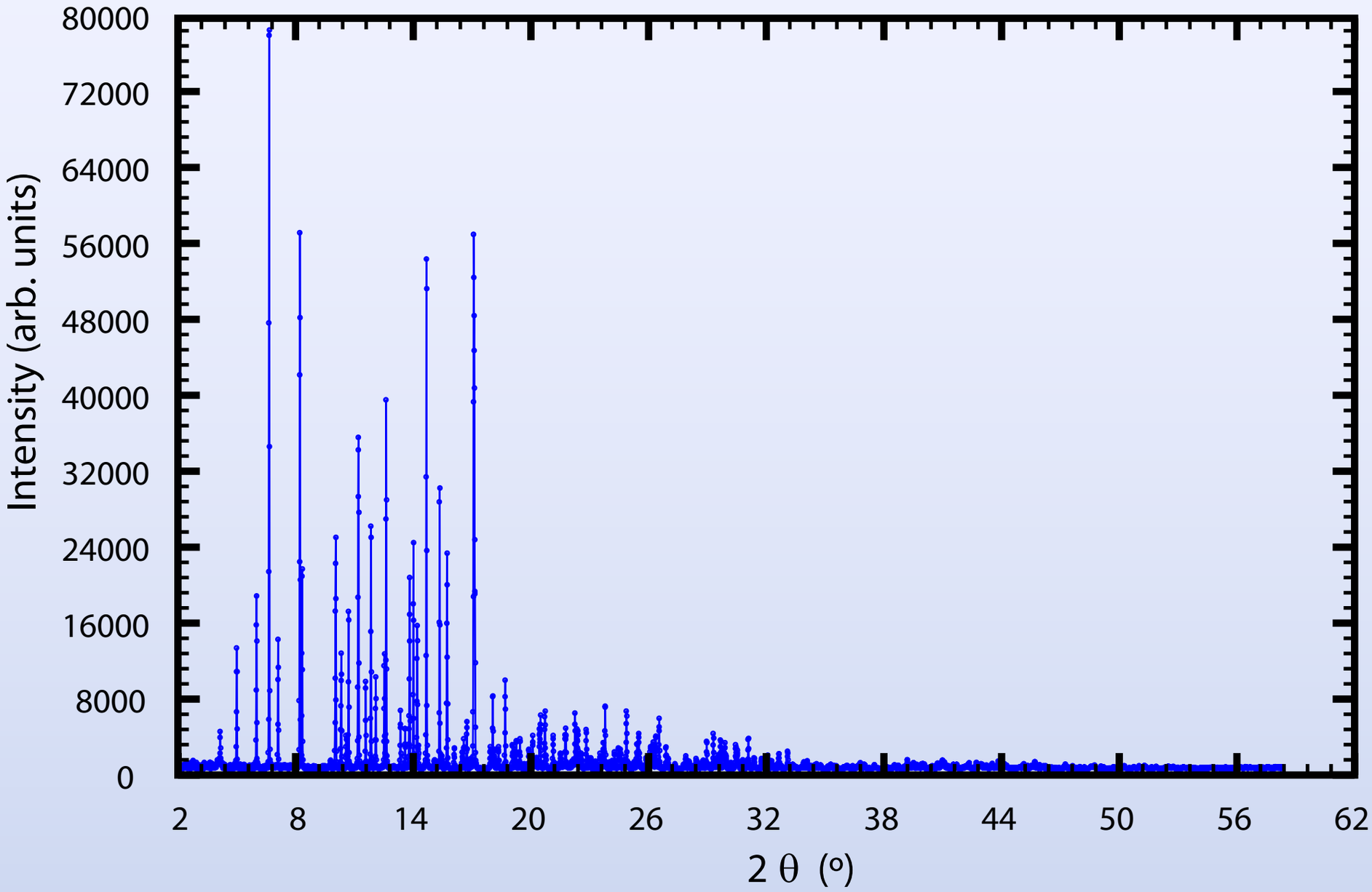
Powder diffraction data from MYTHEN II detector

organic compound

Powder data of (–)-Riboflavin

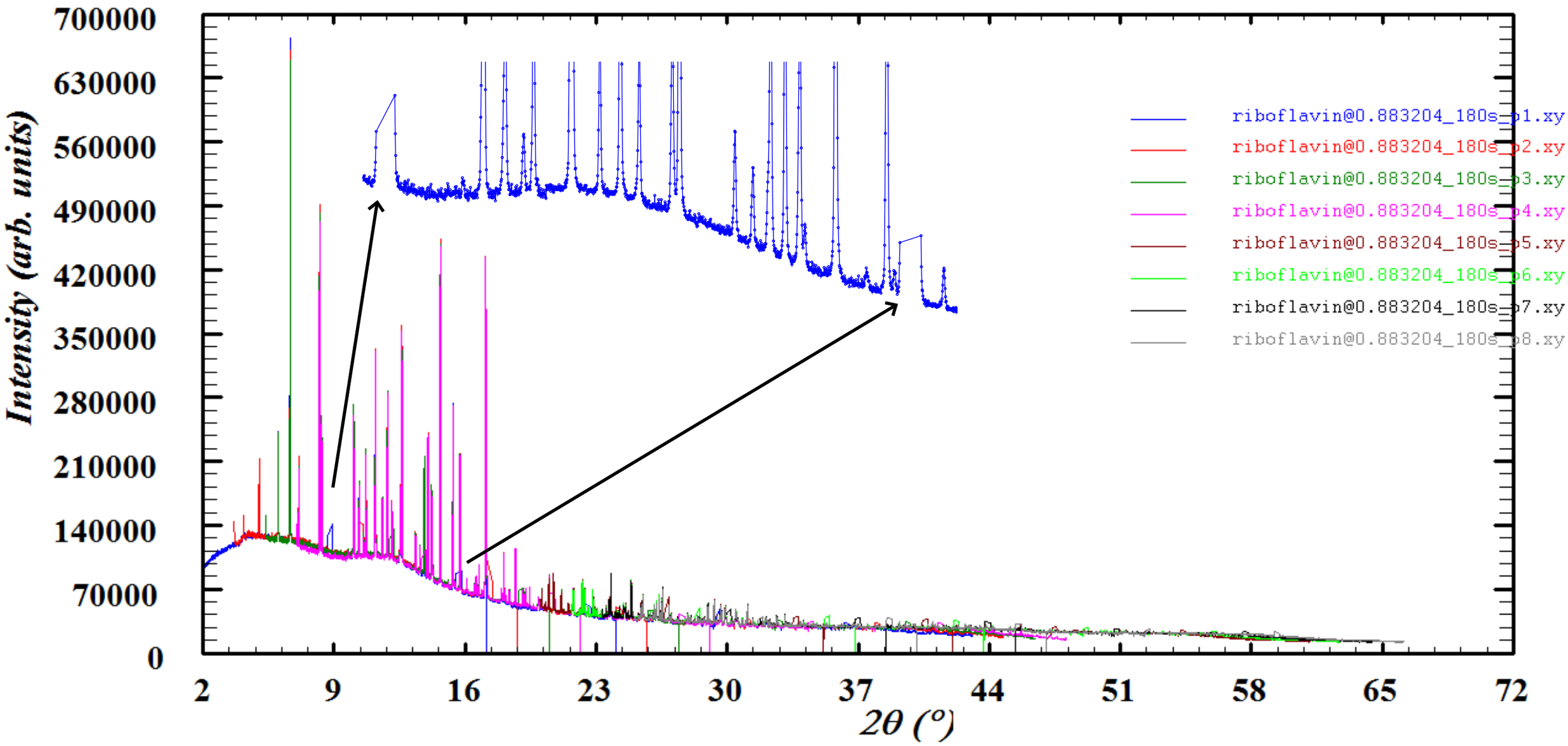
- Capillary Synchrotron data (MYTHEN II)
- $\lambda = 0.88320$ Å
- $C_{17}H_{20}N_4O_6$





Powder data of (–)-Riboflavin - Data preparation

- MERGE and BACKGROUND subtraction
- Manual/automatic (programs)



Powder data of (–)-Riboflavin - Data preparation

- **DMerge** COMBINATION OF POWDER PATTERNS FOR LINEAR MULTISTRIP DETECTORS

Merge control: `param.txt`

```
! === MYTHENII PARAMETERS ===
! DETECTOR SETTINGS:
! Sample-Detector distance (mm)
  552.464
! Number of modules, channels/module and channel size (mm)
  5 1280 0.05
! EXCLUDED ZONES AND EXPERIMENTAL DATA:
! 2T min
  2.00353
! EXCLUDED ZONES
  2.06
  8.56 8.95
  14.47 15.85
  22.40 22.76
  29.31 29.64
  36.16
! DEAD PIXELS (module pixel)
  0
! Wavelength (A)
  0.88320395
! OUTPUT PARAMETERS
! step size (°)
  0.010
! t2ini t2fin
  2.0 58.33
```

- **DMerge file1.xy file2.xy ... fileN.xy**
- Output: **file1-merged.xy**

Indexing

- e.g. DICVOL

```
(...)

   THE SOLUTION IS NOW USED TO TRY TO INDEX ALL INPUT  56 LINES :
   ============================================================
  DIRECT PARAMETERS :    A= 20.17036  B= 15.17811  C=  5.35121   VOLUME= 1638.26
  STANDARD DEVIATIONS :       .00034    .00029    .00010
  REFINED ZERO-POINT SHIFT : 0.0181 deg. 2-theta

    H   K   L    DOBS     DCAL    DOBS-DCAL 2TH.OBS  2TH.CAL  DIF.2TH.

    1   1   0  12.17640 12.18077  -0.00438    4.157    4.155   0.001
    2   0   0  10.12641 10.12167   0.00473    4.999    5.001  -0.002
    2   1   0   8.42660  8.42523   0.00137    6.008    6.009  -0.001
    0   2   0   7.61019  7.60968   0.00051    6.653    6.654   0.000

(...)

          * NUMBER OF LINES
              .- LINES INPUT      =   56
              .- LINES INDEXED    =   56
              .- LINES CALCULATED =  224
          * AVERAGE 2-Theta DIFFERENCE FOR INDEXED LINES =-0.0007
          * MEAN ABSOLUTE DISCREPANCIES
                                          <Q> =0.2522E-04
                              <DELTA(2-THETA)> =0.1880E-02
             MAX. ERROR ACCEPTED (DEG. 2-THETA) =0.4500E-01
          * FIGURES OF MERIT
               1.- M( 20) =   82.2
               2.- F( 20) =  345.4(0.0016,   36)
               3.- F( 56) =  133.0(0.0019,  224)
```

DAjust requires the previous indexing of the pattern to obtain the approximate cell parameters:

a	20.17 Å	α	90°
b	15.18 Å	β	90°
c	5.35 Å	γ	90°

V 1638 Å^3

Orthorhombic

Z=4 Z'=1

DAjust UI

DAjust_UI_v1209

File Options Help

General

Name

Formula

Z

Cycles

Cell parameters

a α 90.000

b β 90.000

c γ 90.000

Metric cubic

Fix cell param.

Use existing LAT file

Symmetry

SG.Num:Symbol : set Lattice P

Centrosimetric

No centrosimetric

Highest symmetry

Symmetry matrices unlock

Instrumental & Data parameters

Pattern type 2 (2T Yobs) nYline 1 2θsup 65.000

Rad. source Synchrotron λ1 λ2

Intensity Extraction NFWHM 20 tolerance 0.5

Sample Flat Capillary

Primary monochromator

Yes No cos 2θ 1.000

Divergence correction

Yes No Fixed slit Variable slit

slit-w (º) 0.000 sample size 0.000 armlenght 0.000

Absorption correction

Yes No

R*mu 0.000 2θRefInt 0.000 Transmi. 0.000

Profile Function

Type Pseudo-Voigt T... zero 0.001 exp 1.000

Lorentzian coef. X 0.001 Y 0.001

Gaussian coef. W 0.000 V 0.000 U 0.000

Pref. Orientation: March-coef 1.000 direction (h k l) 0 0 1

Excluded zones

2θinf Add

2θsup Del.

2Tinf	2Tsup

Background

type Calcula... 2θ + -

<back> 60.000 bg-value File

FWHM 0.150

Iterations 20

2T	bg-value

Asymmetry correction

coef. Add

2θsup Del.

coef	2Tsup

Ghost peaks

value 2θ width

η asym + -

value	2T	width	nu	asym

Run AJUST Stop run open PRF Output window

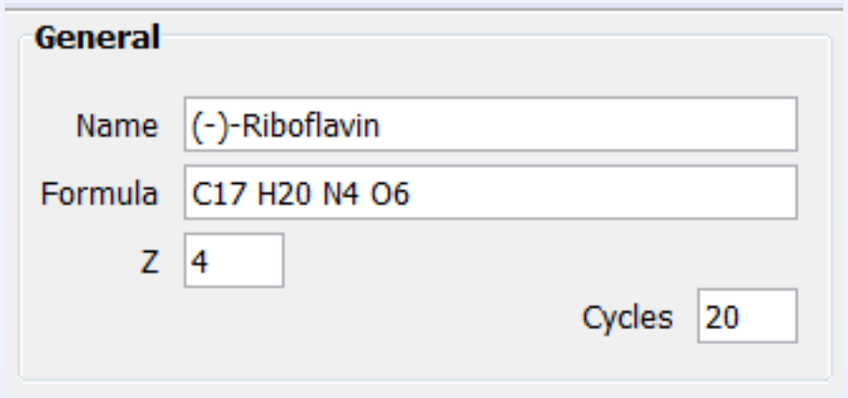
Run SGAid Update fields SGAid window

Work file: no file

Data file: no file

DAjust UI - Cell parameters and symmetry

- (–)-Riboflavin
- $C_{17}H_{20}N_4O_6$

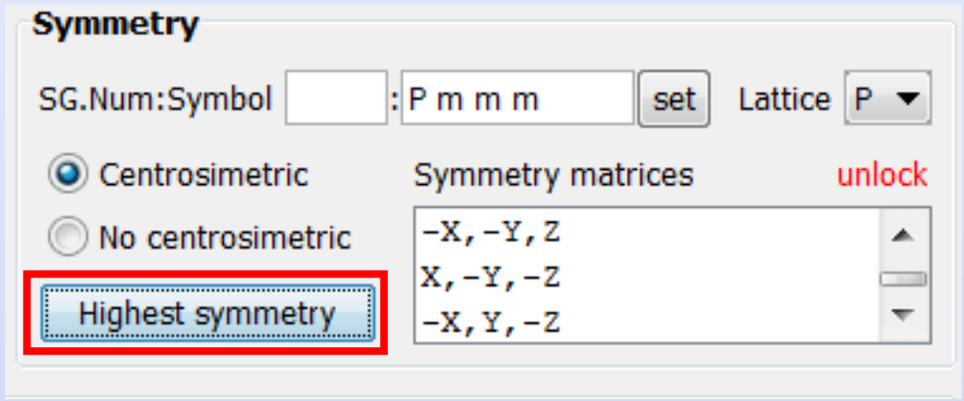


a 20.17 Å α 90°
b 15.18 Å β 90°
c 5.35 Å γ 90°

Orthorhombic

V 1650 Å^3

Z=4 *Z′*=1



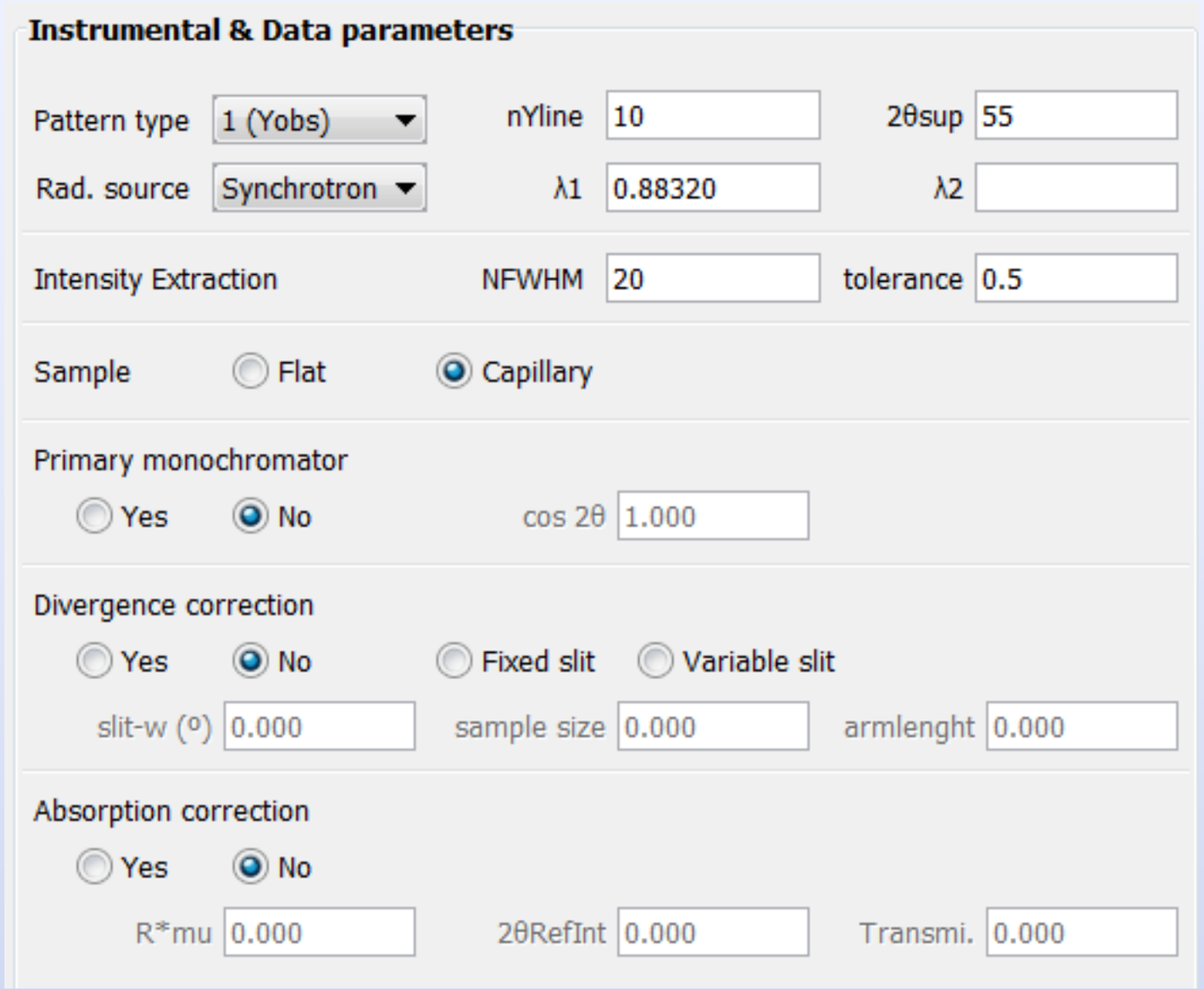
DAjust UI - Instrumental & Data parameters

PXRD data format

The .DAT (or .NET) file has the following structure:

- LINE 1: Title line beginning with !
- LINE 2: 2θmin(deg.) step(deg.) 2θmax(deg.)
- NEXT LINES (free format): Intensity data. Three different options are supported. The choice is indicated in DAjust_UI (Pattern type option):
  1. Only intensity data. Yobs Yobs2 Yobs3 ...
     The number of Yobs values per line must be specified in the **nYline** field of DAjust_UI.
  2. 2θ Yobs
  3. 2θ Yobs sigma(Yobs)

```
! Riboflavin ALBA-MYTHENII
      2.060000       0.010000      58.320000
    10       0     295      26       0      14      91       0     263      68
   196     110      27     145     154     200      20     314     361     151
   244      96       0     269     340     147     444     307     273     150
   ...
```



Pattern type =1

(NYLINE=10)

$2\theta_{sup}$=55°

Synchrotron (λ=0.88320Å)

DAjust UI - Profile function, background,...

Profile Function

Pseudo-Voigt (TCH)

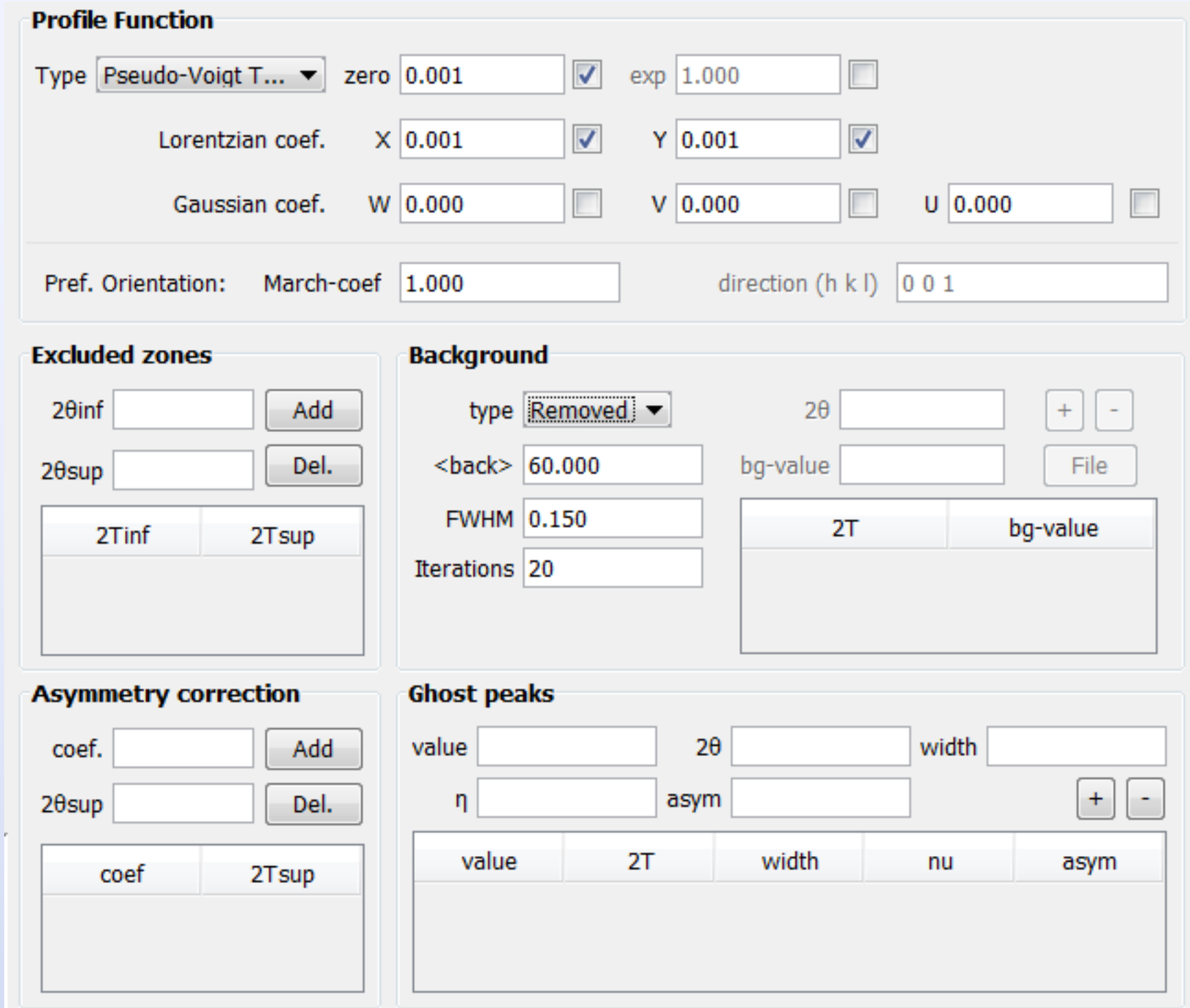
- Zero
- Lorentzian coef. X,Y

Background

Removed (.NET)

Excluded Zones

Asymmetry correction



DAjust UI - Save JST and run DAjust

DAjust_UI_v1209

File Options Help

General

Name (-)-Riboflavin

Formula C17 H20 N4 O6

Z 4

Cycles 20

Cell parameters

a 20.20 α 90.000

b 15.21 β 90.000

c 5.37 γ 90.000

Metric orthorombic

Fix cell param.

Use existing LAT file

Symmetry

SG.Num:Symbol : P m m m set Lattice P

Centrosimetric

No centrosimetric

Highest symmetry

Symmetry matrices unlock

-X,-Y,Z

X,-Y,-Z

-X,Y,-Z

Instrumental & Data parameters

Pattern type 1 (Yobs) nYline 10 2θsup 55

Rad. source Synchrotron λ1 0.88320 λ2

Intensity Extraction NFWHM 20 tolerance 0.5

Sample Flat Capillary

Primary monochromator

Yes No cos 2θ 1.000

Divergence correction

Yes No Fixed slit Variable slit

slit-w (º) 0.000 sample size 0.000 armlenght 0.000

Absorption correction

Yes No

R*mu 0.000 2θRefInt 0.000 Transmi. 0.000

Profile Function

Type Pseudo-Voigt T... zero 0.001 exp 1.000

Lorentzian coef. X 0.001 Y 0.001

Gaussian coef. W 0.000 V 0.000 U 0.000

Pref. Orientation: March-coef 1.000 direction (h k l) 0 0 1

Excluded zones

2θinf Add

2θsup Del.

Background

type Removed 2θ + -

<back> 60.000 bg-value File

Run AJUST Stop run open PRF Output window

Run SGAid Update fields SGAid window

Work file: no file

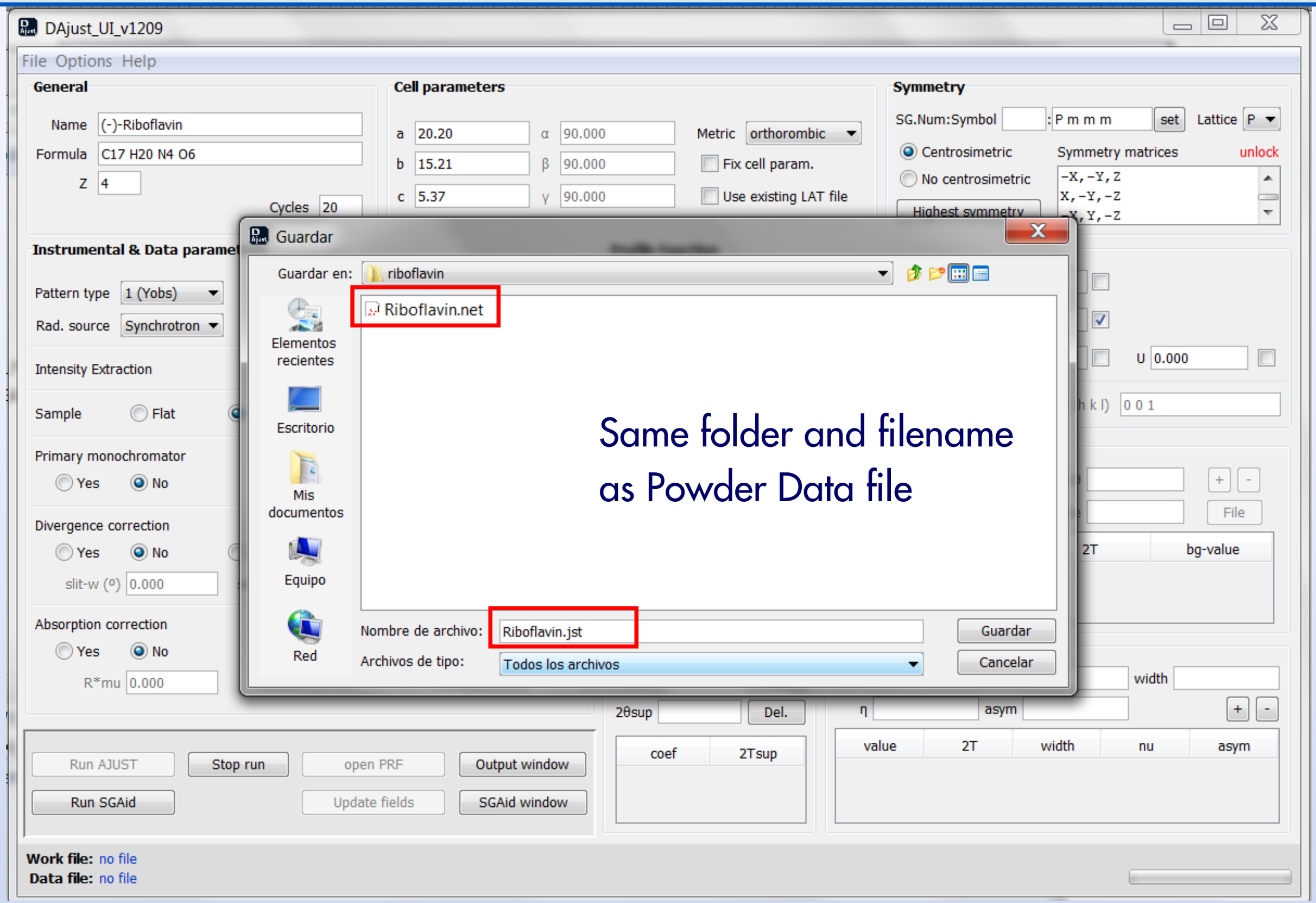
Data file: no file

DAjust_UI Output

Font Size: + - on top

```
    DAjust Software - version 1209
    Report of errors to the authors will be appreciated.

[08:58] bin directory: C:\ovallcorba\UIs\WEB dajust-xlens\DAjust_1209\bin\
```

DAjust UI - Save JST and run DAjust



DAjust UI - Check DAjust result

DAjust_UI Output

Font Size: + - on top

```
[10:49] file saved: O:\ovallcorba\riboflavin\dajust\riboflavin.jst
[10:49] PDD file found: O:\ovallcorba\riboflavin\dajust\riboflavin.net

[10:49]  ************************************************
[10:49]  ****              AJUST OUTPUT:             ****
[10:49]  ************************************************
[10:49]    2.060000      9.9999998E-03   58.32000
[10:49]    2.060000      9.9999998E-03   55.00000
[10:49]   NUM.REFLEXS < T2MAX=          1205
[10:49]    0  0.4275E+01  0.1497E+01  0.1322E+01  0.1214E+03
[10:49]    1  0.1018E+01  0.8890E+00  0.1007E+01  0.2889E+02
[10:49]    2  0.1567E+01  0.9504E+00  0.9611E+00  0.4448E+02
[10:49]    3  0.1799E+01  0.1022E+01  0.1229E+01  0.5108E+02
[10:49]    4  0.1463E+01  0.9440E+00  0.1056E+01  0.4154E+02
[10:49]    5  0.8848E+00  0.7936E+00  0.9234E+00  0.2512E+02
[10:49]    6  0.1069E+01  0.8336E+00  0.1011E+01  0.3036E+02
[10:49]    7  0.8727E+00  0.7605E+00  0.9015E+00  0.2478E+02
[10:49]    8  0.8086E+00  0.7308E+00  0.9036E+00  0.2296E+02
[10:49]    9  0.7899E+00  0.6941E+00  0.8543E+00  0.2242E+02
[10:49]   10  0.7255E+00  0.6464E+00  0.8064E+00  0.2060E+02
[10:49]   11  0.6781E+00  0.5973E+00  0.7567E+00  0.1925E+02
[10:49]   12  0.6381E+00  0.5530E+00  0.6970E+00  0.1811E+02
[10:49]   13  0.6046E+00  0.5187E+00  0.6302E+00  0.1716E+02
[10:49]   14  0.5671E+00  0.4780E+00  0.5612E+00  0.1610E+02
[10:49]   15  0.5295E+00  0.4349E+00  0.4851E+00  0.1503E+02
[10:49]   16  0.4950E+00  0.3951E+00  0.4170E+00  0.1405E+02
[10:49]   17  0.4599E+00  0.3593E+00  0.3697E+00  0.1306E+02
[10:49]   18  0.4261E+00  0.3228E+00  0.3134E+00  0.1210E+02
[10:49]   19  0.3931E+00  0.2914E+00  0.2677E+00  0.1116E+02
[10:49]   20  0.3716E+00  0.2674E+00  0.2259E+00  0.1055E+02
[10:49]
[10:49]   ZERO-SHIFT:
[10:49]   -0.01587   0.00021
[10:49]   FINAL LATTICE PARAMETERS:
[10:49]   20.16345  15.17621   5.35084   90.0000   90.0000   90.0000
[10:49]
[10:49]      Volume=     1637.383
[10:49]
[10:49]   ST. DEVS. OF LATTICE PARAMETERS:
[10:49]     1     0.00046
[10:49]     2     0.00031
[10:49]     3     0.00010
[10:49]   PEAK WIDTH PARAMETERS:
[10:49]     0.540E-01   0.328E-02  -0.339E-03
[10:49]     0.111E-01   0.411E-03  -0.671E-03
[10:49]   SCALA FACTOR:
[10:49]    0.1009E+01  0.6427E-02  0.9414E-02
[10:49]  ------------------------------------------------------------------------
[10:49]  Cycle   Rwp  Rp   RB   Chi(planes) Chi(dist)   Chi(I)
[10:49]   20  0.3716E+00  0.2674E+00  0.2259E+00  0.1055E+02

[10:49] New χ = 10.55  (no previous run to compare with)
[10:49] Better χ, fields updated. To recover old values click on reload JST.
[10:49] file read: O:\ovallcorba\riboflavin\dajust\riboflavin.new
[10:49] dAjust finished
```

more cycles needed

χ=10.55

DAjust_UI_v1209

File Options Help

General

Name (-)-Riboflavin
Formula C17 H20 N4 O6
Z 4
Cycles 20

Cell parameters

a 20.16345 α 90.000
b 15.17621 β 90.000
c 5.35084 γ 90.000
Metric orthorombic
Fix cell param.
Use existing LAT file

Symmetry

SG.Num:Symbol : P m m m set Lattice P
Centrosimetric / No centrosimetric
Symmetry matrices unlock
-X,-Y,Z
X,-Y,-Z
Highest symmetry

Instrumental & Data parameters

Pattern type 1 (Yobs) nYline 10 2θsup 55.0000
Rad. source Synchrotron λ1 0.88320 λ2 0.00000
Intensity Extraction NFWHM 20 tolerance 0.5000
Sample Flat Capillary
Primary monochromator Yes No cos 2θ 1.00000
Divergence correction Yes No Fixed slit Variable slit
slit-w (°) 0.0000 sample size 0.0000 armlenght 0.0000
Absorption correction Yes No
R*mu 0.0000 2θRefInt 0.0000 Transmi. 0.0000

Profile Function

Type Pseudo-Voigt T... zero -0.015873 exp 1.0000
Lorentzian coef. X 0.540E-01 Y 0.111E-01
Gaussian coef. W 0.000E+00 V 0.000E+00 U 0.000E+00
Pref. Orientation: March-coef 1.000 direction (h k l) 0 0 1

Excluded zones

2θinf Add
2θsup Del.
2Tinf 2Tsup

Background

type Removed 2θ
<back> 60.00000 bg-value File
FWHM 0.15000
Iterations 20
2T bg-value

Asymmetry correction

coef. Add
2θsup Del.
coef 2Tsup

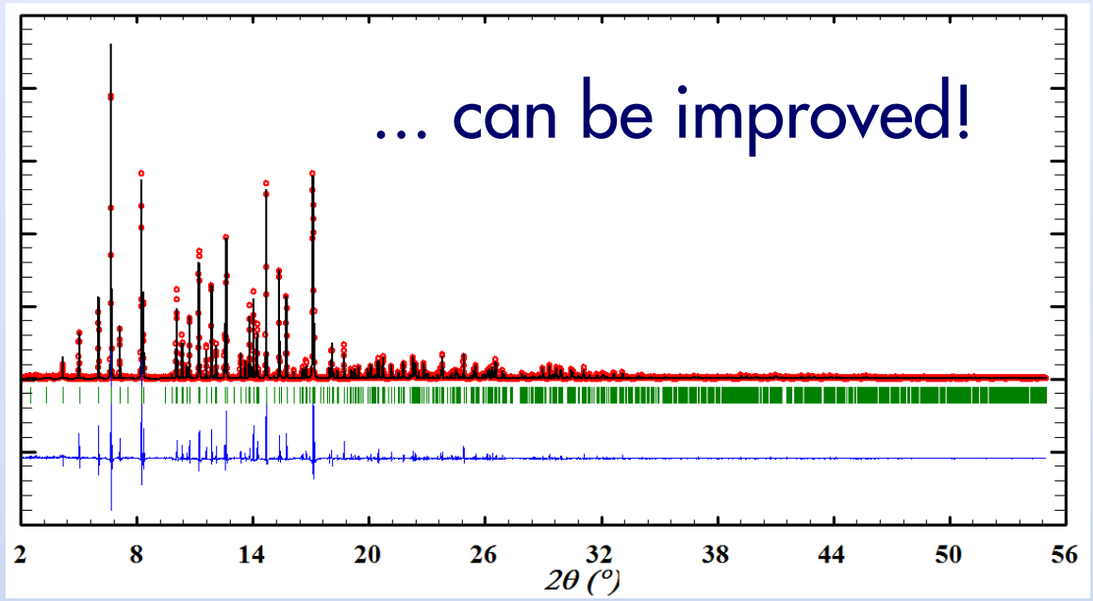
Ghost peaks

value 2θ width
η asym
value 2T width nu asym

Run AJUST Stop run open PRF Output window
Run SGAid Reload JST SGAid window

Work file: O:\ovallcorba\riboflavin\dajust\riboflavin.jst
Data file: O:\ovallcorba\riboflavin\dajust\riboflavin.net

Fields updated



… can be improved!

DAjust UI - Run DAjust (#2)

- 20 extra cycles with new parameters
- 1 Gaussian parameter (W)

DAjust_UI_v1209

File Options Help

General

Name (-)-Riboflavin

Formula C17 H20 N4 O6

Z 4

Cycles 20

Cell parameters

a 20.16345 α 90.000

b 15.17621 β 90.000

c 5.35084 γ 90.000

Metric orthorombic

Fix cell param.

Use existing LAT file

Symmetry

SG.Num:Symbol : P m m m set Lattice P

Centrosimetric

No centrosimetric

Highest symmetry

Symmetry matrices unlock

-X,-Y,Z

X,-Y,-Z

Profile Function

Type Pseudo-Voigt T... zero -0.015873 exp 1.0000

Lorentzian coef. X 0.540E-01 Y 0.111E-01

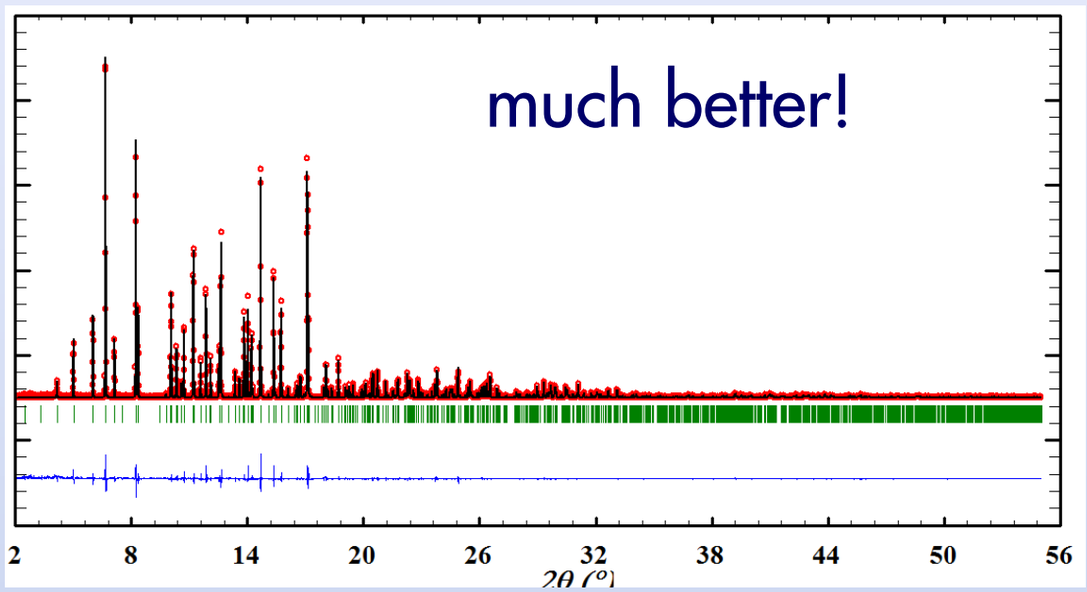
Gaussian coef. W 0.001 V 0.000E+00 U 0.000E+00

DAjust_UI Output

Font Size: + - on top

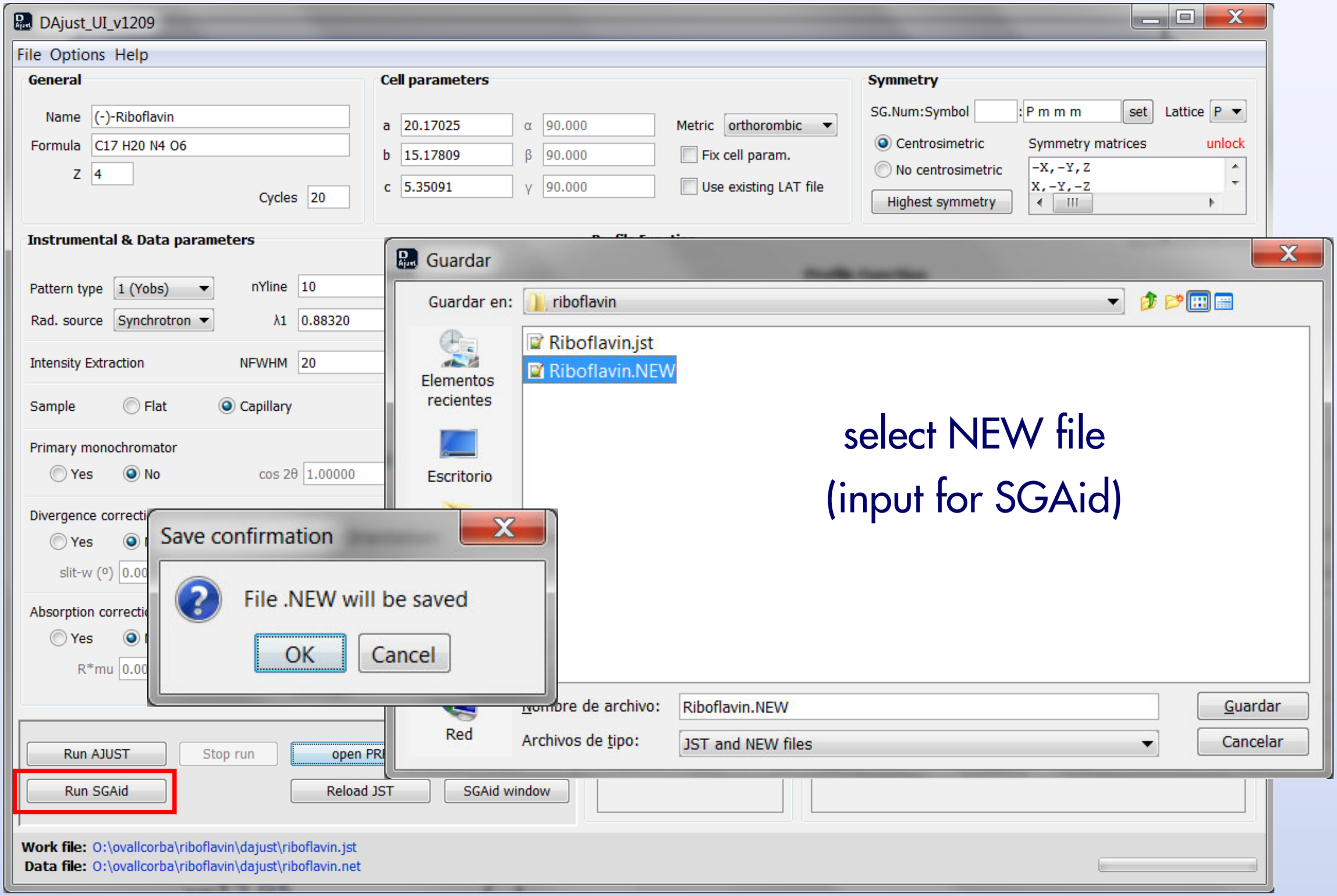
```
[10:55]   16  0.1897E+00  0.1012E+00  0.5403E-01  0.5385E+01
[10:55]   17  0.1896E+00  0.1012E+00  0.5414E-01  0.5382E+01
[10:55]   18  0.1895E+00  0.1012E+00  0.5426E-01  0.5381E+01
[10:55]   19  0.1895E+00  0.1011E+00  0.5434E-01  0.5379E+01
[10:55]   20  0.1894E+00  0.1011E+00  0.5447E-01  0.5379E+01
[10:55]
[10:55]   ZERO-SHIFT:
[10:55]   -0.01853   0.00011
[10:55]   FINAL LATTICE PARAMETERS:
[10:55]   20.17025  15.17809   5.35091   90.0000   90.0000   90.0000
[10:55]
[10:55]      Volume=     1638.159
[10:55]
[10:55]   ST. DEVS. OF LATTICE PARAMETERS:
[10:55]     1     0.00022
[10:55]     2     0.00016
[10:55]     3     0.00005
[10:55]   PEAK WIDTH PARAMETERS:
[10:55]     0.272E-01   0.138E-02  -0.628E-04
[10:55]     0.239E-02   0.179E-03   0.510E-05
[10:55]     0.793E-03   0.809E-05   0.112E-07
[10:55]   SCALA FACTOR:
[10:55]    0.9997E+00  0.2850E-02 -0.2533E-03
[10:55]  ------------------------------------------------------------------
[10:55]  Cycle   Rwp  Rp   RB   Chi(planes) Chi(dist)   Chi(I)
[10:55]   20  0.1894E+00  0.1011E+00  0.5447E-01  0.5379E+01

[10:55] New χ = 5.379  (previous χ = 10.55)
[10:55] Better χ, fields updated. To recover old values click on reload JST.
[10:55] file read: O:\ovallcorba\riboflavin\dajust\riboflavin.new
[10:55] dAjust finished
```

χ=5.38



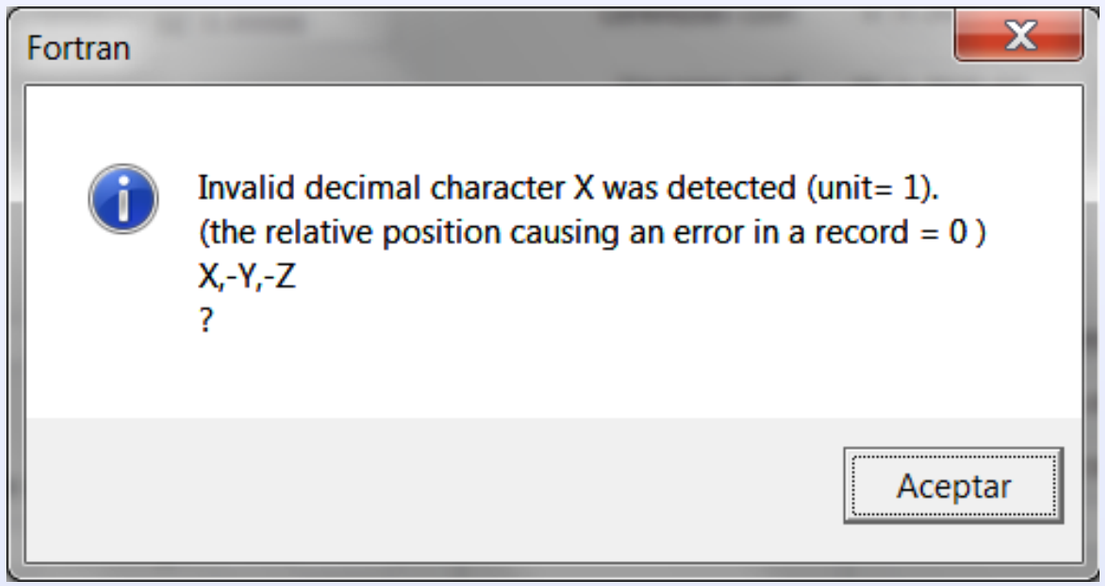
DAjust UI - Run SGAid

- Space group determination



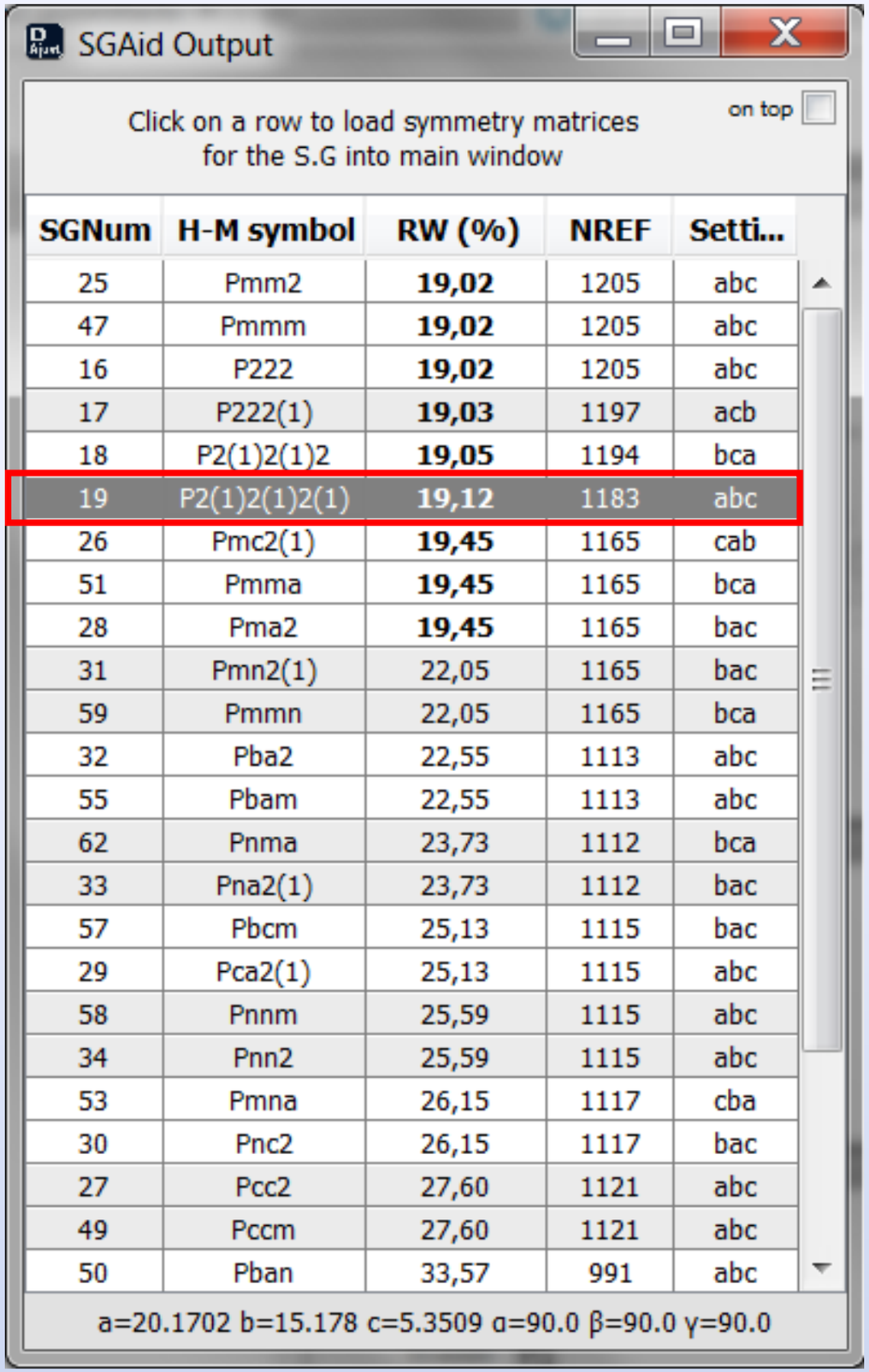
DAjust UI - Run SGAid

(Maybe a Fortran error in some systems)



Just wait a moment and click again **run SGAid**!

DAjust UI - SGAid Output



SGNum	H-M symbol	RW (%)	NREF	Setti...
25	Pmm2	**19,02**	1205	abc
47	Pmmm	**19,02**	1205	abc
16	P222	**19,02**	1205	abc
17	P222(1)	**19,03**	1197	acb
18	P2(1)2(1)2	**19,05**	1194	bca
19	P2(1)2(1)2(1)	**19,12**	1183	abc
26	Pmc2(1)	**19,45**	1165	cab
51	Pmma	**19,45**	1165	bca
28	Pma2	**19,45**	1165	bac
31	Pmn2(1)	22,05	1165	bac
59	Pmmn	22,05	1165	bca
32	Pba2	22,55	1113	abc
55	Pbam	22,55	1113	abc
62	Pnma	23,73	1112	bca
33	Pna2(1)	23,73	1112	bac
57	Pbcm	25,13	1115	bac
29	Pca2(1)	25,13	1115	abc
58	Pnnm	25,59	1115	abc
34	Pnn2	25,59	1115	abc
53	Pmna	26,15	1117	cba
30	Pnc2	26,15	1117	bac
27	Pcc2	27,60	1121	abc
49	Pccm	27,60	1121	abc
50	Pban	33,57	991	abc

Ranked list of possible Space Groups

- Rw(%) in bold are the most probable
- Lowest NREF

(–)-Riboflavin is $P2_12_12_1$

in this case the three SGs with Rw=19.38 considered as probable are not correct (can be tested clicking and running DAjust)

DAjust UI - Final DAjust run

DAjust_UI_v1209

File Options Help

General

Name (-)-Riboflavin

Formula C17 H20 N4 O6

Z 4

Cycles 20

Cell parameters

a 20.1702 α 90.000

b 15.178 β 90.0

c 5.3509 γ 90.000

Metric orthorombic

Fix cell param.

Use existing LAT file

Symmetry

SG.Num:Symbol 19 : P 21 21 21 set Lattice P

Centrosimetric

No centrosimetric

Highest symmetry

Symmetry matrices unlock

X+1/2,-Y+1/2,-Z
-X,Y+1/2,-Z+1/2
-X+1/2,-Y,Z+1/2

Updated!

Instrumental & Data parameters

Pattern type 1 (Yobs) nYline 10 2θsup 55.0000

Rad. source Synchrotron λ1 0.88320 λ2 0.00000

Intensity Extraction NFWHM 20 tolerance 0.5000

Sample Flat Capillary

Primary monochromator

Yes No cos 2θ 1.00000

Divergence correction

Yes No Fixed slit Variable slit

slit-w (º) 0.0000 sample size 0.0000 armlenght 0.0000

Absorption correction

Yes No

R*mu 0.0000 2θRefInt 0.0000 Transmi. 0.0000

Profile Function

Type Pseudo-Voigt T... zero -0.018528 exp 1.0000

Lorentzian coef. X 0.272E-01 Y 0.239E-02

Gaussian coef. W 0.793E-03 V 0.000E+00 U 0.000E+00

Pref. Orientation: March-coef 1.000 direction (h k l) 0 0 1

Excluded zones

2θinf Add

2θsup Del.

2Tinf	2Tsup

Background

type Removed 2θ + -

<back> 60.00000 bg-value File

FWHM 0.15000

Iterations 20

2T	bg-value

Asymmetry correction

coef. Add

2θsup Del.

coef	2Tsup

Ghost peaks

value 2θ width

η asym + -

value	2T	width	nu	asym

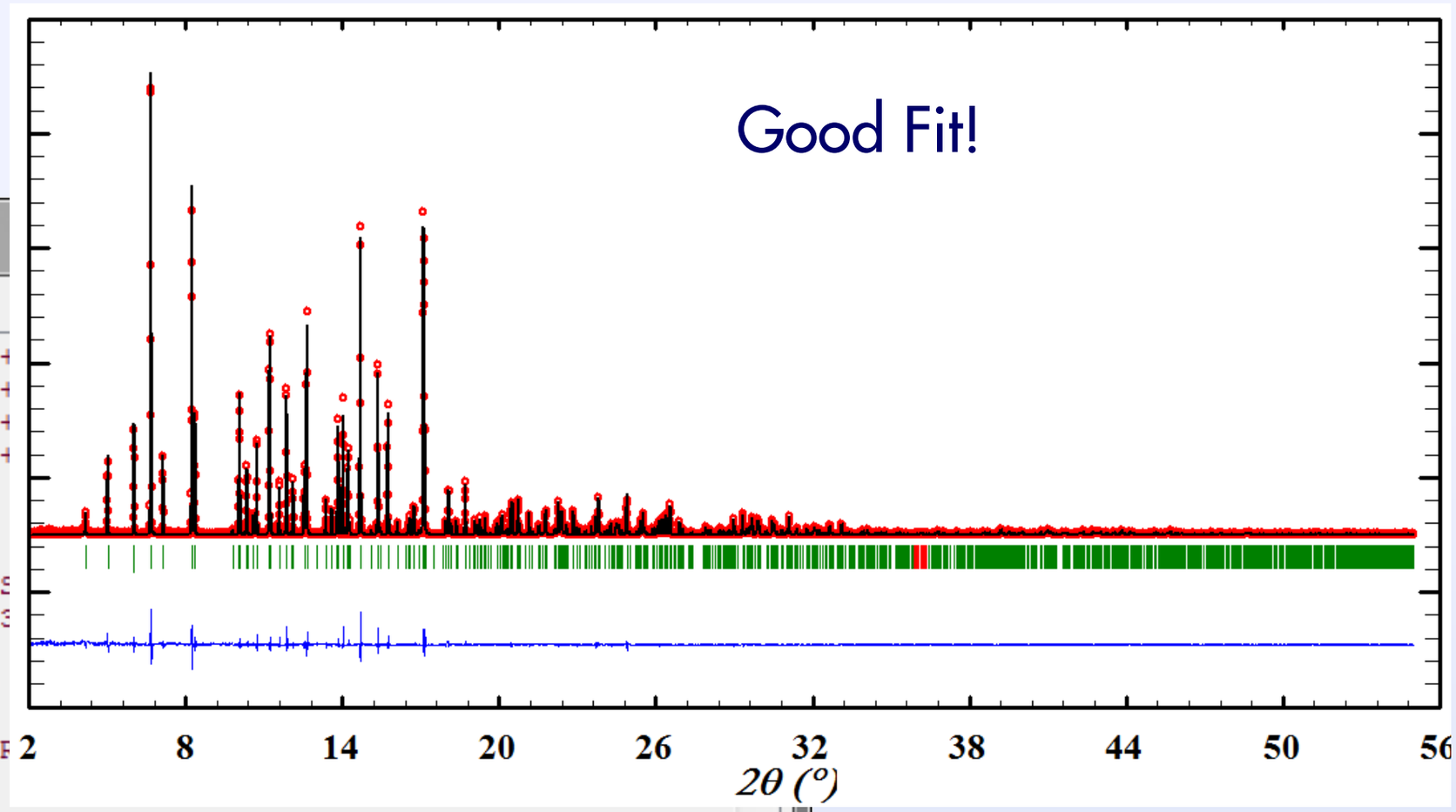
Run AJUST | Stop run | open PRF | Output window

Run SGAid | Reload JST | SGAid window

Work file: O:\ovallcorba\riboflavin\dajust\riboflavin.jst

Data file: O:\ovallcorba\riboflavin\dajust\riboflavin.net

DAjust UI - DAjust Result



DAjust_UI Output

Font Size: + -

```
[12:13]    17   0.1903E+00   0.1017E+
[12:13]    18   0.1903E+00   0.1016E+
[12:13]    19   0.1903E+00   0.1016E+
[12:13]    20   0.1903E+00   0.1016E+
[12:13]
[12:13]    ZERO-SHIFT:
[12:13]    -0.01843    0.00011
[12:13]    FINAL LATTICE PARAMETERS
[12:13]    20.17060  15.17828   5.3
[12:13]
[12:13]       Volume=      1638.209
[12:13]
[12:13]    ST. DEVS. OF LATTICE PAR
[12:13]      1      0.00021
[12:13]      2      0.00016
[12:13]      3      0.00005
[12:13]    PEAK WIDTH PARAMETERS:
[12:13]      0.270E-01    0.138E-02  -0.206E-05
[12:13]      0.242E-02    0.179E-03   0.362E-06
[12:13]      0.792E-03    0.812E-05  -0.137E-07
[12:13]    SCALA FACTOR:
[12:13]     0.9998E+00  0.2864E-02 -0.2065E-03
[12:13]   ------------------------------------------------------------------
[12:13]   Cycle    Rwp   Rp    RB    Chi(planes) Chi(dist)    Chi(I)
[12:13]    20  0.1903E+00  0.1016E+00  0.5543E-01  0.5404E+01

[12:13] New χ = 5.404   (previous χ = 5.381)
[12:13] Worse χ, fields not updated. To load new values click on load NEW.
[12:13] dAjust finished
```

same χ

DAjust UI - Output Files and possibilities

.LST

Relevant information on the refinement.

```
  RIETVELD REFINEMENT OUTPUT:

  ZERO-SHIFT:
  -0.01843   0.00011
  FINAL LATTICE PARAMETERS:
  20.17060  15.17828   5.35091   90.0000   90.0000
90.0000

     Volume=     1638.209

  ST. DEVS. OF LATTICE PARAMETERS:
    1      0.00021
    2      0.00016
    3      0.00005
  PEAK WIDTH PARAMETERS:
    0.270E-01   0.138E-02  -0.206E-05
    0.242E-02   0.179E-03   0.362E-06
    0.792E-03   0.812E-05  -0.137E-07
  SCALA FACTOR:
   0.9998E+00  0.2864E-02 -0.2065E-03
 ------------------------------------------------------
Cycle    Rwp   Rp    RB    Chi(I)
  20  0.1903E+00  0.1016E+00  0.5543E-01  0.5404E+01
```

.NEW

Updated JST file

Structure Solution (tomorrow talks)

.QCK

Input data file for TALP (Structure solution by Direct-Space Methods) [Vallcorba *et al.* 2012]

.POW

Input data file for XLENS (Structure solution by Direct Methods) [Rius, 2011]

.PRF

For visual inspection with WinPLOTR [Roisnel & Rodriguez-Carvajal, 2010]

.LTN, .NOT, .CAL, .OBS, .DIF, .FON

(see DAjust publication or program manual)

DAjust with AJUST & SGAid

Jordi Rius, Oriol Vallcorba, Inma Peral, Carlos Frontera, Carles Miravitlles

PowderXRD 2013

www.icmab.es/crystallography/software

Vallcorba, O., Rius, J., Frontera, C., Peral, I. & Miravitlles, C. (2012). "DAJUST: a suite of computer programs for pattern matching, space-group determination and intensity extraction from powder diffraction data", *J. Appl. Cryst.*, **45**, 844–848

THANK YOU FOR YOUR ATTENTION!!

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CSIC
Consejo Superior de Investigaciones Científicas

ICMAB
Institut de Ciència de Materials de Barcelona
www.icmab.es
Campus de la UAB
08193-Bellaterra (Spain)

ALBA
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