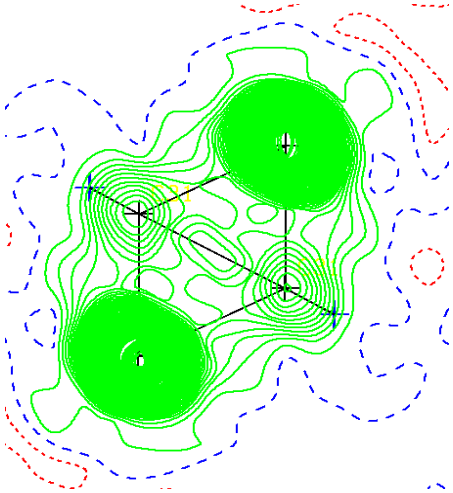
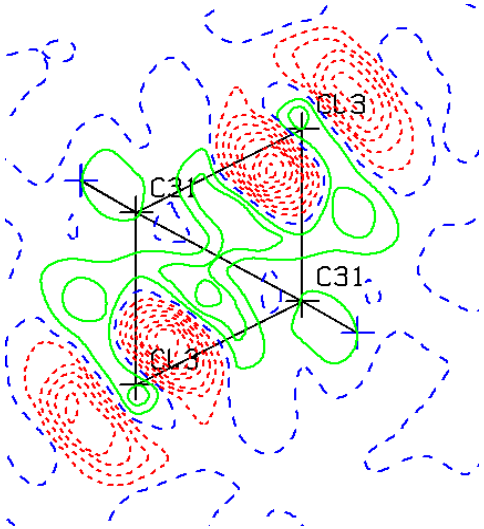
CIF, PLATON-2014, SHELXL-2014, VALIDATION & SQUEEZE



Ton Spek
Utrecht University
The Netherlands



SHELX Workshop, IUCr Congress Aug. 5, 2014 , Montreal

The CIF Data Exchange Standard

- CIF already exists for a quarter of a century
- It was created around 1990 by Syd Hall et al.
- CIF provides a standardized computer readable intermediate between structure refinement software and software that makes use of the resulting structural model (Graphics, Geometry etc.) and data collection and refinement data
- In essence a CIF file consists of a set of records with associations between properly defined data names and their associated values (free format)

EARLY ADOPTERS OF CIF

Refinement Programs

- The, at that time, widely but now rarely used XTAL system program suite (Hall et al.)

- SHELXL92 (The beta follow-up of SHELX-76)

CIF Users

- IUCr/AC-C (Publication, Archival, Checking)

- CCDC/Encifer (Archival/No Retyping)

- Acta: PLATON/Validation (VOIDS/ADDSYM)

The Current Status of CIF

- Most current software can read and/or write CIF
- Hard to keep-up with new CIF items due to new science, changing data collection and refinement techniques (e.g. detectors, constraints/restraints)
- New official data names have been defined for powder studies, twinning & constraints/restraints but not generally implemented in existing software
- In contrast, many more unofficial data names are currently in use starting with _shelx_, _olex2_ etc.
- Regrettably, up to recently, primary reflection data were not generally included in deposited CIF's

CIF-ISSUES

- Unfortunately, The CIF syntax has its problems (no end loop, no loop nesting etc.)
- The realization that when a CIF that does not include the underlying (primary) reflection data, the information is incomplete and thus poor science.
- Many questions about a structural study can be answered only with the availability of reflection data.
- The reflection data may be unique (or hard to obtain) and possibly needed for follow-up studies.
- The historical practice of Fo/Fc deposition is often unsatisfactory (data averaged, 'extinctions' deleted)

Current Solution

- The refinement program specific instruction and reflection files are now soon expected to be at least embedded as comment (under their proper data names) in the CIF
- SHELXL2014 automatically embeds those data with proper checksums for transmission errors etc..
- The embedded data in a SHELXL2014 CIF can be easily extracted and used for alternative refinement purposes or for the creation of an FCF where needed
- PLATON/SQUEEZE makes extensive use of the above

PLATON Tools

Interface: name.cif, .fcf., .ins, .res, .hkl

- Validation - ‘platon –u name.cif’
- SQUEEZE - ‘platon –q name.cif’
- ORTEP - ‘platon –a name.cif’
- ADDSYM - ‘platon –m name.cif
- Etc.
- GUI - ‘platon name.cif’ for CALC, H-Bonds, TwinRotMat, Bijvoet etc.

P L A T O N

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-Plot	Calc Intra	Calc K.P.I	Addsym-EQL	ABSPslScan	Asym-View	fcf2hkl
NewmanPlot	Calc Inter	Squeeze	Addsym-EXT	ABSTompa	FCF-Valid	Expand2P1
Ring-Plots	Calc Coord	Hybrid	Addsym-PLT	ABSGauss	DifFourier	FCF-Gener
Plane-Plot	Calc Metal	CalcFCFsqd	Addsym-SHX	ABSXtal	ANALofVAR	HKL-Gener
Polyhedra	Calc Geom	Contoursqd	Newsym	ABSSphere	ByvoetPair	HKL-Transf
ContourDif	Calc Hbond	Solv F3D	Nonsym	ShxAbs	Asym-Expct	Exor-Res
Contour-Fo	Calc TMA	Solv Plot	LePage	AnomDisVal	Asym-Valid	Anis-Res
AutoMolFit	L.S.-Plane	CavityPlot	DelRed	AnomDisPlt	SupplMater	Rename-RES
hkl2Powder	DihedAngle		Molsym	MuPlot	Expect-hkl	Auto-Renum
SimPowderP	AngleLines	Flip Menu	SPGRfromEX		CSD-Cell	Create-spf
RadDistFun	AngLsplLin	Flip Show	Asym		CSD-Quest	Create-res
Patterson	CremerPopl	Flip Patt	ASYMaverFR		StructTidy	Create-clf
ShelxtPlot	BondValenc	Flipper 25	LePageTwin	XtlPlanAgl	StrainAnal	Create-pdb
PlutONatlv	Hflx - res	Structure?	TwinRotMat	Xtal Habit	LocCIF-acc	clf2shelxl

Xtal Data (CIF14) sl2349_shelxl.clf- Set 1(1): sl2349_s

Refl Data (LIST4) sl2349_shelxl.fcf [FCF] (1): sl2349_s

http://www.platonsoft.nl/PLATON-MANUAL.pdf

Browser - HELP

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

>>

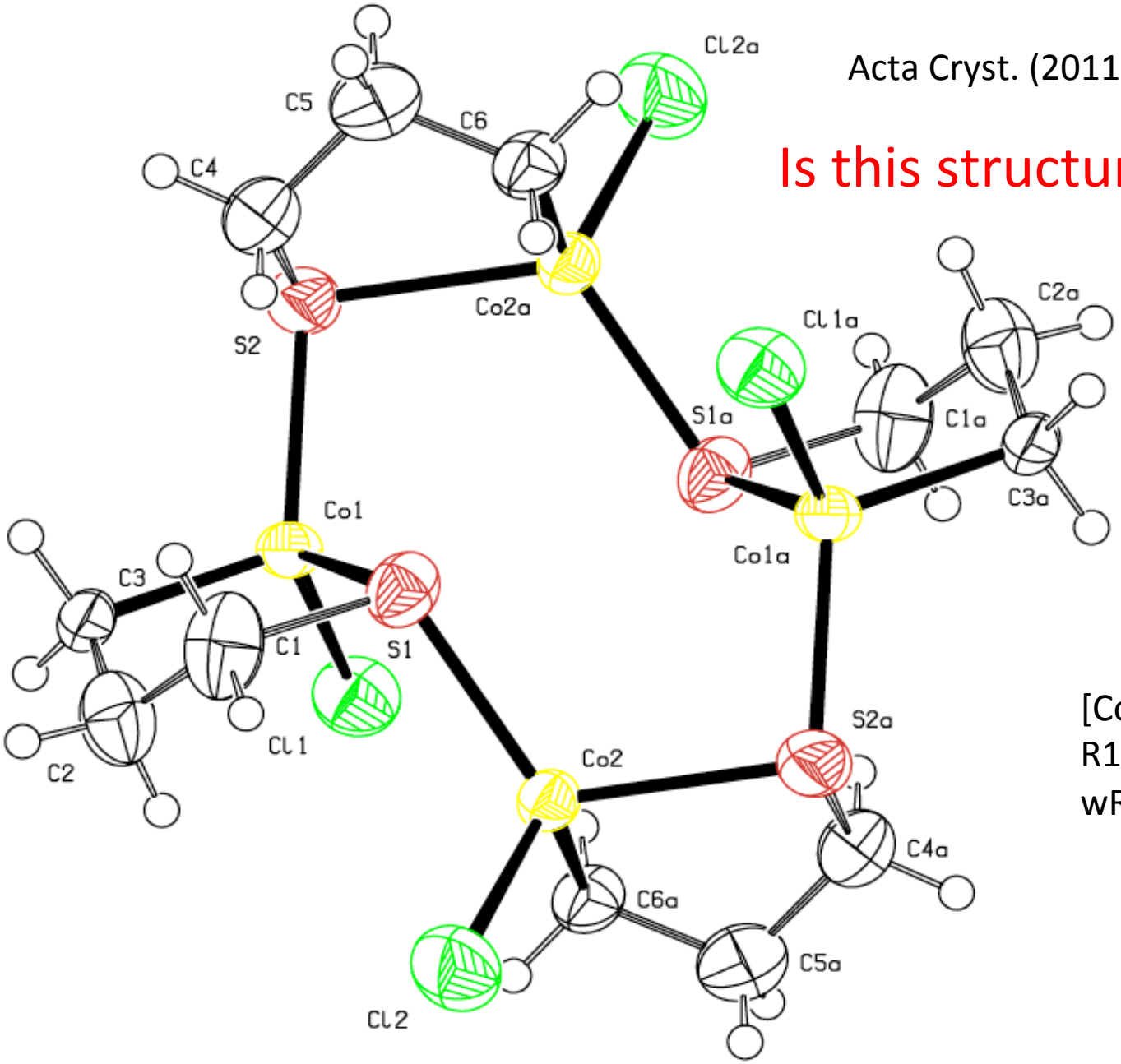
PLA-SP2 12
OptionMenus
Print-Level
EPS-Listing
PDF-Listing
PageHeader
NoMolFitInv
KeepMon-I-n
NoExpand
FCF-Calc
PNG
ReflListing
DebugOutput
SetWindSize
Portrait
GenerRandom
EPS HPGL
Auto-Plot
X-LineWidth
Reverse-B&W
Browser
Reset End
Exit
MenuActive

CIF-Validation

- ALERTS come in levels A,B,C & G
- All A,B,C ALERTS should looked at carefully and acted upon (correct or comment)
- G-ALERTS are info and not necessarily Errors
- The use of constraint/restraints should be commented upon. Their use, just to beautify an ORTEP to hide problems, is poor practice
- IUCr standard is best attainable, not 25 deg
- Next a validation output example based on a SHELXL2014 CIF ➔

```
#==============================================================================
# PLATON/CHECK-(270714) versus check.def version of 240714   for Entry: si2349_s
# Data: si2349_shelxl.cif - Type: CIF14          Bond Precision   C-C = 0.0113 A
# Refl: si2349_shelxl.fcf - Type: LIST4                             Temp = 296 K
# X-Ray                   R(int) = 0.058,  wR2/R(int) =  2.1,  Nref/Npar =  19.7
# Cell 23.6135(12)   7.8465(3)  16.8693(9)          90   130.440(4)          90
# Wavelength 0.71073    Volume Reported     2378.8(2)   Calculated     2378.9(2)
# SpaceGroup from Symmetry C 2/c      Hall: -C 2yc                 monoclinic
#                 Reported C 2/c            -C 2yc                 monoclinic
# MoietyFormula C12 H24 Cl4 Co4 S4
#      Reported ?
#    SumFormula C12 H24 Cl4 Co4 S4
#      Reported C12 H24 Cl4 Co4 S4
# Mr         =    674.07[Calc],    674.07[Rep]
# Dx,gcm-3   =     1.882[Calc],     1.882[Rep]
# Z          =         4[Calc],         4[Rep]
# Mu (mm-1)  =     3.537[Calc],     3.537[Rep]
# F000       =    1344.0[Calc],    1344.0[Rep]  or F000' =   1354.05[Calc]
# Reported   T Limits: Tmin=0.675              Tmax=0.683  AbsCorr=?
# Calculated T Limits: Tmin=0.512 Tmin'=0.424  Tmax=0.609
# Reported   Hmax= 28, Kmax=  9, Lmax= 20, Nref=   2152        , Th(max)= 25.242
# Obs in FCF Hmax= 28, Kmax=  9, Lmax= 20, Nref=   2152[  2152], Th(max)= 25.242
# Calculated Hmax= 28, Kmax=  9, Lmax= 20, Nref=   2152        , Ratio  =  1.000
# Reported   Rho(min) = -0.62, Rho(max) =  0.70 e/Ang**3 (From CIF)
# Calculated Rho(min) = -0.61, Rho(max) =  0.73 e/Ang**3 (From CIF+FCF data)
# w=1/[sigma**2(Fo**2)+(0.0653P)**2+ 15.5359P], P=(Fo**2+2*Fc**2)/3
# R= 0.0413(  1782), wR2= 0.1237(  2152), S = 1.029      (From CIF+FCF data)
# R= 0.0413(  1782), wR2= 0.1236(  2152), S = 1.029      (From FCF data only)
# R= 0.0413(  1782), wR2= 0.1236(  2152), S = 1.029, Npar=  109
#==============================================================================
```

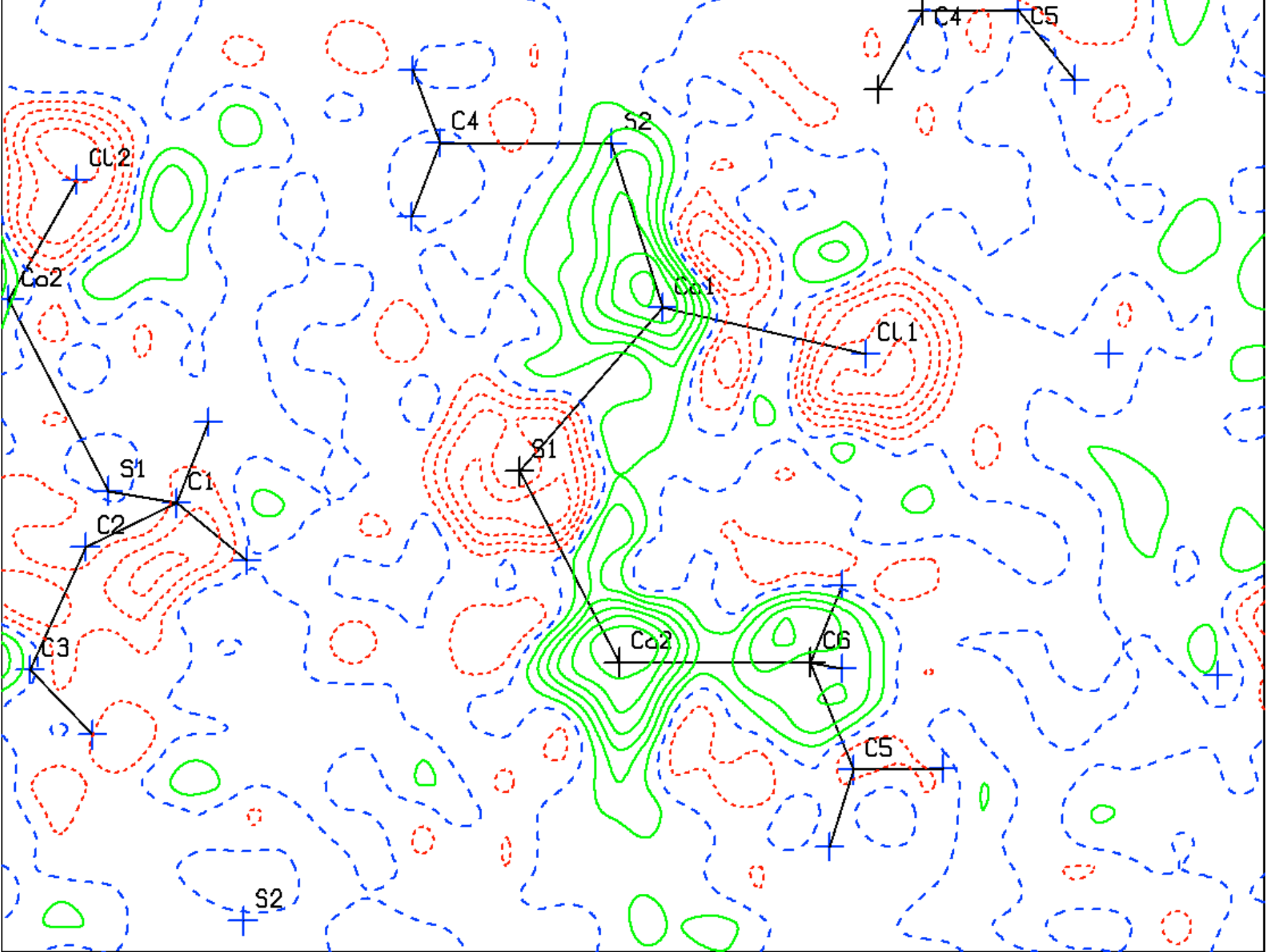
```
232_ALERT_2_B Hirshfeld Test Diff (M-X)  Co1    --  S1      ..       10.1 su
232_ALERT_2_B Hirshfeld Test Diff (M-X)  Co1    --  S2      ..       10.3 su
232_ALERT_2_B Hirshfeld Test Diff (M-X)  Co2    --  S1      ..       11.3 su
232_ALERT_2_B Hirshfeld Test Diff (M-X)  Co2    --  S2_a    ..       11.3 su
#=============================================================================
030_ALERT_1_C _diffrn_reflns_number   <   _reflns_number_total     Please Check
048_ALERT_1_C MoietyFormula Not Given .......................     Please Do !
052_ALERT_1_C Info on Absorption Correction Method Not Given .    Please Do !
057_ALERT_3_C Correction for Absorption Required   RT(exp) ...      1.19 Do !
230_ALERT_2_C Hirshfeld Test Diff for    C2     --  C3      ..       6.0 su
242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       Co2 Check
341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0113 Ang.
790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #         1 Note
              C12 H24 Cl4 Co4 S4
#=============================================================================
083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      15.54 Report
128_ALERT_4_G Alternate Setting for Input Space Group     C2/c      I2/a Note
232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1    --  Cl1     ..       10.4 su
232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co2    --  Cl2     ..        8.9 su
764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.14 Ratio
909_ALERT_3_G Percentage of Observed Data at Theta(Max) still         65 %
#=============================================================================
```

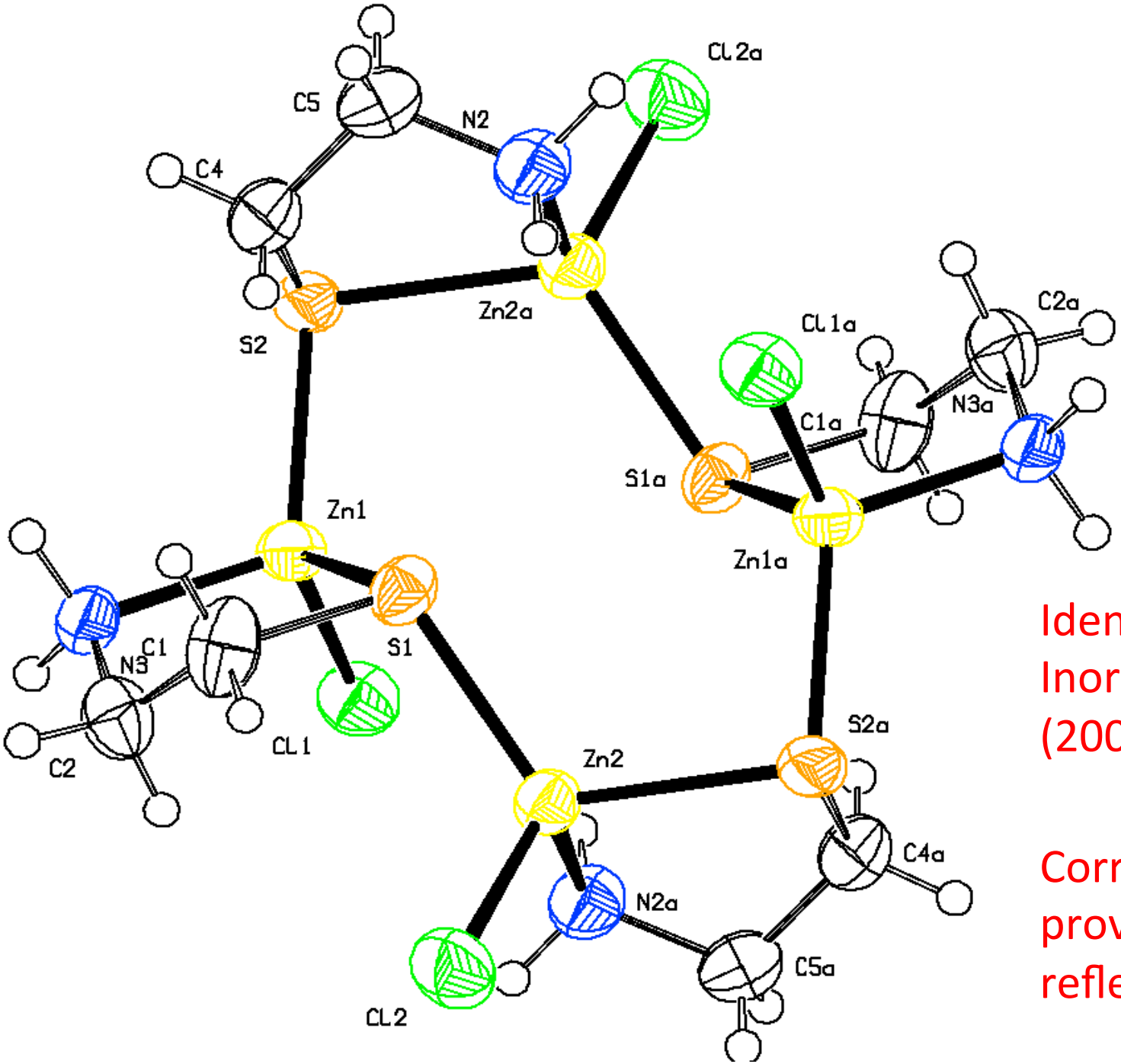


Acta Cryst. (2011). E67, m576-m577

Is this structure correct ?

[Co4Cl4(C3H6S)4]
R1 = 0.041
wR2 = 0.125


C4
C5
S2
C4
Cl2
Co2
Co1
Cl1
S1
C1
S1
C2
C3
Co2
C6
C5
S2



Co → Zn
C3 → N1
C6 → N2
R1 = 0.028
wR2 = 0.072

Identical to:
Inorg. Chem.
(2006) 45, 8318

Correction
proved with
reflection data

FCF-Validation

- Listing of outliers
- Listing of missing reflections
- %observed data versus resolution plot
- Analysis of Variance + Normal Prob. Plot
- TwinRotMat
- Bijvoet Pair Hooft/Parsons analysis
- Difference Fourier peak list (see whether peaks are near heavy atoms or elsewhere)

```
PLATON-(Version  270714)-Mode=2 FCF-File Validation for:I
================================================================================
For Documentation: http://www.platonsoft.nl/FCF-VALIDATION.pdf

Section 1
================================================================================
General Data
================================================================================
Crystal Data From: zl2039.cif
Fo/Fc   Data From: zl2039.fcf FCF-TYPE=LIST4
Space Group      : P21/n
Wavelength (Ang) :   0.71073
Unit Cell (CIF)  :    8.5814  19.4260  10.1180   90.000   96.620   90.000
SHELX WGHT Pars. :    0.0336   0.0000

Section 2
================================================================================
Reflections with abs((I(obs) - I(calc)) / SigW(I) .GT.  3.0
================================================================================
   Nr    H    K    L  Theta     I(obs)    I(calc) Sigma(I)    Ratio  SigW(I) RatioW
--------------------------------------------------------------------------------
    1    8    6    0  20.56      89.20     155.04    20.77    -3.17    21.25  -3.10
    2    4    7    0  12.14     102.88      64.92    11.25     3.37    11.55   3.29
    3   -1    0    3   6.28     782.69     674.72    26.62     4.06    35.76   3.02
    4    0    4    3   7.40     485.61     590.60    24.33    -4.32    30.67  -3.42
    5    8    6    4  23.12     -11.16      29.85    13.62    -3.01    13.64  -3.01
    6    4   13    5  20.48     528.19     400.54    39.70     3.22    42.40   3.01
    7    1   15    7  22.03      94.71     177.93    26.92    -3.09    27.39  -3.04
    8    6    2    9  25.37     723.80    1021.52    91.48    -3.25    96.59  -3.08
                                                             --------         --------
                                                  Average =    -0.77            -0.79
```

Missing Reflections (Asym. Refl. Unit) below sin(th)/lambda = 0.5

Nr	H	K	L	sin(th)/lambda	Theta	I(calc)	I(calc)/I(max)
1	0	2	0	0.051	2.10*	23.09	0.00029
2	1	3	0	0.097	3.95	168.56	0.00209
3	-1	5	1	0.148	6.02	307.55	0.00381
4	6	10	1	0.443	18.37	2760.21	0.03422
5	-1	1	2	0.113	4.59	146.91	0.00182
6	0	1	2	0.103	4.19	1183.75	0.01468
7	-1	3	2	0.134	5.47	1582.16	0.01962
8	-4	14	3	0.446	18.49	30.64	0.00038
9	-5	14	4	0.492	20.47	2085.30	0.02585
10	-3	1	7	0.373	15.35	894.30	0.01109
11	-2	3	7	0.363	14.94	93.44	0.00116

** Note: I(max) is the maximum I(obs) encountered in the fcf-file **

Starred Reflections have a Theta below Theta(Min) = 2.28

From CIF: Theta(Min) = 2.28

Section 4:

Resolution & Completeness Statistics (Cumulative and Friedel Pairs Averaged)

Theta	sin(th)/Lambda	Complete	Expected	Measured	Missing	
20.82	0.500	0.994	1748	1737	11	
23.01	0.550	0.994	2340	2327	13	
25.24	0.600	0.994	3035	3016	19	
						ACTA Min. Res. ---
26.01	0.617	0.994	3300	3280	20	

Section 5

R-Value Statistics as a Function of Resolution (in Resolution Shell)

Theta	sin(Th)/L	#	R1	wR2	S	Rs	av(I/SigW)	av(I)	av(SigW)
12.38	0.302	375	0.018	0.050	1.136	0.013	21.16	5080.87	189.10
15.68	0.380	392	0.019	0.049	0.917	0.025	16.13	1900.87	82.64
18.02	0.435	378	0.025	0.061	0.953	0.039	13.10	1223.39	65.58
19.90	0.479	382	0.031	0.074	0.964	0.056	10.62	867.64	58.41
21.51	0.516	389	0.036	0.086	0.946	0.069	8.47	681.53	54.41
22.94	0.548	387	0.046	0.113	0.944	0.104	6.29	415.97	46.59
24.22	0.577	382	0.059	0.143	0.971	0.135	5.20	322.79	45.47
25.40	0.603	379	0.064	0.161	0.956	0.158	4.38	278.71	45.43
26.01	0.617	216	0.056	0.159	0.815	0.196	3.73	233.41	46.74

R(sig) = sum(sig(I)) / sum(I) = 0.0383

From FCF: R1 = 0.0307(2523), wR2 = 0.0711(3280), S = 1.001
From CIF: R1 = 0.0308(2523), wR2 = 0.0711(3280), S = 1.001, Npar = 229

No (SHELXL) Optimized Weights: wR2 = 0.0474 , S = 1.385

```
Intensity Distribution [Decay of I/Sigma(I) versus sin(theta)/lambda]
=======================================================================
sh  st/l   Ang     #  0.25   1.0   2.0  Percent  Distr. for I .gt. 2.0 * sig(I)
=======================================================================
 1 0.301 1.661   375  98.9  97.1  95.7 ************************************..
 2 0.379 1.318   389  96.1  92.8  88.9 ************************************....
 3 0.434 1.152   371  97.0  92.2  85.2 ************************************......
 4 0.478 1.046   382  95.8  89.0  81.7 ************************************.......
 5 0.515 0.971   395  92.2  86.3  75.4 ************************************.........
 6 0.547 0.914   370  90.0  82.2  69.7 ************************************...........
 7 0.576 0.868   382  91.6  80.4  69.6 ************************************...........
 8 0.602 0.830   385  86.0  71.7  59.2 ************************************.............
 9 0.626 0.798   231  83.1  73.2  60.6 ************************************.............
                                      I                    I                    I
                  Percent Observed:   0                   50                  100


Maximum Percentage of Reflections with I .gt. 2*s(I) in any Resolution Shell 96
.
```

SQUEEZE

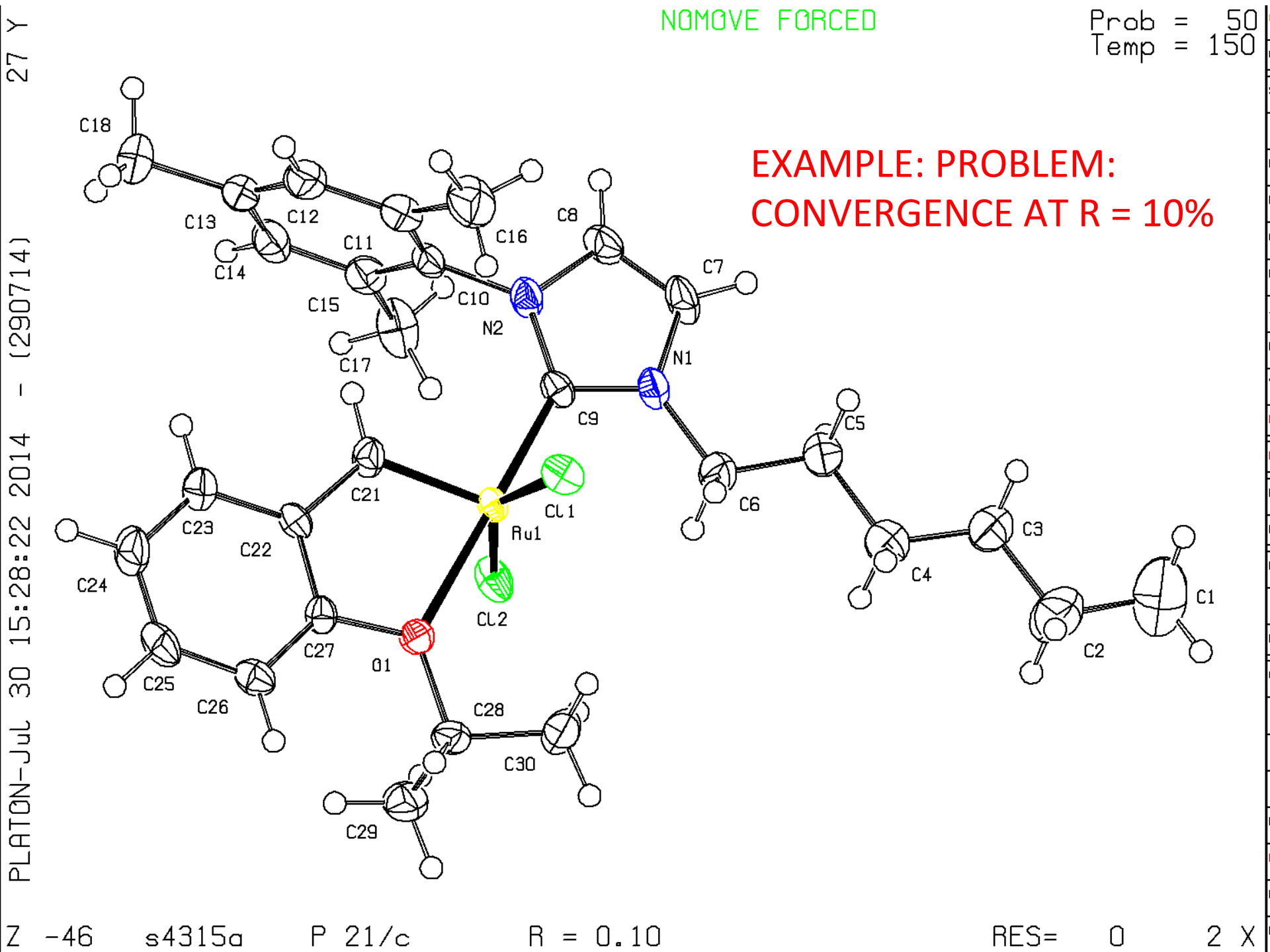
- SQUEEZE is a tool in PLATON that takes care of the disordered solvent contribution to F_{calc} as part of the L.S. refinement.
- It is assumed that the total electron density can be split up into a part that can be parameterized with the usual label,x,y,z,population,Uij model and a part with unimportant substance that can not be parameterized satisfactorily.
- The solvent accessible region is determined automatically and used iteratively as a mask for the back-Fourier transformation of the solvent density in the difference map to F_{calc} (solvent)
- The actual L.S. refinement of the model parameters has to be done with an external program (SHELXL, CRYSTALS)
- SHELXL97 required refinement against I(obs) corrected for the solvent contribution into solvent free data (seen as heresy …)

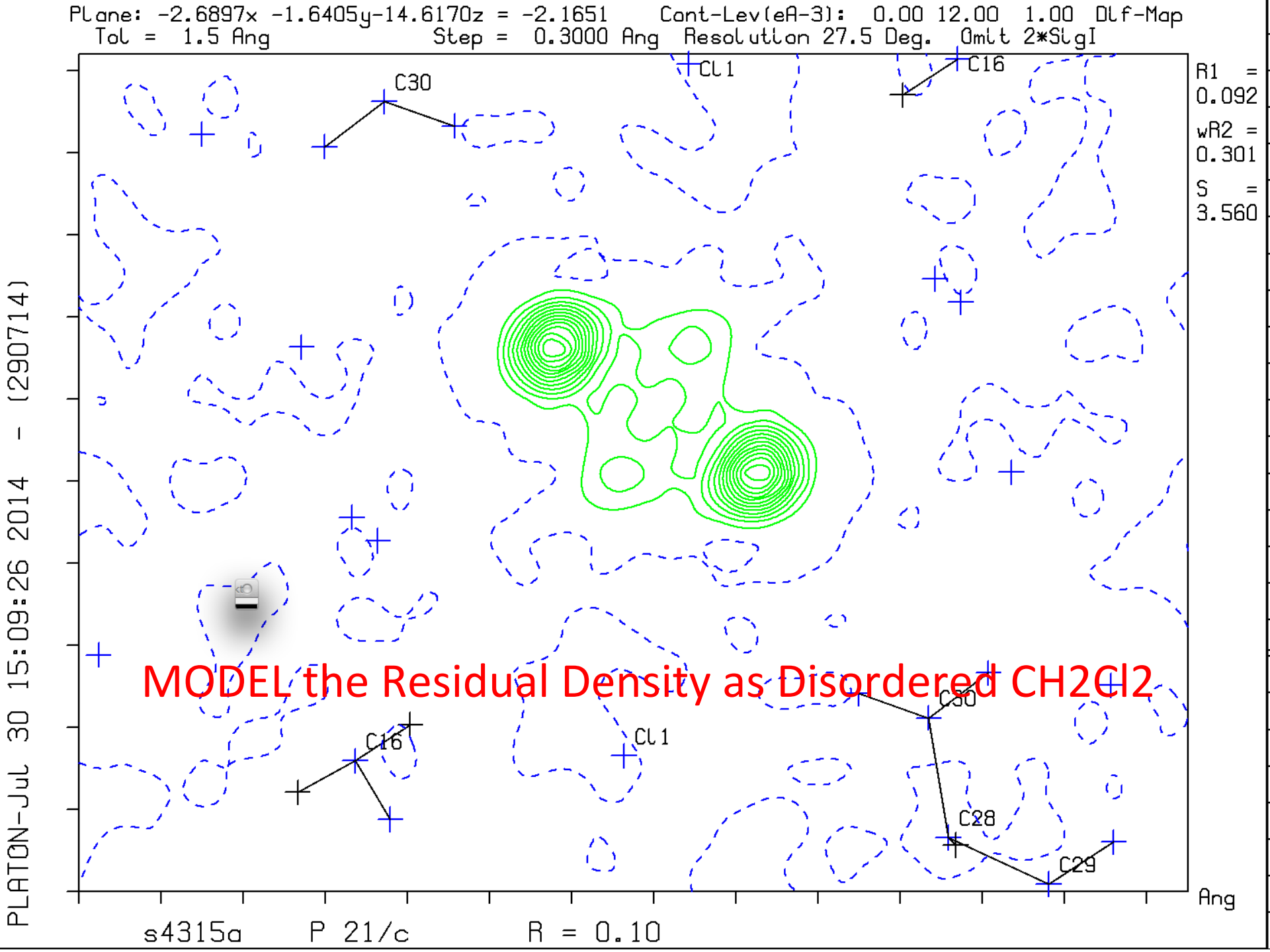
SQUEEZE & SHELXL2014

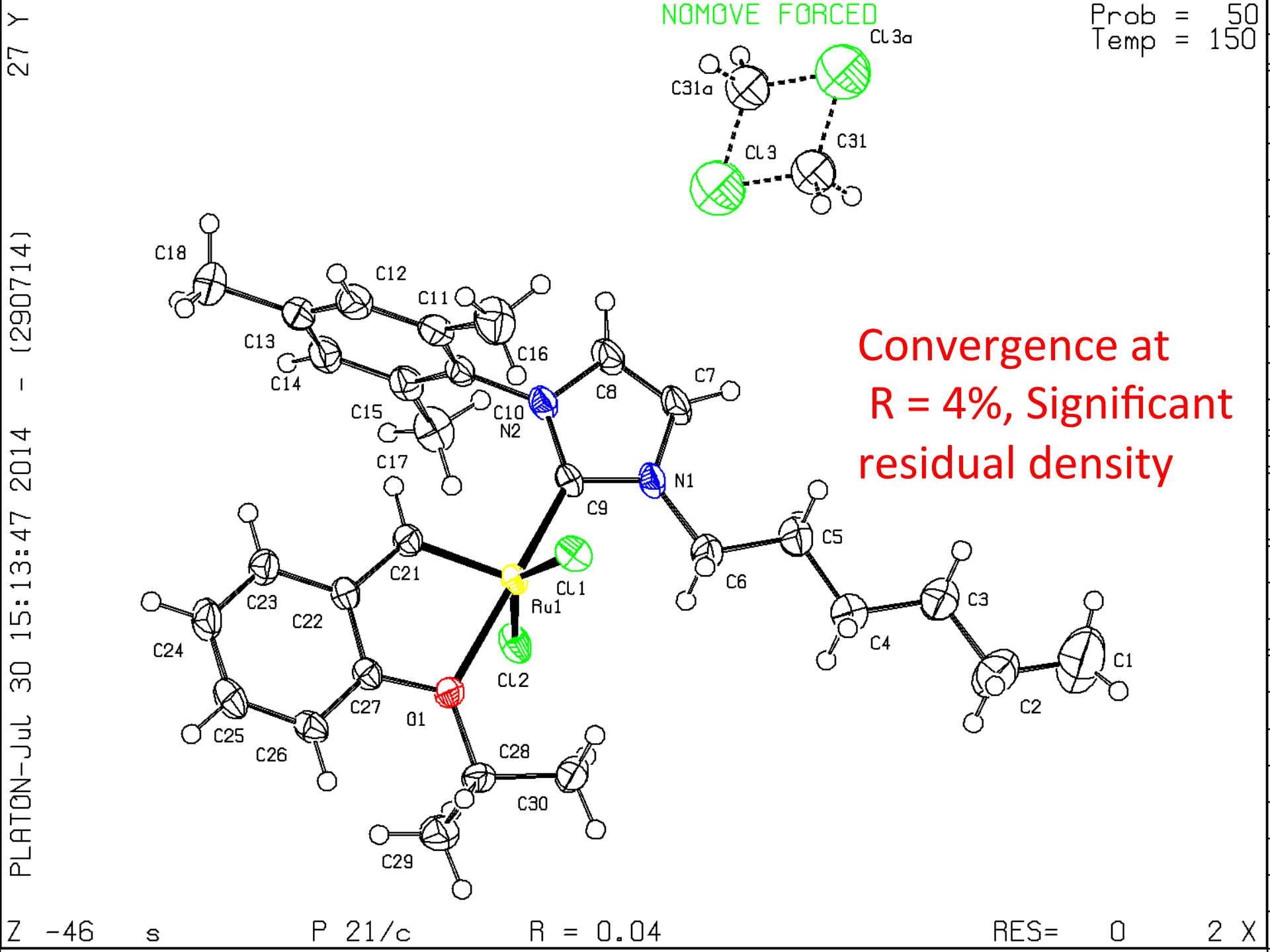
- SHELXL2014 now has a command, ABIN, that instructs to read an externally supplied .fab file with fixed contributions to the calculated structure factors
- PLATON/SQUEEZE supplies such a .fab file with the disordered solvent contribution.
- The new SHELXL2014 CIF file with the embedded .res and .hkl makes the use of SQUEEZE much simpler.
- The recommended input files needed for a SQUEEZE job are a .cif and .fcf from a converged SHELXL2014 refinement job
- SQUEEZE generates _sq.ins, _sq.hkl & _sq.fab for SHELXL2014
- Info on the use of SQUEEZE for archival and validation is automatically embedded in the CIF

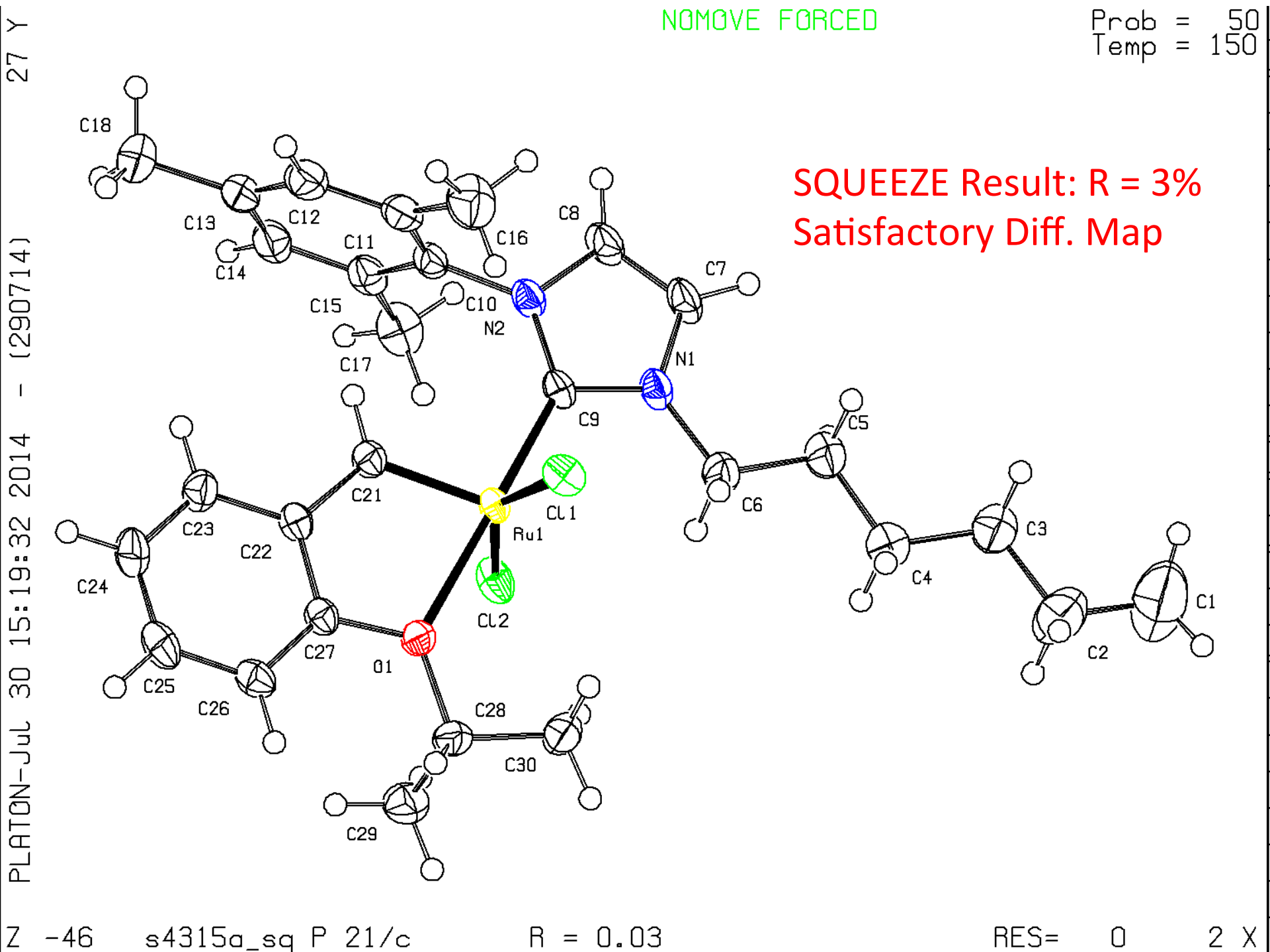
How to SQUEEZE with SHELXL2014

1. Refine non-solvent model (Include ACTA, and in case of twinning, LIST 8 record(s) in the .ins).
2. Run SQUEEZE, based on the *.cif* & *.fcf* from **1** as 'platon –q name.cif'.
3. Continue SHELXL2014 refinement with the files *name_sq.ins,* name_sq.hkl & *name_sq.fab* from **2** as 'shelxl name_sq'
4. Inspect the .lis & .lst files and Validate


NOMOVE FORCED
Prob = 50
Temp = 150
EXAMPLE: PROBLEM:
CONVERGENCE AT R = 10%
C18
C13
C12
C16
C8
C14
C11
C7
C15
C10
N2
N1
C17
C9
C5
C21
CL1
C6
C23
Ru1
C3
C22
C4
C24
CL2
C1
C27
O1
C2
C25
C26
C28
C30
C29
PLATON-Jul 30 15:28:22 2014 - (290714)
27 Y
Z -46 s4315a P 21/c R = 0.10 RES= 0 2 X

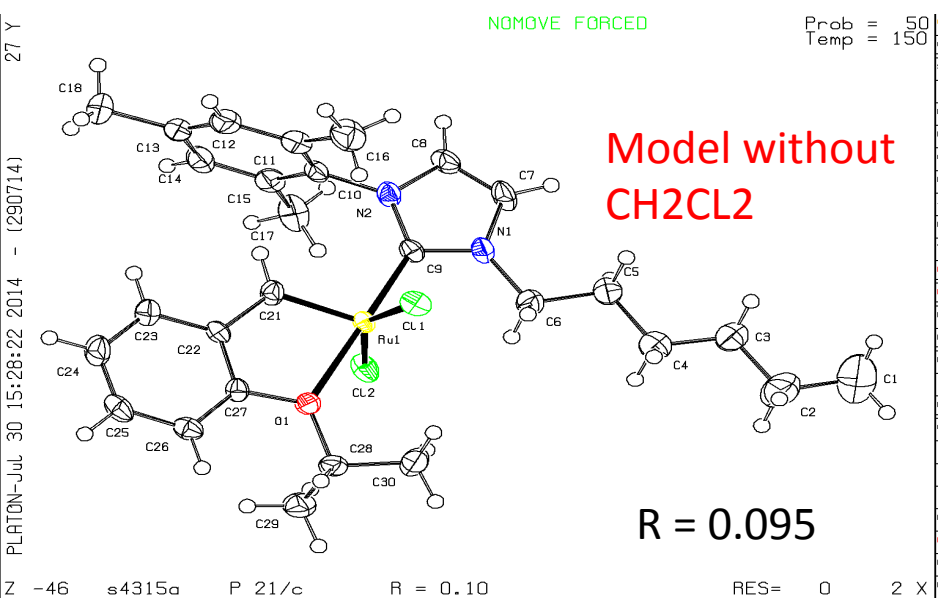

Plane: -2.6897x -1.6405y-14.6170z = -2.1651 Cont-Lev(eA-3): 0.00 12.00 1.00 Dlf-Map
Tol = 1.5 Ang Step = 0.3000 Ang Resolution 27.5 Deg. Omit 2*SigI
R1 = 0.092
wR2 = 0.301
S = 3.560
C30
Cl1
C16
C16
Cl1
C30
C28
C29
MODEL the Residual Density as Disordered CH2Cl2
PLATON-Jul 30 15:09:26 2014 - (290714)
Ang
s4315a P 21/c R = 0.10


NOMOVE FORCED
Prob = 50
Temp = 150
Cl3a
C31a
Cl3
C31
C18
C12
C11
C13
C16
C14
C15
C10
N2
C8
C7
C17
N1
C9
C5
C21
Cl1
C6
C23
Ru1
C3
C22
C24
C4
C1
Cl2
C27
C2
O1
C25
C26
C28
C30
C29
Convergence at
R = 4%, Significant
residual density
PLATON-Jul 30 15:13:47 2014 - (290714)
27 Y
Z -46 s P 21/c R = 0.04 RES= 0 2 X

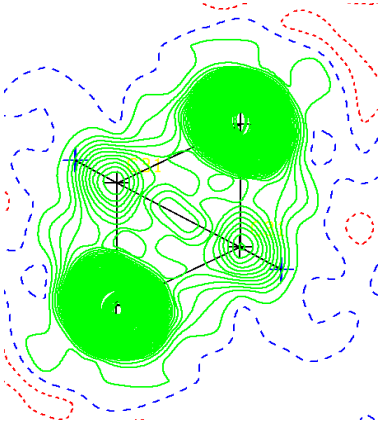

NOMOVE FORCED
Prob = 50
Temp = 150
SQUEEZE Result: R = 3%
Satisfactory Diff. Map
C18
C13
C12
C11
C16
C8
C7
C14
C15
C10
N2
N1
C17
C9
C5
C21
Cl1
Ru1
C6
C3
C23
C22
C4
C1
C24
Cl2
C27
O1
C2
C25
C26
C28
C30
C29
PLATON-Jul 30 15:19:32 2014 - (290714)
27 Y
Z -46 s4315a_sq P 21/c R = 0.03 RES= 0 2 X

Result Summary

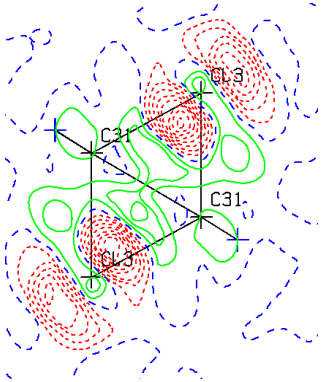
P21/c	2(C28 H38 Cl2 N2 O Ru, x(C H2 Cl2)		
	none	0.69(CH2Cl2)	squeeze
R	0.0954	0.0442	0.0327
wR2	0.3111	0.1315	0.0918
S	3.690	1.050	1.064
rho min/max	-0.80,12.61	-1.59,2.02	-0.43, 1.07
BP (Ang)	0.0137	0.0058	0.0042



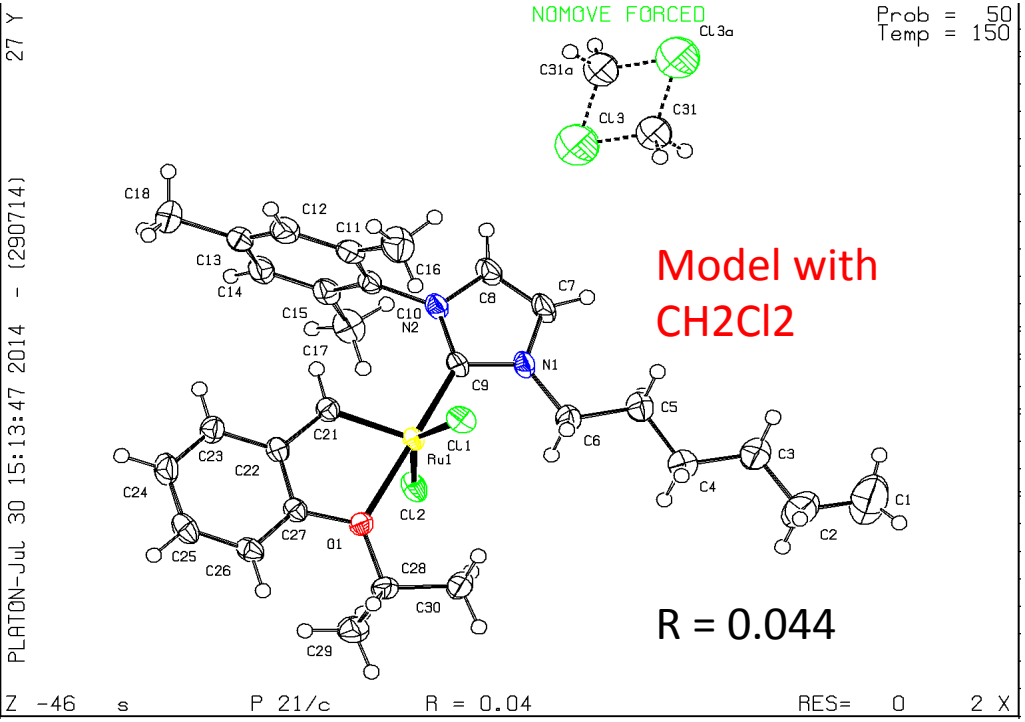
Difference Maps based on Modelled CH2Cl2

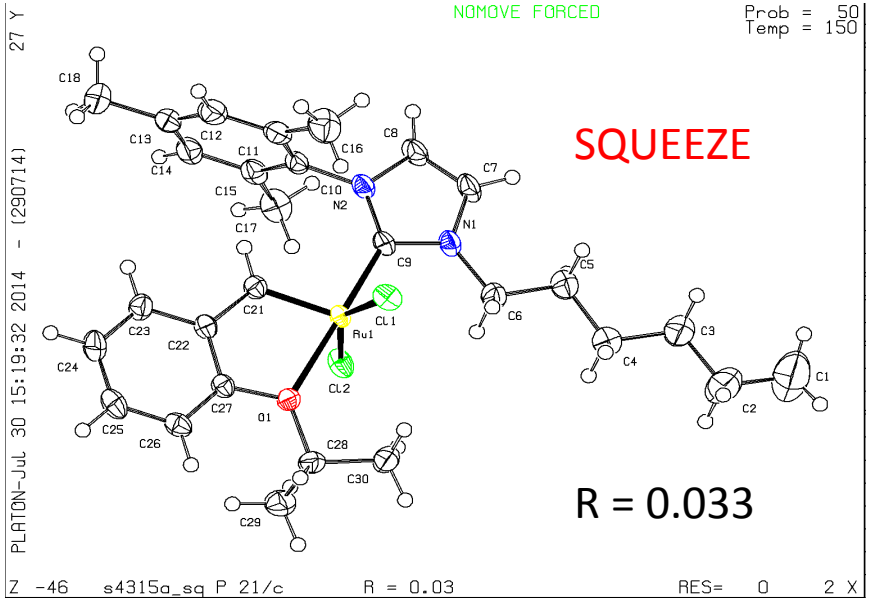


Diff. Map +/- CH2Cl2



Diff.Map + CH2Cl2





The ‘NEXTRA’ Issue

- One of the issues that needs to be addressed is the number of additional parameters to be added in the calculation associated with SQUEEZE on the L.S. Command. The default value is set to: (E x n) / (Z x m) where
- E = the number of recovered electrons in the unit cell
- Z = the number of asymmetric units
- m = the number of electrons in a CH2 fragment (=8)
- n = the number of parameters usually refined for a CH2 fragment (=9)

- This formula has the nice property that it vanishes when there is no residual density in the void

SQUEEZE Requirements

- There should be no residual unresolved density in the parameterized model region of the structure because of its impact in the solvent region.
- The data set should be reasonably complete and with sufficient resolution [i.e. sin(theta)/lambda >0.6]. Low temperature data help a lot.
- There should be no unresolved charge balance issues that might effect the chemistry involved (e.g. The valency of a metal in the ordered part of the structure)

Limitations

- The SQUEEZE technique can not handle cases where the solvent region is not constant but varies due to (coupled) disorder in the discrete part of the model.
- The solvent region is assumed not to contain significant anomalous scatterers (Friedels averaged)
- Designed for ‘small molecule structures’
- The use of SQUEEZE as part of the Fujita et al. MOF soaking method where the interest lies in the solvent region is very tricky and not recommended

SQUEEZE & TWINNING

Thanks to Shelxl2014, SQUEEZE can now handle the combination of solvent disorder and twinning via the LIST 8 option

(Both TWIN/BASF & BASF/HKLF 5)

See

SQUEEZE lecture in MS96.005

Thanks

to

George Sheldrick for his excellent major 2014 update to

SHELXL (and of course SHELXT)

and the

many users who gave their time for useful comments, suggestions and bug reports

(with supporting CIF)

Informal Theory of the SQUEEZE Procedure

$$F_H = \int_V \rho(\vec{r})\, e^{2\pi i \vec{H}\cdot\vec{r}}\, dV$$

$$= \int_V \left(\rho^M(\vec{r}) + \rho^S(\vec{r})\right) e^{2\pi i \vec{H}\cdot\vec{r}}\, dV$$

$$\rho^M(\vec{r}) = \sum_{j=1}^{N} \rho(\vec{r} - \vec{r}_j)$$

$$F_H^M = \sum_{j=1}^{N} f_j\, e^{2\pi i \vec{H}\cdot\vec{r}_j}$$

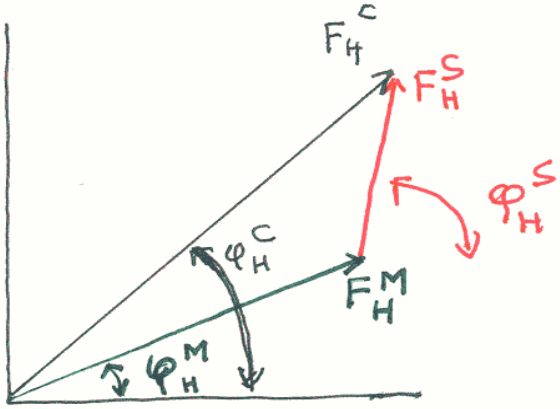
$$\rho^S(\vec{r}) \approx \Delta\rho(\vec{r}_k) \text{ on grid}$$

$$F_H^S = V_q \sum_S \Delta\rho(\vec{r}_k)\, e^{2\pi i \vec{H}\cdot\vec{r}_k}$$

$$F_H^C = F_H^M + F_H^S \Longrightarrow$$

M = Ordered

S = Solvent



Iterate (Initially $\rho_H^S = \rho_H^M$)

$$\Delta\rho(\vec{r}) = \frac{1}{V} \sum_H \left(s|F_H^o| e^{i\varphi_H^C} - |F_H^M| e^{i\varphi_H^M}\right) e^{-2\pi i \vec{H}\cdot\vec{r}} + \frac{F_o^S}{V}$$

Solvent Free ElectronCount

$$F_H^o : F_H^{o'} = |F_H^o| e^{i\varphi^C} - |F_H^S| e^{i\varphi^S}$$

$$: V_q \sum_S \Delta\rho(\vec{r}_k)$$