PLATON, New Options

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Overview of this Presentation

- PLATON development started more than 25 years ago.
- Start of the talk with some historical notes.
- Recent additions to PLATON such as the analysis for TWINNING and the analysis of Bijvoet pairs will be introduced.
- Preliminary results of the new Charge Flipping algorithm for ab-initio structure determination will be shown.
- Some life Demo's

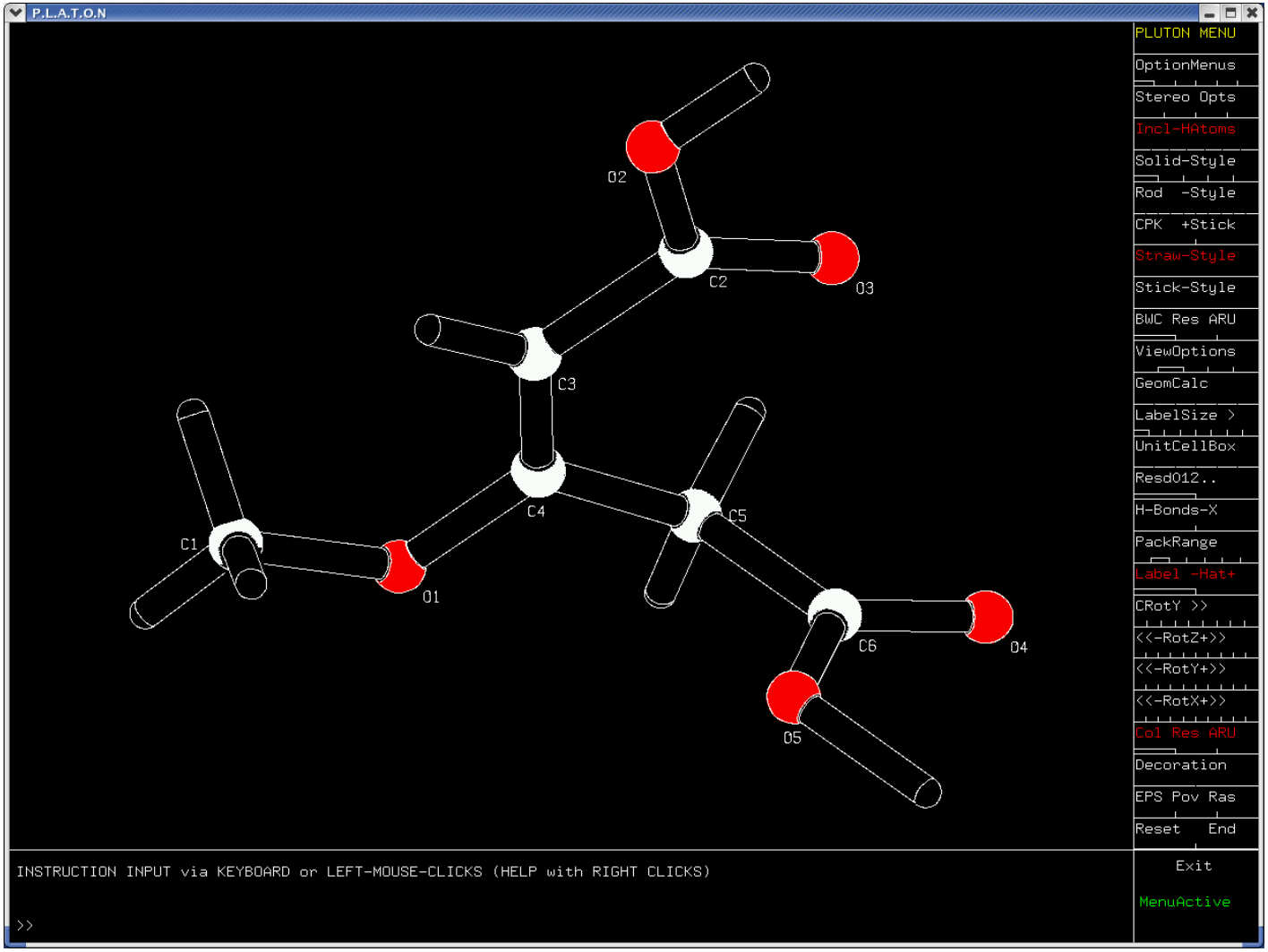
PLATON BACKGROUND

- I started as a student in crystallography in the second half of the 1960th.
- As it happens, that was also the period of the first publication of the FFT algorithm by Cooley & Tukey.
- The relevance of FFT in the context of this talk will become clear later on.

PLATON BACKGROUND

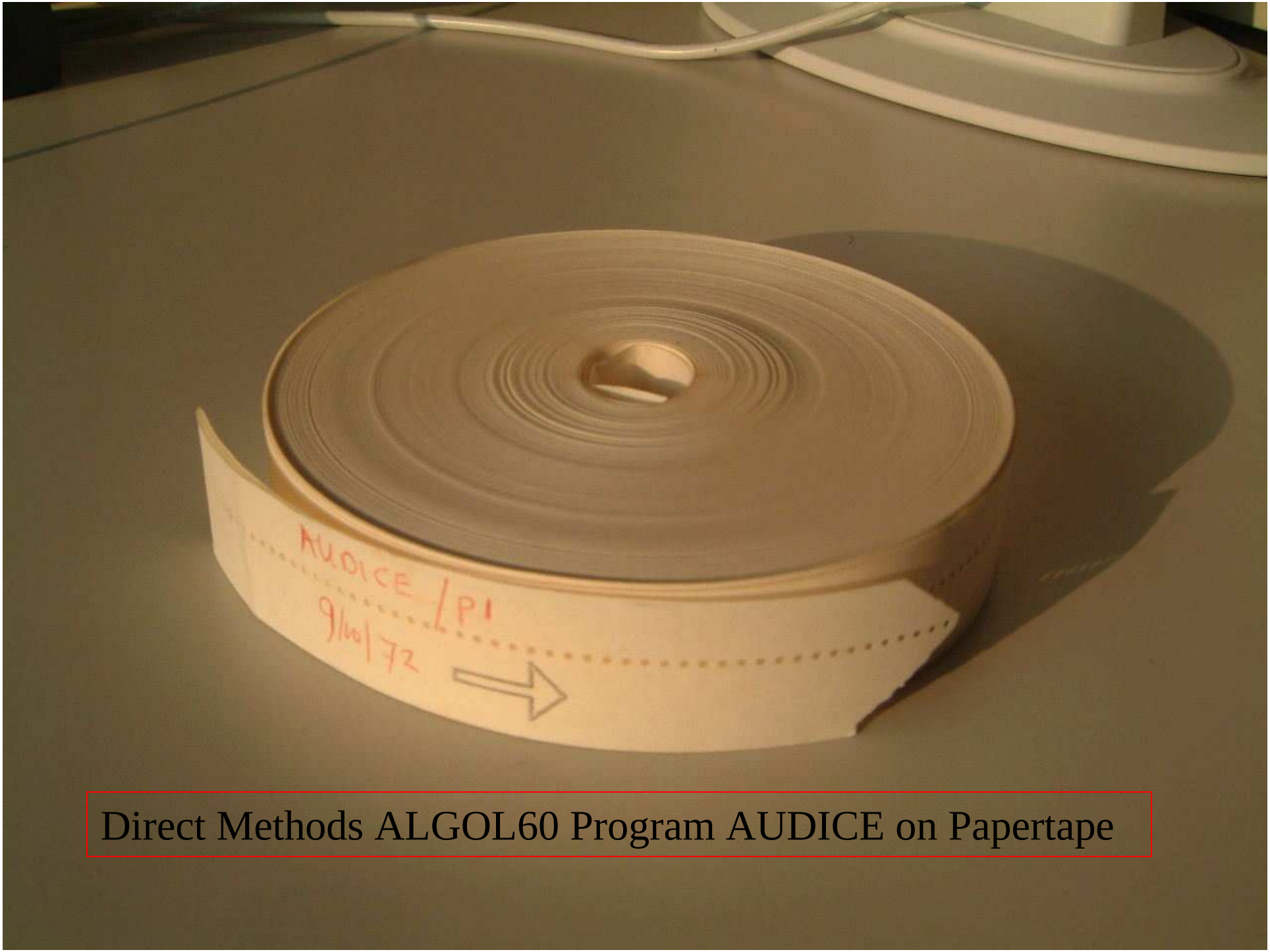
- As a student, I was given a small batch of colorless crystals of a compound **X** of unknown composition.
- The assignment was to find out what was in that sample using X-ray diffraction only.
- It took at that time about half a year to produce an interpretable Fourier map and solve the mystery structure.

Puzzle Solved !



PLATON BACKGROUND

- In order to arrive at a solution, a new Symbolic Addition Method program had to be created, AUDICE, written in ALGOL-60.
- It subsequently also solved other difficult structures in the lab.



Direct Methods ALGOL60 Program AUDICE on Papertape

~1966, Electrologica X8 ALGOL60 ‘Mainframe’ (<1MHz)

Flexowriter for the creation and editing of programs and data

PLATON BACKGROUND

- AUDICE was superseded by MULTAN and later by SHELXS, SIR and DIRDIF with the change of the central university computer to a CDC6400 + FORTRAN.
- Structure refinement moved via XRAY-72, XRAY-76, SHELX76 to the current SHELXL-97.
- Since 1980, virtually everything else needed for our national service was developed or incorporated as part of the PLATON package since around 1980.

What is PLATON

- A Multipurpose Crystallographic Tool.
- Compatible with and Complementary to the SHELX & Bruker-AXS SHELXTL Software. (.res,.hkl,.cif,.fcf)
- ‘Semi Public domain’ (I.e. free-of-charge for academics, but with a License Fee for For Profit Organizations).
- Developed on UNIX/LINUX and available on MS-Windows & MAC-OSX Platforms.

Multipurpose Crystallographic Tool

- Absorption Correction Tools

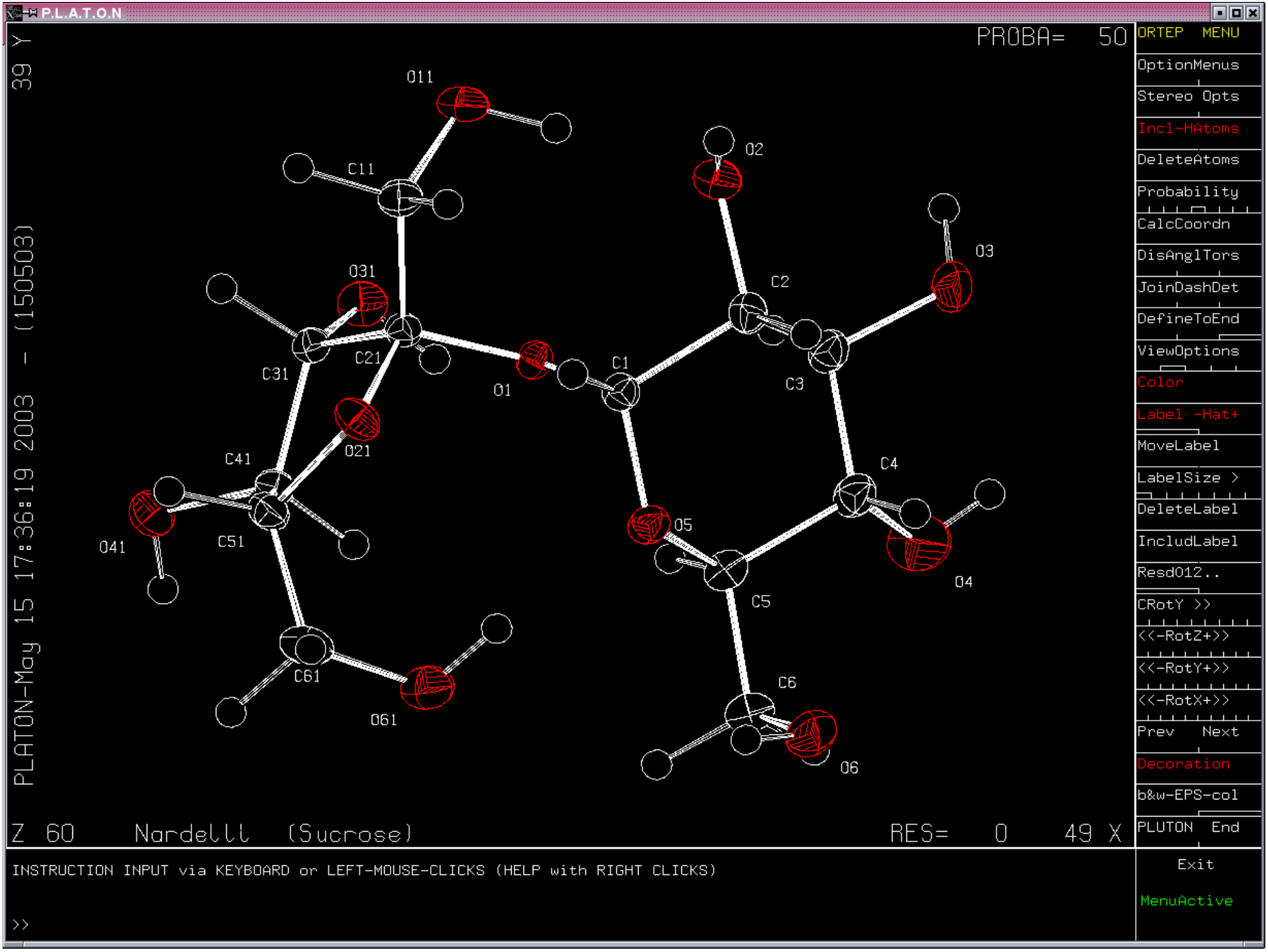
  (e.g. MULABS,TOMPA)
- Space Group Determination from Extinctions.
- ADDSYM - Check for Missed Symmetry.
- SQUEEZE – Disordered Solvent Handling..
- Geometry (Bonds,Angles, Rings etc.).
- Molecular Graphics (ORTEP, PLUTON, Contour)

EXAMPLE ORTEP

- Input Shelx Style: sucrose.res
- (Alternatively: .cif,.pdb,.dat,.spf style)

- Automatic ORTEP style PLOT ➔


P.L.A.T.O.N
PLATON
A Multipurpose Crystallographic Tool
(C) 1980-2005 A.L.Spek - 40M-Version: 130605
GRAPHICS
GEOM-CALC
VOIDS TWIN
SYMMETRY
ABSORPTION
REPORT
MISC-TOOLS
PLUTONauto
ORTEP/ADP
NEWMAN
RING-PLOTS
PLANE-PLOT
POLYHEDRA
CONTOUR-DF
CONTOUR-Fo
AutoMolFit
HKL2Powder
SlmPowderP
RadDistFun
PLUTONativ
CALC ALL
CALC K.P.I
CALC INTER
CALC COORD
CALC METAL
CALC GEOM
CALC HBOND
CALC TMA
L.S.-PLANE
DihedAngle
AngleLines
AngLsplLin
CremerPopl
BondValenc
HFIX - RES
CALC SOLV
SQUEEZE
CALC-FCF
CONTOUR-SQ
SOLV F3D
SOLV PLOT
CAVITY-PLT
LePageTwin
TwinRotMat
ADDSYM
ADDSYM-XCT
ADDSYM-PLT
ADDSYM-SHX
NEWSYM
NONSYM
LEPAGE
DELRED
MOLSYM
ASYM
ASYMoverFR
SPGAfromEX
StructTidy
DELrefABS
ABSPslScan
ABSTompa
ABSGauss
ABSXtal
ABSSphere
MULscanABS
SHXABS
Xtal Habit
VALIDATION
ASYM-VIEW
FCF-VALID
SUPPLEMMAT
ANALofVAR
ByvoetPolr
ASYM-EXPCT
EXPECT-HKL
CSD-CELL
CSD-QUEST
CIF-LOCAL
PATTERSON
FCF2HKL
EXPAND-P1
FCF-GENER
HKL-GENER
HKL-TRANSF
EXOR-RES
ANIS-RES
RENAME-RES
PDB -pdb
SPF -eld
SHELXL-res
CIF -acc
AUTO-RENUM
SYSTEM-S
Xtal Data (SPF) sucrose.spf- Set 1(1): Nardelli
No Refl Data on sucrose.FCF or .hkl
Browser - HELP
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
PLATON MENU
OptionMenus
NoMove
NoDisorder
Organic
Round
Parentheses
Label-Alias
R/S-Determ
Norm-H-bond
NoSymm
Join-Expand
LstARU RCel
LstCellSymm
ListAtoms
ListBonds
LstFlagRadi
MinQPeakHgt
MinQPeakDis
Q-Peak-Incl
KeyInstruct
Prev Next
SAVE-InstrS
ENTRY-LIST
Reset End
Exit
MenuActive


P.L.A.T.O.N
PROBA= 50
O11
C11
O2
O3
O31
C2
C31
C21
O1
C1
C3
O21
C41
C4
O41
C51
O5
O4
C5
C61
C6
O61
O6
Z 60 Nardelli (Sucrose)
RES= 0 49 X
39 Y
PLATON-May 15 17:36:19 2003 - (150503)
ORTEP MENU
OptionMenus
Stereo Opts
Incl-HAtoms
DeleteAtoms
Probability
CalcCoordn
DisAnglTors
JoinDashDet
DefineToEnd
ViewOptions
Color
Label -Hat+
MoveLabel
LabelSize >
DeleteLabel
IncludLabel
Resd012..
CRotY >>
<<-RotZ+>>
<<-RotY+>>
<<-RotX+>>
Prev Next
Decoration
b&w-EPS-col
PLUTON End
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
Exit
MenuActive

Multipurpose Crystallographic Tool – (continued)

- Generation of Powder Patterns (Coordinates, hkl)
- Structure Validation (part of IUCr CHECKCIF).
- Analysis of Fo/Fc data including Bijvoet Pairs for absolute structure determination.
- Analysis of (Pseudo) Merohedral Twinning.
- System-S, Automated Structure Determination.

System S

- Automatic structure determination

  (Space group determination, structure solution, refinement and analysis)
- Build-in in PLATON (Unix version only)
- Calls external programs (including itself) for various functions (e.g. SHELXS, SIR).
- Program runs in either *guided* or *no-questions-asked* mode.
- **LIFE DEMO for ‘mistery structure’ X**

S.Y.S.T.E.M - S

S Y S T E M - S

Status = Refine for x From tm/sg/pn/ = 02/002/011 - SHELXL WEIGHT

Elem	C	H	O
Form	12	14	10
Unit	12	14	10
Cont	12	14	10

StrDetStage DETAILS

SpaceGroup P-1

Z 1

AbsCorrMetd

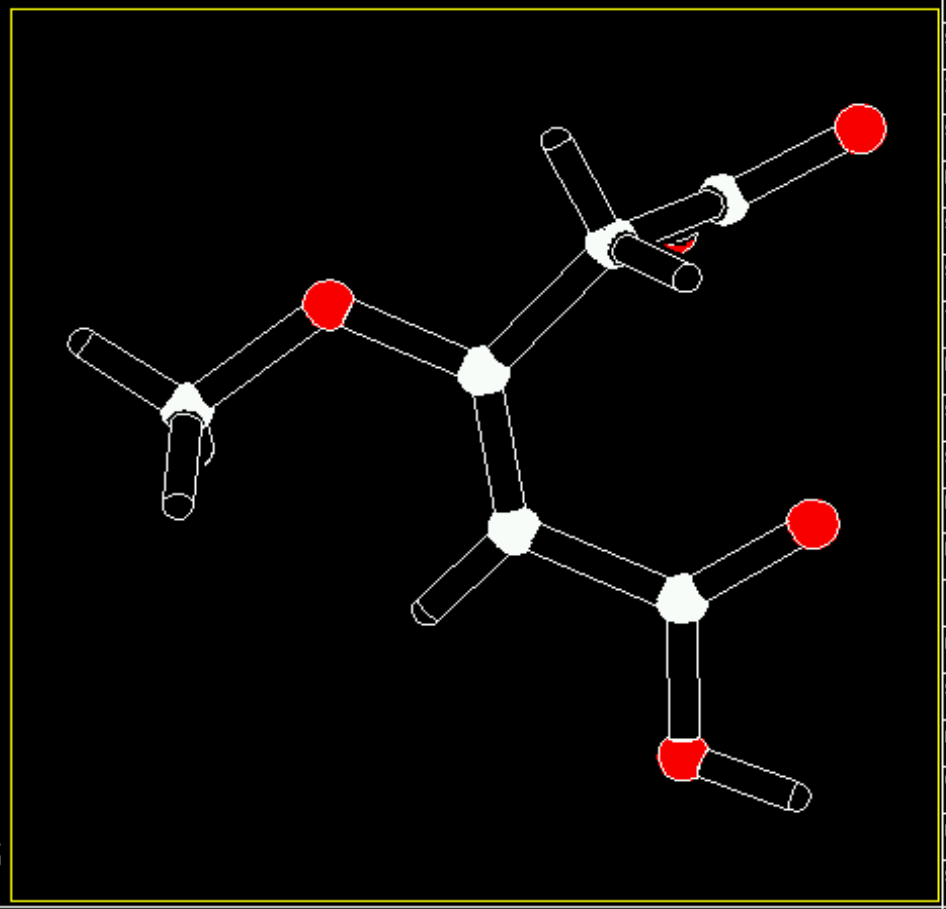
PhasingMetd SHELXS86

Add H-Atoms HDIF

	R	wR2	S
Iso Refin	0.074	0.287	2.53
Aniso Refin	0.072	0.273	2.44
H-AtomRefin	0.002	0.012	0.10
WeightRefin	0.011	0.032	1.06

Valid-Alert 3A, 1B, 4C, 2G

PLATON



INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)

>> Hit RETURN to Continue

SYSTEM - S
OptionMenus
LOG RELINK
DELABS MULA
ABST/P/NONE
TRMX SPGR
FORMULA Z
SHS SHP SHD
DIRDIF ORNT
S86 SIR SR4
EXOR /S /D
SHELXL-ISO
SHELXL-ANIS
TwinRotMat
HDIF HFIX
SHELXL-HATS
SHELXL-WGHT
PLUTON RENM
PLATON ADP
INVRT HFREE
ASYM VIEW
SQUEEZE FCF
ADDSYM SOLV
VALI REPORT
AutoRenum
SKIP ACCEPT
Exit
MenuActive

Twinning

- Twinning results in overlap of reflections with different hkl indices.
- Twinning can be detected in some cases during the data collection experiment
- Cases of (Pseudo) Merohedral twinning are generally detected during the structure determination

(Pseudo)Merohedral Twinning

- Options to handle twinning in L.S. refinement available in SHELXL, CRYSTALS etc.
- Problem: Determination of the Twin Law that is in effect.
- Partial solution: coset decomposition, try all possibilities

  (I.e. all symmetry operations of the lattice but not of the structure)
- ROTAX (S.Parson et al. (2002) J. Appl. Cryst., 35, 168.

  (Based on the analysis of poorly fitting reflections of the type F(obs) >> F(calc))
- TwinRotMat Automatic Twinning Analysis as implemented in PLATON (Based on a similar analysis but implemented differently)

Example

- Structure refined to R= 20% in P-3
- Run TwinRotMat on CIF/FCF
- Result: Twinlaw with estimate of the twinning fraction and drop in R-value

TwinRotMat

Analysis of Fo/Fc Data for Unaccounted (Non)Merohedral Twinning for: twin

Cell: 0.71073 20.983 20.983 7.644 90.00 90.00 120.00 Spgr: P-3

Criteria: DeltaI/SigmaI .GT. 16.0, DeltaTheta 0.10 Deg., NselMin = 50

N(refl) = 4445, N(selected) = 50, IndMax = 25, CritI = 0.3, CritT = 0.10

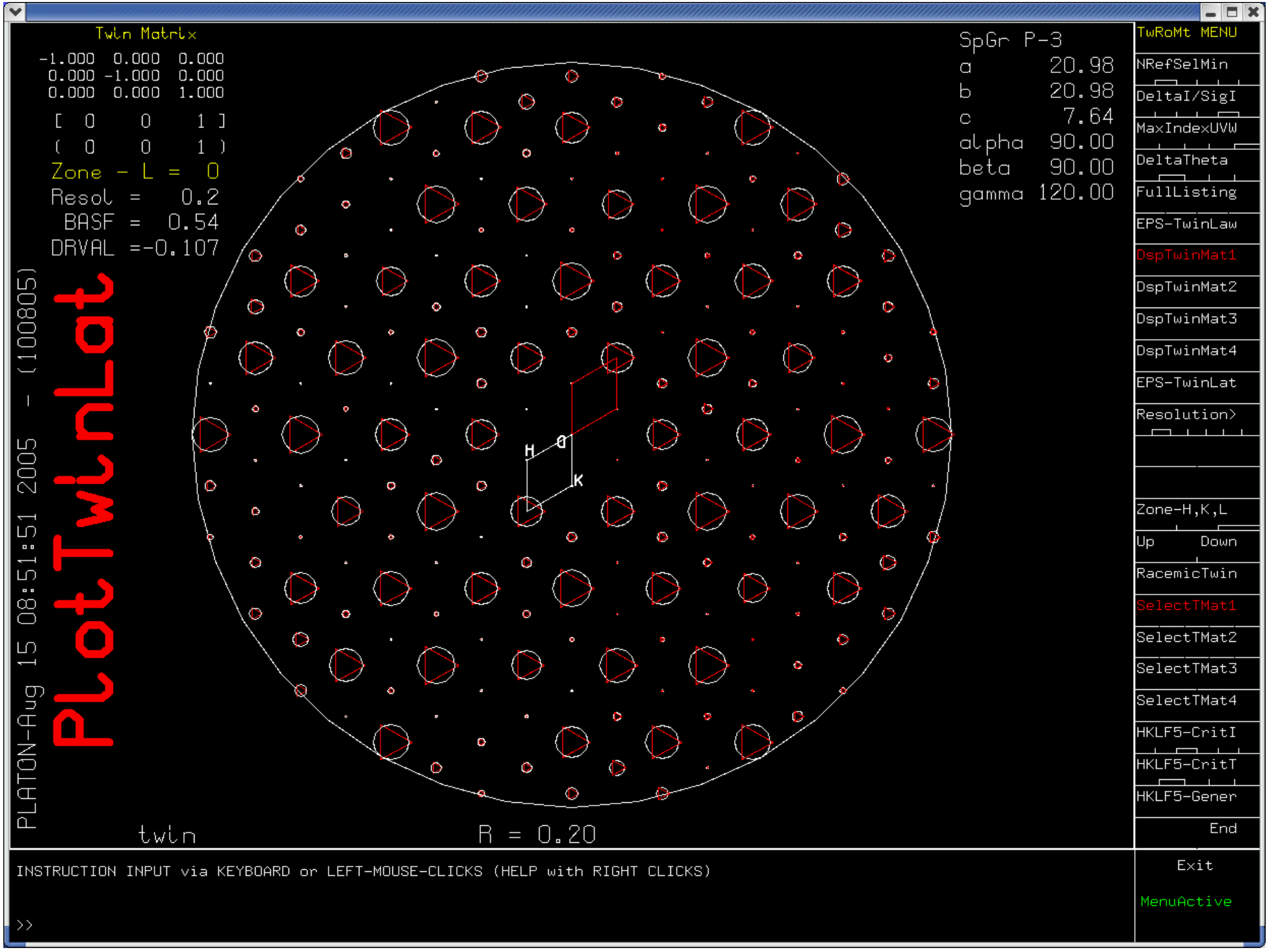
PLATON-Aug 8 17:21:12 2005 - (80805)

2-axis (0 0 1) [0 0 1], Angle () [] = 0.00 Deg, Freq = 47		1
(-1.000 0.000 0.000) (h1) (h2)	Nr Overlap = 4445	
(0.000 -1.000 0.000) * (k1) = (k2)	BASF = 0.54	
(0.000 0.000 1.000) (l1) = (l2)	DEL-R =-0.107	
2-axis (1 -1 0) [1 -1 0], Angle () [] = 0.00 Deg, Freq = 48		2
(0.000 -1.000 0.000) (h1) (h2)	Nr Overlap = 4445	
(-1.000 0.000 0.000) * (k1) = (k2)	BASF = 0.01	
(0.000 0.000 -1.000) (l1) = (l2)	DEL-R =-0.001	
2-axis (2 -1 0) [1 0 0], Angle () [] = 0.00 Deg, Freq = 36		3
(1.000 0.000 0.000) (h1) (h2)	Nr Overlap = 4445	
(-1.000 -1.000 0.000) * (k1) = (k2)	BASF = 0.01	
(0.000 0.000 -1.000) (l1) = (l2)	DEL-R =-0.001	
2-axis (1 3 -1) [10 14 -23], Angle () [] = 0.45 Deg, Freq = 10		4
(-0.732 0.375 -0.606) (h1) (h2)	Nr Overlap = 576	
(0.804 0.126 -1.818) * (k1) = (k2)	BASF = 0.02	
(-0.268 -0.375 -0.394) (l1) = (l2)	DEL-R = 0.000	
twin	R = 0.20	

INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)

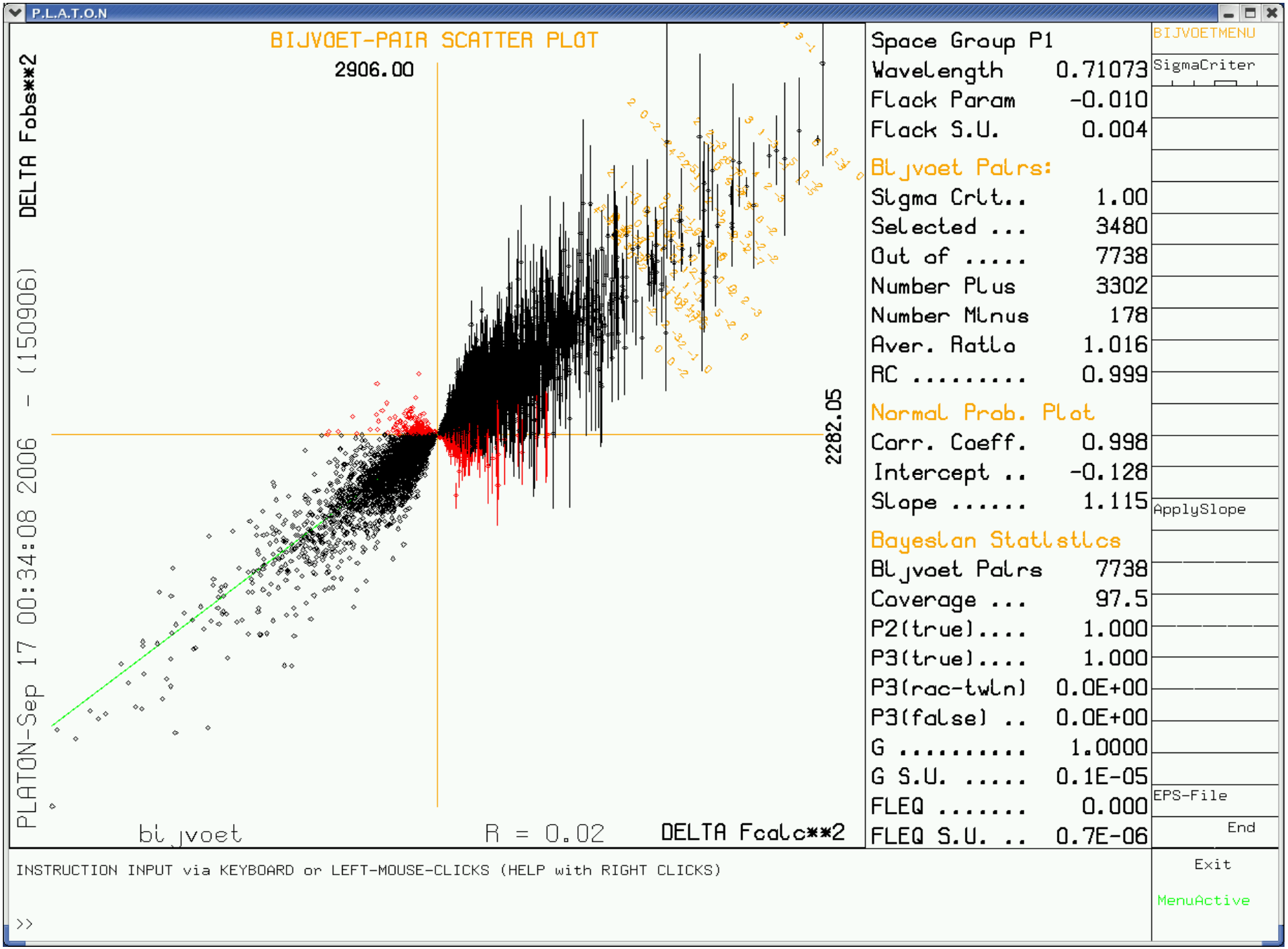
>>

TwRoMt MENU
NRefSelMin
DeltaI/SigI
MaxIndexUVW
DeltaTheta
FullListing
EPS-TwinLaw
DspTwinMat1
DspTwinMat2
DspTwinMat3
DspTwinMat4
EPS-TwinLat
Resolution>
Zone-H,K,L
Up Down
RacemicTwin
SelectTMat1
SelectTMat2
SelectTMat3
SelectTMat4
HKLF5-CritI
HKLF5-CritT
HKLF5-Gener
End
Exit
MenuActive


Twln Matrix
-1.000 0.000 0.000
0.000 -1.000 0.000
0.000 0.000 1.000
[0 0 1]
(0 0 1)
Zone - L = 0
Resol = 0.2
BASF = 0.54
DRVAL =-0.107
SpGr P-3
a 20.98
b 20.98
c 7.64
alpha 90.00
beta 90.00
gamma 120.00
PLATON-Aug 15 08:51:51 2005 - (100805)
PlotTwinLat
H
O
K
twln
R = 0.20
TwRoMt MENU
NRefSelMin
DeltaI/SigI
MaxIndexUVW
DeltaTheta
FullListing
EPS-TwinLaw
DspTwinMat1
DspTwinMat2
DspTwinMat3
DspTwinMat4
EPS-TwinLat
Resolution>
Zone-H,K,L
Up Down
RacemicTwin
SelectTMat1
SelectTMat2
SelectTMat3
SelectTMat4
HKLF5-CritI
HKLF5-CritT
HKLF5-Gener
End
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
Exit
MenuActive

Absolute Structure

- The absolute structure of a compound is normally determined with the refinement of the Flack parameter.
- The value of the Flack parameter can be inconclusive in view of a high su.
- A detailed scatter-plot may be more conclusive.


P.L.A.T.O.N
BIJVOET-PAIR SCATTER PLOT
2906.00
DELTA Fobs**2
PLATON-Sep 17 00:34:08 2006 - (150906)
2282.05
bijvoet
R = 0.02
DELTA Fcalc**2
Space Group P1
Wavelength 0.71073
Flack Param -0.010
Flack S.U. 0.004
Bijvoet Pairs:
Sigma Crit.. 1.00
Selected ... 3480
Out of 7738
Number Plus 3302
Number Minus 178
Aver. Ratio 1.016
RC 0.999
Normal Prob. Plot
Corr. Coeff. 0.998
Intercept .. -0.128
Slope 1.115
Bayesian Statistics
Bijvoet Pairs 7738
Coverage ... 97.5
P2(true).... 1.000
P3(true).... 1.000
P3(rac-twin) 0.0E+00
P3(false) .. 0.0E+00
G 1.0000
G S.U. 0.1E-05
FLEQ 0.000
FLEQ S.U. .. 0.7E-06
BIJVOETMENU
SigmaCriter
ApplySlope
EPS-File
End
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
Exit
MenuActive

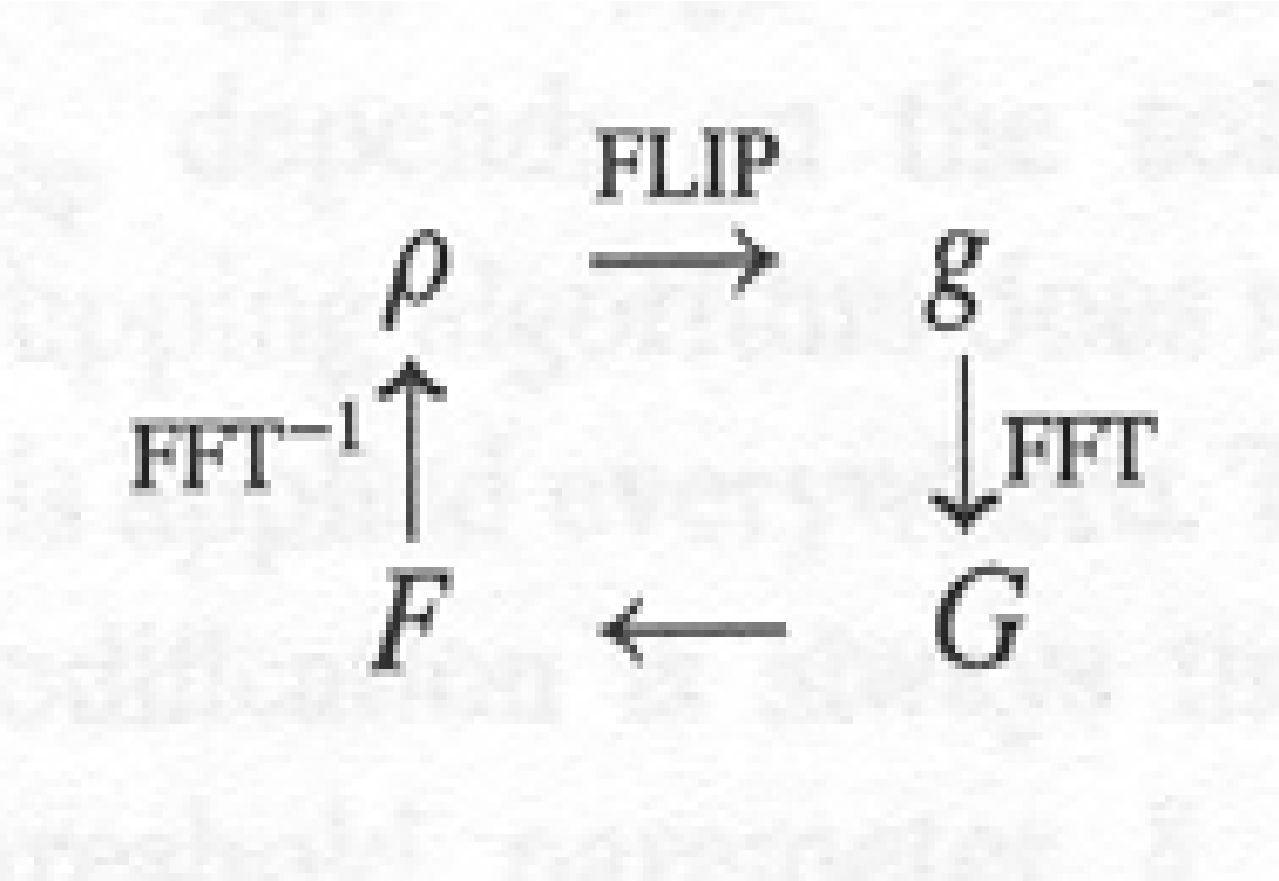
New: Charge Flipping

- *Ab Initio structure solution by charge flipping*
- See G.Oszlanyi & A. Suto, (2004). Acta Cryst. A60,134.
- The approach does not use Direct or Patterson methods to solve structures, just number crunching via FFT transforms.

Procedure

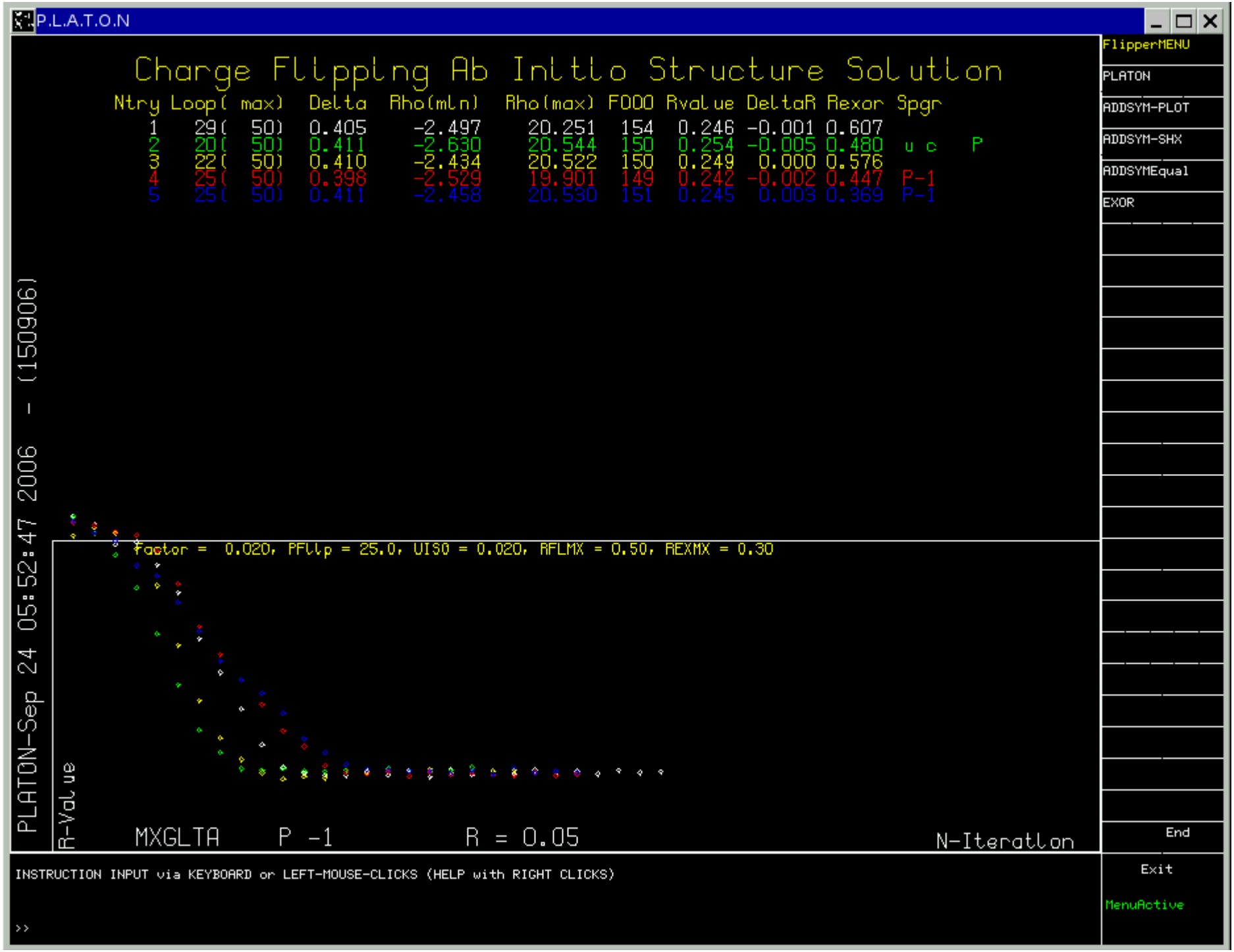
- Expand the reflection set to P1 from the assumed Laue symmetry.
- Assign random starting phases to all reflections.
- Calculate a Fourier map. Change sign of all density below a given level. Do a back-Fourier transformation to get calculated structure factors. Assign the calculated phases to the observed data. Recycle to convergence.
- After convergence: Interprete the map in terms of atom types and determine the correct symmetry.

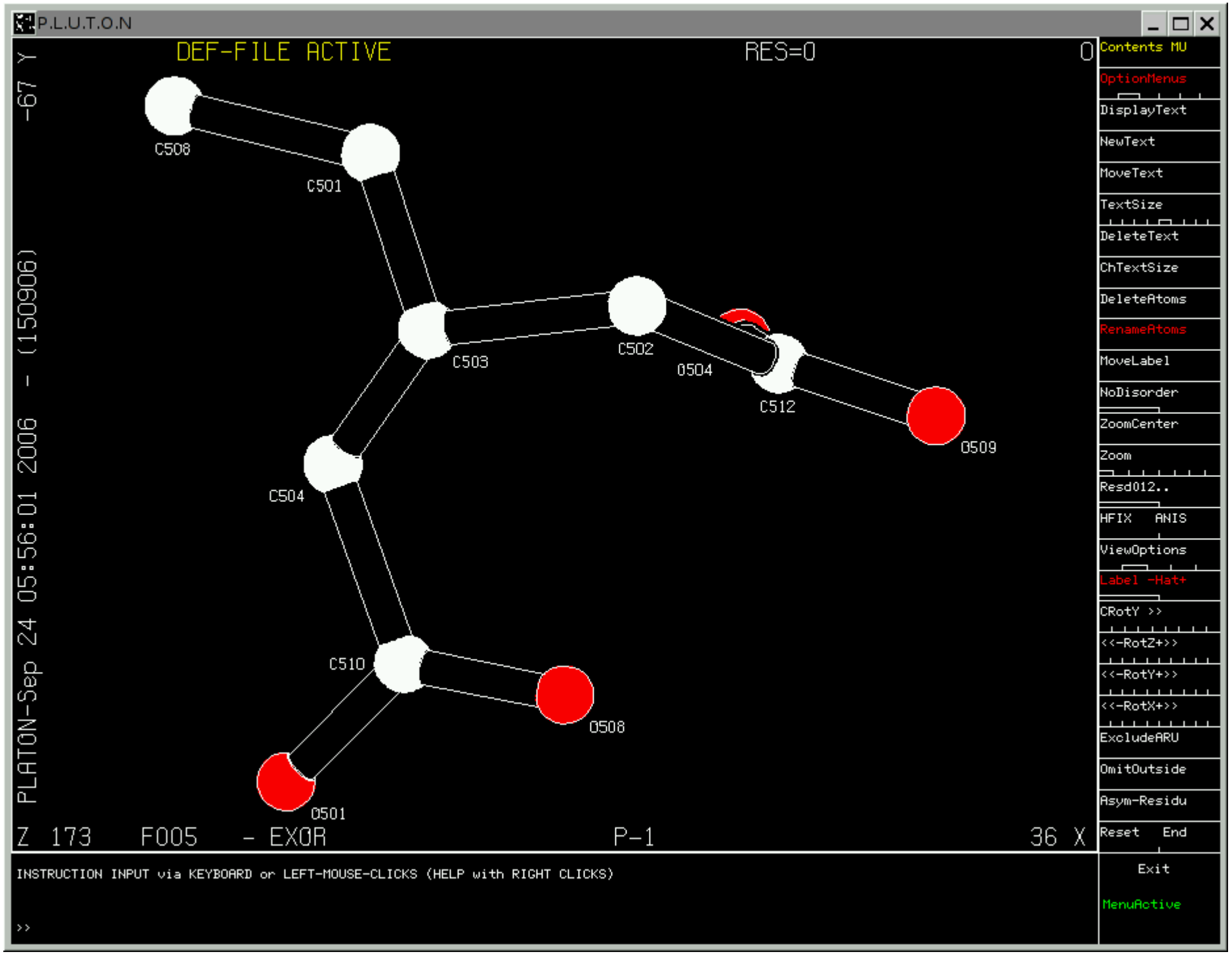
Procedure



Applications

- Structure determination of powders.
- Structure determination of incommensurate structures.
- Routine structure determinations. (Preliminary implementation of the algorithm in PLATON with a routine named FLIPPER).
- **LIFE DEMO for Stucture X ➔**


P.L.A.T.O.N
Charge Flipping Ab Initio Structure Solution
Ntry Loop(max) Delta Rho(min) Rho(max) FOOO Rvalue DeltaR Rexor Spgr
1 29(50) 0.405 -2.497 20.251 154 0.246 -0.001 0.607
2 20(50) 0.411 -2.630 20.544 150 0.254 -0.005 0.480 u c P
3 22(50) 0.410 -2.434 20.522 150 0.249 0.000 0.576
4 25(50) 0.398 -2.529 19.901 149 0.242 -0.002 0.447 P-1
5 25(50) 0.411 -2.458 20.530 151 0.245 0.003 0.369 P-1
PLATON-Sep 24 05:52:47 2006 - (150906)
Factor = 0.020, PFlip = 25.0, UISO = 0.020, RFLMX = 0.50, REXMX = 0.30
R-Value
MXGLTA P -1 R = 0.05
N-Iteration
FlipperMENU
PLATON
ADDSYM-PLOT
ADDSYM-SHX
ADDSYMEqual
EXOR
End
Exit
MenuActive
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>


P.L.U.T.O.N
DEF-FILE ACTIVE
RES=0
0
-67 Y
Z PLATON-Sep 24 05:56:01 2006 - (150906)
C508
C501
C503
C502
O504
C512
O509
C504
C510
O508
O501
Z 173 F005 - EXOR P-1 36 X
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
Contents MU
OptionMenus
DisplayText
NewText
MoveText
TextSize
DeleteText
ChTextSize
DeleteAtoms
RenameAtoms
MoveLabel
NoDisorder
ZoomCenter
Zoom
Resd012..
HFIX ANIS
ViewOptions
Label -Hat+
CRotY >>
<<-RotZ+>>
<<-RotY+>>
<<-RotX+>>
ExcludeARU
OmitOutside
Asym-Residu
Reset End
Exit
MenuActive

Conclusions

- Charge Flipping solves structures ab-initio !
- Very limited a-priori info on the structure is needed and no a-priori choise of space-group is required.
- Theoretical background is limited.
- Room for improvement and extension of the algorithm.
- Comparison of the applicability with alternative techniques still limited.

Thanks

Info: www.cryst.chem.uu/platon

Thanks to users for:

- Complaints
- Bug reports (‘undocumented features ..)
- Suggestions for extensions
- And you for your attention