PLATON, AN OVERVIEW

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Platon Workshop

Chicago, 24-July-2010

What is PLATON About

- PLATON is a collection of tools for single crystal structure analysis bundled within a single SHELX and CIF compatible program.
- The tools are either unique to the program (e.g. Validation) or adapted and extended versions of existing tools (e.g. ORTEP).
- The program was developed over of period of over 30 years in the context of the needs of our National Single Crystal Service Facility in the Netherlands.

DESIGN HISTORY

- PLATON started out in 1980 as a program 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 (e.g. SQUEEZE).

DESIGN FEATURES

- As hardware independent as possible
- Limited dependence on external libraries
- Single routine for all graphics calls
- Single routine for all symmetry handling
- Sharing of the numerical routines by the various tools
- Single Fortran source, simple compilation
- Small C routine for interface to X11 graphics
- Hardcopy standards: PostScript (and HPGL)

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 issues that are reported in need of attention.
- Current Platforms:

  UNIX/LINUX, MAC-OSX, MS-WINDOWS

PLATON Organization

- The program is invoked with the file(s) to work with (UNIX: platon name.cif)
- The tools available in PLATON are listed as clickable objects on the opening menu
- Main menu and tool options are clickable in submenu's.
- Input can be either in a keyboard entry area or by clicking
- 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

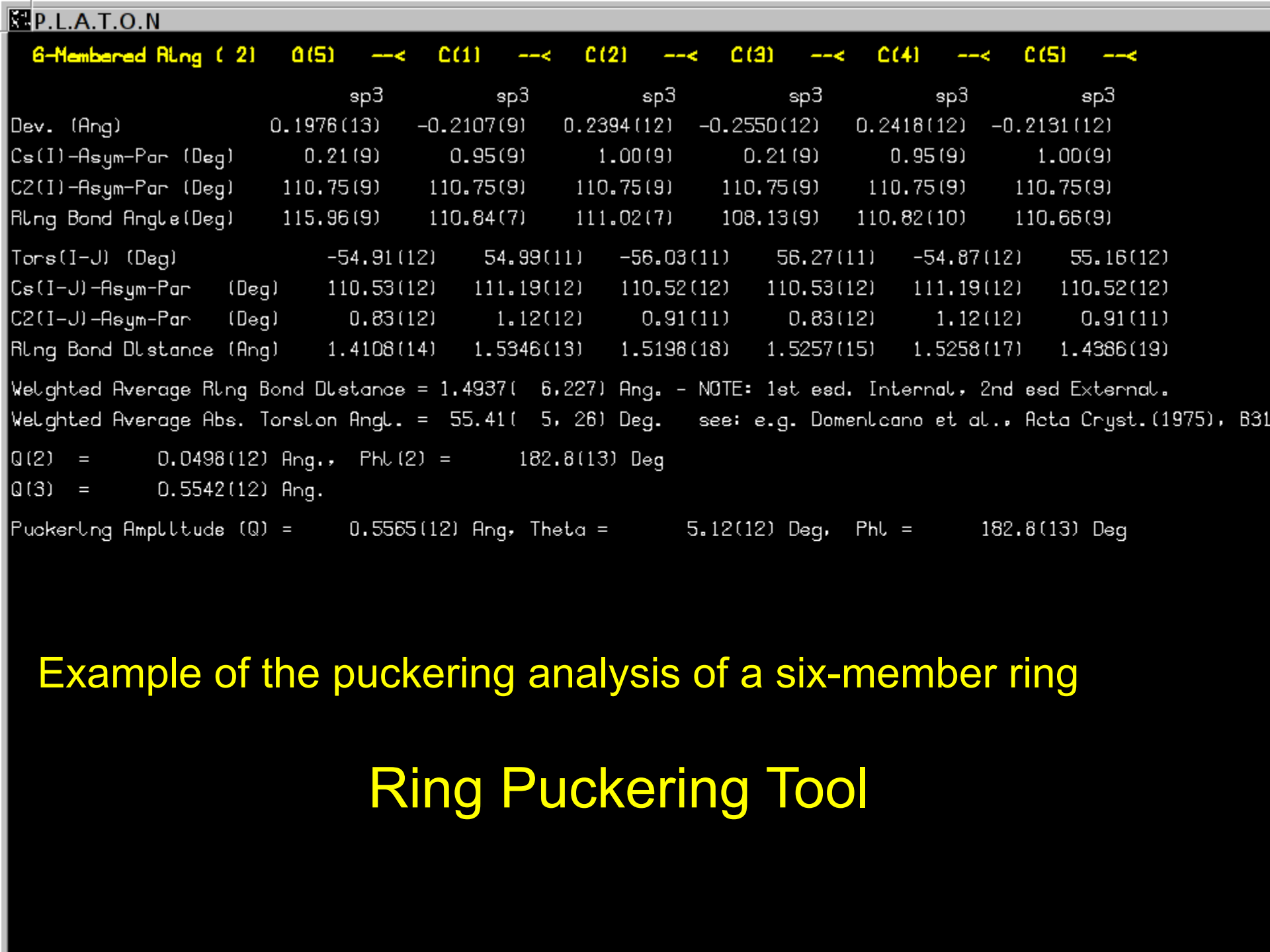
Reset End

Exit

MenuActive

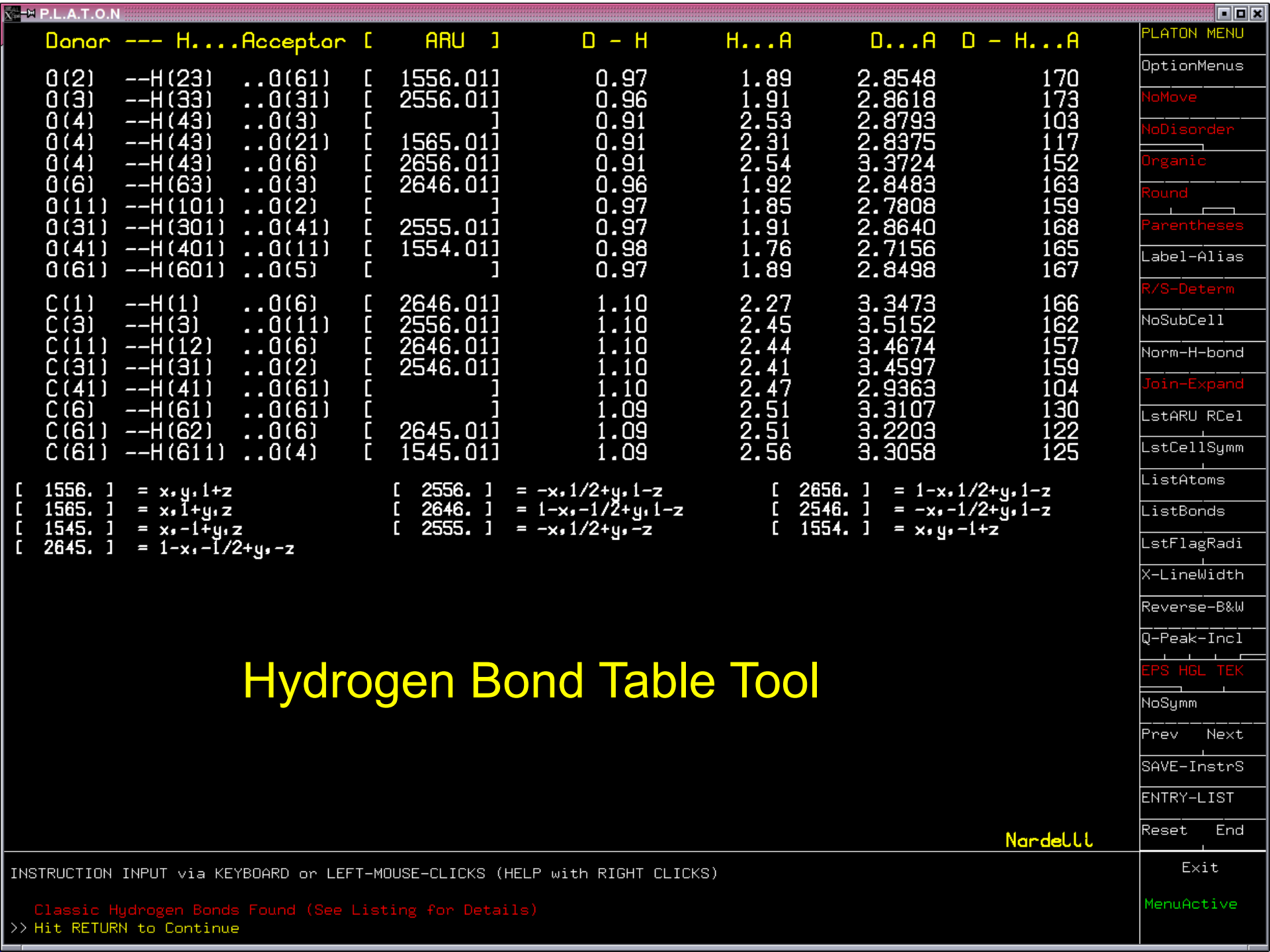
The Geometry Tool

- Extensive Output Listing:
- CALC INTRA - bonds, angles, torsion angles, ring, 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



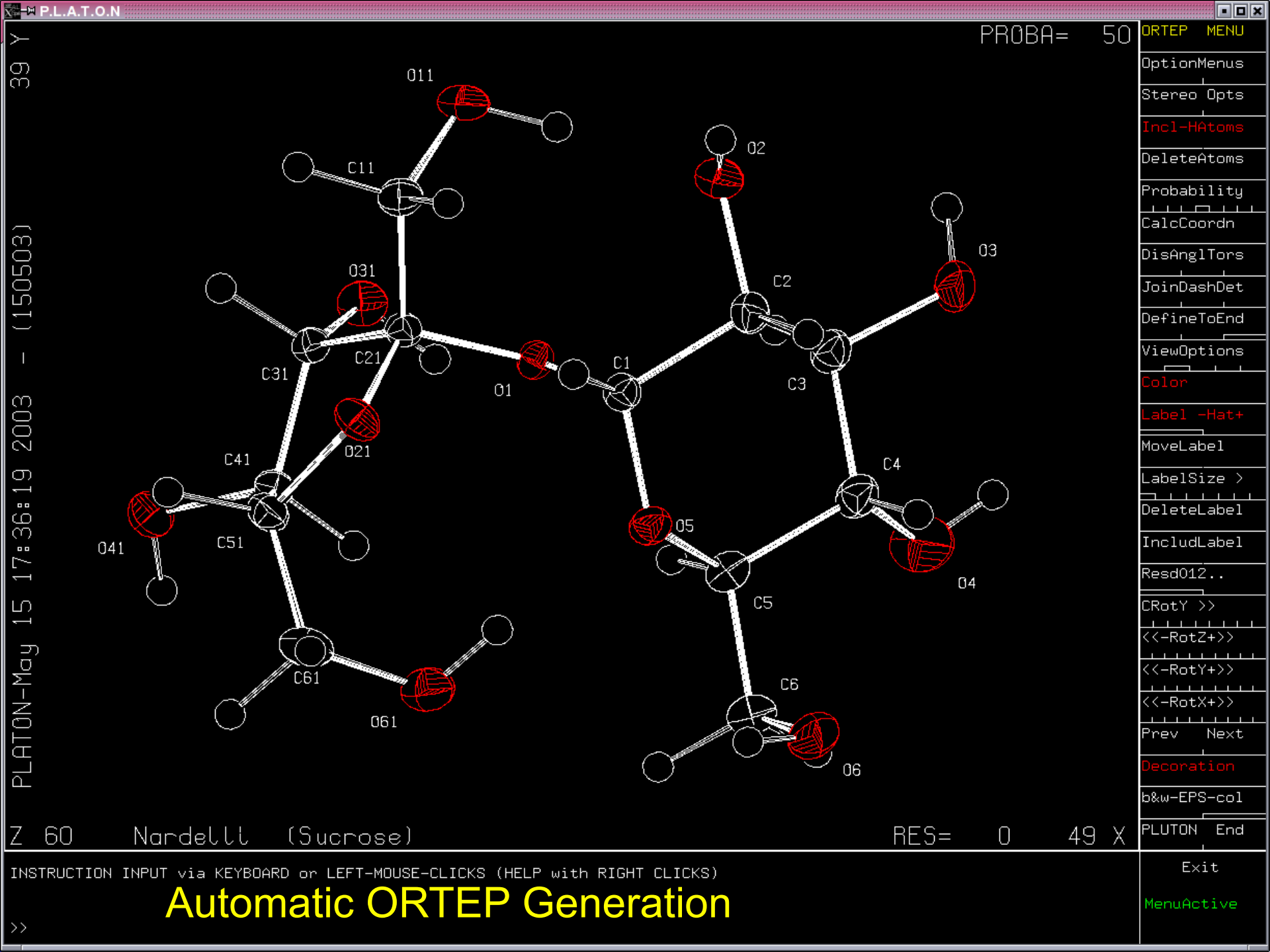
Example of the puckering analysis of a six-member ring

Ring Puckering Tool


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
[2556.] = -x,1/2+y,1-z
[2656.] = 1-x,1/2+y,1-z
[1565.] = x,1+y,z
[2646.] = 1-x,-1/2+y,1-z
[2546.] = -x,-1/2+y,1-z
[1545.] = x,-1+y,z
[2555.] = -x,1/2+y,-z
[1554.] = x,y,-1+z
[2645.] = 1-x,-1/2+y,-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

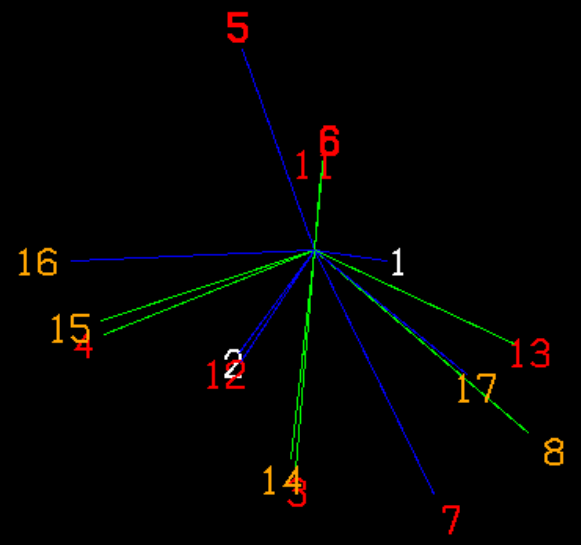
The ORTEP Tool

- Automatic Display of Molecular Geometry and Displacement Parameters
- Interactive tool for least squares plane, 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

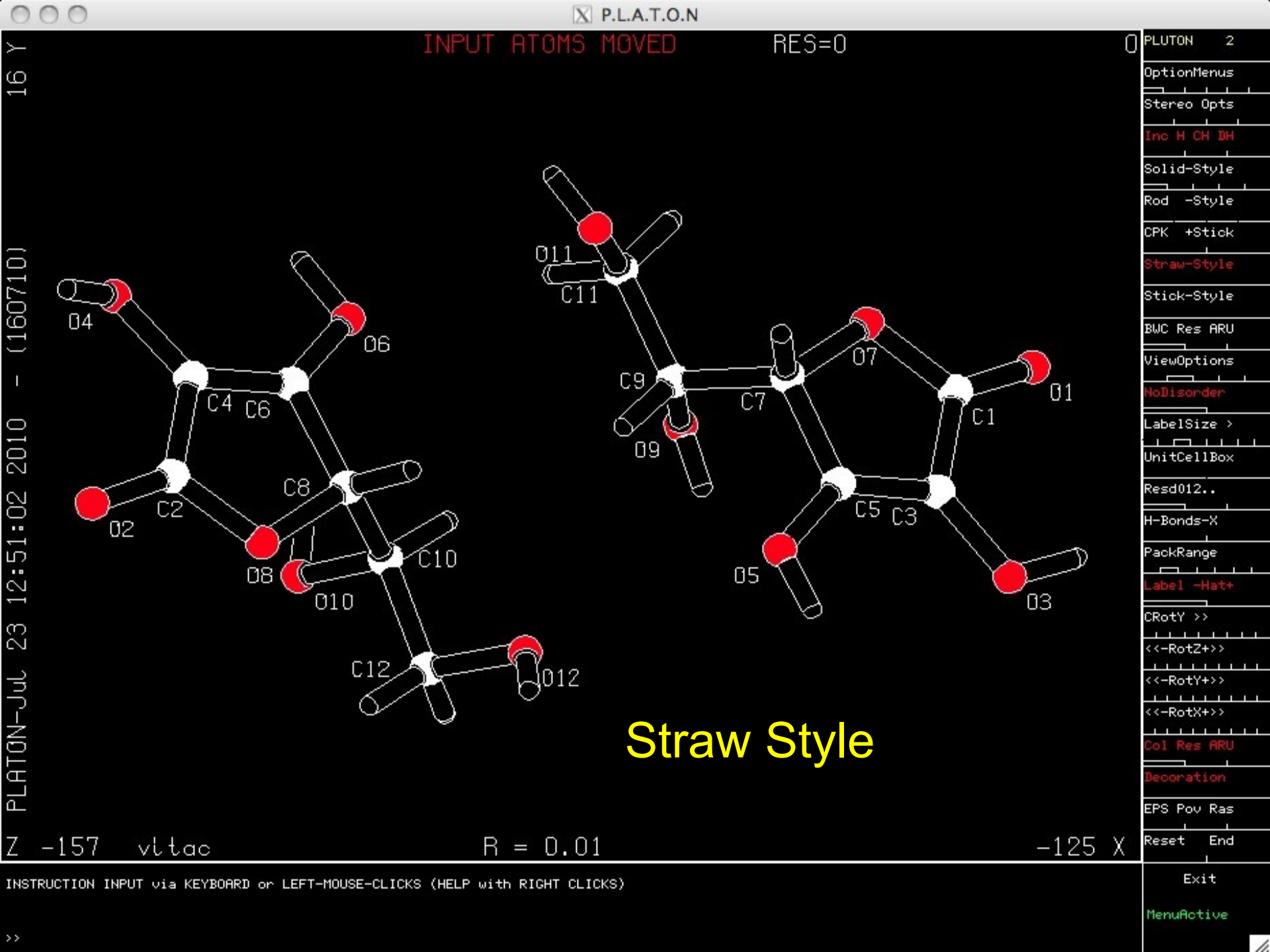
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)

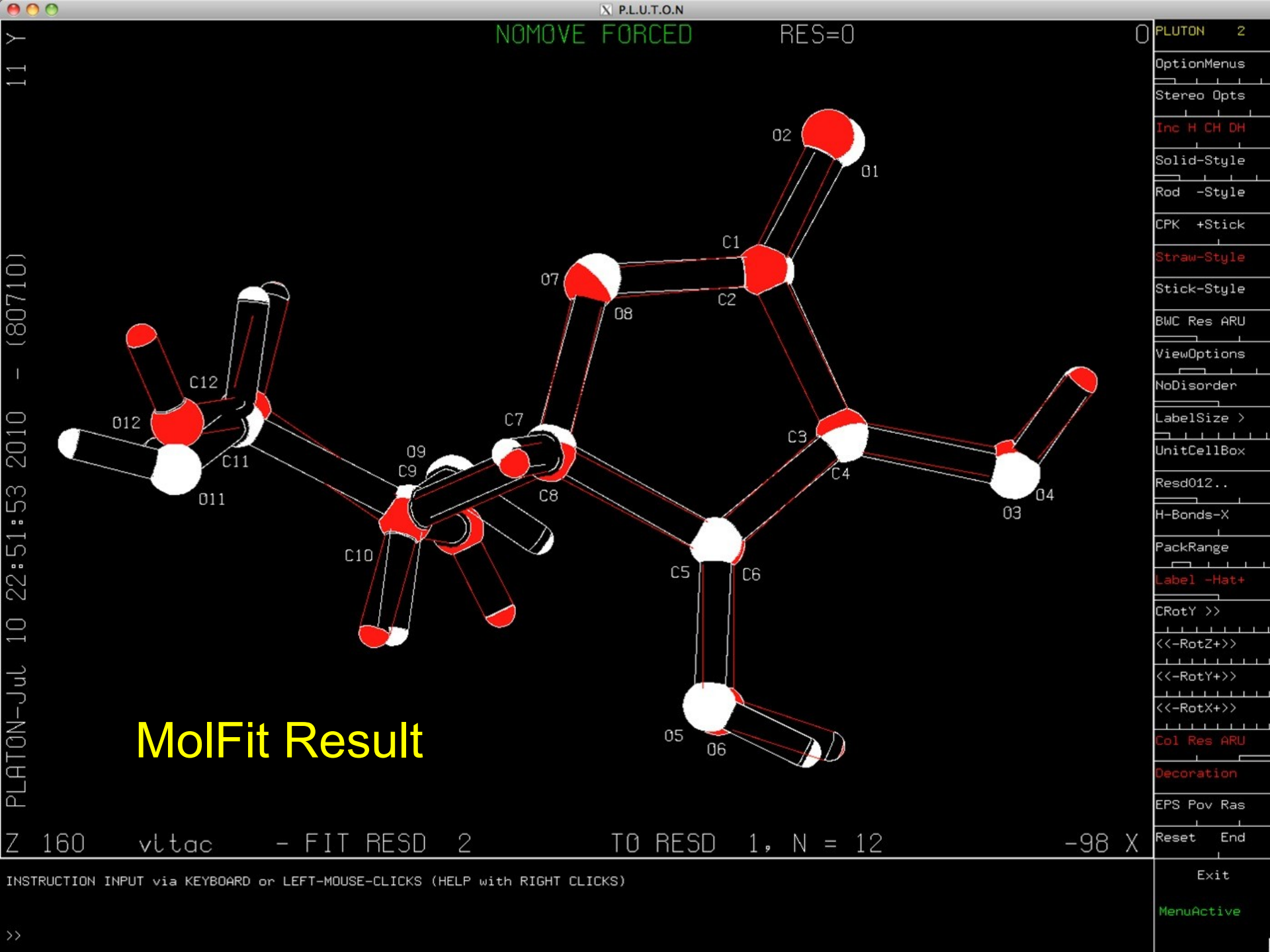
Click on ARU-Code to ADD ARU to ORTEP PLOT
>> Hit RETURN to Continue

Exit
MenuActive

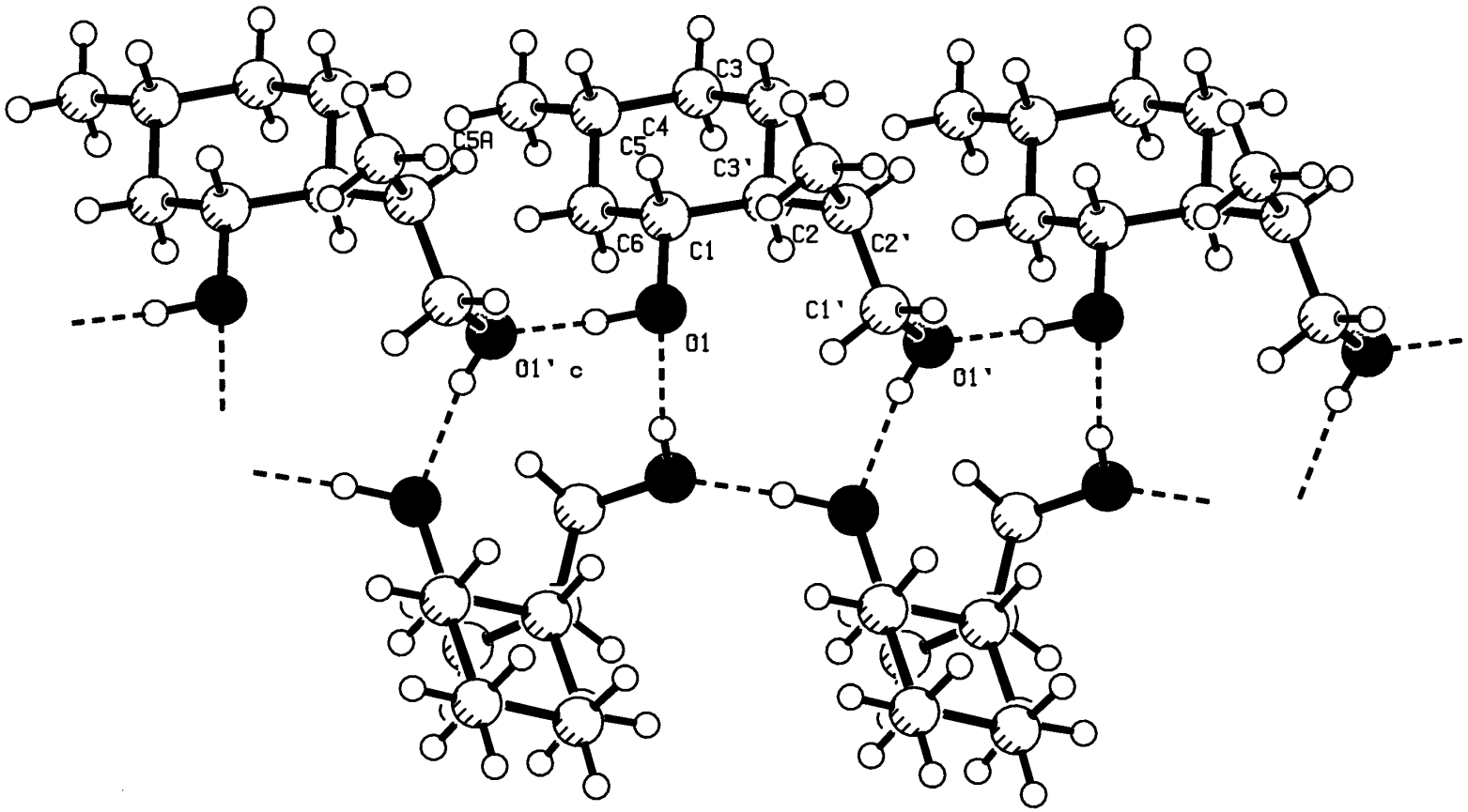
The PLUTON Tool

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


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)
>>

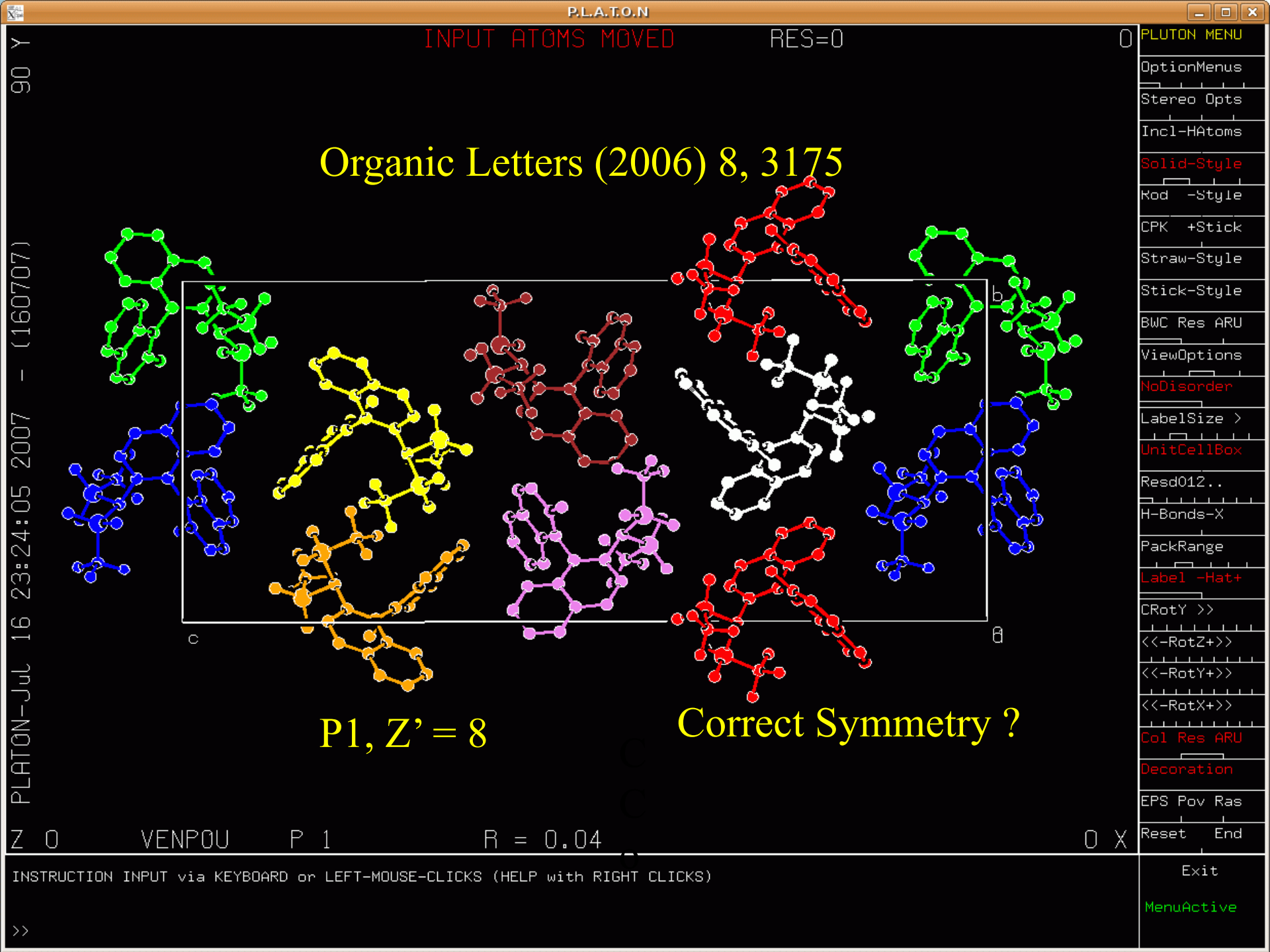

P.L.U.T.O.N
NOMOVE FORCED
RES=0
0
PLUTON 2
OptionMenus
Stereo Opts
Inc H CH DH
Solid-Style
Rod -Style
CPK +Stick
Straw-Style
Stick-Style
BWC Res ARU
ViewOptions
NoDisorder
LabelSize >
UnitCellBox
Resd012..
H-Bonds-X
PackRange
Label -Hat+
CRotY >>
<<-RotZ+>>
<<-RotY+>>
<<-RotX+>>
Col Res ARU
Decoration
EPS Pov Ras
Reset End
Exit
MenuActive
O2
O1
C1
O7
C2
O8
C12
O12
C7
C3
O9
C9
C11
C4
O4
O11
C8
O3
C10
C5
C6
O5
O6
MolFit Result
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)
>>

Hydrogen Bonding Network



The ADDSYM Tool

- Automatic search for (missed) higher symmetry in a crystal structure
- Creation of a RES file to continue refinement in the higher symmetry
- 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
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
Organic Letters (2006) 8, 3175
P1, Z' = 8
Correct Symmetry ?
PLATON-Jul 16 23:24:05 2007 - (160707)
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

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

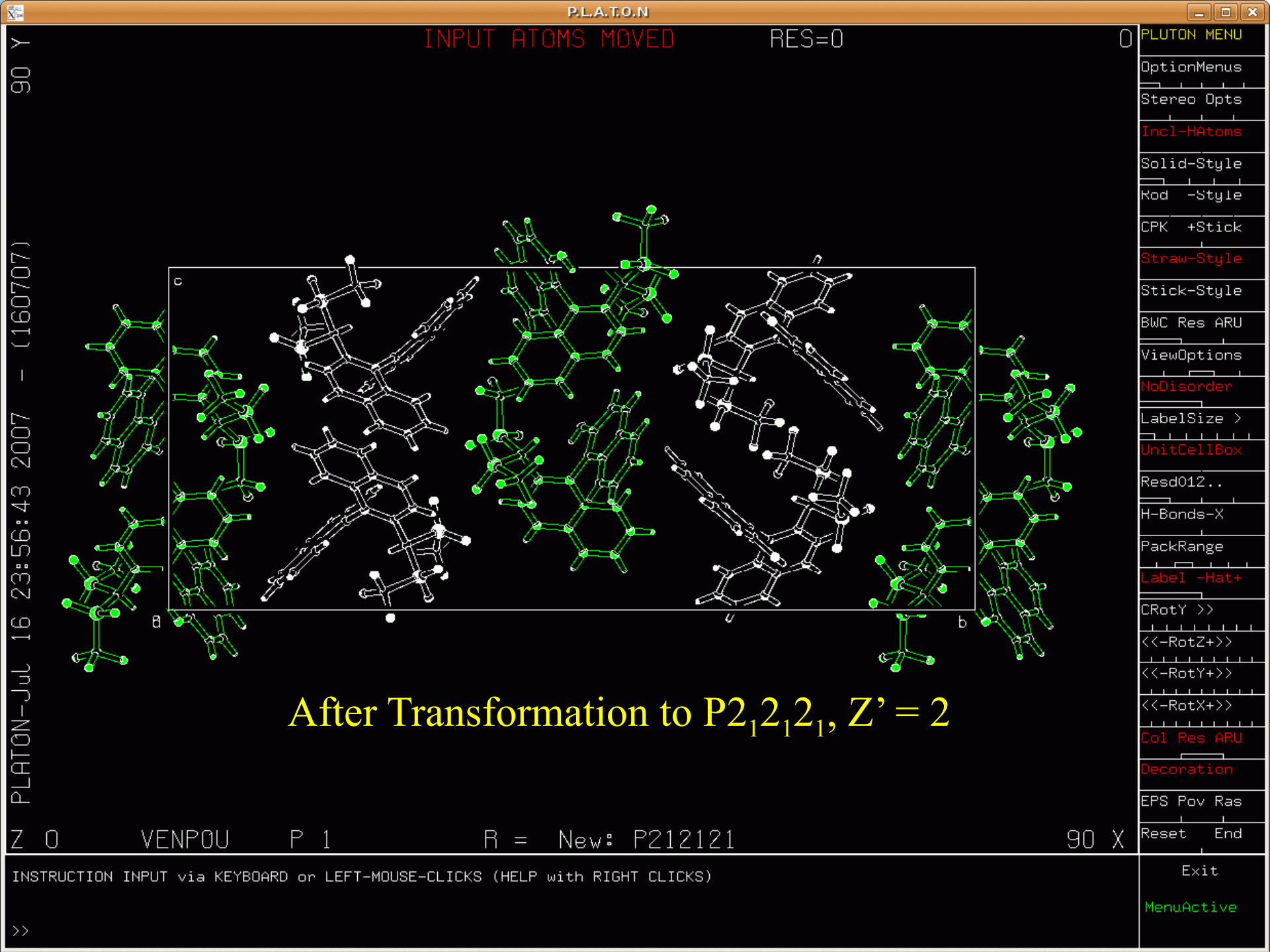
Cell	Lattice	a	b	c	Alpha	Beta	Gamma	Volume	CrystalSystem	Laue
Input	aP	8.079	15.672	36.082	90.13	90.01	90.06	4569	Triclinic	-1
Reduced	P	8.079	15.672	36.082	90.13	90.02	90.05	4569		
Convent	oP	8.079	36.082	15.672	89.87	89.94	90.01	4569	Orthorhombic	mmm

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)
>>

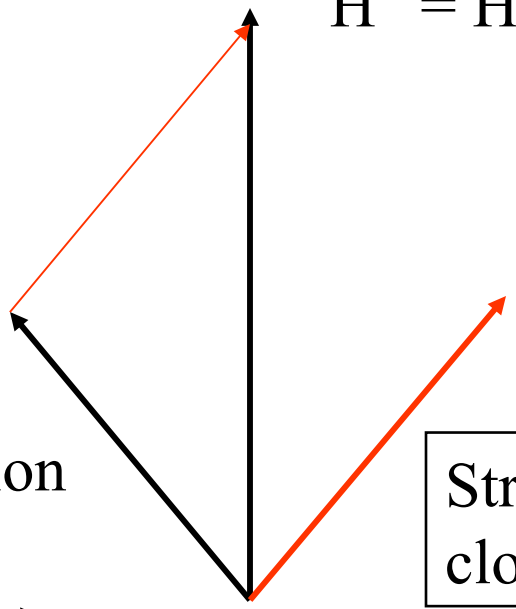


After Transformation to $P2_12_12_1$, $Z' = 2$

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

Possible Twin Axis



H” = H + H’

Candidate twinning axis
(Normalize !)

H’

H

Reflection
with
F(obs) >>
F(calc)

Strong reflection H’ with theta close to theta of reflection H

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)

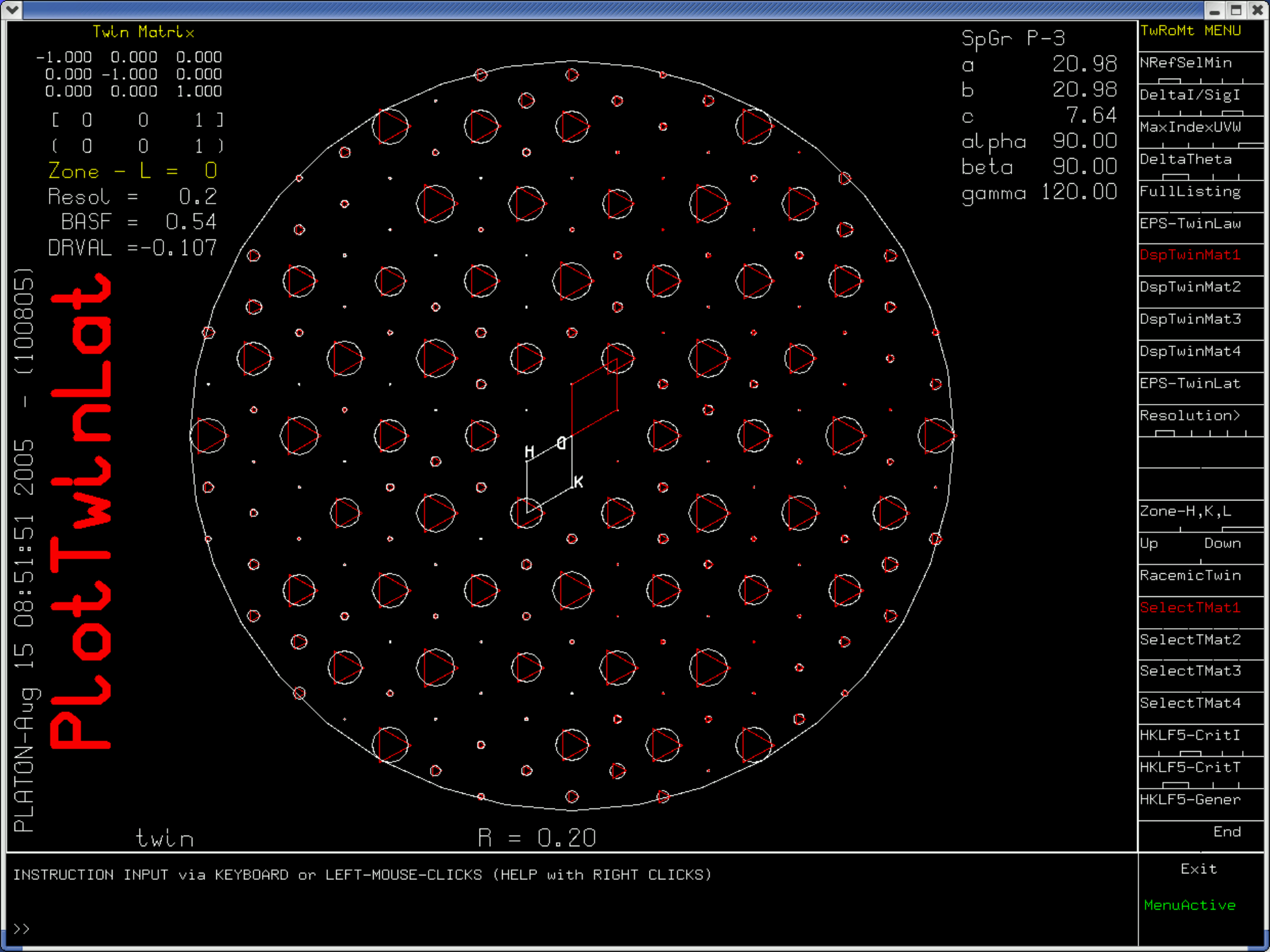
2-axis (0 0 1) [0 0 1], Angle () [] = 0.00 Deg, Freq = 47 (-1.000 0.000 0.000) (h1) (h2) Nr Overlap = 4445 (0.000 -1.000 0.000) * (k1) = (k2) BASF = 0.54 (0.000 0.000 1.000) (l1) = (l2) DEL-R =-0.107	1	
2-axis (1 -1 0) [1 -1 0], Angle () [] = 0.00 Deg, Freq = 48 (0.000 -1.000 0.000) (h1) (h2) Nr Overlap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

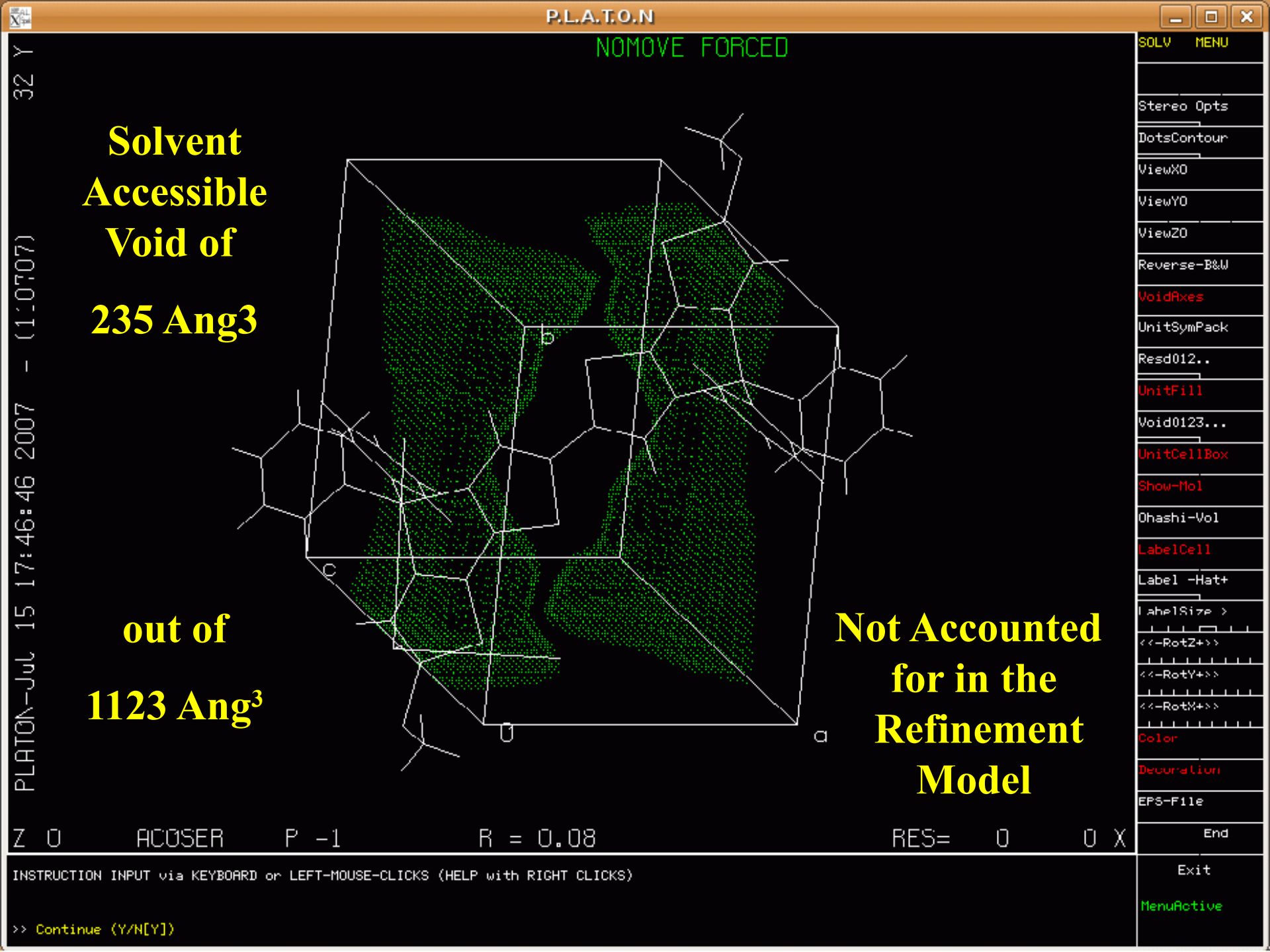
>>

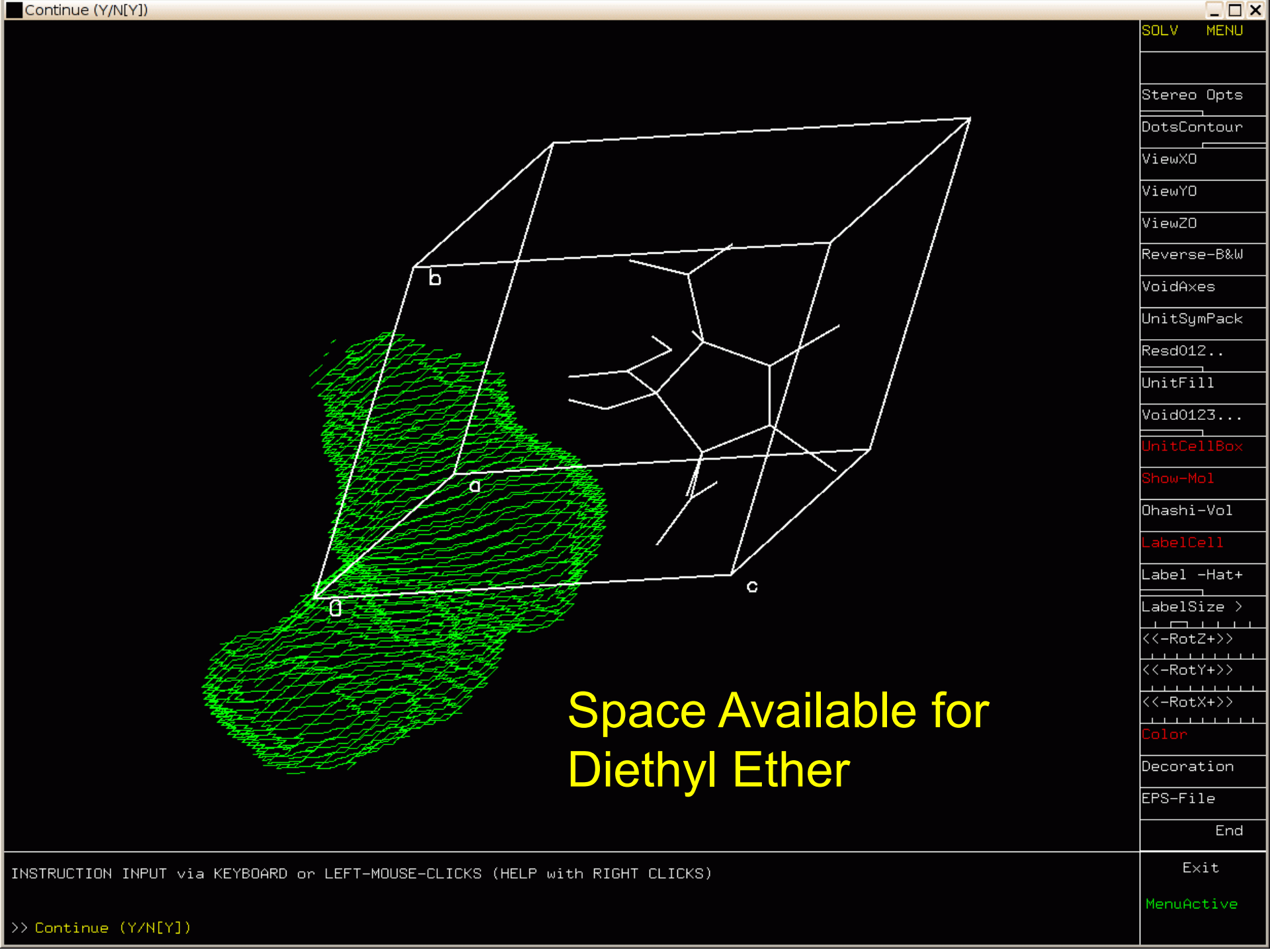
Exit
MenuActive

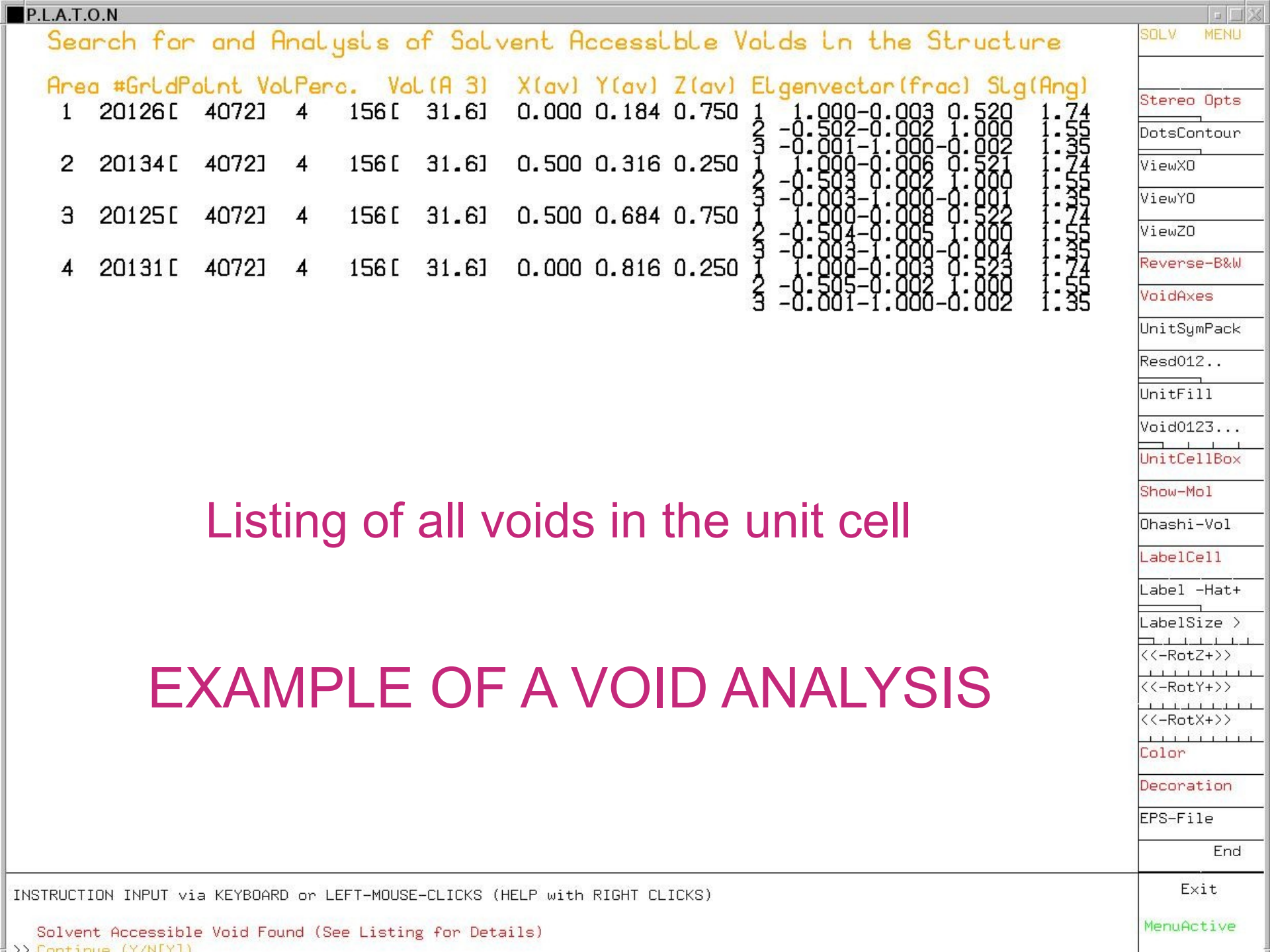

Twin Matrix
-1.000 0.000 0.000
0.000 -1.000 0.000
0.000 0.000 1.000
[0 0 1]
(0 0 1)
Zone - L = 0
Resol = 0.2
BASF = 0.54
DRVAL =-0.107
SpGr P-3
a 20.98
b 20.98
c 7.64
alpha 90.00
beta 90.00
gamma 120.00
PLATON-Aug 15 08:51:51 2005 - (100805)
PlotTwinLat
H
O
K
twin
R = 0.20
TwRoMt MENU
NRefSelMin
DeltaI/SigI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


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])


Continue (Y/N[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+
LabelSize >
<<-RotZ+>>
<<-RotY+>>
<<-RotX+>>
Color
Decoration
EPS-File
End
b
a
c
0
Space Available for
Diethyl Ether
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>> Continue (Y/N[Y])
Exit
MenuActive

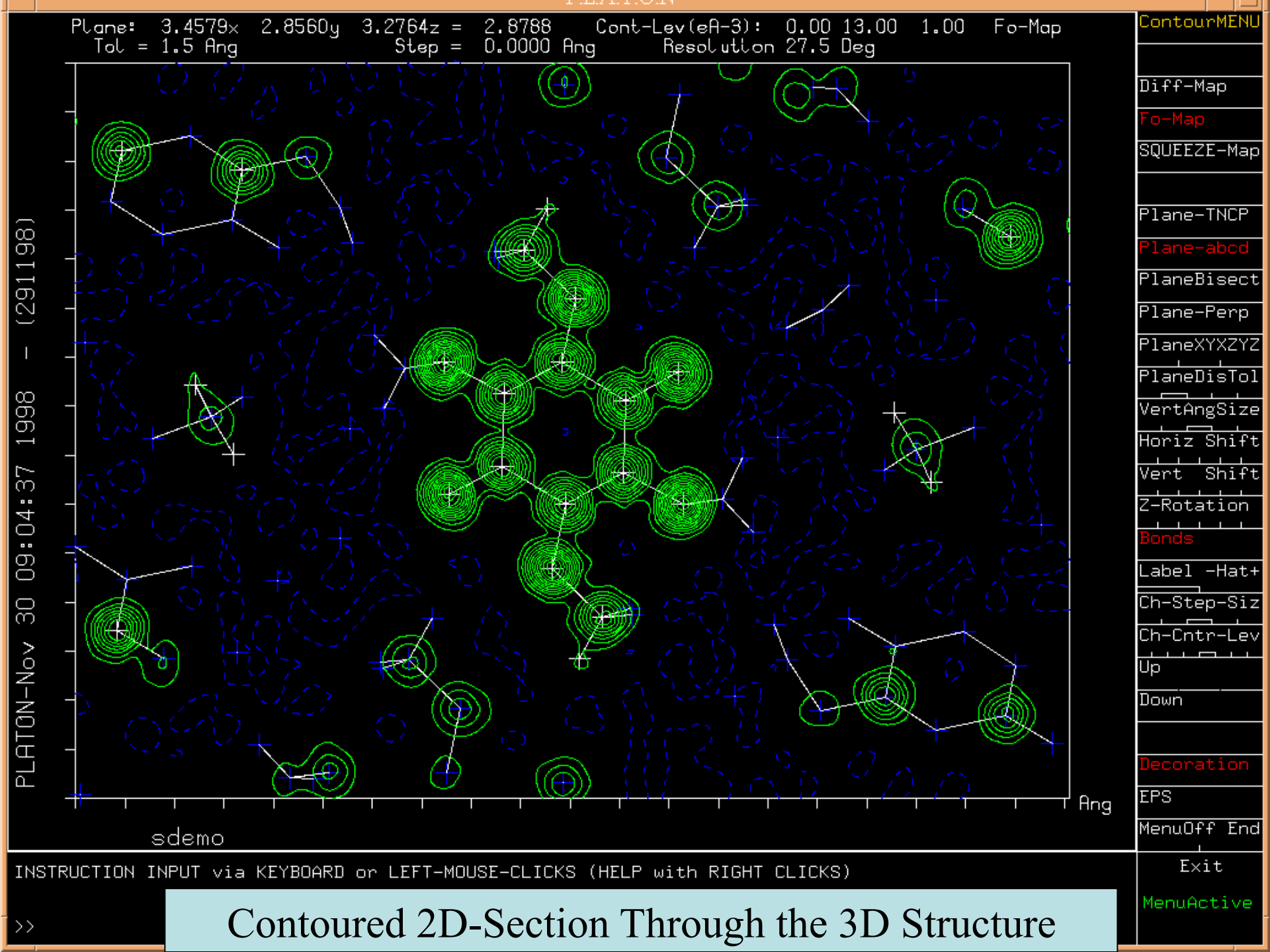


Listing of all voids in the unit cell

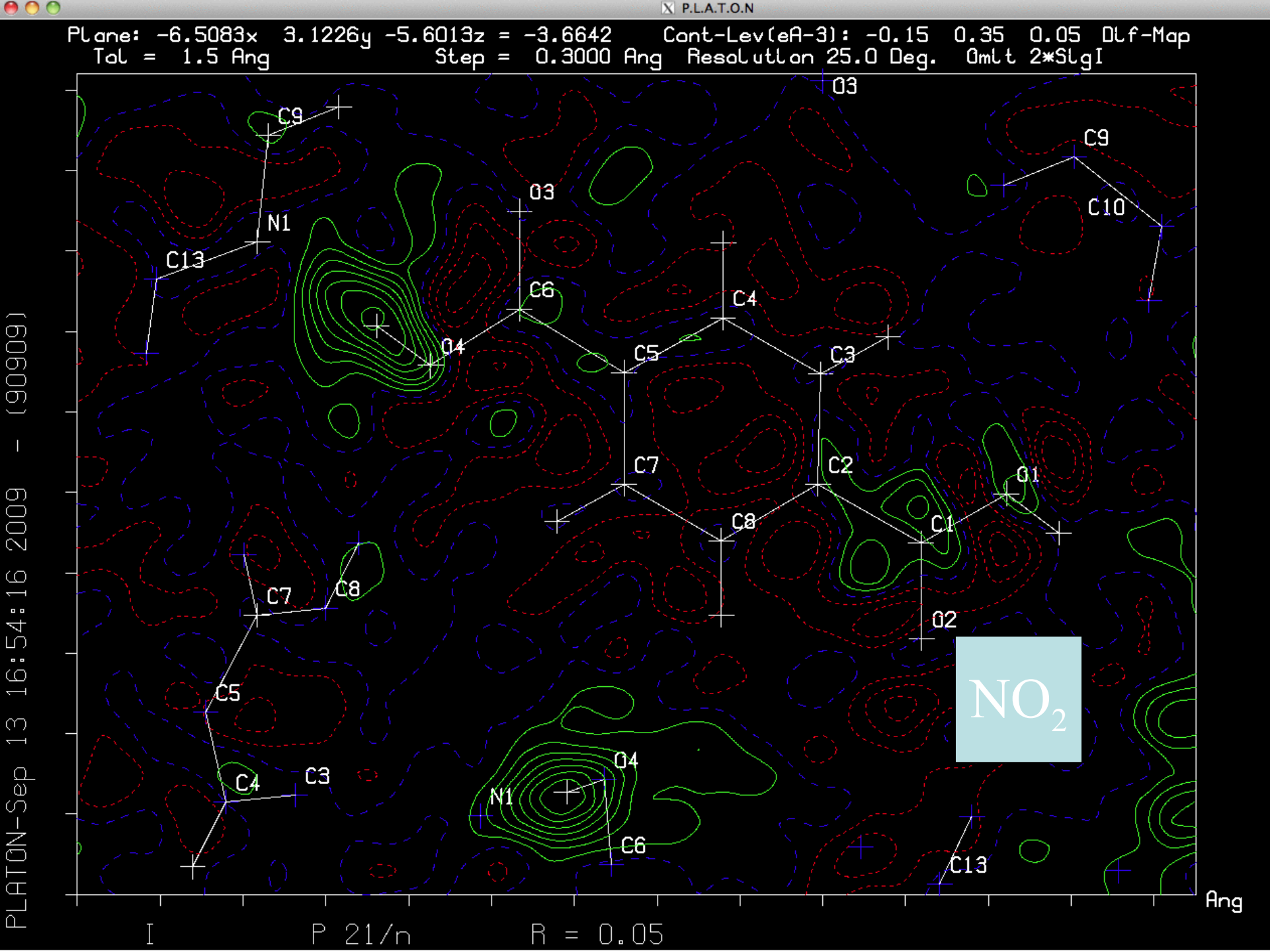
EXAMPLE OF A VOID ANALYSIS

The Fourier Contour Tool

- Contoured display of sections through electron density and difference electron density maps.
- Difference maps can be calculated with some atoms left out of the structure factor calculation testing purposes
- Missing atoms show up green and misplaced atoms show up with red contours.



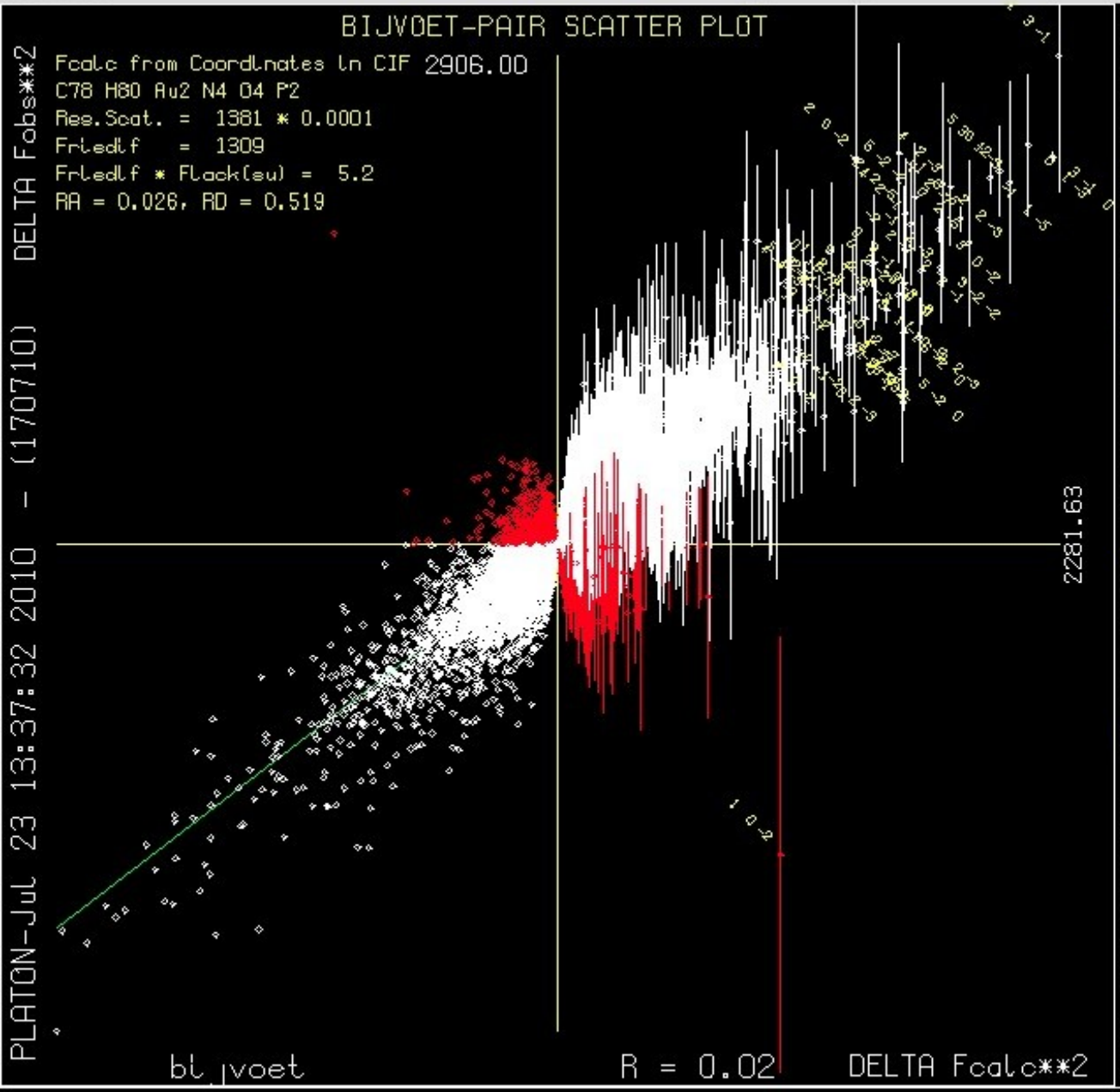
Contoured 2D-Section Through the 3D Structure


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*Sig(I)
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)

>>

The Structure Validation Tool

- Part of the IUCr CheckCif Suite
- CIF-Validation
- FCF-Validation
- Shortcut: platon –U name.cif
- Output on *name.chk* and *name.ckf*
- ALERTS are documented in *check.def* and www.cryst.chem.uu.nl/platon/CIF-VALIDATION.pdf
- www.cryst.chem.uu.nl/platon/FCF-VALIDATION.pdf

The SYSTEM S Tool

- Guided or Automatic structure determination (UNIX/LINUX only)
- Originally (1990) developed around a serial detector system (1 data set a day)
- Used for early structure determination with incomplete data sets for evaluation
- Interfaces to SHELX, SIR, DIRDIF etc. for structure solution

The FLIPPER Tool

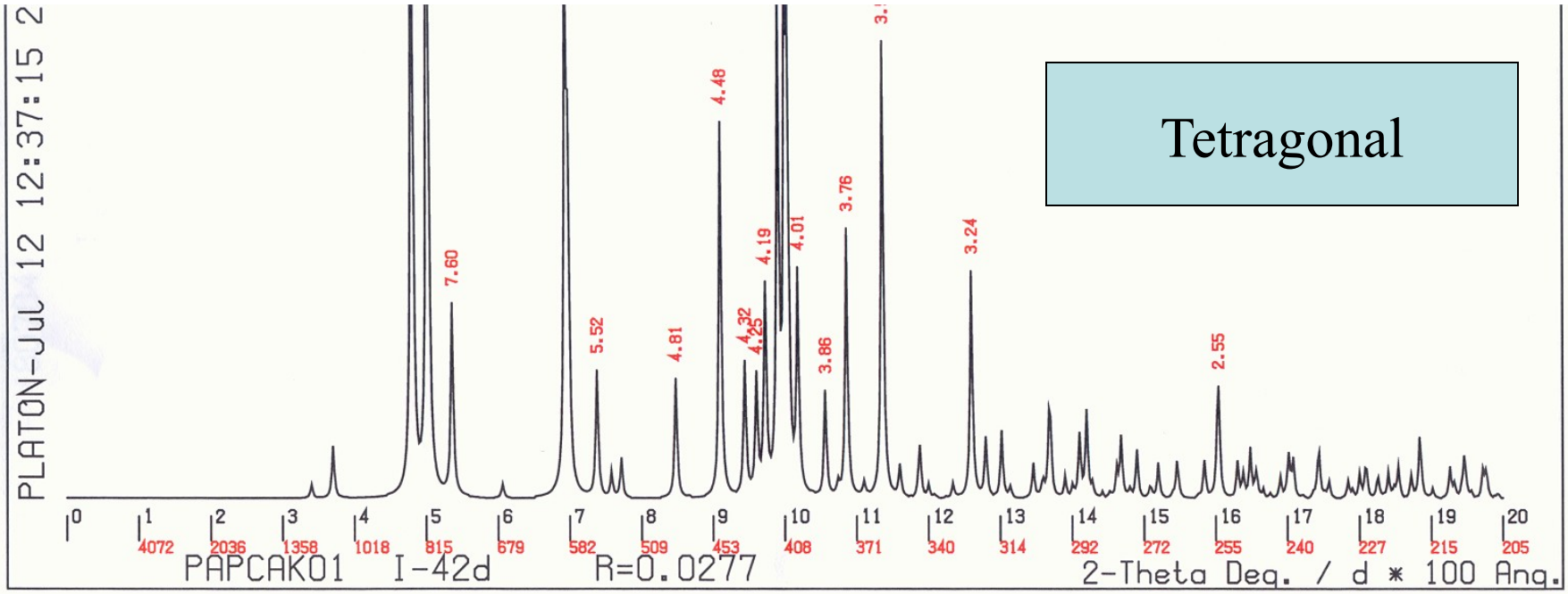
Ab-initio structure determination based on a local implementation of the Charge Flipping technique (Oszlanyi & Suto) in space group P1

There are three main options:

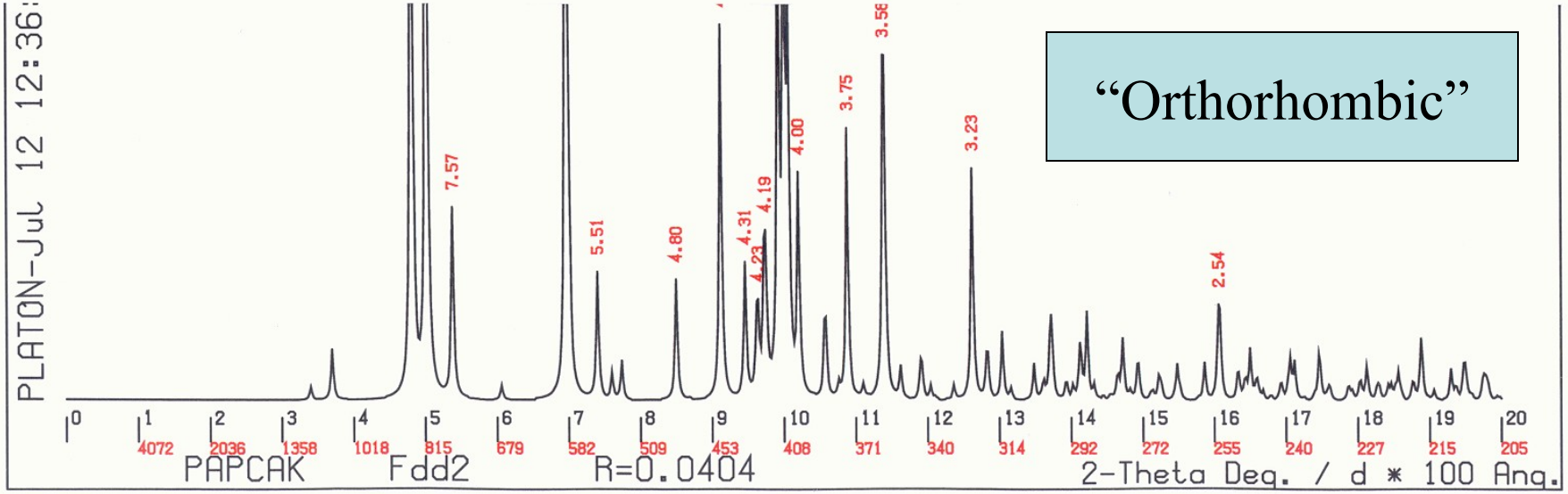
1. 25 random phase starting point attempts
2. A single solution attempt starting from all phases set to zero (the PATT option)
3. Same as 2 with subsequent L.S. refinement

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



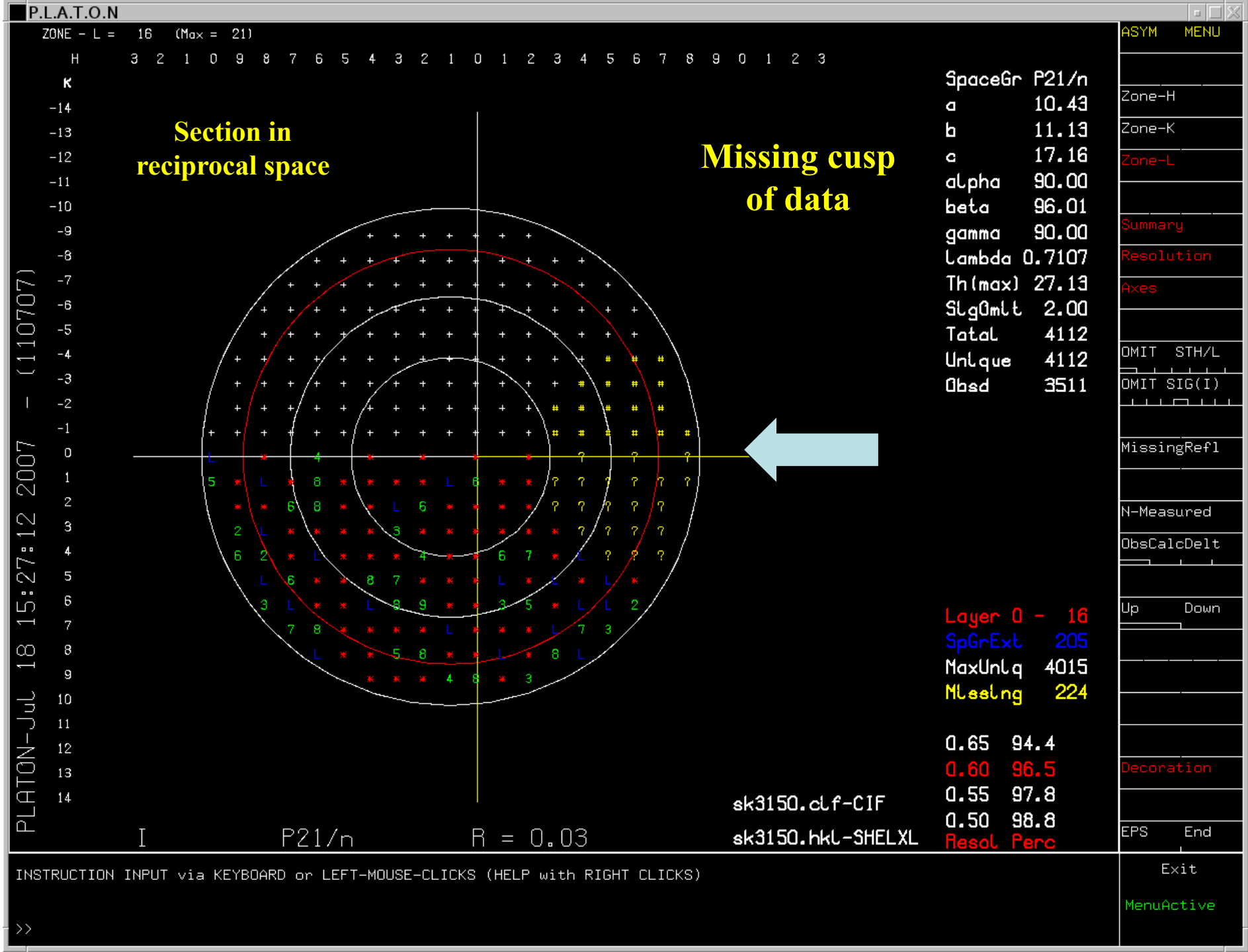
Tetragonal



"Orthorhombic"

The ASYM VIEW Tool

- Display of the data resolution, data completeness, data multiplicity, intensity, etc. as artificial reciprocal lattice plane views
- The view may point to the presence of additional (pseudo) extinctions
- The view may visualize systematically missing parts of the reflection sphere


P.L.A.T.O.N
ZONE - L = 16 (Max = 21)
H 3 2 1 0 9 8 7 6 5 4 3 2 1 0 1 2 3 4 5 6 7 8 9 0 1 2 3
K
-14 -13 -12 -11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14
Section in reciprocal space
Missing cusp of data
PLATON-Jul 18 15:27:12 2007 - (110707)
SpaceGr P21/n
a 10.43
b 11.13
c 17.16
alpha 90.00
beta 96.01
gamma 90.00
Lambda 0.7107
Th(max) 27.13
SlgOmlt 2.00
Total 4112
Unique 4112
Obsd 3511
Layer 0 - 16
SpGrExt 205
MaxUnlq 4015
Mlssing 224
0.65 94.4
0.60 96.5
0.55 97.8
0.50 98.8
Resol Perc
sk3150.clf-CIF
sk3150.hkl-SHELXL
I P21/n R = 0.03
ASYM MENU
Zone-H
Zone-K
Zone-L
Summary
Resolution
Axes
OMIT STH/L
OMIT SIG(I)
MissingRefl
N-Measured
ObsCalcDelt
Up Down
Decoration
EPS End
INSTRUCTION INPUT via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
Exit
MenuActive

Correction for Absorption

- HKL file should include SHELX style direction cosines
- Multi-scan (Blessing)
- Analytical (de Meulenaer & Tompa)
- Gaussian integration (Coppens)
- Spherical correction

File Creation Tools

- Conversion of SHELXL *.ins* and *.hkl* files from *.cif* and *.fcf* files. This can be useful to do further calculations with data from Acta Cryst. publications
- Conversion to CIF, RES, SPF, PDB style files
- Creation of a P1 coordinate set for the input data set
- Creation of a *.hkl* from coordinate data

Other Tools

- ASYM – Averaging of Reflection Data
- SPGRfromEx – Space group determination
- NEWSYM – Space group determination from calculated (model derived) data
- LePage – Determination of the metrical symmetry of a lattice
- Auto-renumbering of the labels in a *.res* file
- Bond Valence Calculation
- Structure Tidy – Standardization of Inorganic structures.
- Comparison of two FCF files (Scatter Plot)

FINALLY …

A current PLATON Manual can be found on

www.cryst.chem.uu.nl/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)

Thanks to the users for taking time for valuable suggestions and bug reports