BLAND: A Stimulating Method for the Analysis of Diffraction Patterns

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Overview

Crystal Structure
Model Refinement
Bayesian Data Analysis

UNIT CELL

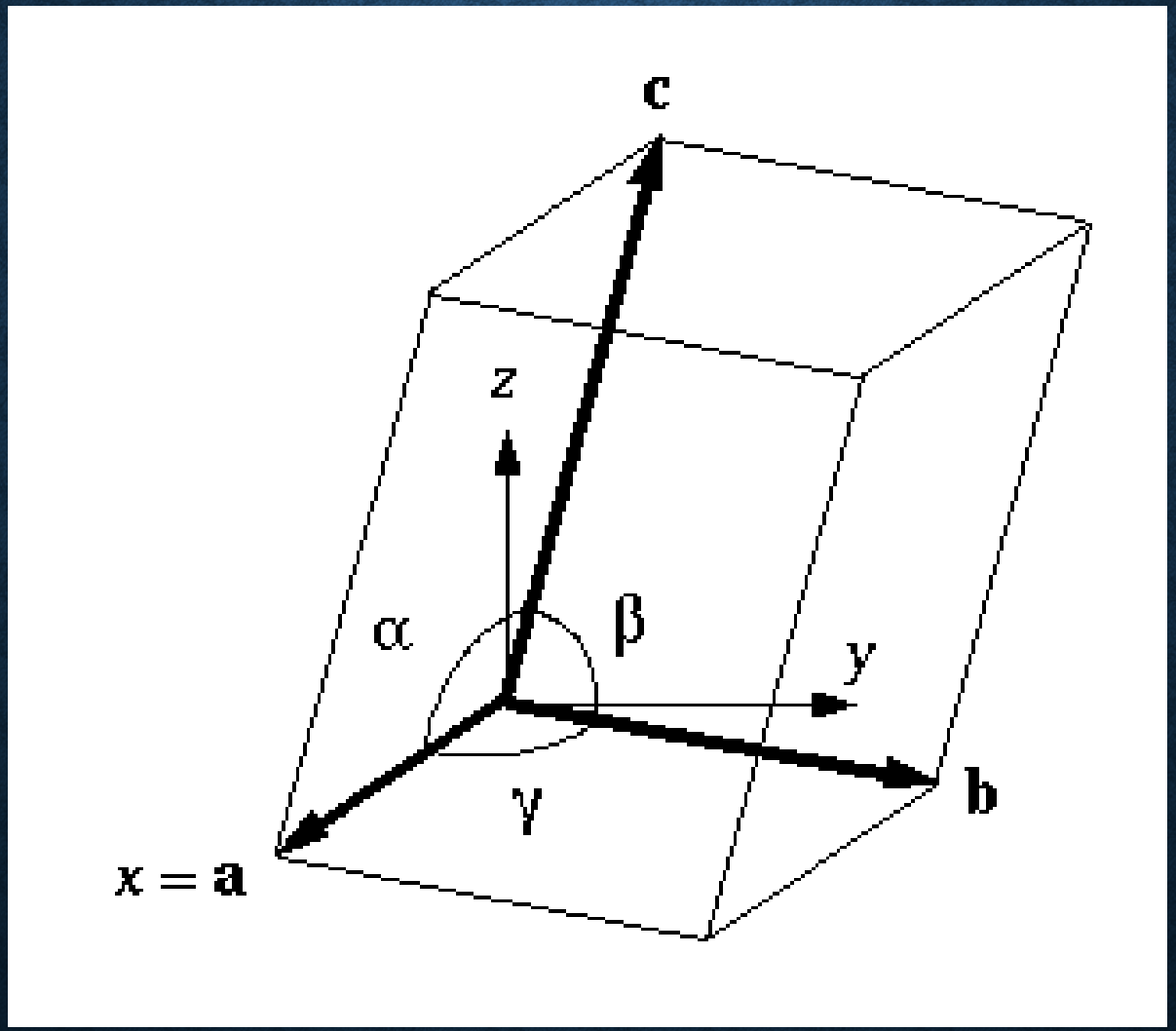


Image: ctcms.nist.gov

Unit Cell Types

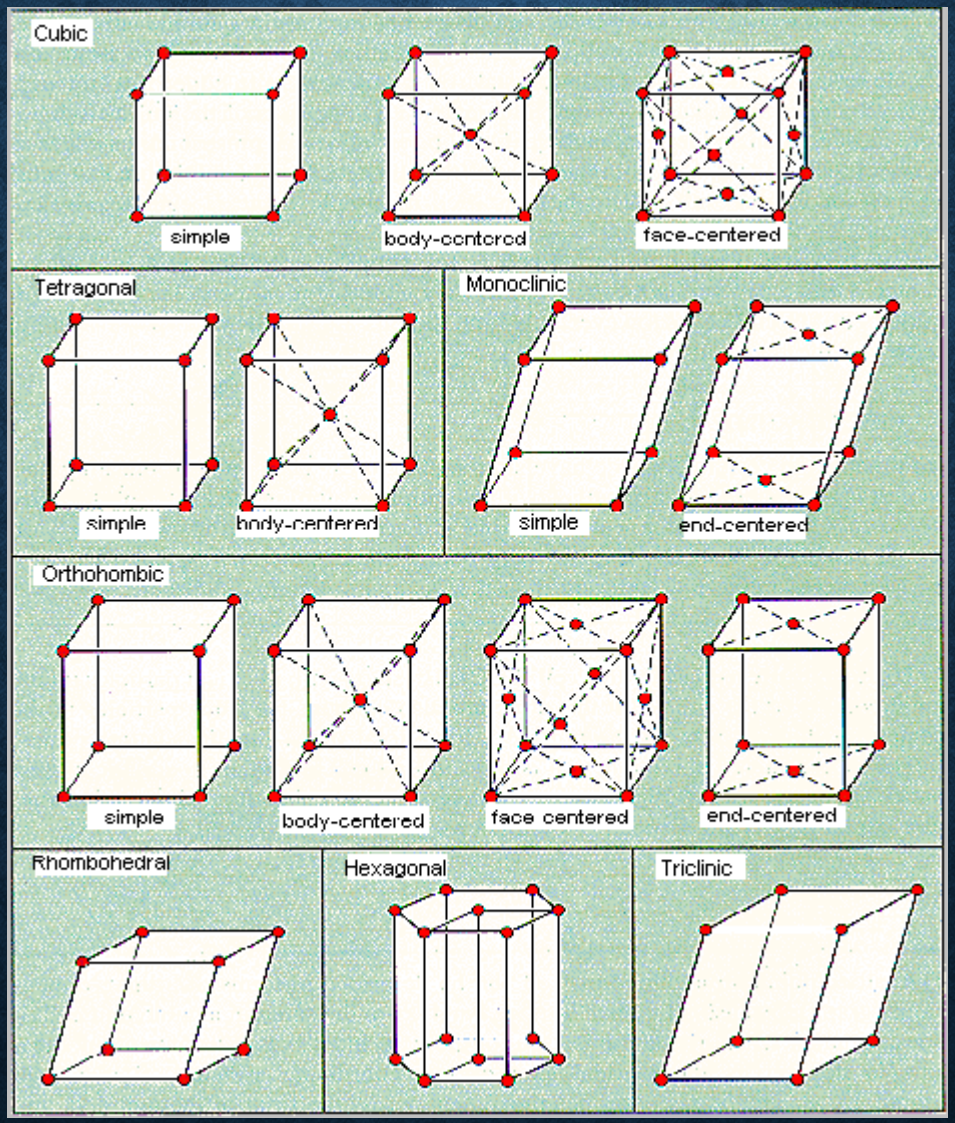


Image: chem.purdue.edu

Bragg Diffraction

Bragg's Law: $2d \sin\theta = \lambda$

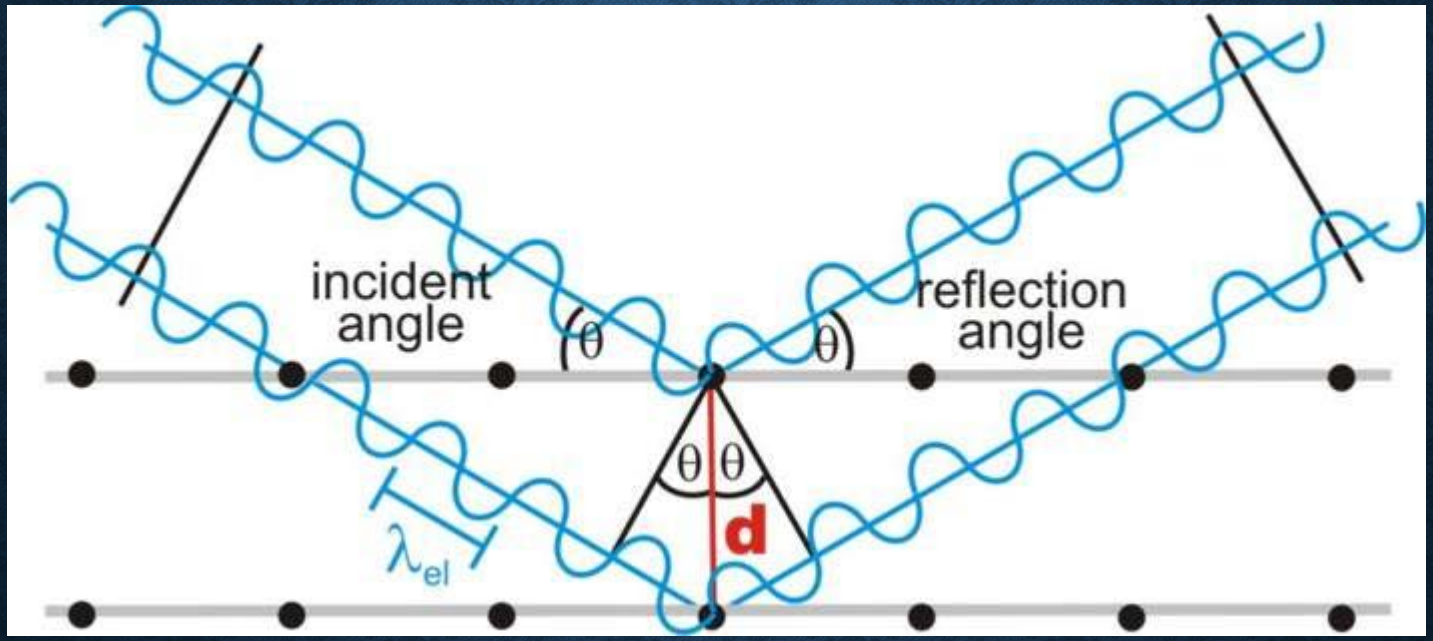
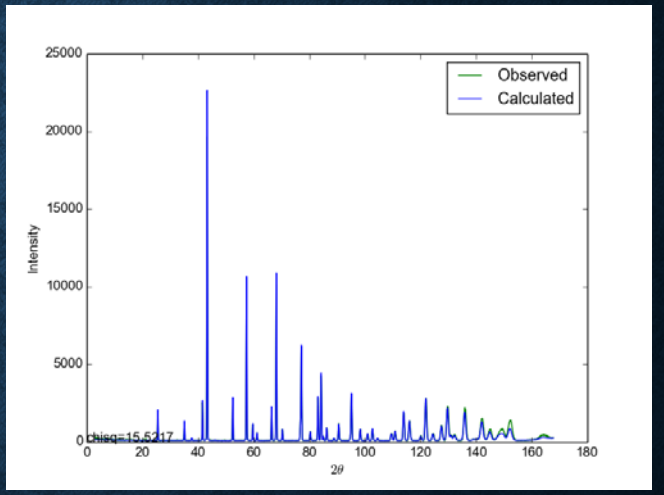


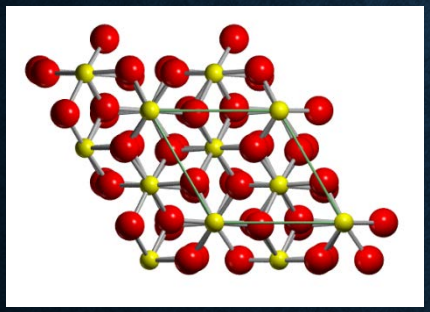
Image: microscopy.ethz.ch

Diffractometer

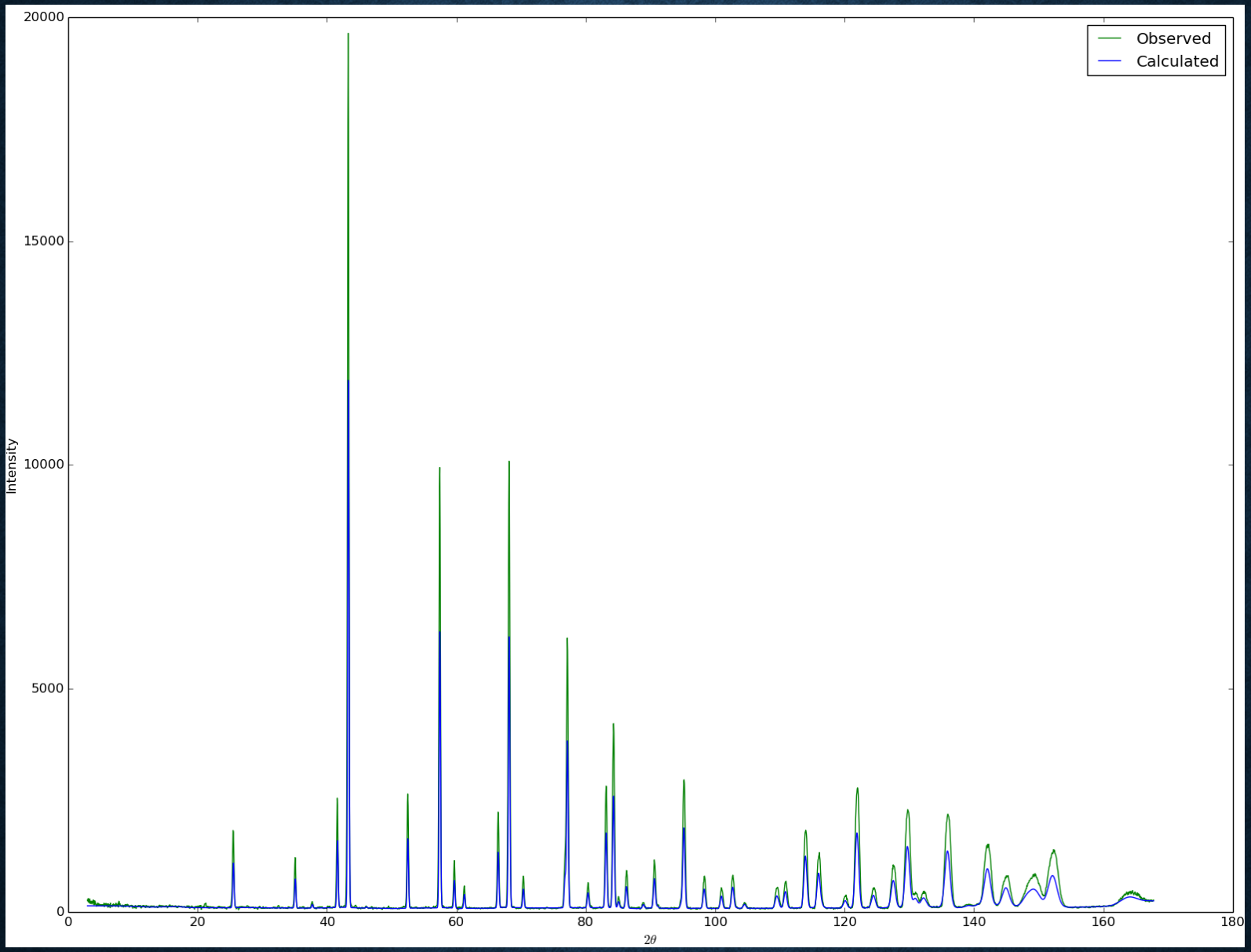
Ideally give same diffraction pattern



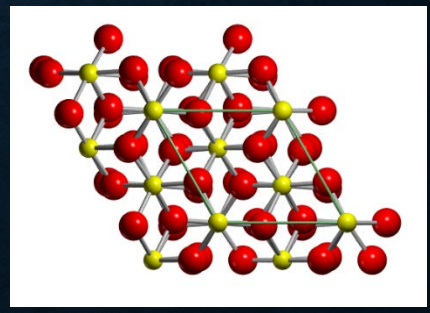
Crystalline powder



Images: ncnr.nist.gov, theochem.unito.it



Reality



Images: ncnr.nist.gov, theochem.unito.it

FullProf Suite

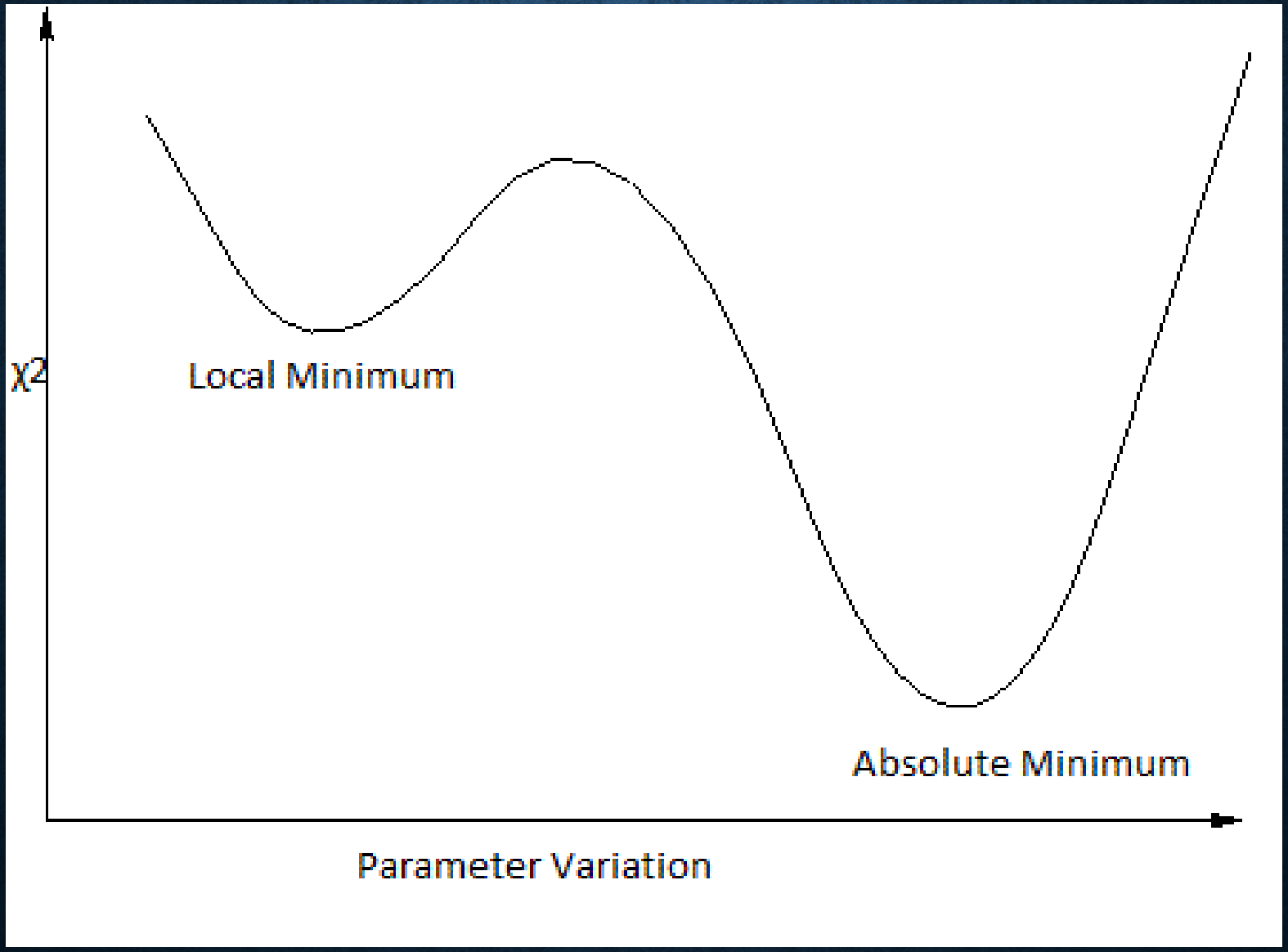
Crystallographic tools for Rietveld, profile matching & integrated intensity refinements of X-Ray and/or neutron data

(Juan Rodríguez-Carvajal)

- Allows hand fitting using Gauss-Newton Algorithm
- Similar to GSAS, TOPAS, etc.
- Uses PCR files to handle fits
- Powered by CrysFML Library

```
COMM  Test G.Courbion data on Na2Ca3Al2F14  3T2 (Diam: 6mm H=50mm)
! Current global Chi2 (Bragg contrib.) =      3.265
! Files => DAT-file: ncaf_3t2.dat,  PCR-file: ncaf_3t2
!Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
  1   7   2 -1   2   0   1   0   0   0   1   0   0   0   0   0   0   0   1
!
!Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho Ana
  0   2   1   2   1   0   4   0   0   1   6 -1   1   0   0   0   0
!
! Lambda1  Lambda2    Ratio    Bkpos    Wdt    Cthm     muR   AsyLim   Rpolarz  2nd-muR -> Patt# 1
 1.225300 1.225300  0.00000   30.000 10.0000  0.0000  0.0000   35.00    0.0000  0.0000
!
!NCY  Eps  R_at  R_an  R_pr  R_gl     Thmin      Step      Thmax    PSD    Sent0
  8  0.05  1.00  1.00  1.00  1.00      0.0000   0.050000   125.4500   0.000   0.000
!
! Excluded regions (LowT  HighT) for Pattern#  1
       0.00       5.00
     125.00      180.00
!
!
    51    !Number of refined parameters
```

Gauss-Newton Algorithm



Bayesian Data Analysis

Dream Fitting Algorithm

- Markov Chain
- Monte Carlo
- Differential Evolution

BUMPS

Bayesian Uncertainty Modeling of Parametric Systems

```
step 10206 cost 3.85175379008
                                    O1 x ....|.....   0.909055 in (-0.1,2)
                                    O1 z .....|....   0.595744 in (-0.5,1.6)
                                    O2 x .....|....   0.192831 in (-0.9,1.2)
                                    O2 z ....|.....   0.542582 in (-0.5,1.6)
                                    O3 x .....|....   0.081153 in (-1,1.1)
                                    O3 y ....|.....  0.0282213 in (-1,1.1)
                                    O3 z ....|.....   0.807125 in (-0.2,1.9)
                                    Pb B |.........   0.374014 in (0,10)
                                    Pb x .....|....    0.18723 in (-0.9,1.2)
                                    Pb z .....|....   0.167179 in (-0.9,1.2)
                                     S x .....|....  0.0648723 in (-1,1.1)
                                     S z .....|....   0.685412 in (-0.4,1.7)
                                   base .....|....    213.475 in (-80,430)
                                      a .....|....    8.47816 in (7.9,9)
                                      b .....|....    5.39688 in (4.8,5.9)
                                      c .....|....    6.95831 in (6.4,7.5)
                                    eta ....|.....   0.451881 in (0,1)
                                  scale .|........    1.14508 in (0,10)
                                      u |.........   0.155385 in (0,2)
                                      v ........|.  -0.361573 in (-2,0)
                                      w .|........   0.374667 in (0,2)
                                   zero ...|......  -0.138759 in (-0.3,0.11)
step 10207 cost 3.85175379008
```

BLAND

Bayesian Library for Analysis of Neutron Diffraction data

Origin

- Pain-staking hand written wrapper code
- Wrapped only a small portion of Fortran library
- Unstable due to unsafe assumptions concerning memory layout of Fortran derived types

✓ Automated Global Fitting

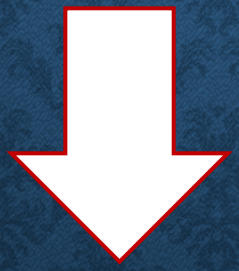
✓ Eliminate need for intuition

Assumption

1	2	3	4

Possible Reality

1	2	3	//	4



```
jel@jel-VirtualBox:~/Pycrysfml/Data$ python Al2O3.py
Segmentation fault (core dumped)
jel@jel-VirtualBox:~/Pycrysfml/Data$
```

PyCrysfml Library

- Uses custom version of FortWrap (fortwrap.sourceforge.net) to generate C++ wrapper for use with SWIG (swig.org)
- Automatic build script wraps entire library into native python module
- Greater stability
- Adaptable to changes in library

GOALS

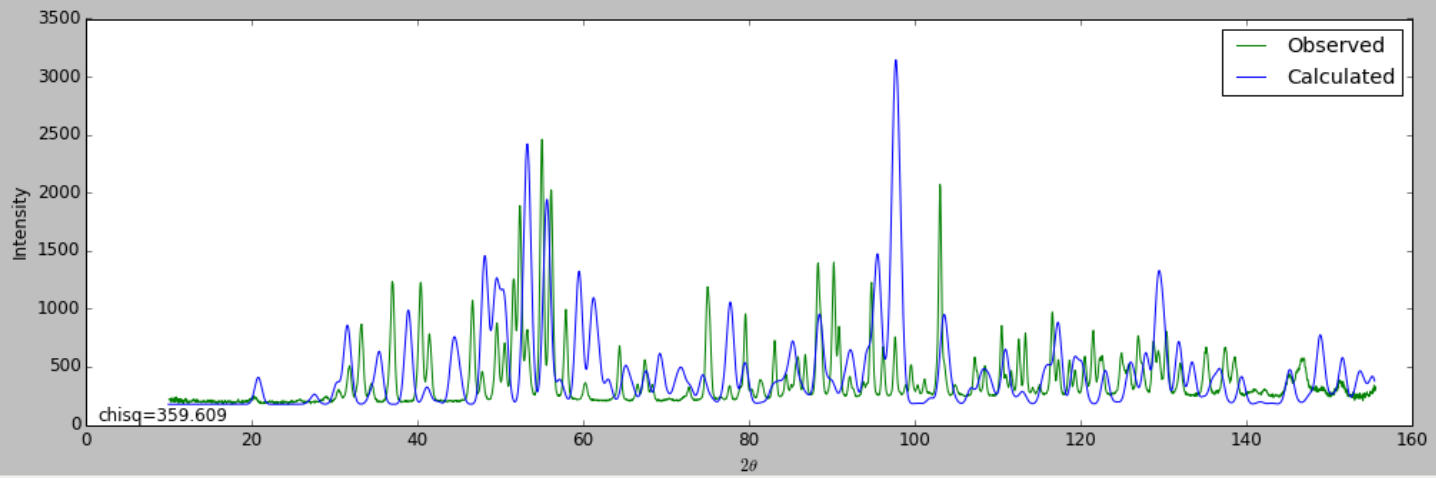
- ✓ Automated Global Fitting
- ✓ Eliminate need for intuition
- ✓ Reliability
- ✓ Adaptability
- ❑ Magnetism
- ❑ Single Crystal Patterns

EXAMPLE FITS

$PBSO_4$ Pre-fit

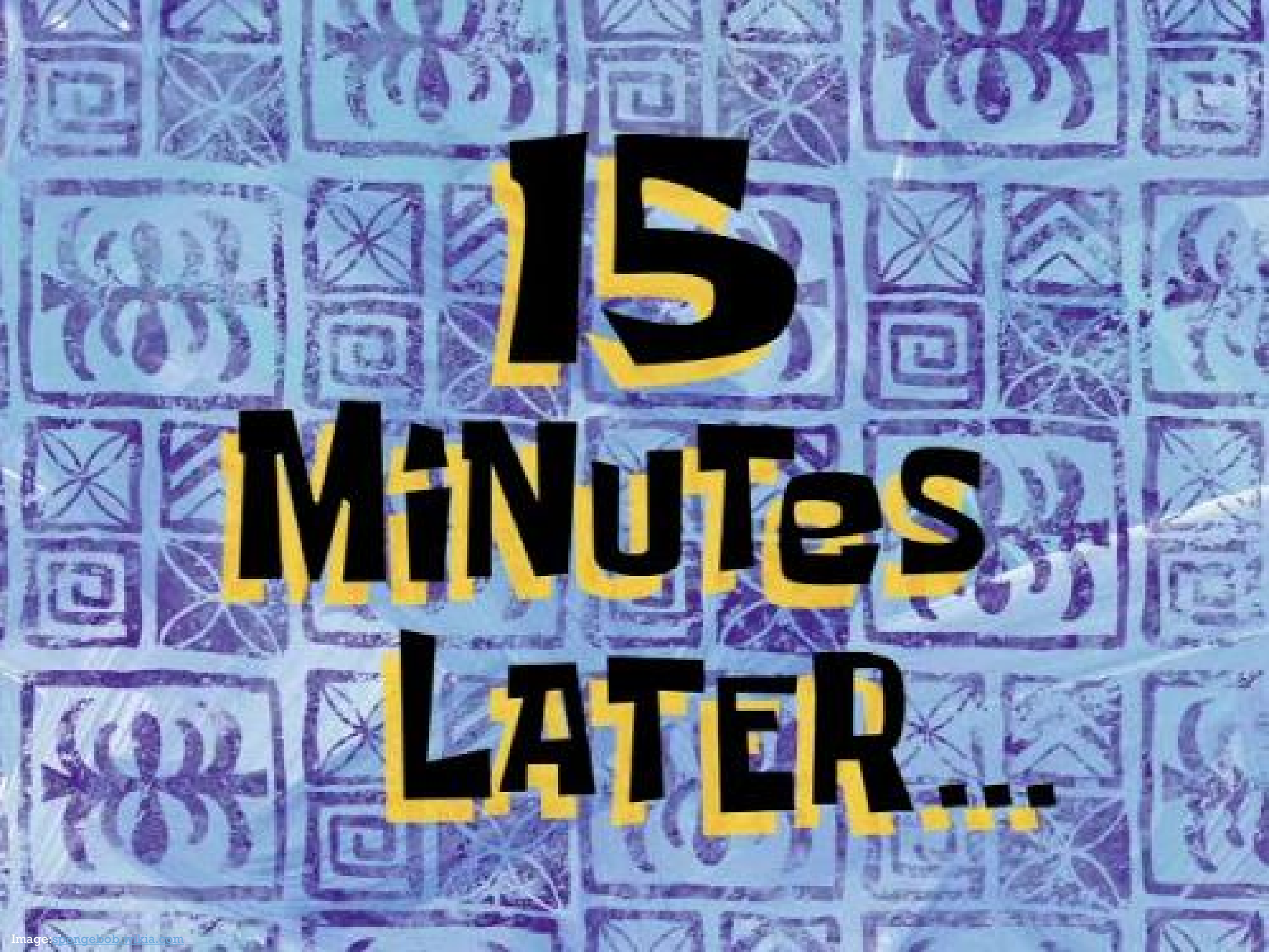
Bumps: PbSO4

Data

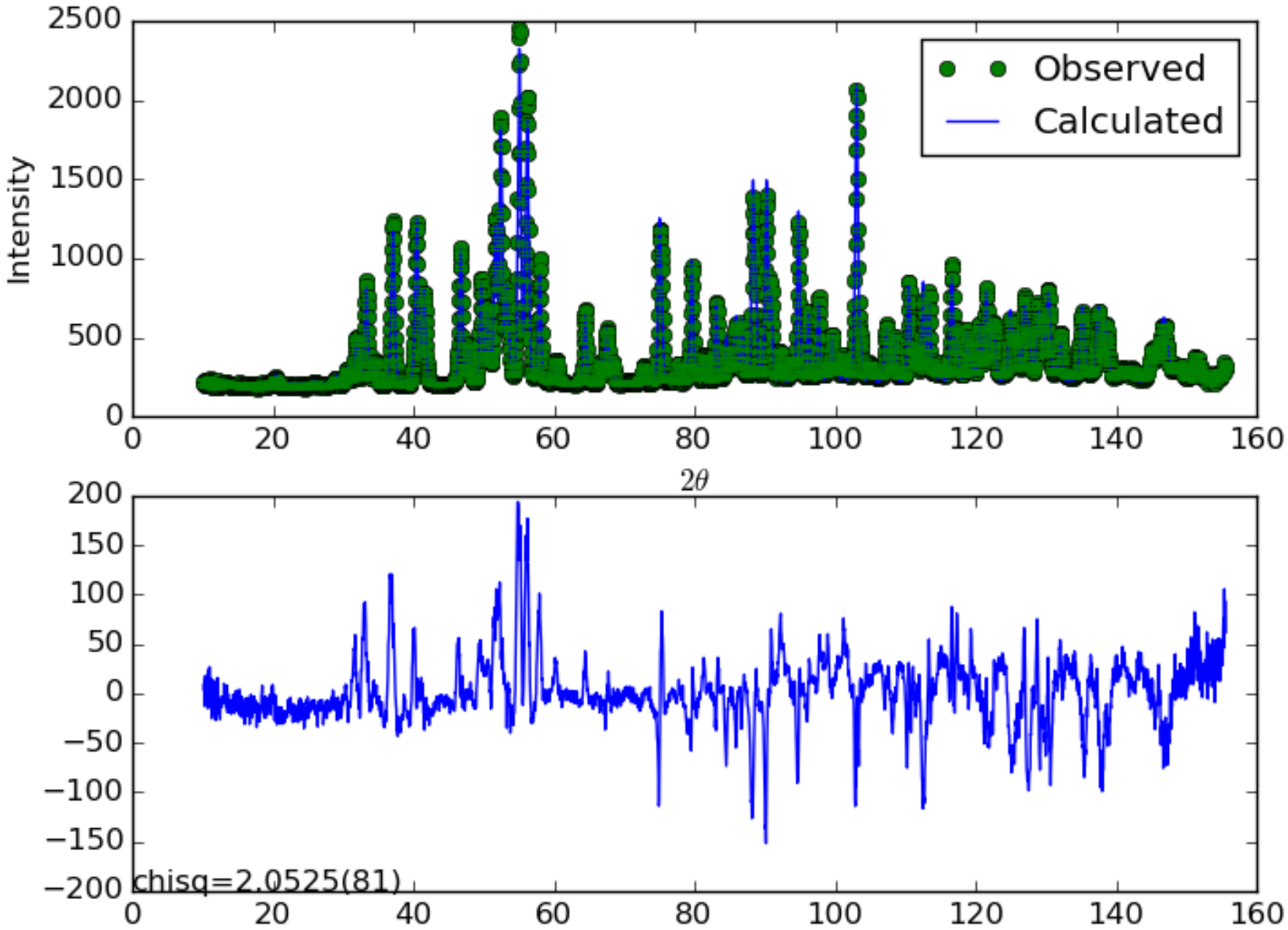


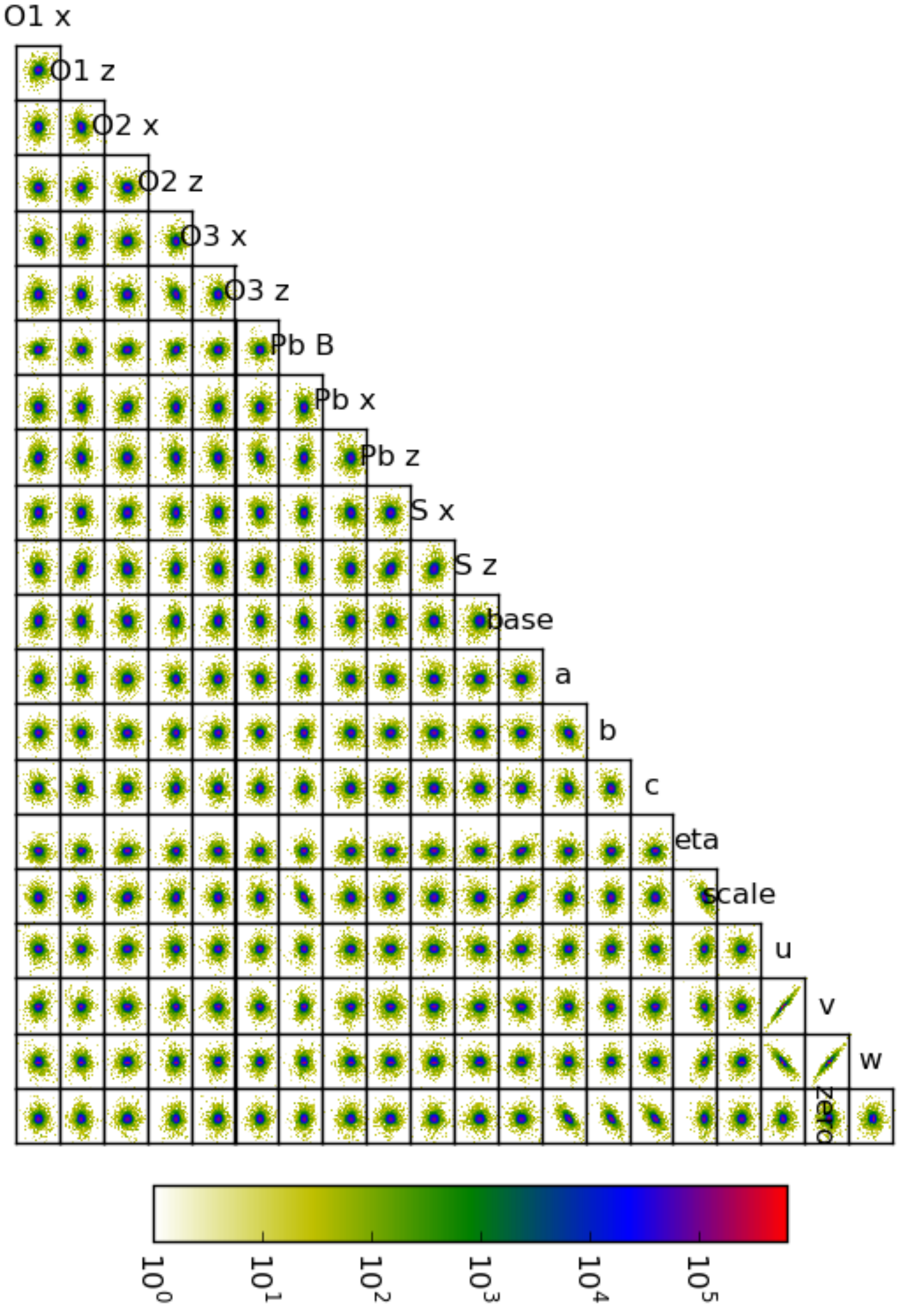
Parameters | Summary | Log | Convergence | Uncertainty | Correlations | Parameter Trace | Model Uncertainty

Model	Parameter	Value	Minimum	Maxim...	Fit?
Model					
atoms					
O1					
O1 B	O1 B	0.5			No
O1 occ	O1 occ	1.0			No
O1 x	O1 x	0.8861	0.8	1.01	Yes
O1 y	O1 y	0.25			No
O1 z	O1 z	0.553	0.49	0.7	Yes
O2					
O2 B	O2 B	0.5			No
O2 occ	O2 occ	1.0			No
O2 x	O2 x	0.2139	0.09	0.3	Yes
O2 y	O2 y	0.25			No
O2 z	O2 z	0.5618	0.44	0.65	Yes
O3					
O3 B	O3 B	0.5			No
O3 occ	O3 occ	1.0			No
O3 x	O3 x	0.085	-0.02	0.19	Yes
O3 y	O3 y	0.02709	-0.08	0.13	Yes



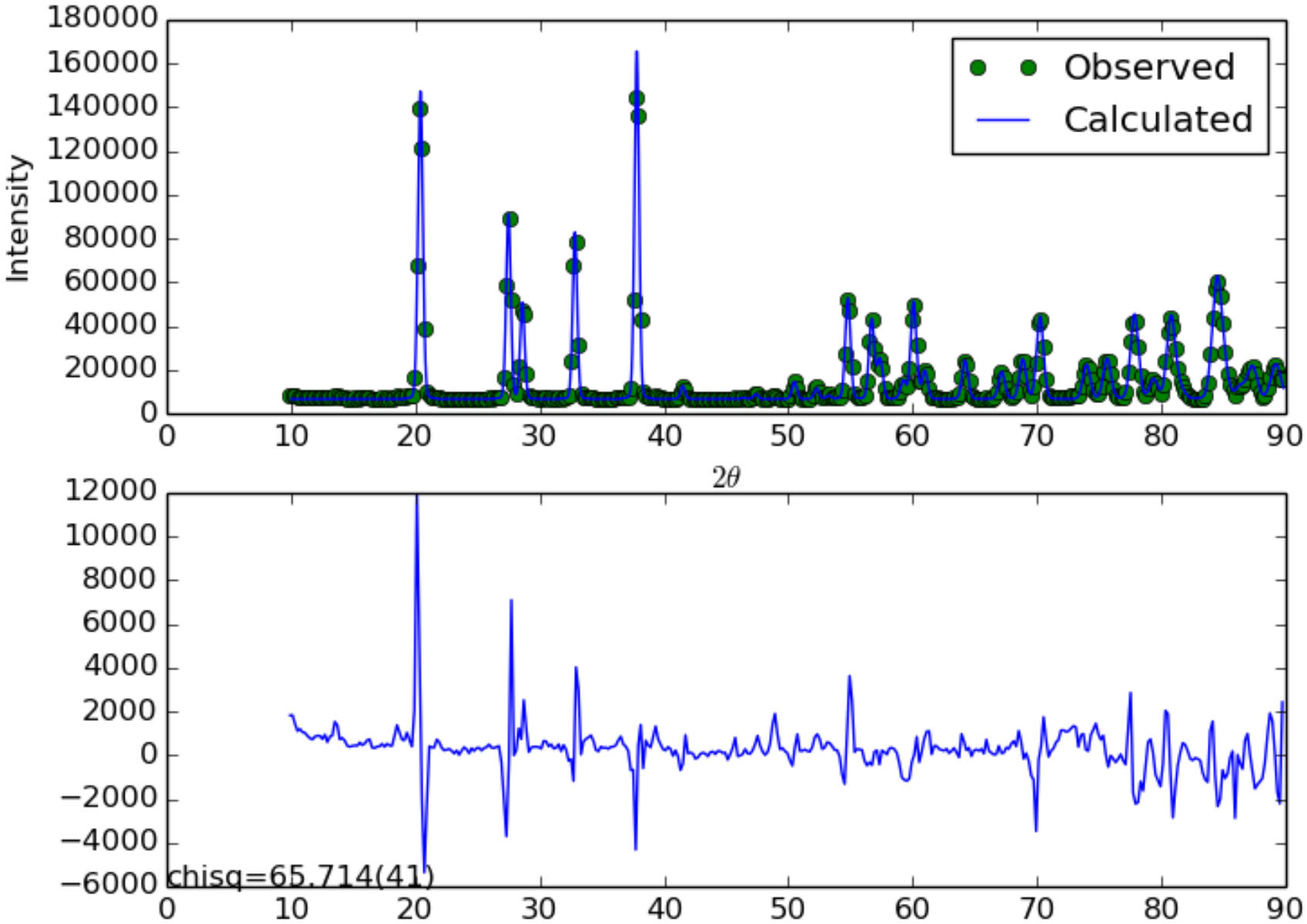
$PbSO_4$

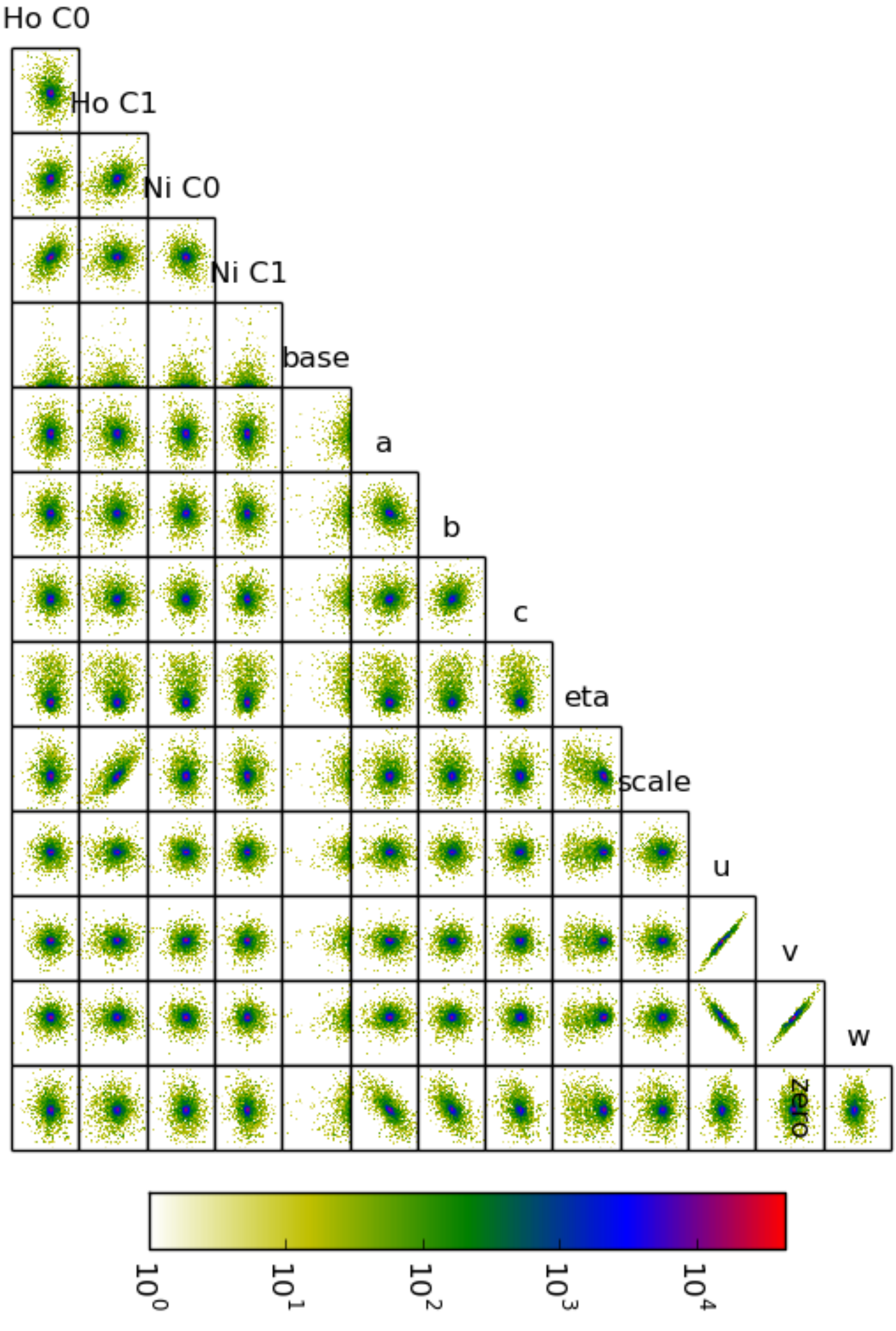



O1 x
O1 z
O2 x
O2 z
O3 x
O3 z
Pb B
Pb x
Pb z
S x
S z
base
a
b
c
eta
scale
u
v
w
zero
PbSO4
10^0
10^1
10^2
10^3
10^4
10^5

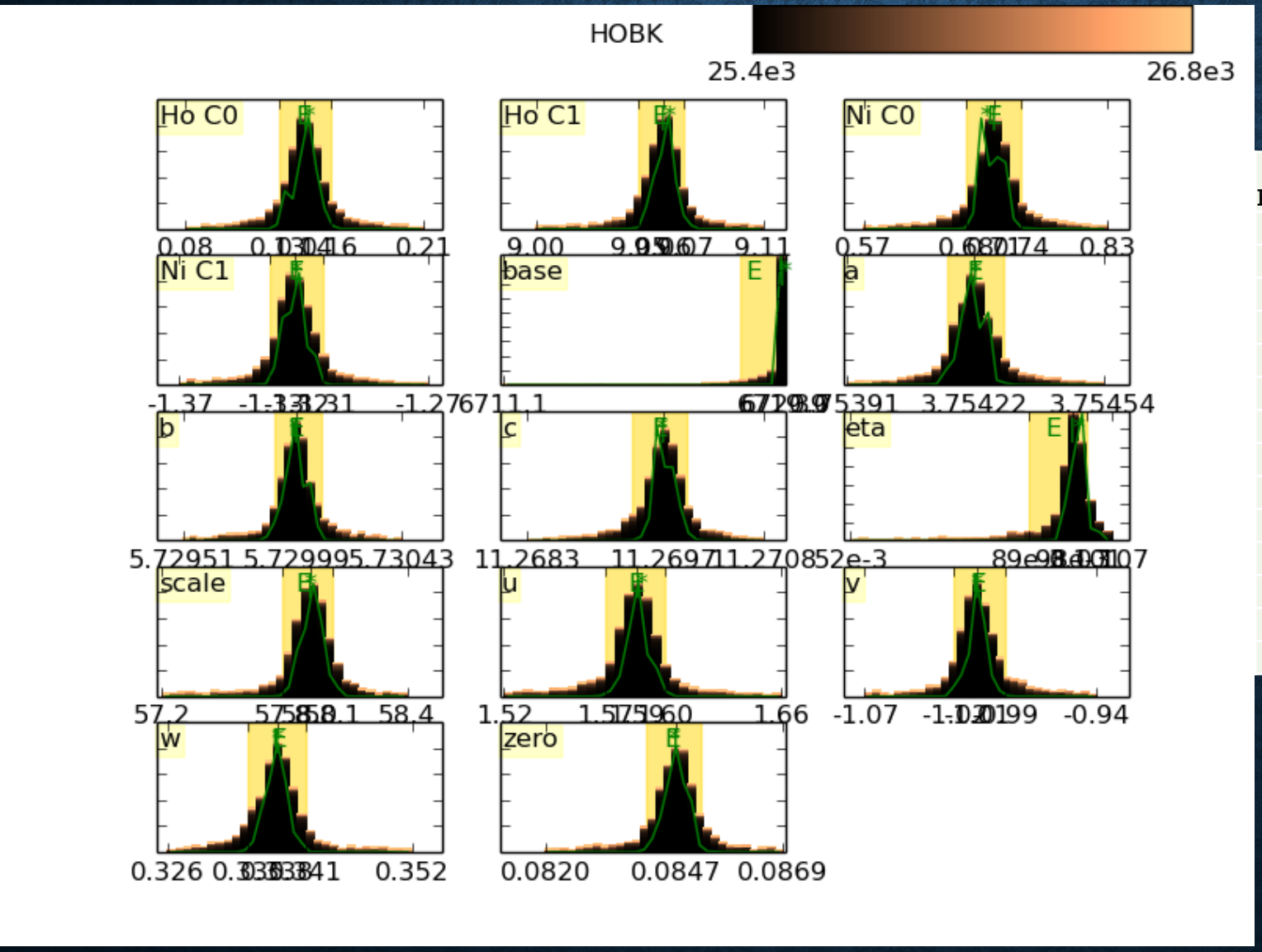
Parameter	Value	95% Interval
O1 x	0.90905528	[0.9082, 0.9095]
O1 z	0.59574381	[0.5951, 0.5964]
O2 x	0.19283123	[0.1924, 0.1937]
O2 z	0.54258205	[0.5418, 0.5434]
O3 x	0.08115299	[0.08077, 0.08152]
O3 y	0.02822131	[0.0277, 0.0288]
O3 z	0.80712467	[0.80669, 0.80758]
Pb B	0.37401401	[0.32, 0.51]
Pb x	0.18722964	[0.18689, 0.18752]
Pb z	0.16717933	[0.16676, 0.16767]
S x	0.06487234	[0.0641, 0.0663]
S z	0.68541183	[0.6839, 0.6866]
base	213.475422	[212.53, 217.71]
a	8.47815771	[8.47788, 8.47844]
b	5.39688196	[5.39672, 5.39710]
c	6.95830693	[6.95801, 6.95853]
eta	0.45188095	[0.03, 0.47]
scale	1.14508016	[1.065, 1.152]
u	0.15538536	[0.142, 0.163]
v	-0.3615733	[-0.380, -0.330]
w	0.37466735	[0.361, 0.412]
zero	-0.1387589	[-0.1420, -0.1359]

Ho_2BaNiO_5



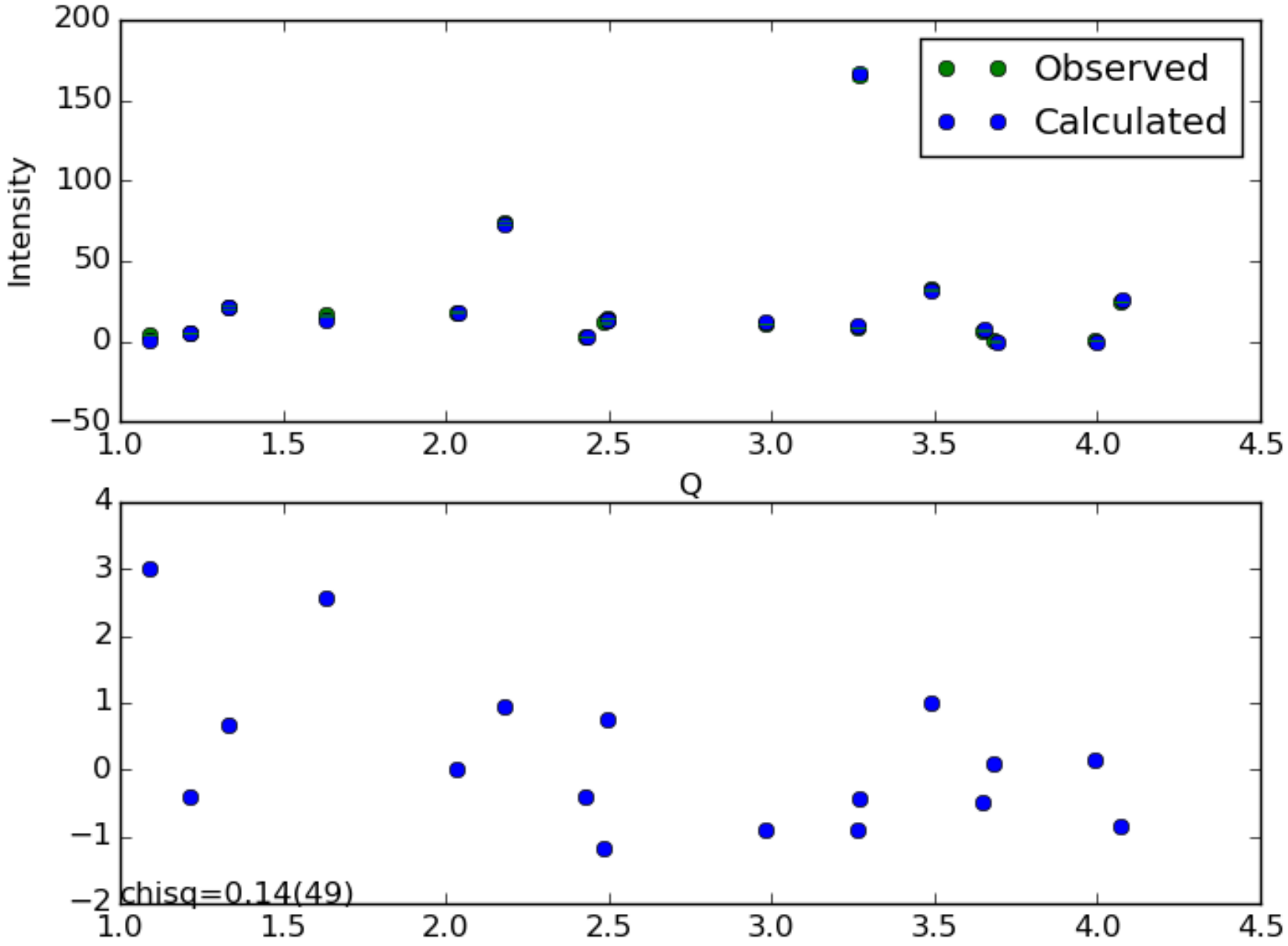

Ho C0
Ho C1
Ni C0
Ni C1
base
a
b
c
eta
scale
u
v
w
zero
HOBK
10^0
10^1
10^2
10^3
10^4

Ho_2BaNiO_5 Results

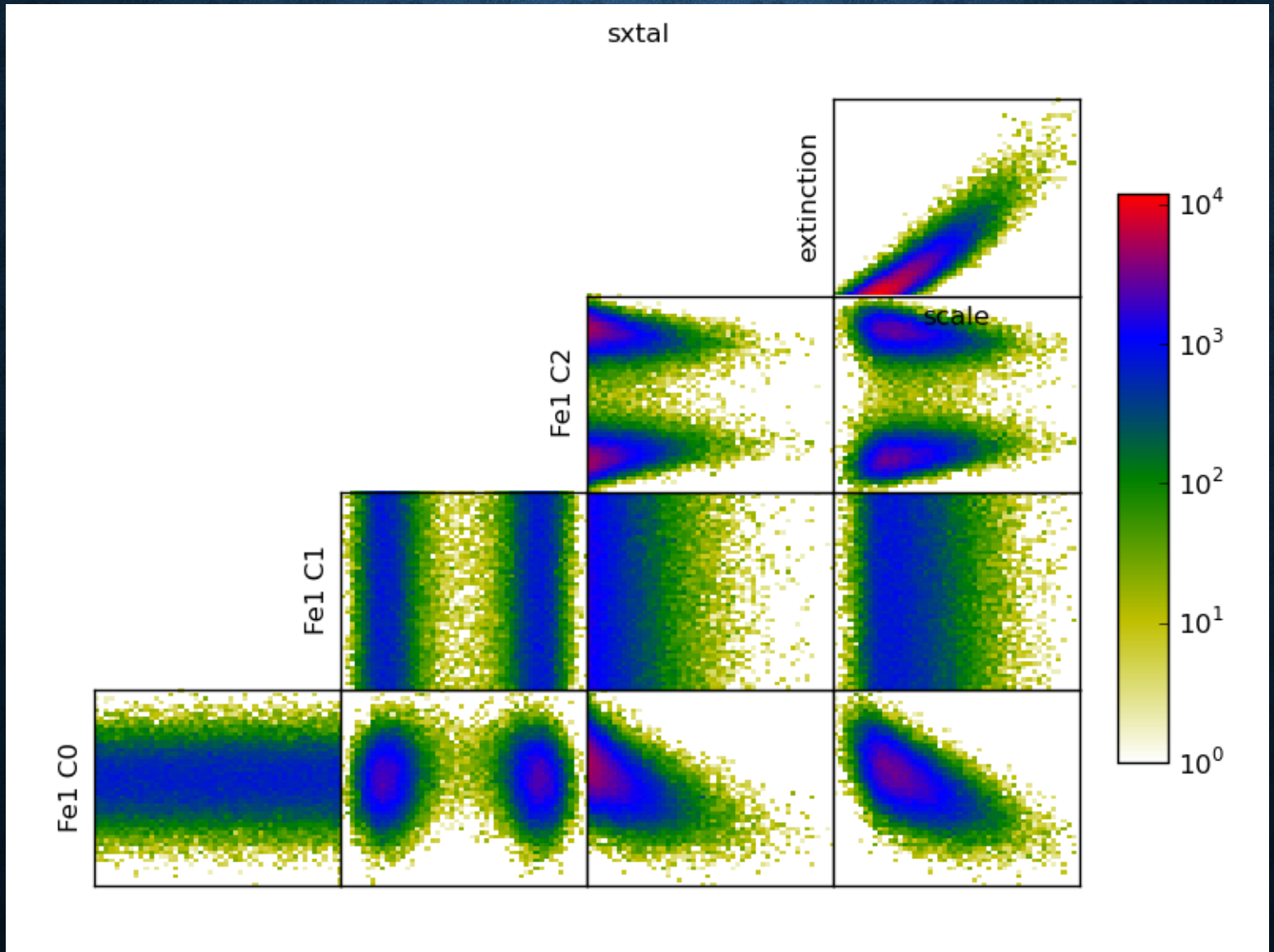


Parameter	Value	[95% interval]
Ho C0	0.145	[0.08 0.21]
Ho C1	9.063	[9.00 9.11]
Ni C0	0.699	[0.57 0.83]
Ni C1	-1.321	[-1.37 -1.27]
base	6719.97	[6711.10 6720.00]
a	3.7542	[3.75391 3.75454]
b	5.7299	[5.72951 5.73043]
c	11.26	[11.2683 11.2708]
eta	0.0993	[0.052 0.107]
scale	57.949	[57.23 58.43]
u	1.589	[1.52 1.66]
v	-1.006	[-1.07 -0.94]
w	0.3375	[0.326 0.352]
zero	0.08465	[0.0820 0.0869]

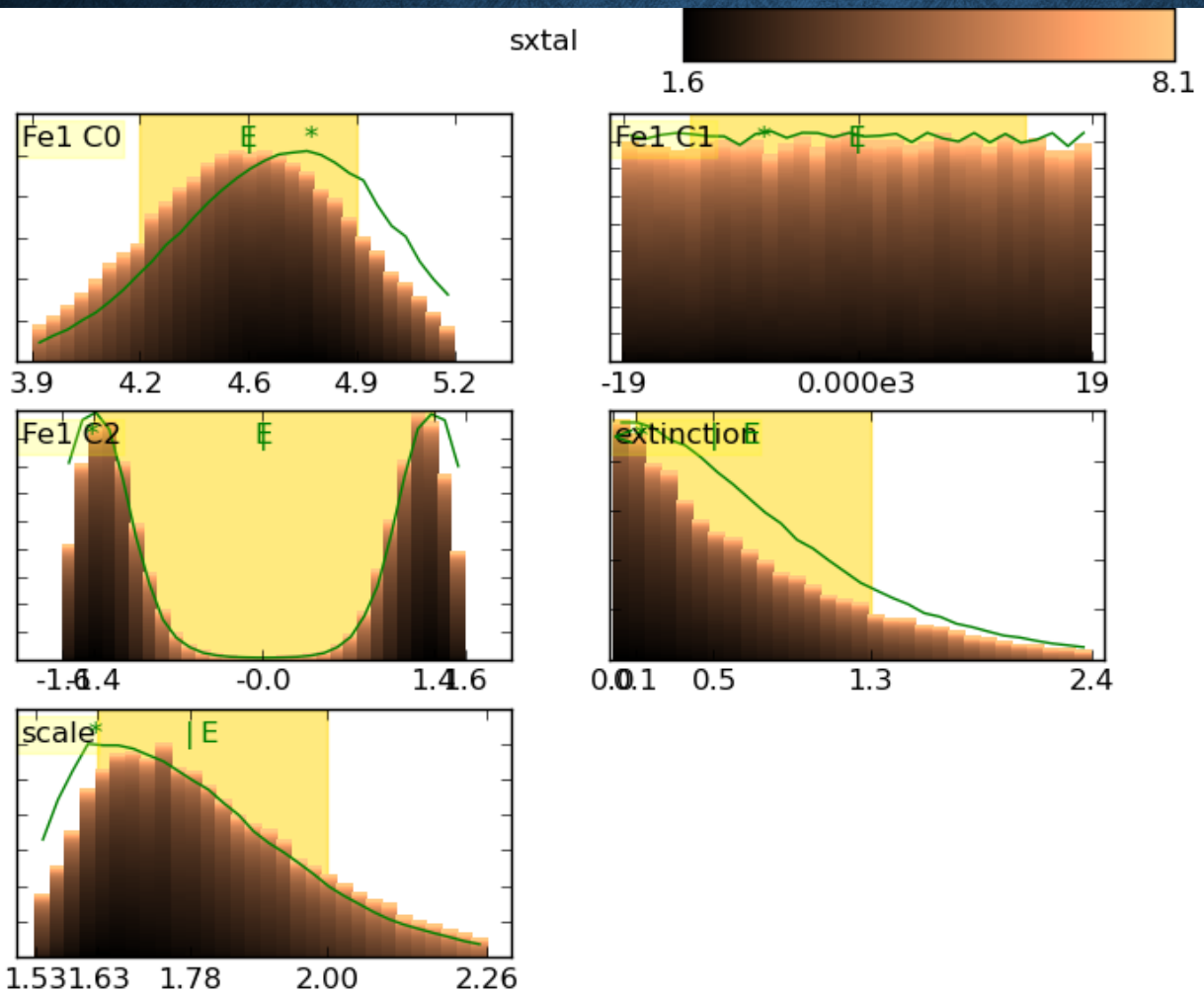
$LuFe_{0.66}Mn_{0.33}O_3$



$LuFe_{0.66}Mn_{0.33}O_3$



$LuFe_{0.66}Mn_{0.33}O_3$ Results



Parameter	value	[95% interval]	
Fe1 C0	4.752	[3.85	5.22]
Fe1 C1	-7.56	[-19.0	19.0]
Fe1 C2	-1.392	[-1.63	1.63]
extinction	0.002	[0.02	2.44]
scale	1.626	[1.53	2.26]

FUTURE GOALS

- ❑User-friendly interface
- ❑Model fitting
- ❑NICE integration
- ❑Take over the world

Acknowledgements

William Ratcliff
Paul Kienzle
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SURF directors