The PLATON Toolbox
History and Applications

Ton Spek

Utrecht University,

The Netherlands.

Goettingen, 6-Sep-2011

What is PLATON About

PLATON is a program with a development history of more than 30 years in the context of the needs of our National Single Crystal Service Facility in the Netherlands and our Acta Cryst. C co-editor activities.

PLATON is a collection of tools for single crystal structure analysis bundled within a single SHELXL and CIF compatible program.

The tools in PLATON are either unique to the program (e.g. TwinRotMat, Validation, Hooft y) or adapted and extended versions of existing tools (e.g. ORTEP, MISSYM).

DESIGN HISTORY

- PLATON started out in 1980 as a companion program to SHELX76 for the automatic generation of an extensive molecular geometry analysis report to be given to the clients of our service. (The CALC ALL mode)
- Soon molecular graphics functionality was added (e.g. PLUTON, ORTEP)
- Over time many other tools were included, many of which also require the reflection data as well (e.g. Validation & Hooft y parameter value).
- Structure validation and automated structure determination were added in the 1990s.

Design Features

- As hardware independent as possible.
- Limited dependency on external libraries.
- Single Fortran source (150000 lines).
- Single routine for all graphics calls.
- Small C routine for interface to X11 graphics.
- Hardcopy standard PostScript (and HPGL)
- Keyboard Input & Point+Clicking.
- Shell command line options.

Design and Development Legacy

- Pre-SHELXL solutions for the handling of disorder, labels and symmetry (i.e. no PART).
- Originally designed to execute in terminal mode on a limited memory CDC mainframe + Tektronix & HPGL graphics.
- Later: Migration to the in-house (micro)VAX Platform.
- Current development on the UNIX/X-Windows Platform.

PLATON Usage

- Today, the PLATON functionality is most widely used in its validation incarnation as part of the IUCr checkCIF facility.
- Tools are available in PLATON to analyze and address/solve many of the validation issues that are reported in need of attention.
- PLATON reads/writes .ins, .res, .hkl, .cif, .fcf
- Current Platforms:

  UNIX/LINUX, MAC-OSX,

  MS-WINDOWS (Louis Farrugia)

PLATON Organization

- The program is invoked with the file(s) to work with (UNIX: platon name.cif; MS-WINDOWS from GUI PWT)
- The tools available in PLATON are listed as clickable objects on the opening menu
- Various tool options are clickable in sub-menu's.
- Input can be either in a keyboard entry area or by clicking on menu items.
- Frequently used tools can also be invoked with command line options (e.g. platon –U name.cif)

PLATON

A Multipurpose Crystallographic Tool

GRAPHICS	GEOM-CALC	VOIDS FLIP	SYMMETRY	ABSORPTION	REPORT	MISC-TOOLS
PLUTONauto	Calc All	Calc Solv	ADDSYM	MULscanABS	Validation	SYSTEM-S
ORTEP/ADP	Calc Intra	Calc K.P.I	ADDSYM-EQL	ABSPsiScan	ASYM-VIEW	FCF2HKL
NewmanPlot	Calc Inter	SQUEEZE	ADDSYM-EXT	ABSTompa	FCF-Valid	Expand2P1
Ring-Plots	Calc Coord	CALC-FCF	ADDSYM-PLT	ABSGauss	DifFourier	FCF-Gener
Plane-Plot	Calc Metal	Contour-SQ	ADDSYM-SHX	ABSXtal	ANALofVAR	HKL-Gener
Polyhedra	Calc Geom	SOLV F3D	NEWSYM	ABSSphere	ByvoetPair	HKL-Transf
ContourDif	Calc Hbond	SOLV PLOT	NONSYM	SHXABS	ASYM-EXPCT	EXOR-RES
Contour-Fo	Calc TMA	CavityPlot	LePage		ASYM-Valid	ANIS-RES
AutoMolFit	L.S.-PLANE		DelRed		SupplMater	Rename-RES
HKL2Powder	DihedAngle		MOLSYM		EXPECT-HKL	Auto-Renum
SimPowderP	AngleLines	FLIP MENU	SPGRfromEX		CSD-CELL	SPF -eld
RadDistFun	AngLsplLin	FLIP SHOW	ASYM		CSD-QUEST	SHELXL-res
Patterson	CremerPopl	FLIP PATT	ASYMaverFR		StructTidy	CIF -acc
	BondValenc	FLIPPER 25	LePageTwin		StrainAnal	PDB -pdb
PLUTONatlv	HFIX - RES	STRUCTURE?	TwinRotMat	Xtal Habit	LocCIF-acc	CIF2SHELXL

Xtal Data (CIF) vitac.cif- Set 1(1): vitac

Refl Data (SHELXL) vitac.fcf [NO-DIRC] (1): vitac

http://www.cryst.chem.uu.nl/spek/platon/PLATON-MANUAL.pdf

Browser - HELP

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

>>

PLATON 10

OptionMenus

NoMove

Join-Expand

Organic

Round

Parentheses

Label-Alias

R/S-Determ

Norm-H-bond

NoSymm

NoDisorder

LstARU RCel

LstCellSymm

ListAtoms

ListBonds

LstFlagRadi

Exclude H

MinQPeakHgt

MinQPeakDis

Q-Peak-Incl

KeyInstruct

Prev Next

SAVE-InstrS

ENTRY-LIST

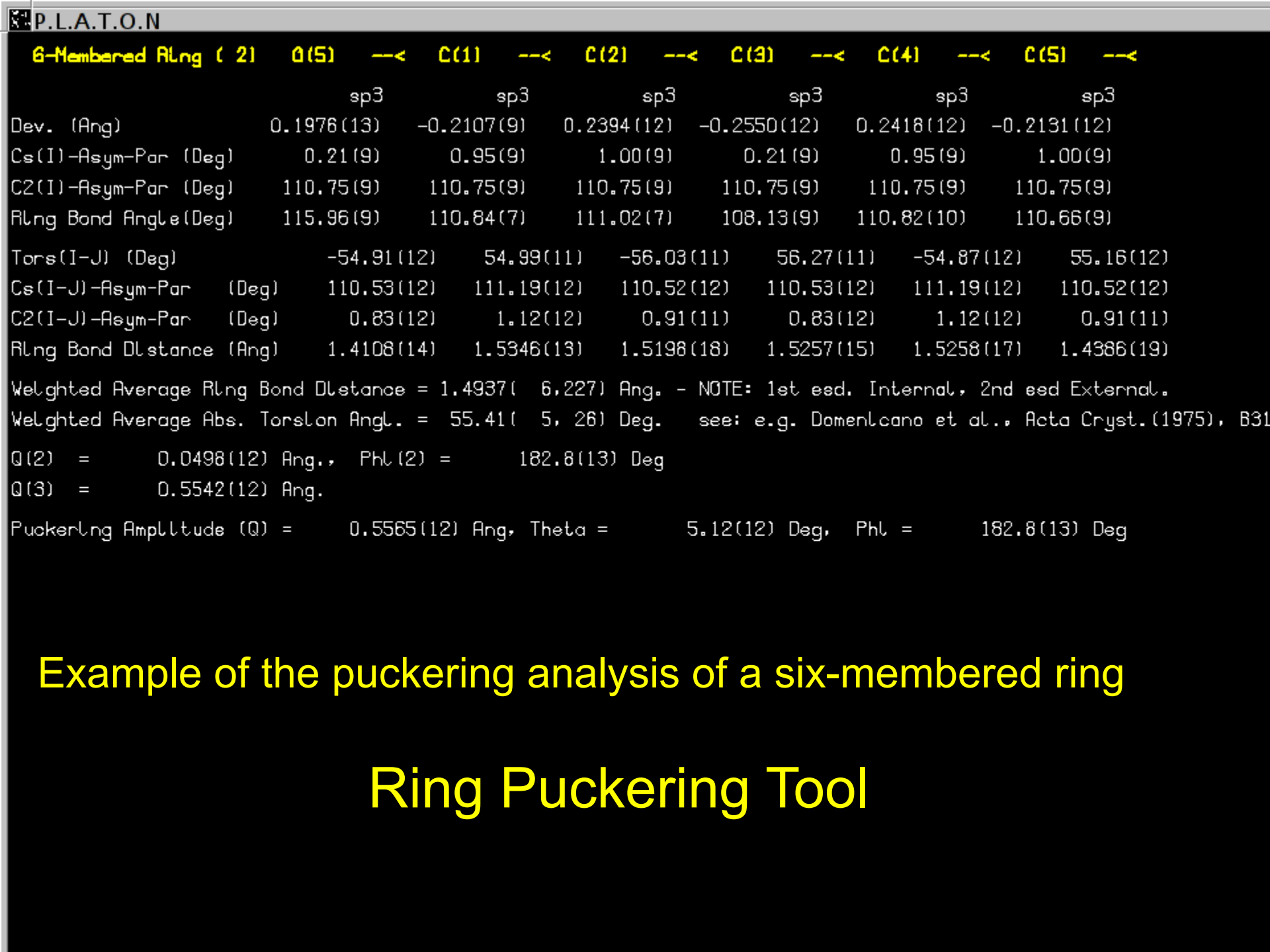
Reset End

Exit

MenuActive

The Geometry Tool

- Extensive Output Listing: 'CALC ALL'
- CALC INTRA - bonds, angles, torsion angles, rings, planes, Cremer and Pople puckering analysis, TLS Rigid body analysis, R/S assignments
- CALC INTER – Short contacts, H-bonds, networks, pi-pi interactions
- CALC Coordination - Berry pseudo-rotation path, Bond Valence

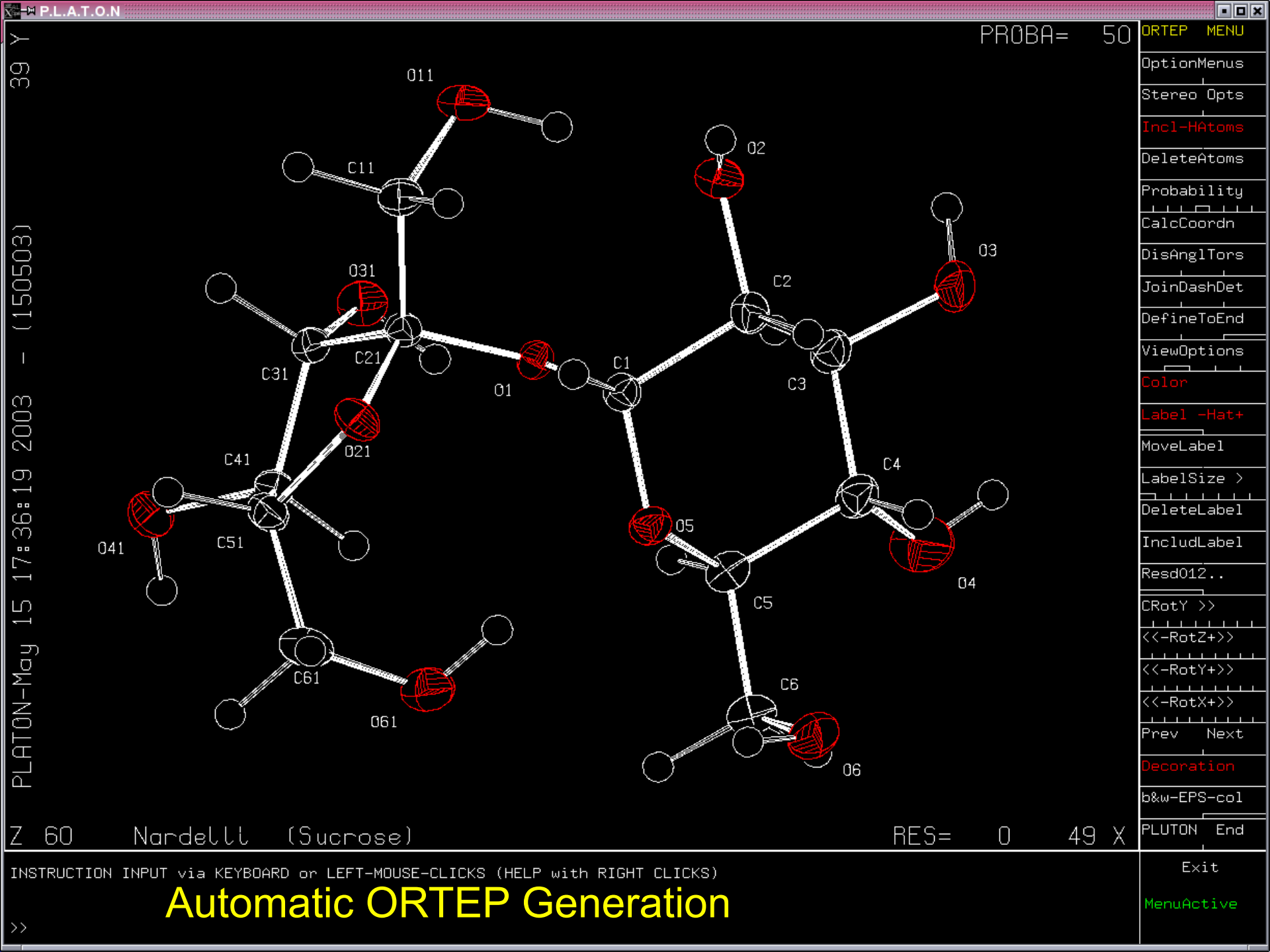


Example of the puckering analysis of a six-membered ring

Ring Puckering Tool

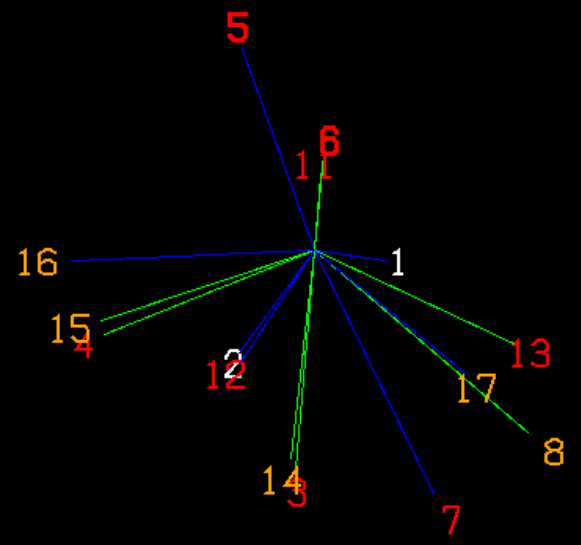
The ORTEP Tool

- Automatic Display of Molecular Geometry and Displacement Parameters (CheckCIF).
- Interactive tool for least squares plane and angle between planes calculations.
- Interactive molfit options.
- Interactive tool to investigate the environment (coordination) of an atom.


P.L.A.T.O.N
PROBA= 50
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
Exit
MenuActive
39 Y
PLATON-May 15 17:36:19 2003 - (150503)
Z 60 Nardelll (Sucrose)
RES= 0 49 X
O11
C11
O31
C31
C21
O21
C41
O41
C51
C61
O61
O1
C1
O2
C2
O3
C3
C4
O4
O5
C5
C6
O6
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
Automatic ORTEP Generation

3.6 Ang. Coordination Sphere around O1 Green = Above, Blue = Below Plane

1	0.8208	--	H1		=	
2	1.428(4)	--	C1		=	
3	2.399(4)	<<	C2		=	
4	2.413(4)	<<	C6		=	
5	2.653(3)	<<	O1' b	1565.01	=	x,1+y,z
6	2.702(3)	<<	O1' a	2656.01	=	1-x,1/2+y,1-z
7	2.944(4)	<<	C2'		=	
8	3.120(4)	.<	C1'		=	
9	3.228(4)	..	C3'		=	
10	3.531(4)	..	C1' a	2656.01	=	1-x,1/2+y,1-z
11	1.8894	<<	H1' a	2656.01	=	1-x,1/2+y,1-z
12	1.9705	<<	H1A		=	
13	2.4952	<<	H1'2		=	
14	2.5846	.<	H2		=	
15	2.5947	.<	H6B		=	
16	2.6051	.<	H6A		=	
17	2.6886	.<	H3'1		=	
18	2.9907	..	H5A2 c	1655.01	=	1+x,y,z
19	3.0745	..	H1' b	1565.01	=	x,1+y,z
20	3.2448	..	H1'2 a	2656.01	=	1-x,1/2+y,1-z



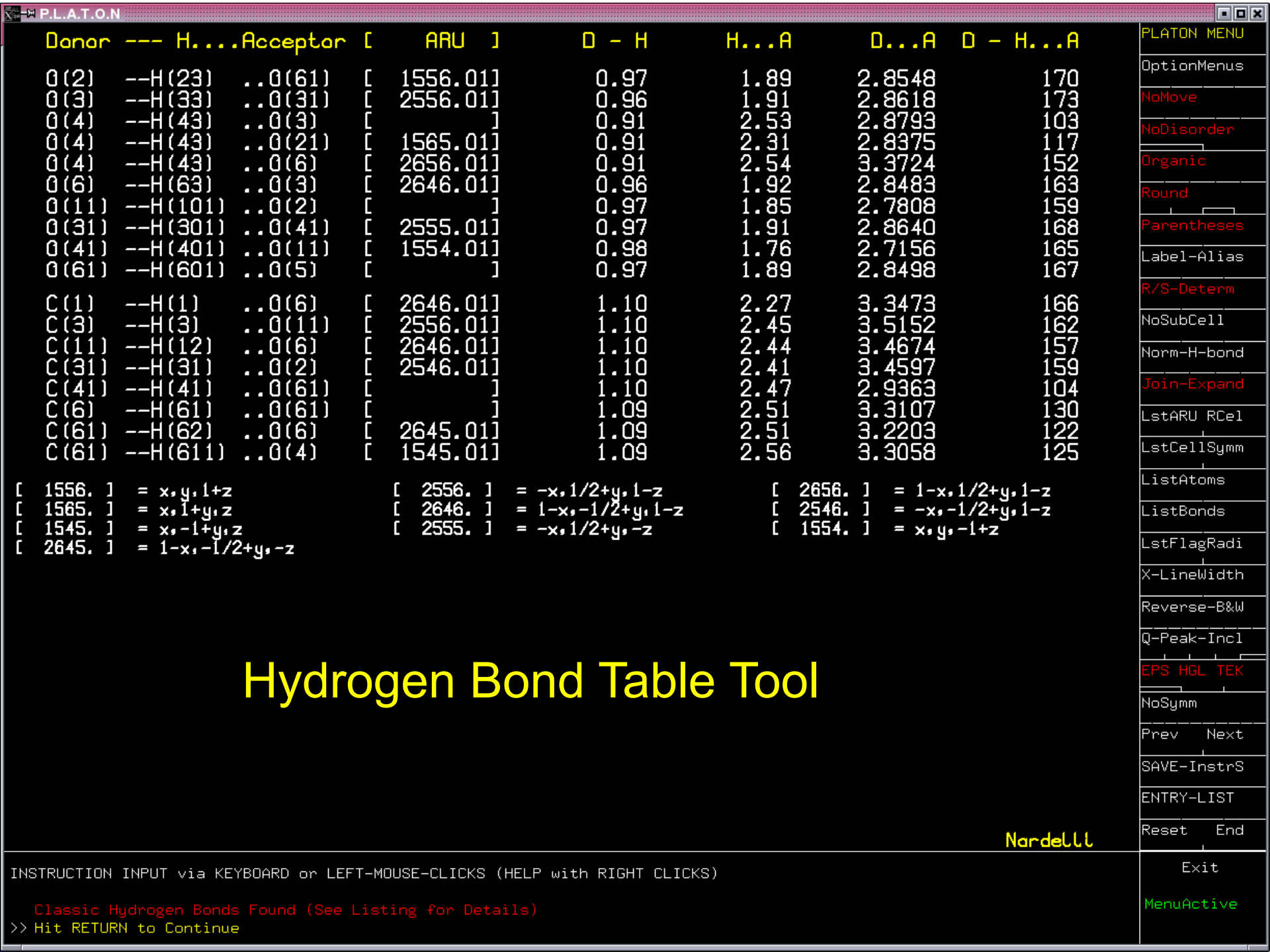
Clicking on an atom in the ORTEP display produces Information on the coordination

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)

Click on ARU-Code to ADD ARU to ORTEP PLOT
>> Hit RETURN to Continue

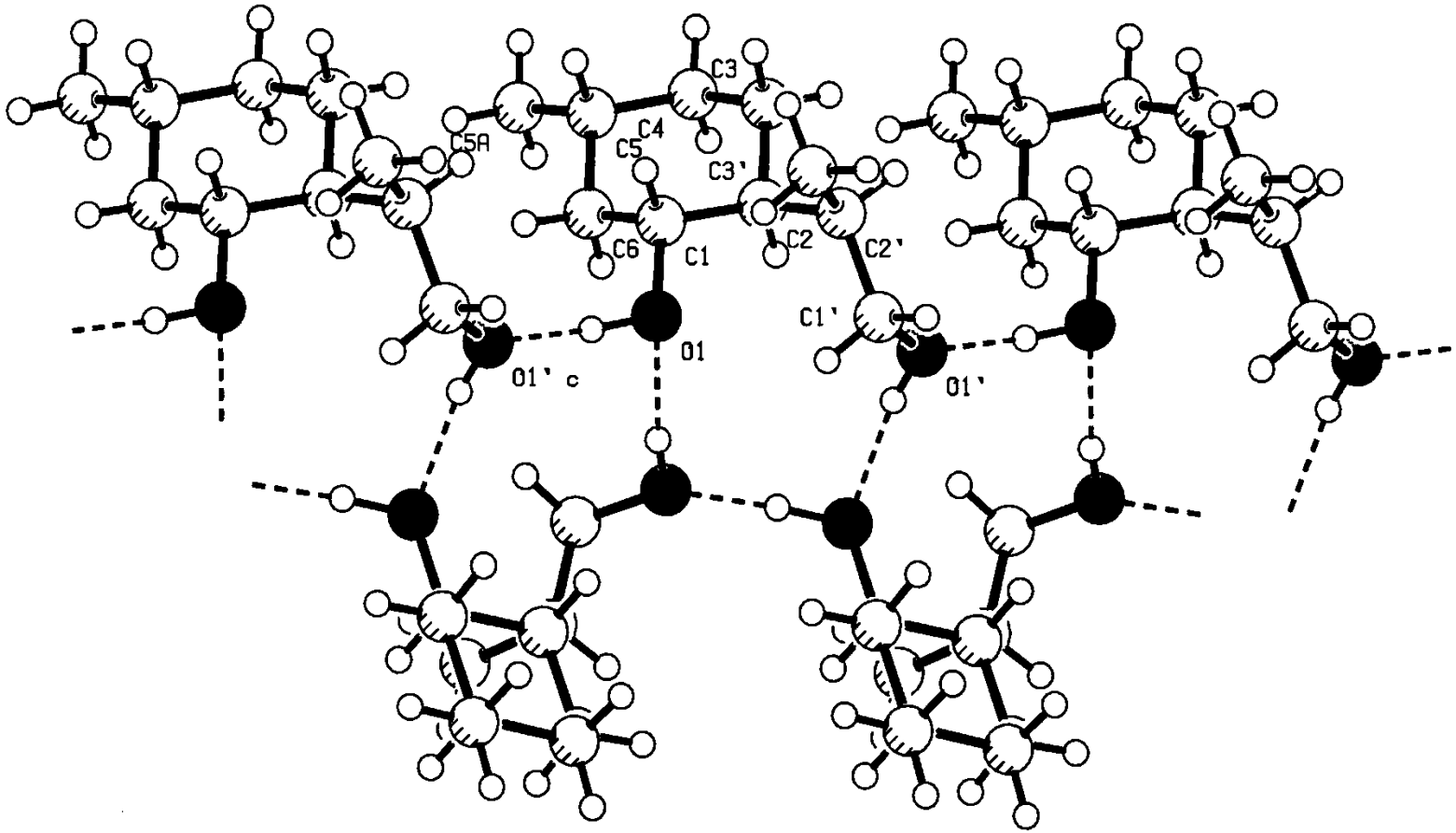
Exit
MenuActive

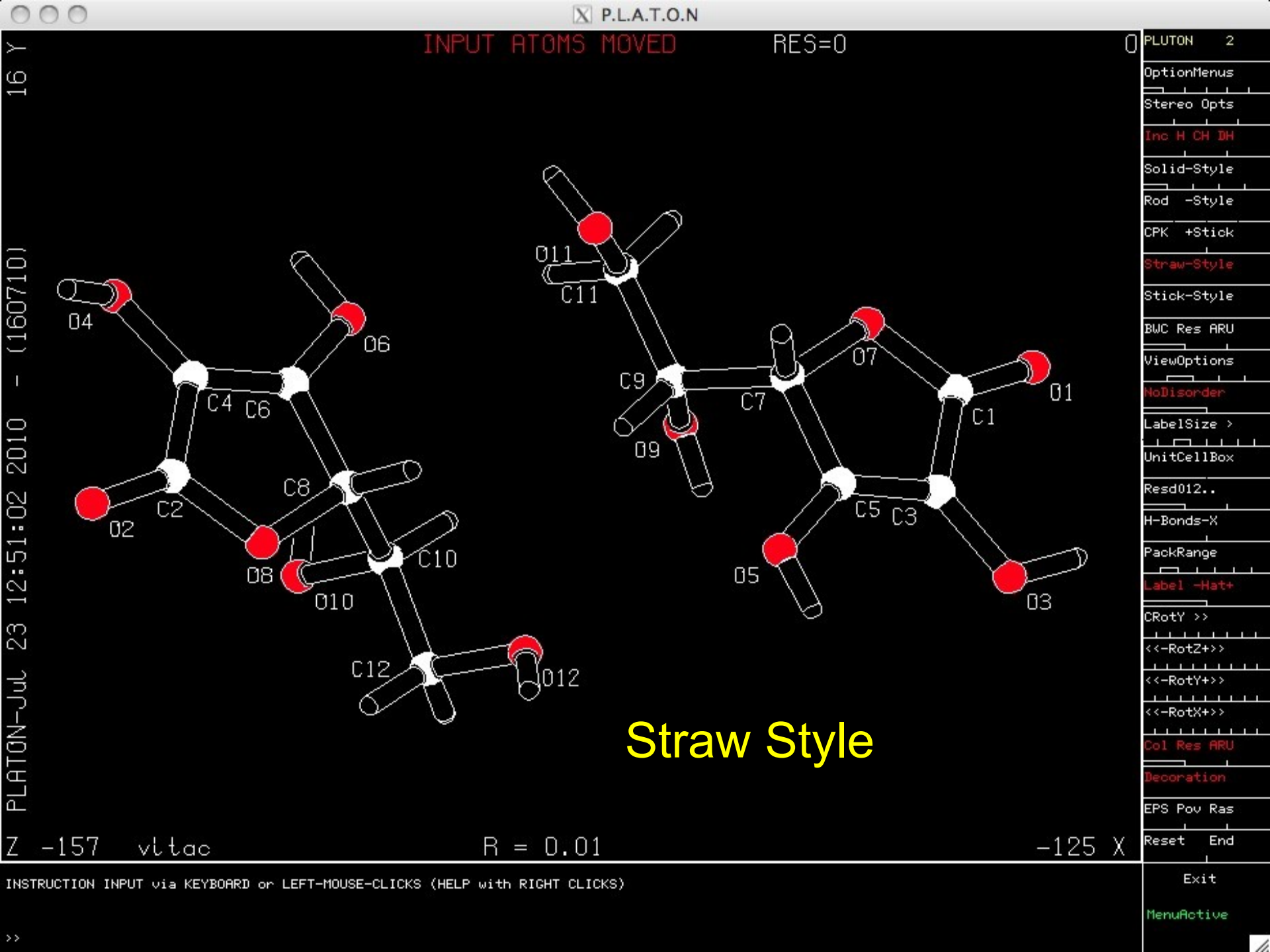

P.L.A.T.O.N
Donor --- H....Acceptor [ARU] D - H H...A D...A D - H...A
O(2) --H(23) ..O(61) [1556.01] 0.97 1.89 2.8548 170
O(3) --H(33) ..O(31) [2556.01] 0.96 1.91 2.8618 173
O(4) --H(43) ..O(3) [ ] 0.91 2.53 2.8793 103
O(4) --H(43) ..O(21) [1565.01] 0.91 2.31 2.8375 117
O(4) --H(43) ..O(6) [2656.01] 0.91 2.54 3.3724 152
O(6) --H(63) ..O(3) [2646.01] 0.96 1.92 2.8483 163
O(11) --H(101) ..O(2) [ ] 0.97 1.85 2.7808 159
O(31) --H(301) ..O(41) [2555.01] 0.97 1.91 2.8640 168
O(41) --H(401) ..O(11) [1554.01] 0.98 1.76 2.7156 165
O(61) --H(601) ..O(5) [ ] 0.97 1.89 2.8498 167
C(1) --H(1) ..O(6) [2646.01] 1.10 2.27 3.3473 166
C(3) --H(3) ..O(11) [2556.01] 1.10 2.45 3.5152 162
C(11) --H(12) ..O(6) [2646.01] 1.10 2.44 3.4674 157
C(31) --H(31) ..O(2) [2546.01] 1.10 2.41 3.4597 159
C(41) --H(41) ..O(61) [ ] 1.10 2.47 2.9363 104
C(6) --H(61) ..O(61) [ ] 1.09 2.51 3.3107 130
C(61) --H(62) ..O(6) [2645.01] 1.09 2.51 3.2203 122
C(61) --H(611) ..O(4) [1545.01] 1.09 2.56 3.3058 125
[1556.] = x,y,1+z
[1565.] = x,1+y,z
[1545.] = x,-1+y,z
[2645.] = 1-x,-1/2+y,-z
[2556.] = -x,1/2+y,1-z
[2646.] = 1-x,-1/2+y,1-z
[2555.] = -x,1/2+y,-z
[2656.] = 1-x,1/2+y,1-z
[2546.] = -x,-1/2+y,1-z
[1554.] = x,y,-1+z
Hydrogen Bond Table Tool
Nardelll
PLATON MENU
OptionMenus
NoMove
NoDisorder
Organic
Round
Parentheses
Label-Alias
R/S-Determ
NoSubCell
Norm-H-bond
Join-Expand
LstARU RCel
LstCellSymm
ListAtoms
ListBonds
LstFlagRadi
X-LineWidth
Reverse-B&W
Q-Peak-Incl
EPS HGL TEK
NoSymm
Prev Next
SAVE-InstrS
ENTRY-LIST
Reset End
Exit
MenuActive
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
Classic Hydrogen Bonds Found (See Listing for Details)
>> Hit RETURN to Continue

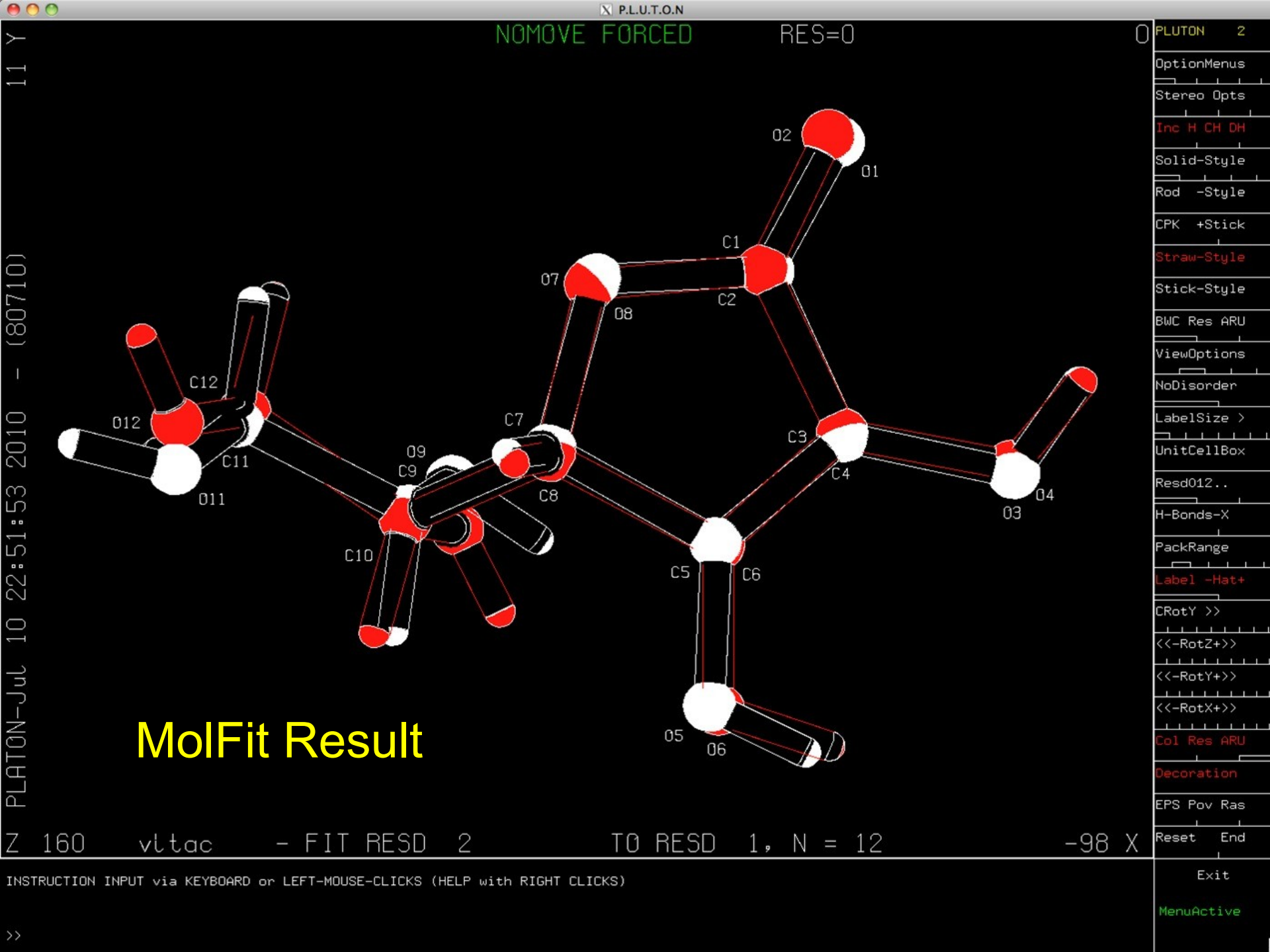
The PLUTON Tool

- PLUTO style ball-and-stick and CPK plots
- Packing plots
- Display of Hydrogen bond networks
- Interactive renaming of atom labels
- Display of molfit results

Automatically Generated Hydrogen Bond Network Display

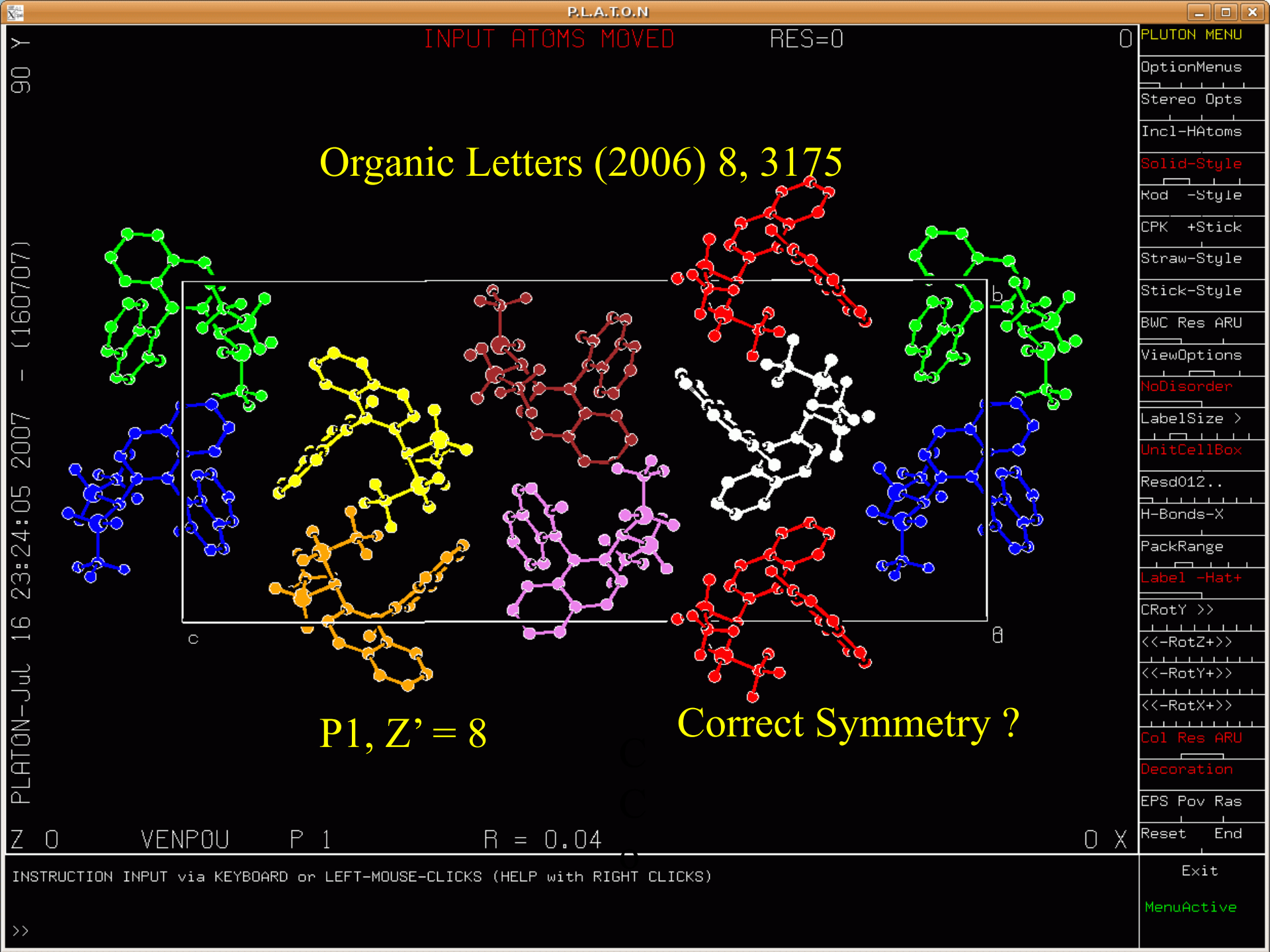



P.L.A.T.O.N
INPUT ATOMS MOVED
RES=0
0
16 Y
PLATON-Jul 23 12:51:02 2010 - (160710)
O4
O6
C4
C6
C8
C2
O2
O8
O10
C10
C12
O12
O11
C11
C9
O9
C7
O7
C1
O1
C5
C3
O5
O3
Straw Style
Z -157 vltac
R = 0.01
-125 X
PLUTON 2
OptionMenus
Stereo Opts
Inc H CH DH
Solid-Style
Rod -Style
CPK +Stick
Straw-Style
Stick-Style
BWC Res ARU
ViewOptions
NoDisorder
LabelSize >
UnitCellBox
Resd012..
H-Bonds-X
PackRange
Label -Hat+
CRotY >>
<<-RotZ+>>
<<-RotY+>>
<<-RotX+>>
Col Res ARU
Decoration
EPS Pov Ras
Reset End
Exit
MenuActive
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>


P.L.U.T.O.N
NOMOVE FORCED
RES=0
0
PLUTON 2
OptionMenus
Stereo Opts
Inc H CH DH
Solid-Style
Rod -Style
CPK +Stick
Straw-Style
Stick-Style
BWC Res ARU
ViewOptions
NoDisorder
LabelSize >
UnitCellBox
Resd012..
H-Bonds-X
PackRange
Label -Hat+
CRotY >>
<<-RotZ+>>
<<-RotY+>>
<<-RotX+>>
Col Res ARU
Decoration
EPS Pov Ras
Reset End
Exit
MenuActive
Y 11 - (80710) 10-Jul-2010 22:51:53 PLATON
Z 160 vltac - FIT RESD 2 TO RESD 1, N = 12 -98 X
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
O1
O2
C1
C2
O7
O8
C3
C4
O3
O4
C5
C6
O5
O6
C7
C8
O9
C9
C10
O11
C11
O12
C12
MolFit Result

The ADDSYM Tool

- Automatic search for (missed) higher symmetry in a crystal structure.
- Creation of a RES file to continue SHELXL refinement in the higher symmetry.
- ADDSYM is an extended implementation of the MISSYM algorithm by Yvon LePage.
- Part of IUCr CheckCIF.


P.L.A.T.O.N
INPUT ATOMS MOVED
RES=0
0
PLUTON MENU
OptionMenus
Stereo Opts
Incl-HAtoms
Solid-Style
Rod -Style
CPK +Stick
Straw-Style
Stick-Style
BWC Res ARU
ViewOptions
NoDisorder
LabelSize >
UnitCellBox
Resd012..
H-Bonds-X
PackRange
Label -Hat+
CRotY >>
<<-RotZ+>>
<<-RotY+>>
<<-RotX+>>
Col Res ARU
Decoration
EPS Pov Ras
Reset End
Exit
MenuActive
90 Y
PLATON-Jul 16 23:24:05 2007 - (160707)
Organic Letters (2006) 8, 3175
P1, Z' = 8
Correct Symmetry ?
b
c
a
Z 0
VENPOU
P 1
R = 0.04
0 X
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>

PLATON/ADDSYM for VENPOU P 1

ADDSYM Search on ALL NON-H Chemical Types [Max NonFit 20 Perc]
Criteria: 1.00 Deg (Metric), 0.25 Ang (Rot.), 0.45 Ang (Inv), 0.45 Ang (Transl)

Symm. Elem	Input Cell Row	Reduced Cell Row	(Ang) d	Typ	Dot	(Deg) Angle	( ) Flt	(Ang) MaxDev.		Input Cell x	y	z
2 *	[1 0 0]	[1 0 0]	8.08	2	1	0.06	100	0.024	Through	0	0.302	0.266
1							F36	-F28	Screw =	1/2	0	0
2 *	[0 0 1]	[0 0 1]	36.08	2	1	0.13	100	0.016	Through	0.415	0.552	0
1							F28	-F3	Screw =	0	0	1/2
2 *	[0 1 0]	[0-1 0]	15.67	2	1	0.14	100	0.025	Through	0.665	0	0.516
1							F10	-F28	Screw =	0	1/2	0

Reduced-to-Convent Input-to-Reduced T = Input-to-Convent: a' = T a

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \times \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \quad \text{Det(T)} = 1.000$$

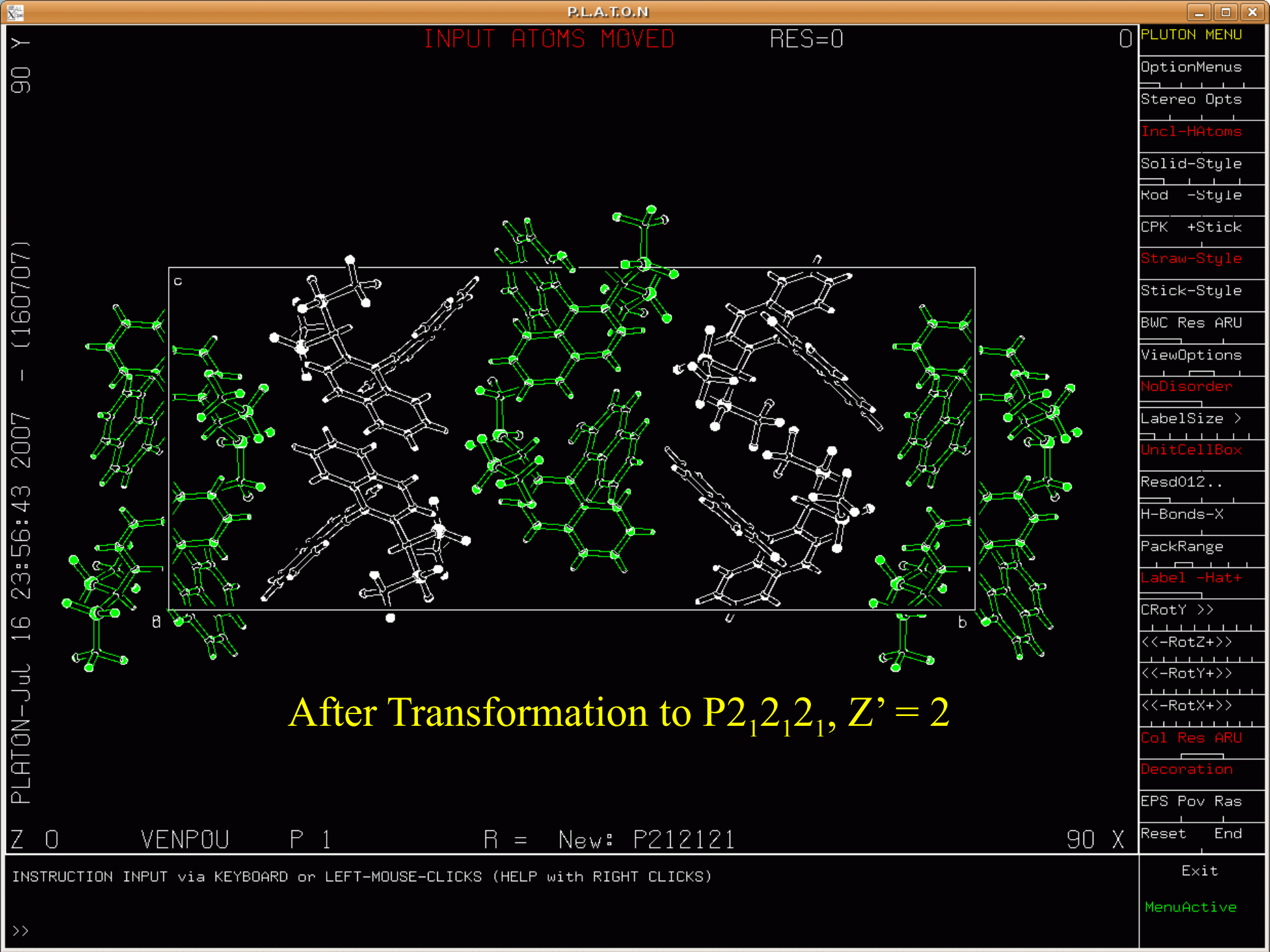
Cell	Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input	aP	8.079	15.672	36.082	90.13	90.01	90.06	4569	Triclinic	-1
Reduced	P	8.079	15.672	36.082	90.13	90.02	90.05	4569		
Convent	oP	8.079	36.082	15.672	89.87	89.94	90.01	4569	Orthorhombic	mmm

Origin shifted to: 0.415,-0.484,-0.302 after transformation
Missed/Additional Symmetry : Suggested SPGR = P212121 (No 19)

ADDSYM MENU
NonFitPerc
TolMetric
TolRotAxis
TolInvers
TolTransl
NFTPercImpl
NoSubCell
KeepMon-I-n
ListDetails
ADDSYMEqual
ADDSYMElmnt
ADDSYMExact
ADDSYM-PLOT
ADDSYM-SHX
End
Exit
MenuActive

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

Additional (Pseudo)Symmetry Found (See Listing for details)
>>



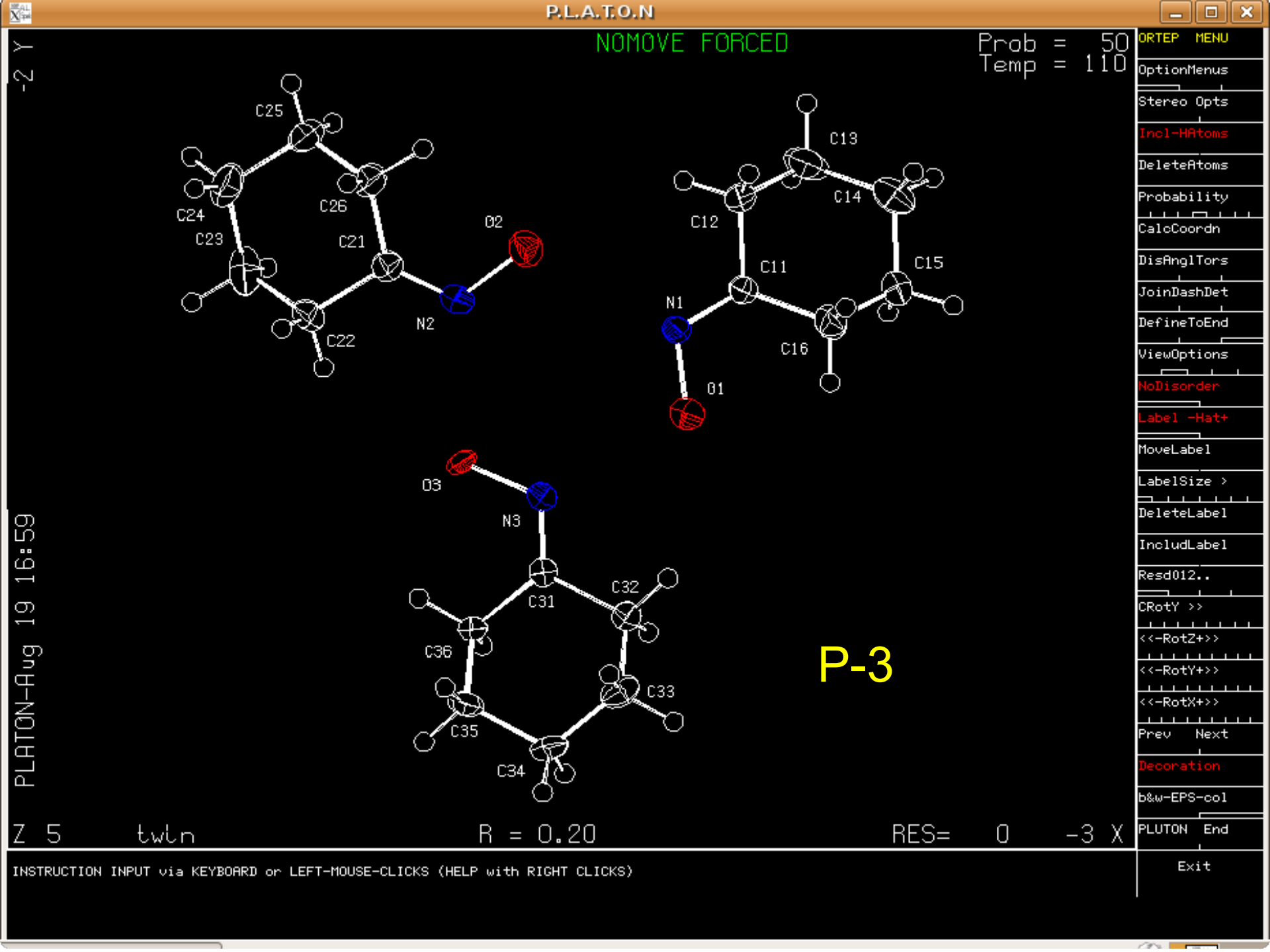
After Transformation to $P2_12_12_1$, $Z' = 2$

The TwinRotMat Tool

- Inspired by but not identical with the ROTAX tool (Parsons et al. (2002) J. Appl. Cryst., 35, 168)
- Reflections effected by twinning show-up in the least-squares refinement with F(obs) >> F(calc)
- Overlapping reflections necessarily have the same Theta value within a certain tolerance.
- Generate a list of implied possible twin axes based on the above observations.
- Test each proposed twin law for its effect on R.
- Part of CheckCIF

TwinRotMat Example

- Originally published as disordered in P3.
- Correct Solution and Refinement in the trigonal space group P-3 ➔R= 20%.
- Run PLATON/TwinRotMat on CIF/FCF
- Result: Twin law with an the estimate of the twinning fraction and the estimated drop in R-value
- Example of a Merohedral Twin ➔


P.L.A.T.O.N
NOMOVE FORCED
Prob = 50
Temp = 110
-2 Y
PLATON-Aug 19 16:59
C25
C24
C26
C23
C21
O2
N2
C22
C13
C12
C14
C11
C15
N1
C16
O1
O3
N3
C31
C32
C36
C33
C35
C34
P-3
Z 5 twin
R = 0.20
RES= 0 -3 X
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
ORTEP MENU
OptionMenus
Stereo Opts
Incl-HAtoms
DeleteAtoms
Probability
CalcCoordn
DisAnglTors
JoinDashDet
DefineToEnd
ViewOptions
NoDisorder
Label -Hat+
MoveLabel
LabelSize >
DeleteLabel
IncludLabel
Resd012..
CRotY >>
<<-RotZ+>>
<<-RotY+>>
<<-RotX+>>
Prev Next
Decoration
b&w-EPS-col
PLUTON End
Exit

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)

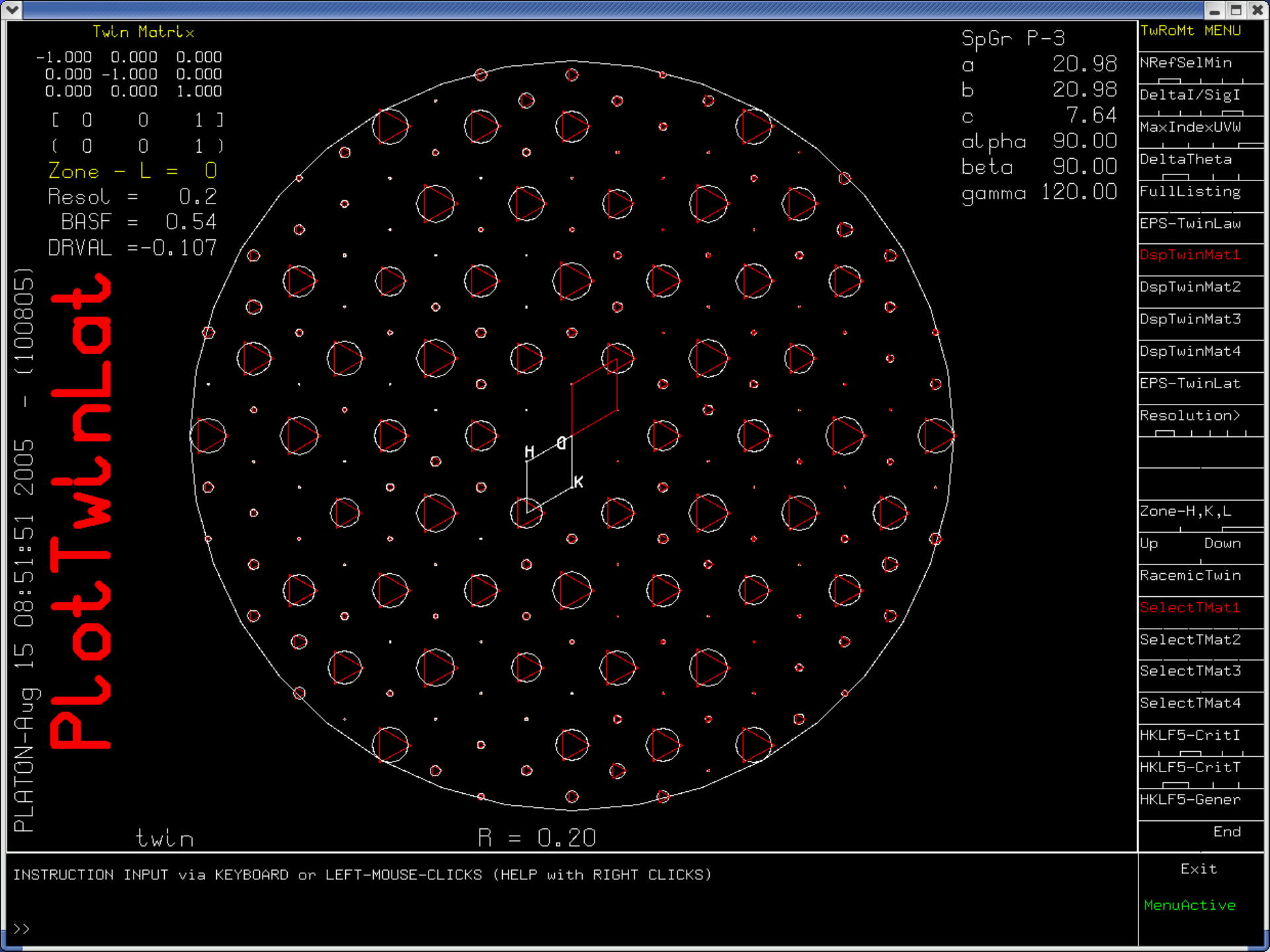
2-axis (0 0 1) [0 0 1], Angle () [] = 0.00 Deg, Freq = 47 (-1.000 0.000 0.000) (h1) (h2) Nr Overlap = 4445 (0.000 -1.000 0.000) * (k1) = (k2) BASF = 0.54 (0.000 0.000 1.000) (l1) = (l2) DEL-R =-0.107	1	
2-axis (1 -1 0) [1 -1 0], Angle () [] = 0.00 Deg, Freq = 48 (0.000 -1.000 0.000) (h1) (h2) Nr Overlap = 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	
2-axis (2 -1 0) [1 0 0], Angle () [] = 0.00 Deg, Freq = 36 (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	3	
2-axis (1 3 -1) [10 14 -23], Angle () [] = 0.45 Deg, Freq = 10 (-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	4	
twin 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)

>>

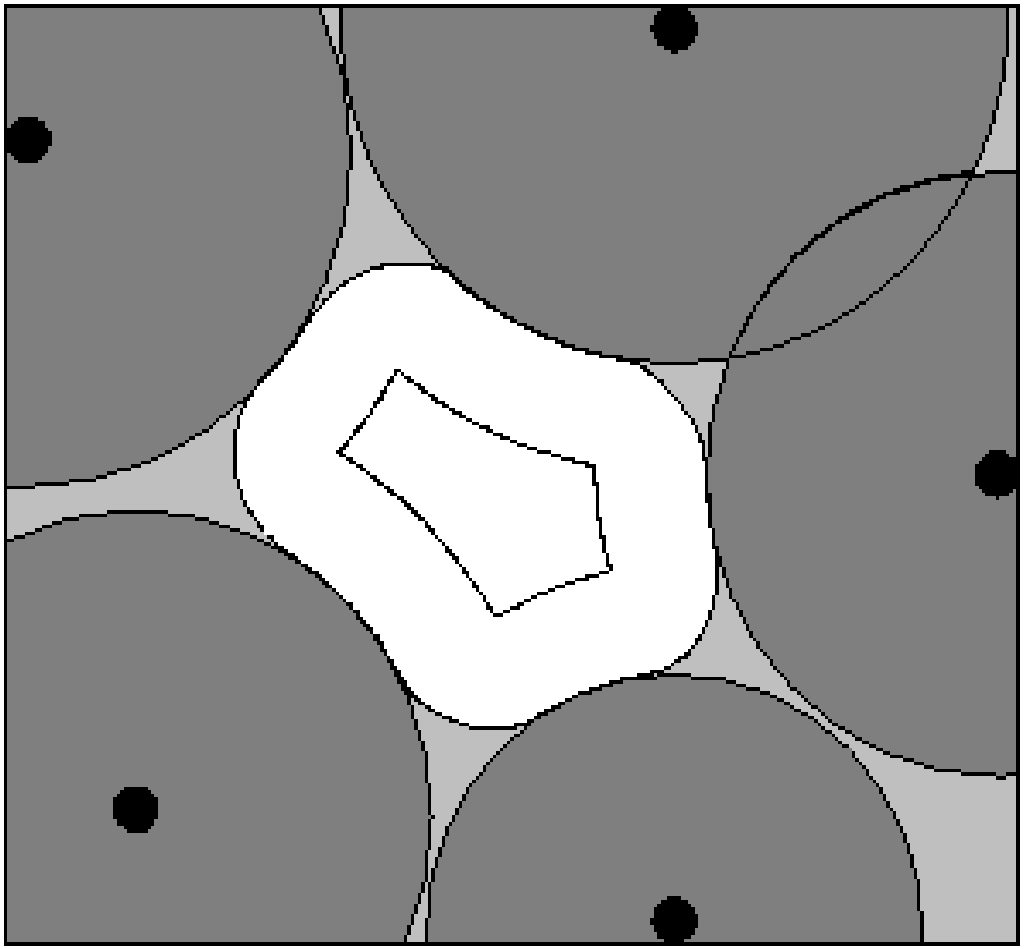
Exit
MenuActive

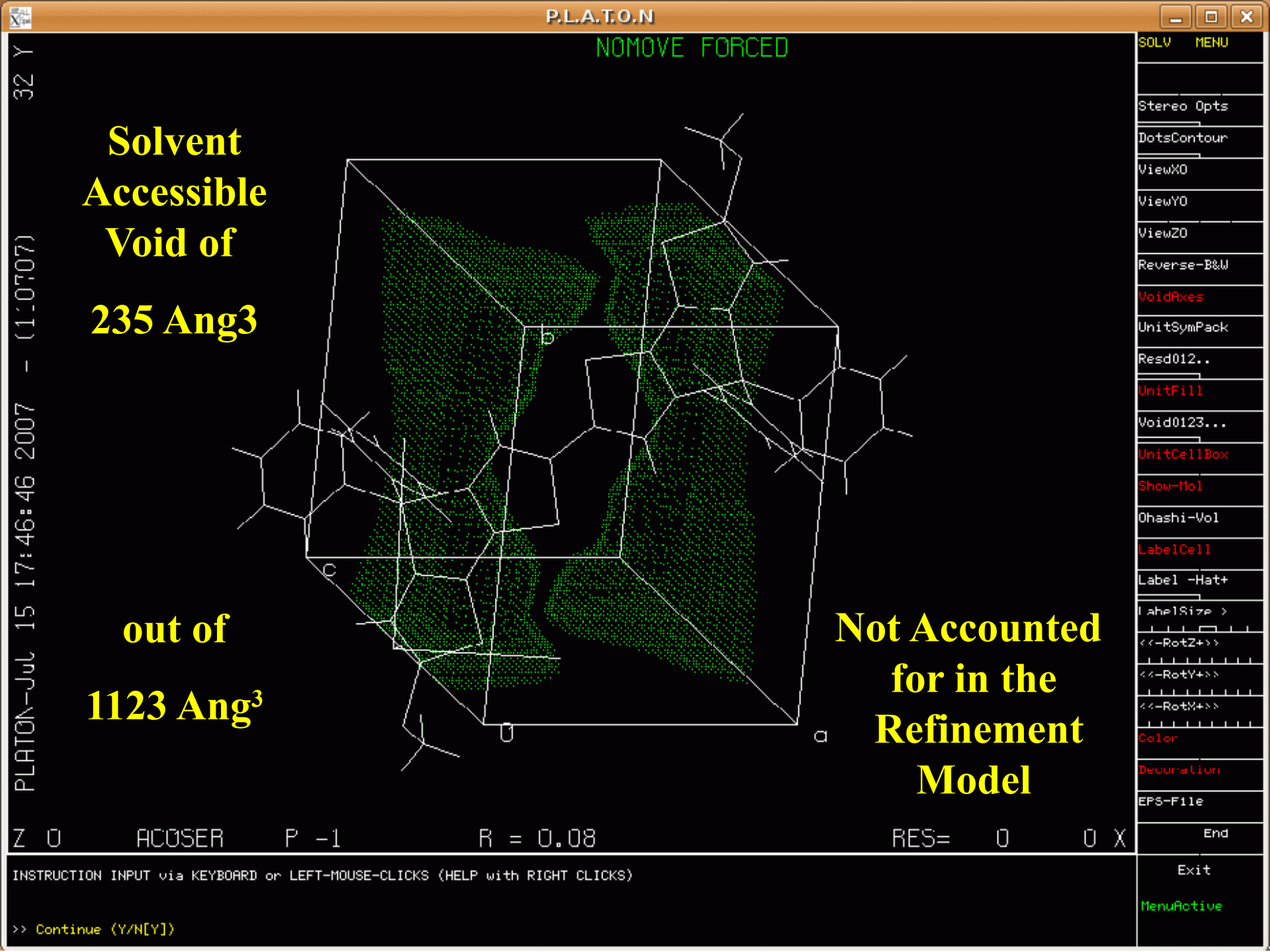

Twin Matrix
-1.000 0.000 0.000
0.000 -1.000 0.000
0.000 0.000 1.000
[0 0 1]
(0 0 1)
Zone - L = 0
Resol = 0.2
BASF = 0.54
DRVAL =-0.107
SpGr P-3
a 20.98
b 20.98
c 7.64
alpha 90.00
beta 90.00
gamma 120.00
PLATON-Aug 15 08:51:51 2005 - (100805)
PlotTwinLat
H
O
K
twin
R = 0.20
TwRoMt MENU
NRefSelMin
DeltaI/SigI
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

The SOLV,VOID & SQUEEZE Tool

- Detection and display of solvent accessible voids in a structure
- Determination of the Kitaigorodskii packing index
- Handling disordered solvent contribution in the structure refinement (SQUEEZE)
- Determination of the available space in solid state reactions (Ohashi)
- Determination of pore volumes, pore shapes and migration paths in microporous crystals
- VOID detection is part of CheckCIF

SOLVENT ACCESSIBLE VOID




P.L.A.T.O.N
NOMOVE FORCED
Solvent Accessible Void of
235 Ang3
out of
1123 Ang3
Not Accounted for in the Refinement Model
PLATON-Jul 15 17:46:46 2007 - (1:0707)
32 Y
SOLV MENU
Stereo Opts
DotsContour
ViewXO
ViewYO
ViewZO
Reverse-B&W
VoidAxes
UnitSymPack
Resd012..
UnitFill
Void0123...
UnitCellBox
Show-Mol
Ohashi-Vol
LabelCell
Label -Hat+
<<-RotZ+>>
<<-RotY+>>
<<-RotM+>>
Color
Decoration
EPS-File
End
Exit
MenuActive
Z 0 ACOSER P -1 R = 0.08 RES= 0 0 X
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>> Continue (Y/N[Y])

P.L.A.T.O.N

Search for and Analysis of Solvent Accessible Voids in the Structure

Area	#GridPoint	VolPerc.	Vol(A^3)	X(av)	Y(av)	Z(av)	Eigenvector(frac)			Sig(Ang)
1	20126[4072]	4	156[31.6]	0.000	0.184	0.750	1	1.000	-0.003	0.520	1.74
							2	-0.502	-0.002	1.000	1.55
							3	-0.001	-1.000	-0.002	1.35
2	20134[4072]	4	156[31.6]	0.500	0.316	0.250	1	1.000	-0.006	0.521	1.74
							2	-0.503	0.002	1.000	1.55
							3	-0.003	-1.000	-0.001	1.35
3	20125[4072]	4	156[31.6]	0.500	0.684	0.750	1	1.000	-0.008	0.522	1.74
							2	-0.504	-0.005	1.000	1.55
							3	-0.003	-1.000	-0.004	1.35
4	20131[4072]	4	156[31.6]	0.000	0.816	0.250	1	1.000	-0.003	0.523	1.74
							2	-0.505	-0.002	1.000	1.55
							3	-0.001	-1.000	-0.002	1.35

Listing of all voids in the unit cell

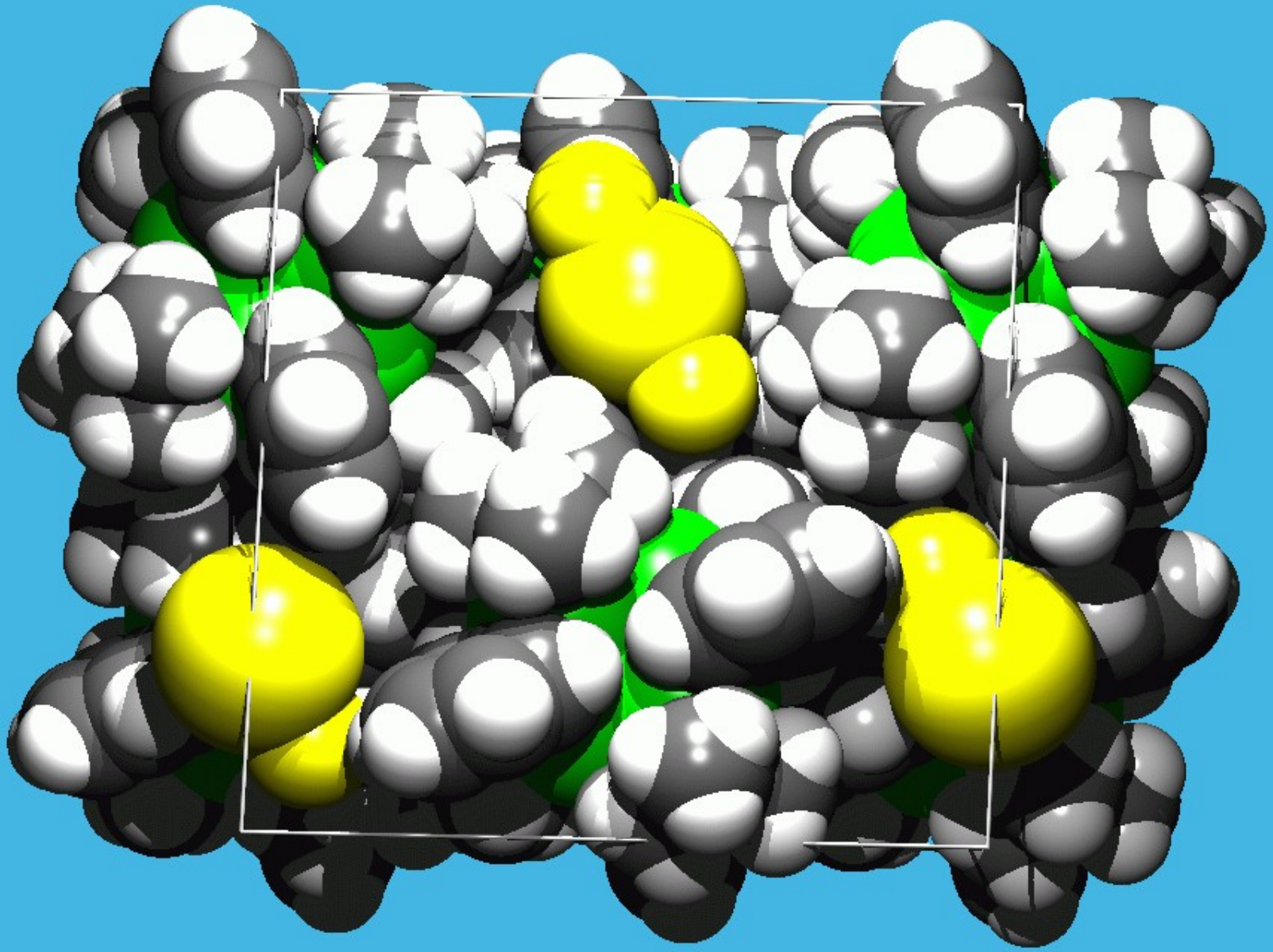
EXAMPLE OF A VOID ANALYSIS

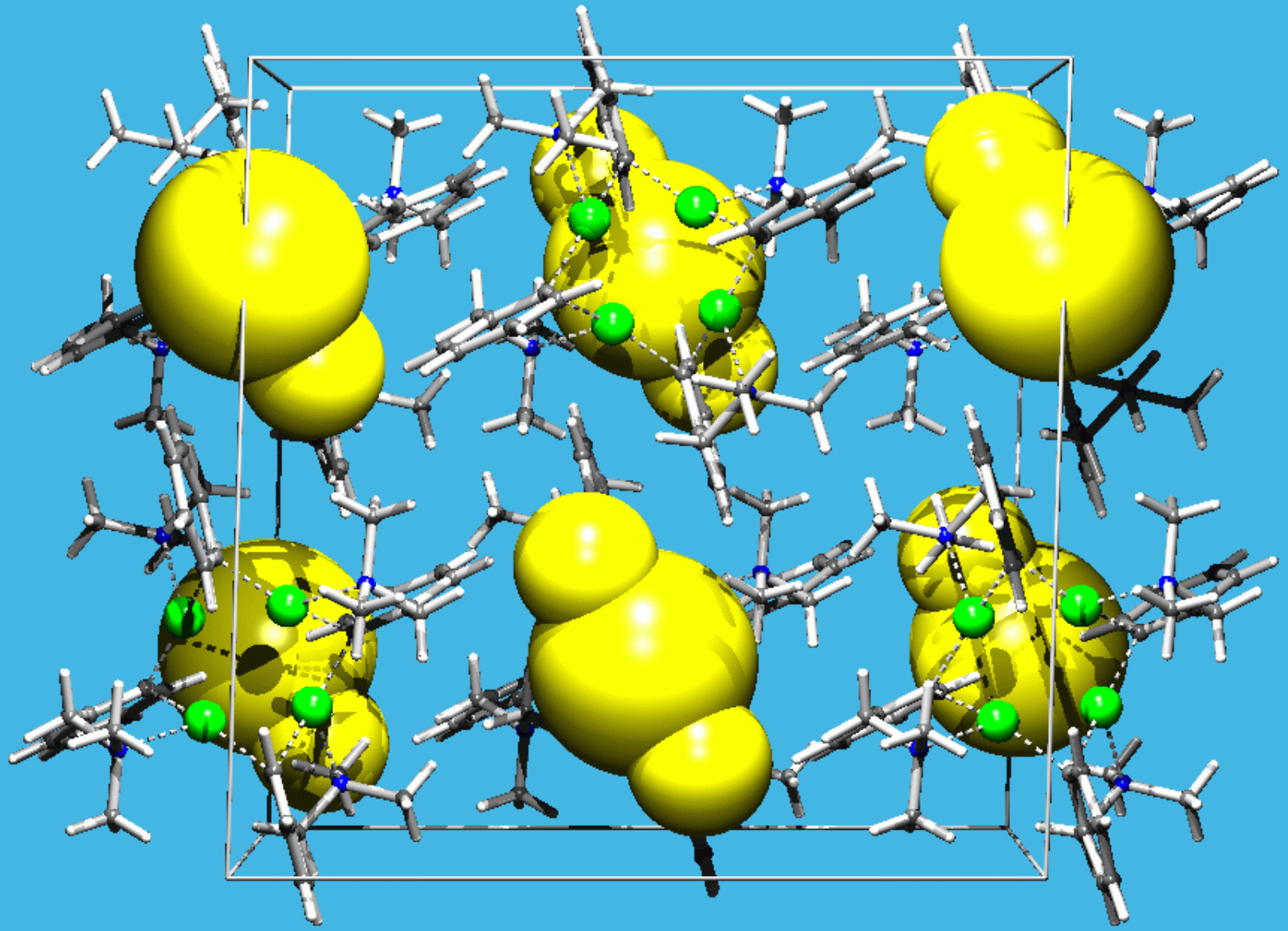
SOLV MENU
Stereo Opts
DotsContour
ViewX0
ViewY0
ViewZ0
Reverse-B&W
VoidAxes
UnitSymPack
Resd012..
UnitFill
Void0123...
UnitCellBox
Show-Mol
Ohashi-Vol
LabelCell
Label -Hat+
LabelSize >
<<-RotZ+>>
<<-RotY+>>
<<-RotX+>>
Color
Decoration
EPS-File
End

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

Solvent Accessible Void Found (See Listing for Details)
>> Continue (Y/N[Y])

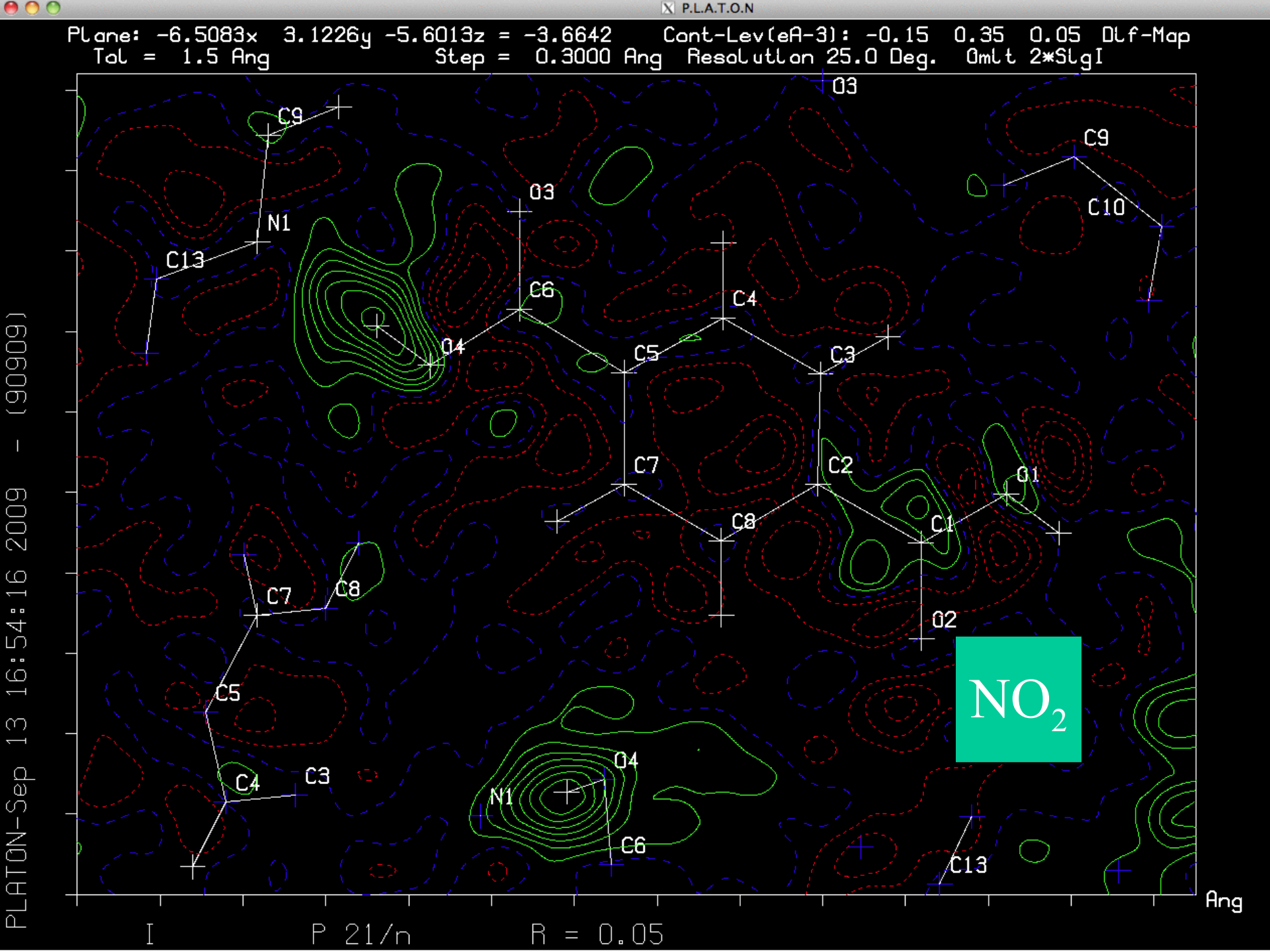
Exit
MenuActive





The Fourier Contour Tool

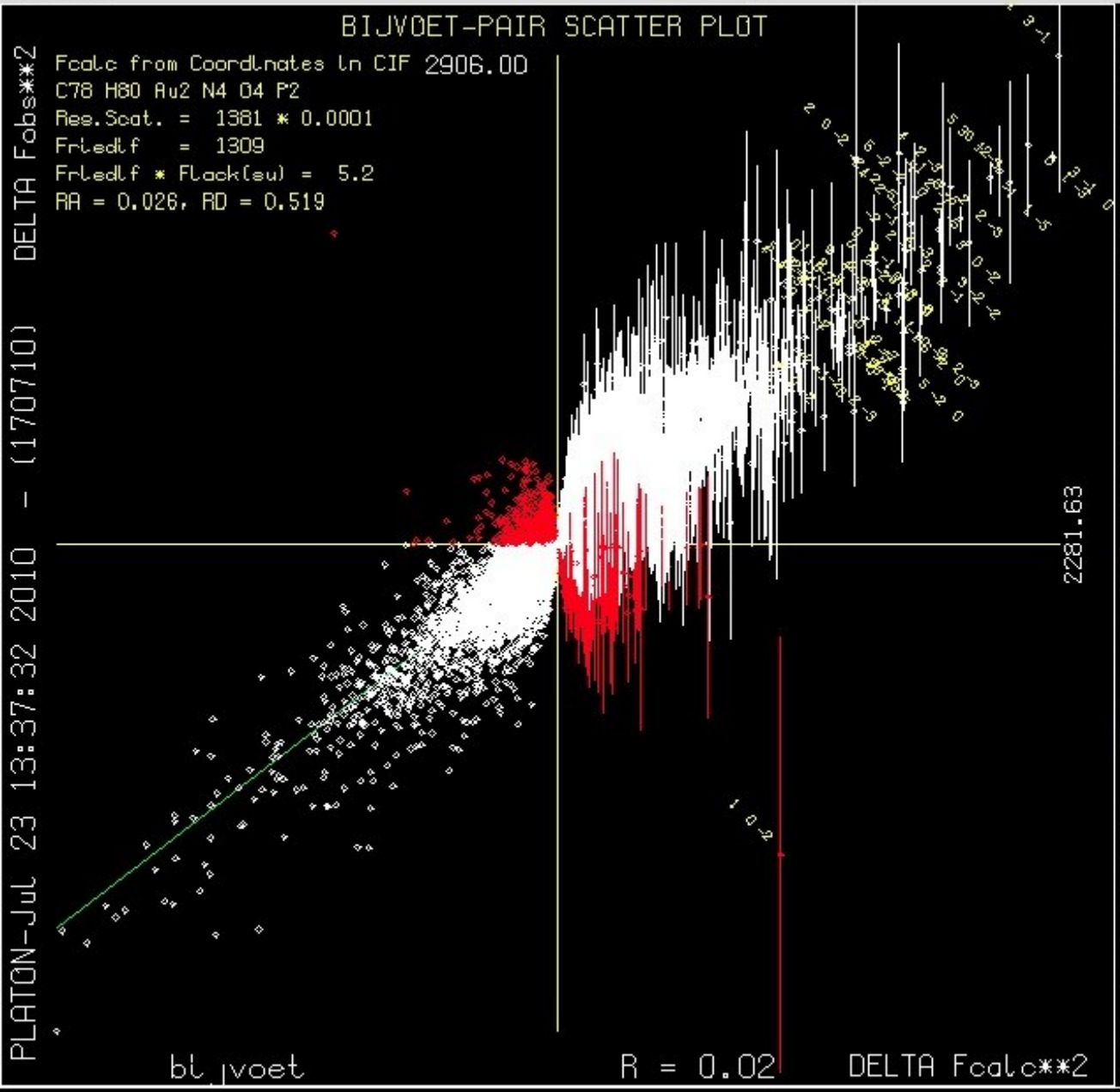
- Display of contoured sections of difference density maps defined by three atoms.
- Difference maps can be calculated with some atoms left out of the SF-calculation.
- Missing atoms show up as green contours.
- Used to check H-atom positions.
- Inspection on coordination planes.


P.L.A.T.O.N
Plane: -6.5083x 3.1226y -5.6013z = -3.6642 Cont-Lev(eA-3): -0.15 0.35 0.05 Dlf-Map
Tol = 1.5 Ang Step = 0.3000 Ang Resolution 25.0 Deg. Omit 2*SigI
PLATON-Sep 13 16:54:16 2009 - (90909)
O3
C9
C10
N1
C13
C6
C4
O4
C5
C3
C7
C2
O1
C8
C1
O2
NO_2
Ang
I P 21/n R = 0.05

The Bijvoet Pair Tool

- Scatter Plot of observed and calculated Friedel/Bijvoet pair differences
- Comparison of Flack and Hooft parameters for absolute structure analysis
- Application to low anomalously scattering compounds
- Part of IUCr CheckCIF

P.L.A.T.O.N



Space Group	P1
Wavelength	0.71073
Flack x	-0.010
Flack (su) .	0.004
Bijvoet Pairs	7738
Coverage ...	98
DiffCalcMax.	2281.63
Outlier Crit	4563.26
Scatter Plot	
Sigma Crit..	0.25
Select Pairs	6416
Number Plus	5441
Number Minus	975
Aver. Ratio	1.026
RC	1.000
Normal Prob. Plot	
Sample Size.	7738
Corr. Coeff.	0.998
Intercept ..	-0.128
Slope	1.115
Bayesian Statistics	
Type	Gaussian
Select Pairs	7738
P2(true)....	1.000
P3(true)....	1.000
P3(rac-twin)	0.0E+00
P3(false) ..	0.0E+00
G	1.0000
G (su)	0.1E-05
Hooft y	0.000
Hooft (su) .	0.1E-02

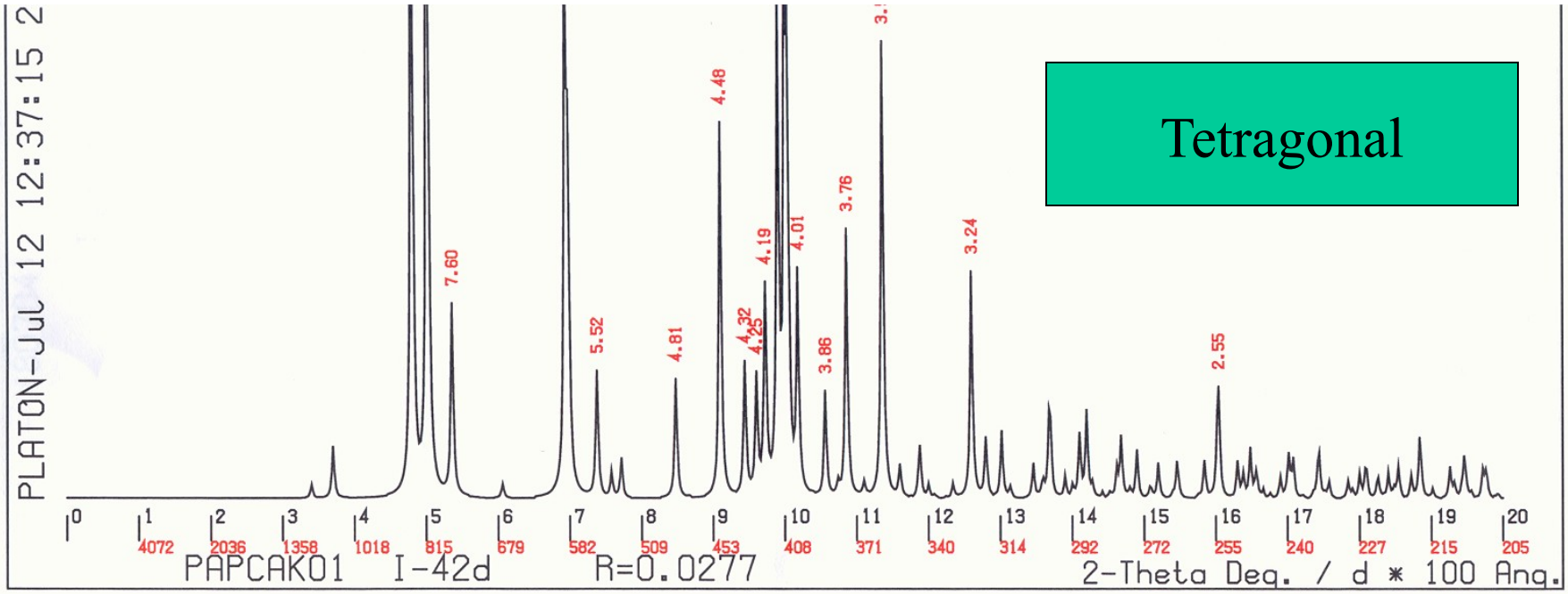
BIJVOET 29
IcalFromFCF
InclWghtPar
OutlierCrit
SigmaCriter
NPP-Bijvoet
ApplySlope
NU-Value
Gaussian
HKL-Display
s.u.-Bar
EPS-File
End
Exit
MenuActive

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

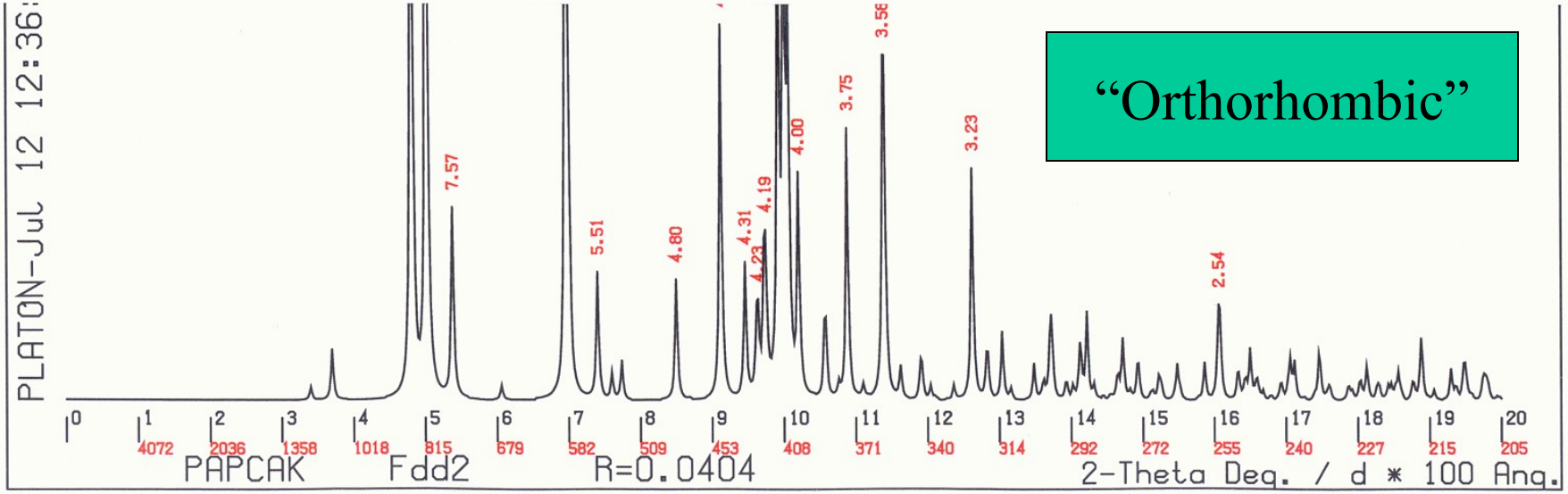
>>

Simulated Powder Patterns

- Powder patterns can be simulated both from observed reflection data or from calculated reflection data
- Easy tool to compare two data sets for the same structure in different settings etc.
- Example: Two published ‘polymorphs’ taken from the CSD



Tetragonal



"Orthorhombic"

FINALLY …

A current PLATON Manual can be found on

'www.cryst.chem.uu.nl/platon/PLATON-MANUAL.pdf'

(Note: do not print the PLATON MANUAL. The current document still needs more details to be added to the already 240 pages)