Fourty Years of Marshing: Is the Missed Symmetry Problem now Solved?

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My Connection with Dick

- My early interest in the 'Missed Symmetry Problem' was aroused by Dick's 1979 paper: Richard E. Marsh & Verner Schomaker, Inorg. Chem. (1979) 18, 2331-2336, *Some Incorrect Space groups in Inorg. Chem, Volume 16 (1977)*
- That paper inspired me, as a service crystallographer, and others to work on software to be routinely aware of this space group problem.
- On the basis of that software I had a nice one-time joint 'internet based' collaborative paper in Acta Cryst. with corrections to the literature.

The Missed Symmetry Problem

- Correct space group assignment to a crystal structure is not always trivial (in particular concerning the centro/non-centro choice case).
- As a result, many (and still uncorrected) errors can be found in the literature and databases.
- Some errors are harmful in having their impact on the presented chemistry, others can be of a more esthetic nature.
- Pseudo-symmetry, disorder, poor data and twinning may confuse the issue.

Space Group Corrections

Space group corrections include:

- Change of crystal system
- Change of Laue group
- Non-Centro to centrosymmetric
- Missed translation symmetry

The last two cases are the more problematic ones since they may lead to structure artefacts in addition to less optimal refinement results.

The Problem

- The problem is that the correct space group assignment is often only possible after the structure is preliminary ‘solved’ in a lower symmetry group, e,g. P1.
- Authors do often not know how to manage a transformation to higher symmetry space groups. E.g. the needed origin shift (P-1) or origin choice (C2/c) problems. Education & Experience needed!
- In addition, for proper evaluation of a proposed space group assignment, we will need the primary reflection data on which the study is based.
- Those data are not always archived for published papers, making ‘correction reports’ based purely on coordinates tricky.

More Correction Papers since 1979

- More erroneous structure reports, due to inexperience, started to appear in the literature, in particular in non-crystallographic journals (Inorg Chem, JACS). Often no crystalographic referees involved.
- The 1979 ‘missed symmetry’ paper was the first in a series of similar papers by Dick, often in collaboration with other ‘senior’ scientists. Other authors soon picked up the same subject as well.
- The procedure that was used by Dick was to look by hand for special relations in the coordinates of similar ‘independent’ atoms. Published ORTEPS are helpfull to spot problems.

How Large is the Problem ?

- An under-bound can be gleaned from the searchable information available in the CSD
- Searching the CSD for the tekst ‘REINT_OF’, that stands for ‘reinterpretation’, reports 1800 entries (89 between 2013-2017) (2018 version)
- 1061 of those indicated as re-interpretations are (co)authored by Dick Marsh
- However, there are many more not marked yet (and corrected) in the CSD (e.g. those reported in Dick’s last Acta Cryst. (2014). C70, 834 paper).

The 156 updated structures, including the CSD refcode, the reported space group, and the revised space group.

Refcode	Reported space group	Revised space group	Refcode	Reported space group	Revised space group	Refcode	Reported space group	Revised space group
APONOJ	$P1$	$P\bar{1}$	IGEKIP	$P1$	$P\bar{1}$	PUBTEM	$P\bar{1}$	$C2/c$
APOPAX	$P1$	$P\bar{1}$	IMOMUT	$P\bar{1}$	$P2_1/n$	PUBTOW	$P2_1$	$P2_1/n$
APOPOL	$P1$	$P\bar{1}$	IQATEA	$P1$	$P2_1$	PUBTUC	$P1$	$P\bar{1}$
APORIH	$P1$	$P\bar{1}$	ISECOZ	$P1$	$P\bar{1}$	QAMLEX	$P\bar{1}$	$P2_1/n$
AQINIY	$P\bar{1}$	$C2/c$	ITEXUB01	Cc	$C2/c$	QANCEP	$P1$	$P\bar{1}$
ATANEP	$P2_1$	$P2_12_12_1$	ITIREJ	$P1$	$P2_12_12$	QAPWUB	$P1$	$P\bar{1}$
ATIWIK	Cc	$P2_1/c$	ITUMIU	$P\bar{1}$	$P2_1/n$	QASLUT	$P4_3$	$P4_322$
AVATIB	Cc	$C2/c$	IVEMUS	$P\bar{1}$	$P2_1/n$	QUDNAF	Cc	$C2/c$
AWEMEV	$P\bar{1}$	$C2/c$	IXUGUE	$P\bar{1}$	$C2/c$	QUHNUD	$P1$	$P\bar{1}$
AYEJUK	Cc	$C2/c$	IZIGII	$P2_12_12_1$	$Pbca$	QUJHOT	$P1$	$P\bar{1}$
AZEKEW	$P2_1/c$	$Pccn$	KAZRIO	$P1$	$P\bar{1}$	QUMKEP	Cc	$C2/c$
BAHHUP	$P1$	$P\bar{1}$	KEFNIU	$P2_1$	$C222_1$	RUGDON	$P\bar{1}$	$P\bar{1}$
BAZYOS	Pn	$P2_1/n$	KETDEU	Pc	$P2_1/c$	RUHGAD	Pn	$P2_1/n$
BOXNOS	$P\bar{1}$	$C2/c$	KUBCOA	$P\bar{1}$	$Cmca$	RUHKOV	$P2_1$	$Pbca$
BOYFIF	$P1$	$P\bar{1}$	KUFLED	$P1$	$P\bar{1}$	SAQHOJ	$P1$	$P\bar{1}$
BOYZIZ	Cc	$C2/c$	KUGPOS	$P2/c$	$Pbcm$	SAWKUY	Cc	$C2/c$
BULCIV	$P\bar{1}$	$P2/c$	KUJLUX	$I4$	$I4/m$	SEFQEB	$P\bar{1}$	$P2_1/c$
CACMEA	$P1$	$P\bar{1}$	LAYNOQ	$P2_1$	$P2_12_12_1$	SELGIB	$P\bar{1}$	$P2_1/c$
CAFWIR	$P\bar{1}$	$C2/c$	LEPMEZ03	$P2_1/n$	$P2_1/n$	SUJWIE	$P\bar{1}$	$P2_1/n$
CAJCAT	$P4_3$	$P4_322$	LUKDEB	$P\bar{1}$	$P2_1/n$	TASTEO	$P3_1$	$P3_121$
CASXEB	$P1$	$P\bar{1}$	LULSUH	$P2_1$	$P2_12_12_1$	TAWYOH	$P2_1/c$	$Pbca$
CEBYIT	Cc	$C2/c$	MAMXEF	$P\bar{1}$	$P2_1/c$	TECLEU	$P\bar{1}$	$P2_1/c$
CEBZAM	$P1$	$P\bar{1}$	MAMXOP	$P1$	$P\bar{1}$	TEJLUR	$P\bar{1}$	$C2m$
CUGKAR	$P\bar{1}$	$C2/c$	MAMXUV	Cc	$C2/c$	TUFTUK	$P1$	$P\bar{1}$
CUMSEJ	$P1$	$P\bar{1}$	MAMYAC	$P2_1$	$P2_1/c$	TUHBEE	$P2_1$	$P2_1/c$
CUNBET	$P1$	$P2_1$	MAVDAQ	$P1$	$P\bar{1}$	UCABOR	$P1$	$P\bar{1}$
DABVIN	$P\bar{1}$	$P\bar{1}$	MAVZUG	$P1$	$P2_1/c$	UHANUN	$P\bar{1}$	$R\bar{3}c$
DAQWOJ	Cc	$C2/c$	MEBGEH	$P2_1/c$	$Pbcn$	UQUDUG	$P\bar{1}$	$P2_1/n$
DEDVEO	Pa	$Pca2_1$	MEDRIY	Cc	$C2/c$	UROPIB	$P2_1/n$	$Pnnm$
DELFIL	$P1$	$P\bar{1}$	MEDXAW	$C2$	$Aba2$	UROPUN	Pc	$P2_1/c$
DUKYIS	Cc	$C2/c$	MOVWIE	$P\bar{1}$	$P\bar{1}$	UWAVOE	$P2_1/n$	$Pnma$
EMOCEP	$P2_1ab$	$Pbca$	MOXDUZ	$P\bar{1}$	$C2/c$	UWIKUH	$C2$	$Fdd2$
ENEKUE	$P\bar{1}$	$P2_1/n$	MUKGEF	$P\bar{1}$	$C2/c$	UWUFEY	$P\bar{1}$	$C2/c$
EQEDAG	$P1$	$P\bar{1}$	NARMAW	$P\bar{1}$	$P2/c$	VASBUO	$P\bar{1}$	$P2_1/n$
ERAZAZ	$P2_1/m$	$Pnma$	NUCSUA	$P1$	$P\bar{1}$	VATHIJ	Pn	$P2/c$
EZIQEK	$P4_3$	$P4_32_12$	NUCTAH	$P1$	$P\bar{1}$	VAVHEH	$P1$	$Pna2_1$
EZOZEZ	$Pna2_1$	$Pccn$	OHAPOD	$P1$	$P\bar{1}$	VUHBEG	Cc	$C2/c$
FAMYUP	$P\bar{1}$	$P\bar{1}$	OMOCAV	$P1$	$P2_12_12$	WEHPUW	$P1$	$P\bar{1}$
FAZGIY	$P3$	$P321$	OMOCUP	$P\bar{1}$	$P2_1/n$	WUGKAL	$P1$	$C2$
FEPGOY	$P1$	$P\bar{1}$	ONILIH	$P1$	$P\bar{1}$	WULCEM	Pa	$P2_1/n$
FOXTIW	$P2_1$	$C222_1$	OQEVOW	$P1$	$P\bar{1}$	WUNLUN	$P1$	$P\bar{1}$
FUDMIB	$P2_1$	$P2_12_12$	OTAPOP	$P\bar{1}$	$P2_1/c$	WUQQEF	$P2_1$	$P2_12_12_1$
FUFCEP	$P\bar{1}$	$P2_1/c$	OWEDAW	$P\bar{1}$	$P2_1/a$	WUSVUC	$I4_1$	$I4_122$
FUNHIG	$R3$	$R32$	OXEJIL	$P\bar{1}$	$P2_1/n$	WUSWAJ	$I4_1$	$I4_122$
GEGVAR	$P\bar{1}$	$P2_1/n$	OXERAL	$P2_1$	$Pmn2_1$	XEHYUG	$P\bar{1}$	$P2_1/c$
GENHUE	$P\bar{1}$	$P2_1/c$	PAKMUL	Cc	$C2/c$	XESPOC	$P2_1$	$P2_1/n$
GUHTAF	$P2_1$	$P2_1$	PAZOXN12	Pn	$P2_1/n$	XOTYOV	Pc	$P2_1/c$
HATCAI	$P1$	$P\bar{1}$	PECPIY	$P\bar{1}$	$P2_1/c$	XOTYUB	$P2_1$	$P2_1/n$
HOGDUD	Cc	$C2/c$	POPPAM	Ia	$I2/a$	YOSFES	$I4_1$	$I4_122$
HORTEO01	$P1$	$P\bar{1}$	POSWOK	$P1$	$P\bar{1}$	YUHCAG	$P1$	$P\bar{1}$
HOXLEM	$P1$	$I2$	POTBAC	$P1$	$P2_1$	YUNWIO	Cc	$C2/c$
IBIXEY	$P1$	$P\bar{1}$	POYXIL	$P\bar{1}$	$P2_1/c$	ZAQKAF	Cc	$C2/c$

Last 2014 Acta Cryst. C70, 834-836 paper with 156 new corrections In recent Papers.

No warning Info added in the 2018 CSD

Will be handledi In the 2019 Release.

Why Bother ?

- Space group re-interpretation papers have always been controversial (and sometimes considered pedantic ..) Dick's early rebuttal on this is already given in the Acta Cryst. (1979) B35, 1094-1099 paper:
- "Some will argue that the mishap was harmless; afterall, the reported structure is essentially correct, as far as we know, except for the symmetry and the divergent lengths and angles. We can understand, but hardly agree."

New Computer Based Algorithms

- 1982: CREDUC, Y Le Page J.Appl.Cryst.,**15**,255.
- Determination of the Metrical Symmetry of the lattice from the number of compatible two-fold axes. E.g. 1 → monoclinic, 5 → tetragonal, 9 → cubic
- Two-axis = coinciding low-index (0,1,2) direct and reciprocal lattice vectors within a tolerance.
- Actual symmetry can be lower, not higher than the metrical symmetry.
- The PLATON/LEPAGE tool is Modelled on CREDUC
- Does the cell content support the lattice symmetry ?

The MISSYM Algorithm

- In 1987, Y. Le Page published an extention to CREDUC called MISSYM (J.Appl.Cryst.,**20**,264).
- MISSYM Looks for support in the actual structure (I.e. coordinate set) for the proposed metrical symmetry elements of the lattice found by the CREDUC algorithm.
- Liberal tolerances are used in general to catch outliers due to refinement divergence and pseudo-symmetry cases.

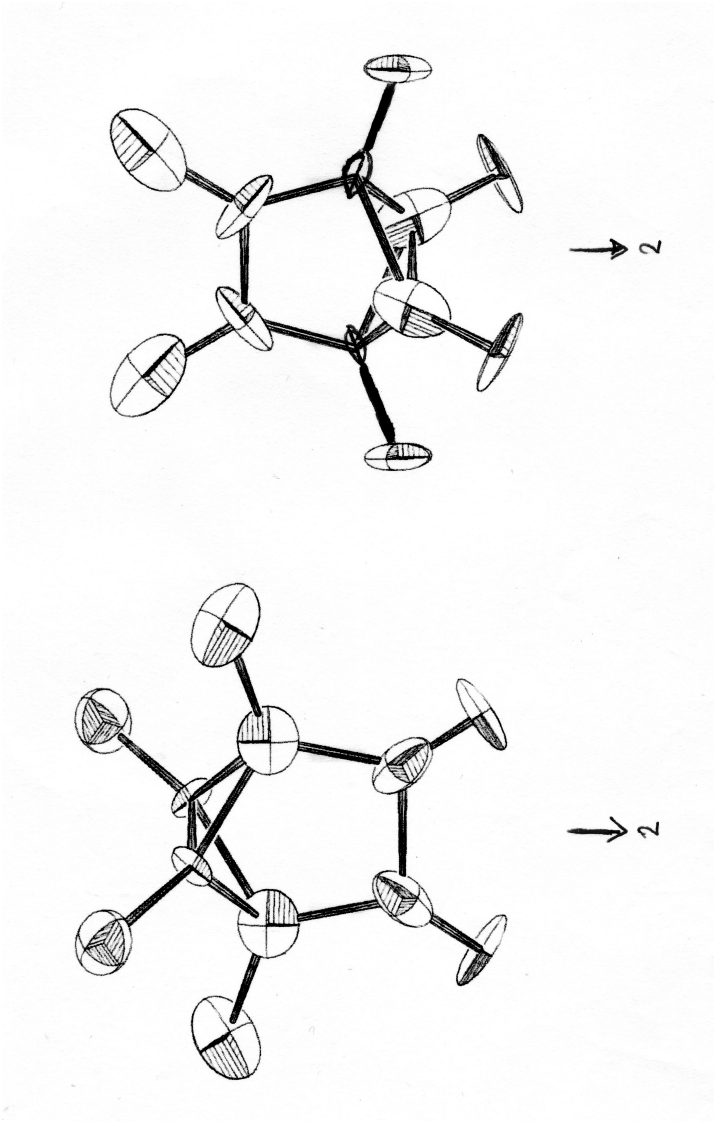
MISSYM Implementation

- Originally as part of the NRCVAX package.
- That version reports additional symmetry elements but leaves their evaluation and implementation into the proper space group to the educated researcher.
- In PLATON as the ADDSYM routine along with a work-up to the suggested new space group.
- ADDSYM is also part of the IUCr/checkCIF tool

PLATON/ADDSYM Extensions

- Suggests automatically a revised space group, unit cell and origin transformation.
- May Generate a new ‘.res’ file for subsequent SHELXL refinement.
- Allows for a percentage of non-fitting atoms in order to catch interesting pseudo-symmetry cases.
- Handles sub-cells (originating from structure prediction)
- Accepts input data in ‘.res’ and ‘.cif’ format.
- Runs on files with multiple entries (CSD/CIF).
- Display of the revised (averaged) structure.

Retro Check of my own Early Publications with the ADDSYM Tool



One Hit ! in papers published in 1977, prior to the Marsh & Schomaker (1979) paper.

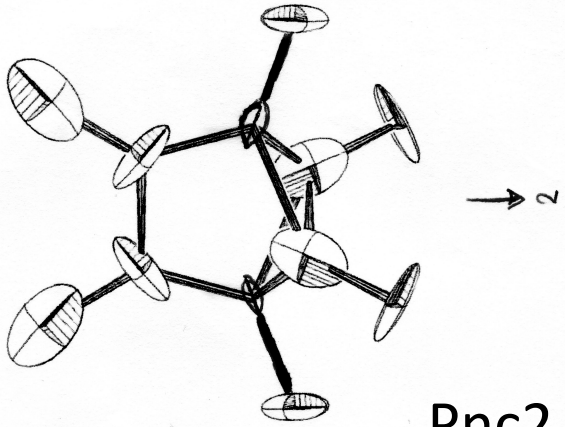
Cryst. Struct. Commun. (1977) 6, 259-262
(Journal was the forerunner of Acta Cryst. C)

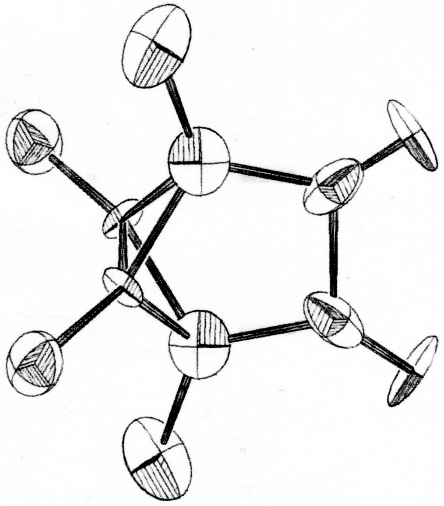
Refined with XRAY76 in the Non-Centro Space Group Pnc2. Poor structure: R_F =0.08

No inversion implemented in view of hk0, h=2n+1 outliers up to 30 sigma(I)

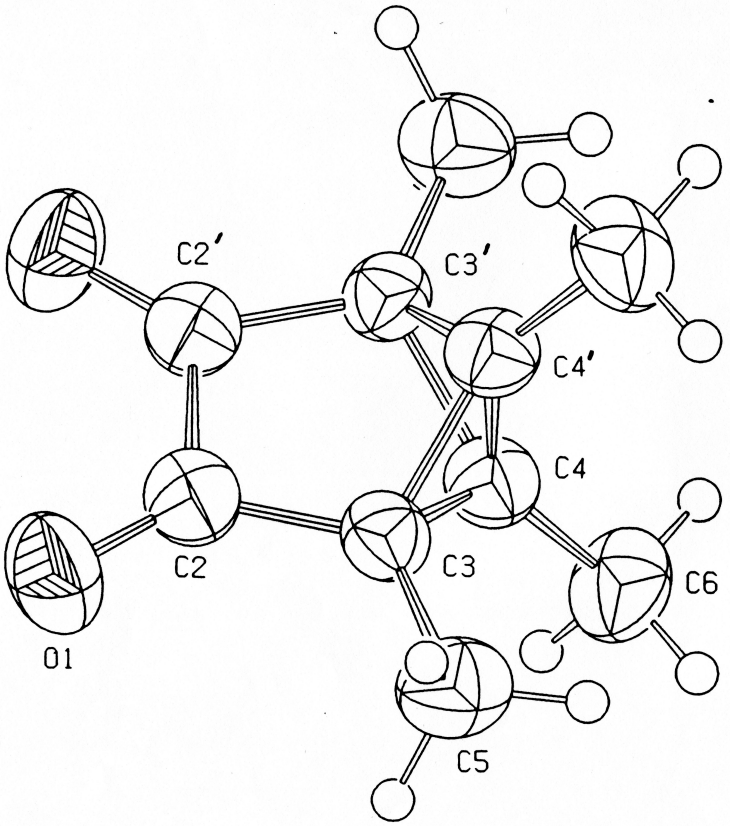
Re-Refined with SHELX76 in Space Group Pnca.
R_F = 0.049, wR_F = 0.077

Refinement Result with the Proper Space Group Assignment



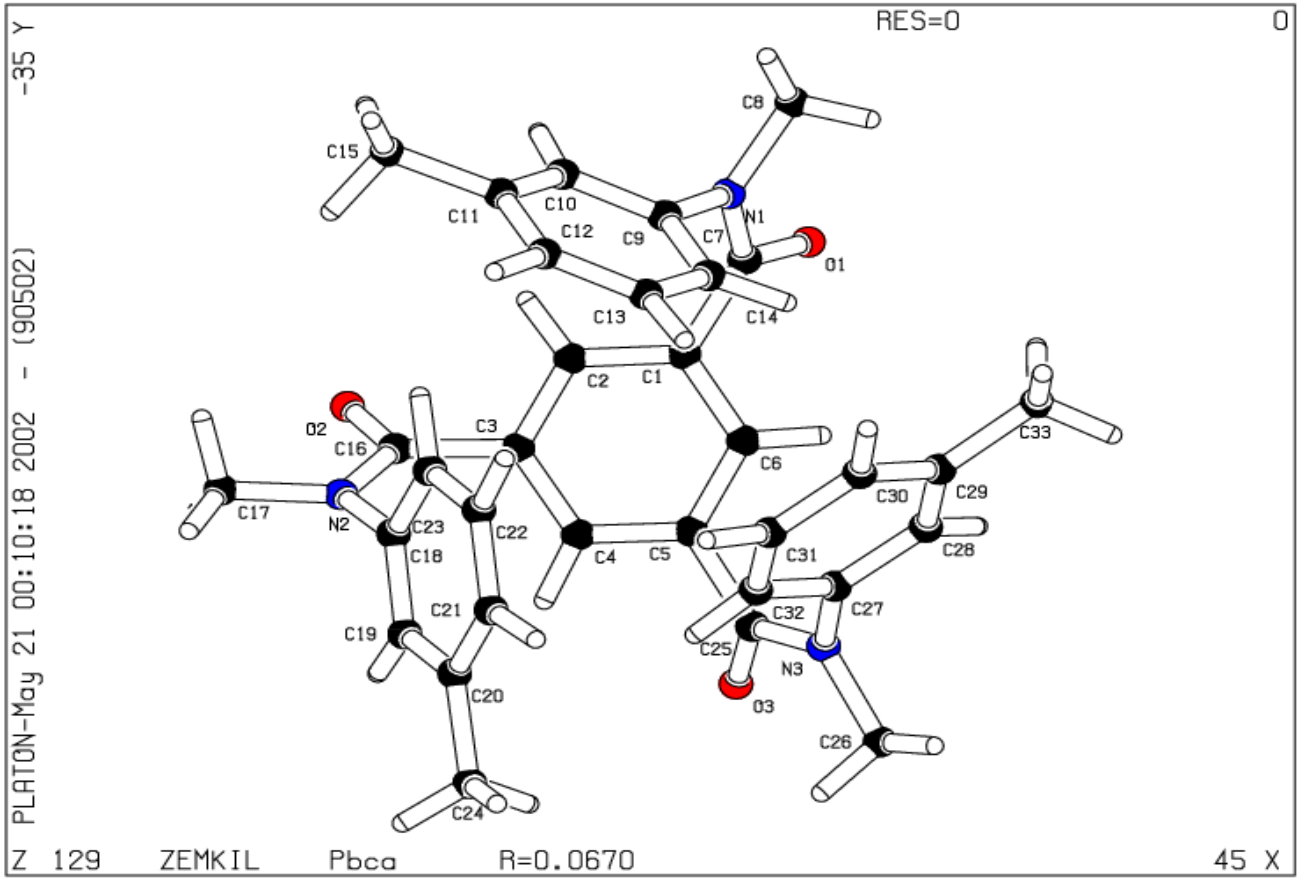


Pnc2 ==> Pnca



Acta Cryst. (1990). C46, 1357-1358
Better geometry and Displacement Parameters

Change of Crystal System Example proposed by ADDSYM



Asymmetric Unit in Pbca

P.L.A.T.O.N

PLATON/ADDSYM for ZEMKIL Pbca

ADDSYM Search on ALL NON-H Chemical Types [Max NonFit 20 Perc]
The Structure Implies the Following Symmetry Elements Subject to the Criteria:
1.00 Deg (Metric), 0.25 Ang (Rotations), 0.45 Ang (Inv), 0.45 Ang (Transl)

Symm. Elem	Input Cell Row	Reduced Cell Row	(Ang) d	Typ	Dot	(Deg) Angle	( ) Fit	(Ang) MaxDev.		Input Cell x	y	z
b	[1 0 0]	[1 0 0]	17.86	4	1	0.00	100	0	through	1/4	0	0
									Glide =	0	1/2	0
c	[0 1 0]	[0-1 0]	17.86	4	1	0.00	100	0	through	0	1/4	0
									Glide =	0	0	1/2
a	[0 0 1]	[0 0 1]	17.86	4	1	0.00	100	0	through	0	0	1/4
									Glide =	1/2	0	0
3 *	[1-1-1]	[-1-1-1]	30.93	3	3	0.00	100 C15	0.009 -C33	through	1/2	0	1/2
3 *	[1 1 1]	[1-1-1]	30.93	3	3	0.00	100 C33	0.009 -C15	through	2/3	1/6	1/6
3 *	[1-1 1]	[1 1-1]	30.93	3	3	0.00	100 C15	0.009 -C33	through	1/3	2/3	1/3
3 *	[1 1-1]	[-1 1-1]	30.93	3	3	0.00	100 C33	0.009 -C15	through	1/6	1/6	1/3
-1	==========						100	0	at	0	0	0

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

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

Cell	Lattice	a	b	c	Alpha	Beta	Gamma	Volume	Crystal System	Laue
Input	oP	17.860	17.860	17.860	90.00	90.00	90.00	5697	Orthorhombic	mmm
Reduced	P	17.860	17.860	17.860	90.00	90.00	90.00	5697		
Convent	cP	17.860	17.860	17.860	90.00	90.00	90.00	5697	Cubic	m-3

Origin shifted to: 0.000, 0.500, 0.000 after transformation

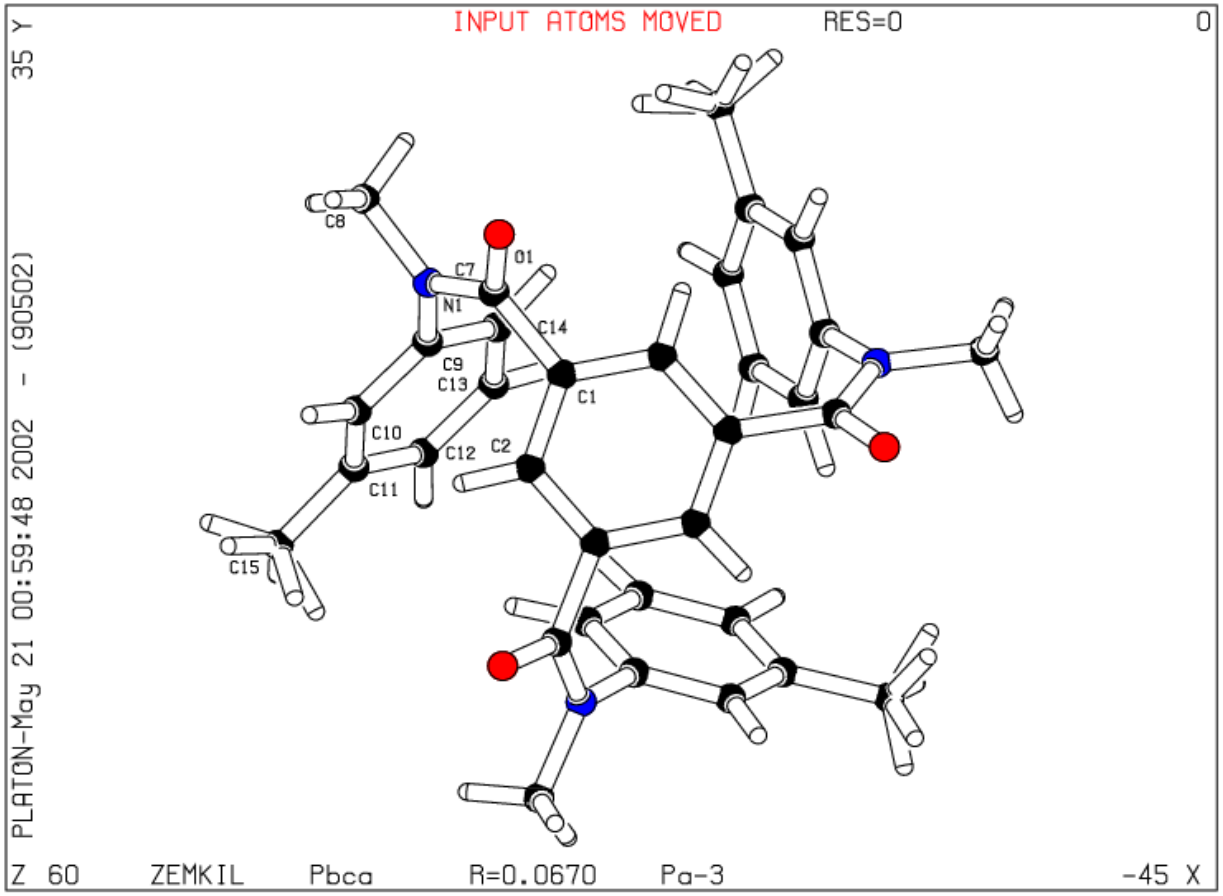
Missed/Additional Symmetry : Suggested SPGR = Pa-3 (No 205)

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

Additional (Pseudo)Symmetry Found (See Listing for details)
>> Hit RETURN to Continue

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

Orthorhombic Pbca ➔ Cubic Pa-3



Molecule on three fold axis

Early Survey's of the Missed Symmetry Issue

- A survey by Dick Marsh in 1997 of all structures published in space group Cc showed that about 10% of the assignments were wrong.
- A new survey by Dick Marsh in 2004 surprisingly showed that this percentage was still around 10%.
- Note: none of the additional 164 corrected assignments were from Acta Cryst. journals.
- Common revisions were to C2/c, Fdd2, R-3c etc.

Centro or Non-centrosymmetric ?

- Correct assignment is not always trivial.
- Refinement of (close to) centrosymmetric structures in P1 is mathematically unstable.
- Mis-assignment -> geometry artifacts.
- **Dick Marsh**: Borderline cases are best treated as centro-symmetric (static/dynamic disorder)
- Inspect Fo/Fc of weak reflection data.
- In general: chiral molecules-> non-centro SpGr.

Interesting Story

- ADDSYM can automatically analyse a CIF file containing multiple entries exported from the CSD.
- In 1999, in response to the paper "P1 or P-1 or something else" I send Dick my larger automatically created "P1" list. He immediately started to work on that list and indeed found some more missed symmetry cases.
- Interestingly, one of the entries (NAXQAM) that he had previously updated to Cc was 'Marshed' again to Fdd2. I did not realize that when I supplied my list.
- I was told that he enjoyed being Marshed.

Joint Paper

- As a follow-up, Dick asked me to send him my automatically generated list for space group corrections to structures published in C2.
- This resulted in a one time long distance internet based collaboration and the paper:
- "*Use of software to seach for higher symmetry: space group C2*". Acta Cryst. (2001). B57, 800-805.
- It was an honor and an enjoyable experience

ADDSYM runs for all 2013-2018 CSD Entries: Is the problem solved ?

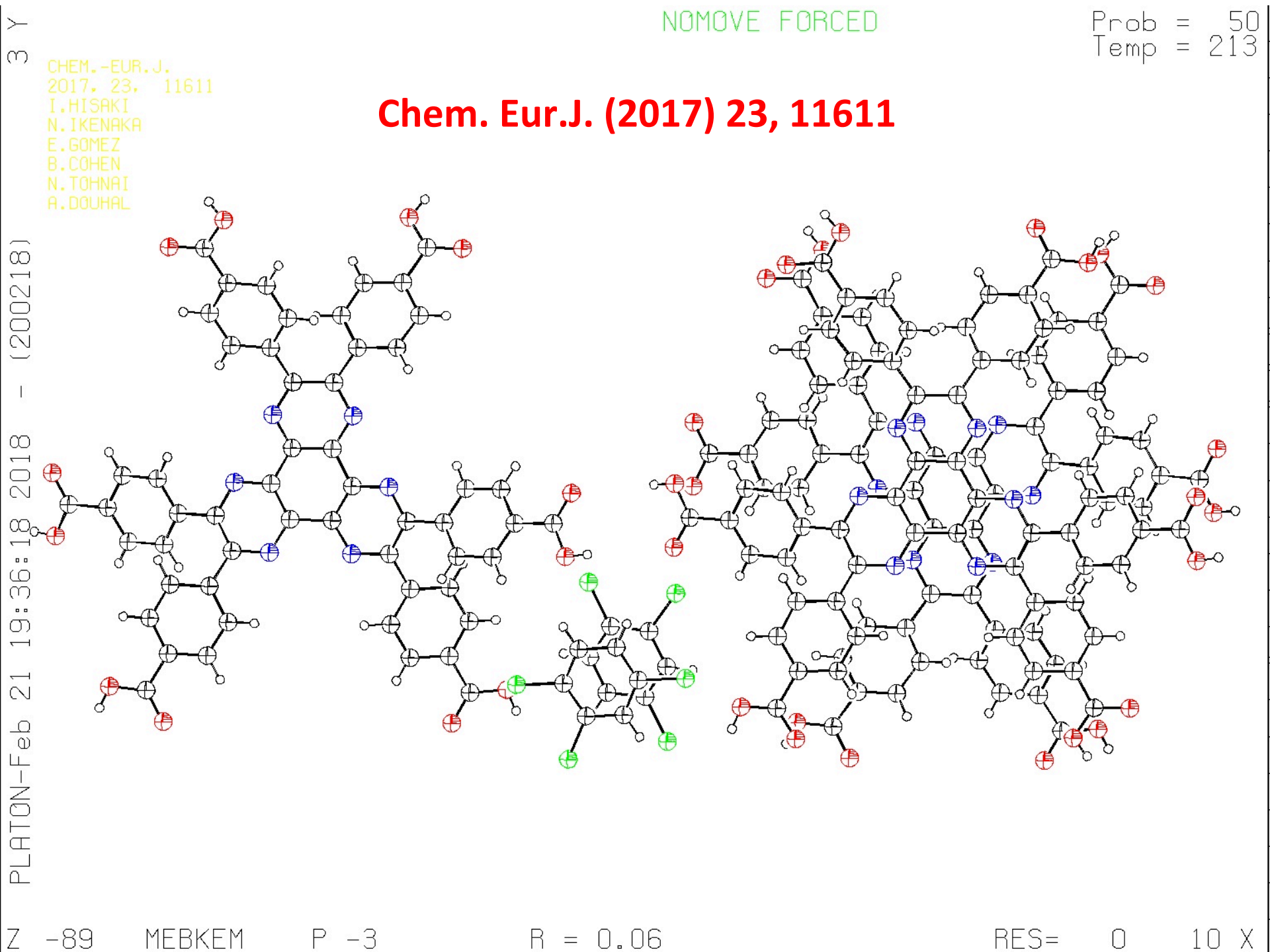
Year	#New ENTRIES	ADDSYM HITS		100% FIT	
2013	47233	797	(1.7%)	364	(0.77%)
2014	49546	890	(1.8)	416	(0.84)
2015	52652	860	(1.6)	390	(0.74)
2016	54333	832	(1.5)	343	(0.63)
2017	40496	618	(1.5)	253	(0.62)
2018	16546	258	(1.6)	93	(0.56)

'HITS' = Number of entries satisfying the default ADDSYM criteria for closer inspection (Not necessarily an Error)

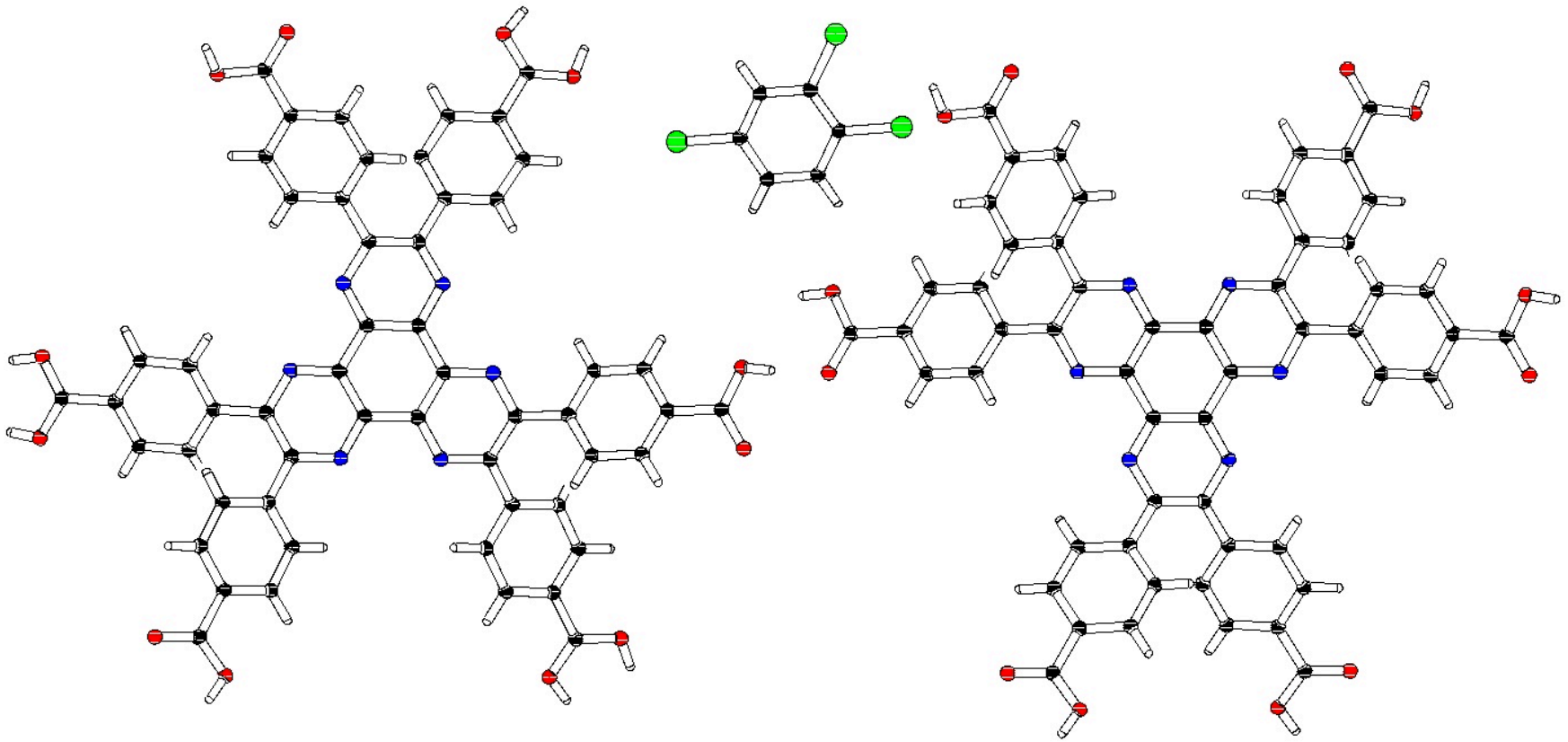
ADDSYM Criteria

- Default criteria are set to values to also catch large outliers (in cell dimensions or near singular refinement parameters), pseudo-symmetry, incorrectly assigned atom types etc.
- All reported cases of additional symmetry should be investigated, acted upon, reported and discussed in a structure report.
- Next: subset of hits for 2017 as illustration

LEJCUB		P n	mP=>mP	0.0	0	0	0.000	0.00	0.204		100%	P21/n
LEJDAI		P n	mP=>mP	0.0	0	0	0.000	0.00	0.236		100%	P21/n
MANNUN		P 21	mP=>mP	0.0	0	0	0.000	0.00	0.000		82%	P21/c
MANQEA		P 21/n	mP=>mP	0.0	0	0	0.000	0.00	0.239	S	100%	P21/m
MAPFER		I 4	tI=>tI	0.0	0	0	0.000	0.00	0.138		100%	I422
MAPXEJ		P b a 2	oP=>oP	0.0	0	0	0.000	0.00	0.000		84%	Pcca
MAQHEU	*	P -1	aP=>aP	0.0	0	0	0.000	0.00	0.000	S	100%	P-1
MASWIP		P 21	mP=>mP	0.0	0	0	0.000	0.00	0.248		87%	P21/c
MAVYAM		P 21	mP=>mP	0.0	0	0	0.000	0.00	0.000		87%	P21/c
MAVZER		P 65	hP=>hP	0.0	0	0	0.000	0.00	0.174		100%	P6522
MAWLII		P 21	mP=>oP	0.0	0	0	0.000	0.15	0.032		100%	Pmc21
MAXVEP		P -1	aP=>mP	0.0	0	0	0.000	0.11	0.007		100%	P21/c
MAXWUG		P 1	aP=>aP	0.0	0	0	0.000	0.00	0.000		89%	P-1
MAXXER		P 21/c	mP=>oP	0.0	0	0	0.000	0.09	0.012		100%	Pbca
MAZDAV		P 21/n	mP=>oP	0.0	0	0	0.000	0.36	0.241		95%	Pnma
MAZSOY		I 2	mI=>mI	0.0	0	0	0.000	0.00	0.000		93%	I2/c
MAZTAL		P 1	aP=>aP	0.0	0	0	0.000	0.00	0.000		97%	P-1
MAZTOZ		P 1	aP=>aP	0.0	0	0	0.000	0.00	0.000		92%	P-1
MEBBIH		P 21	mP=>mP	0.0	0	0	0.000	0.00	0.000		96%	P21/n
MEBKEM	*	P -3	hP=>hP	0.0	0	0	0.000	0.00	0.006		100%	P-3c1
MEBKIQ		R -3	hR=>hR	0.0	0	0	0.000	0.00	0.010		100%	R-3c
MEBRET		P 21/c	mP=>oP	0.0	0	0	0.000	0.86	0.248		95%	Pnma
MEDKIS		P c	mP=>mP	0.0	0	0	0.000	0.00	0.249		99%	P21/c
MEDNER		P c	mP=>mP	0.0	0	0	0.000	0.00	0.249		99%	P21/c
MEDXAX		P -3	hP=>hP	0.0	0	0	0.000	0.00	0.217		100%	P-3m1
MEGMAP		P -4	tP=>tP	0.0	0	0	0.000	0.00	0.231		98%	P-42m
MEHQAU		C 2	mC=>mC	0.0	0	0	0.000	0.00	0.042		100%	C2/c
MEHQEY01		C 2	mC=>mC	0.0	0	0	0.000	0.00	0.051		100%	C2/c
MEJZIL03		P -1	aP=>mP	0.0	0	0	0.000	0.15	0.240	S	100%	P21/c
MEJZIL04		P -1	aP=>mP	0.0	0	0	0.000	0.05	0.244	S	100%	P21/c
MEJZIL05		P -1	aP=>mP	0.0	0	0	0.000	0.15	0.247	S	100%	P21/c

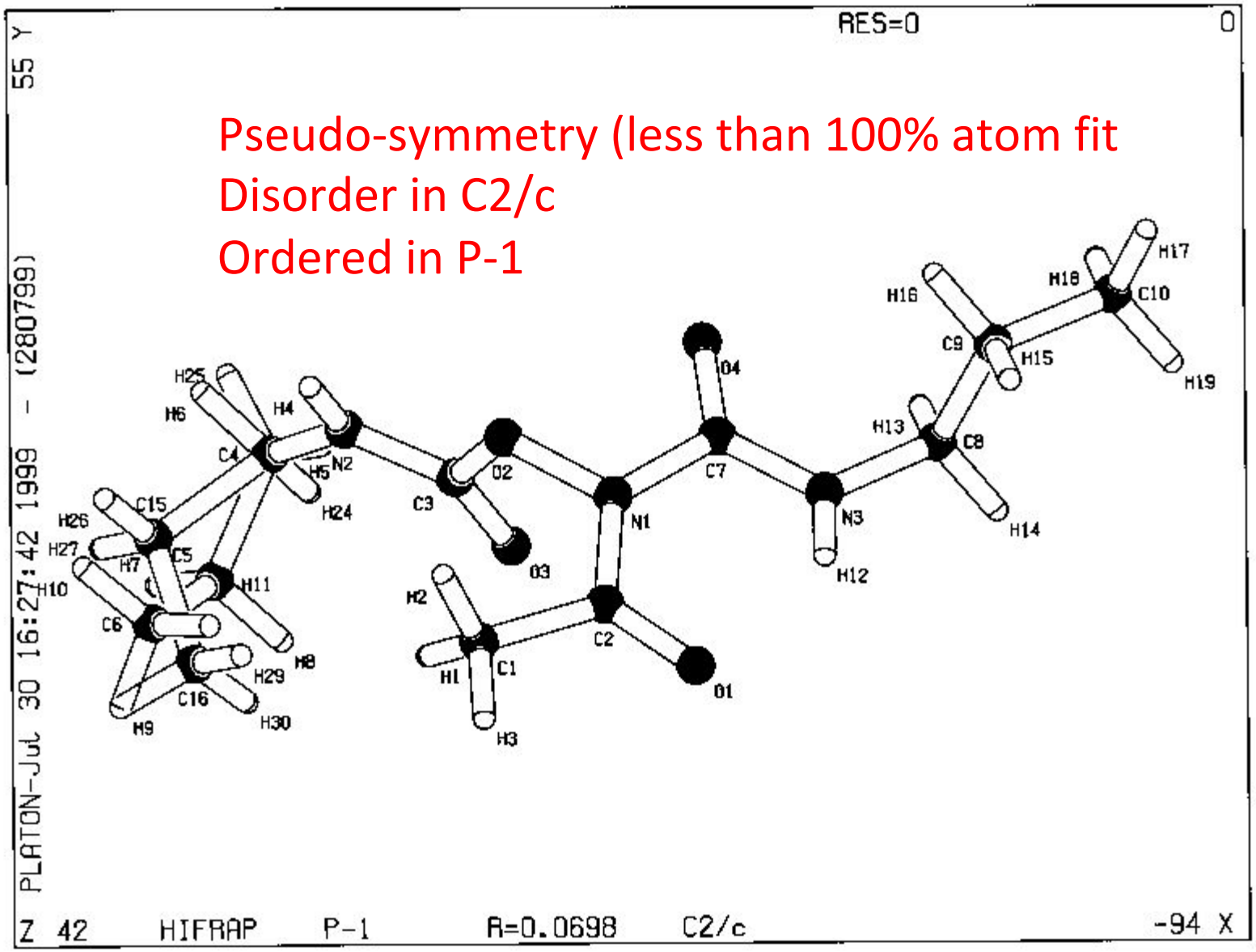

3 Y
CHEM.-EUR.J.
2017, 23, 11611
I.HISAKI
N.IKENAKA
E.GOMEZ
B.COHEN
N.TOHNAI
A.DOUHAL
NOMOVE FORCED
Prob = 50
Temp = 213
Chem. Eur.J. (2017) 23, 11611
PLATON-Feb 21 19:36:18 2018 - (200218)
Z -89 MEBKEM P -3 R = 0.06 RES= 0 10 X

Change of LAUE class: Low to high trigonal -3 ➔ -3m1 , P-3 ➔ P-3c1



The Problem of too High Symmetry

- In particular with point detector data, it was easy to miss weak diffraction spots, resulting in artificial disorder (i.e. averaged structures)
- Pseudo-symmetry may lead to structure solutions in too high symmetry groups and artificial disorder.
- Twinning may lead to similar issues
- A pseudo-symmetry case next:


RES=0
0
55 Y
PLATON-Jul 30 16:27:42 1999 - (280799)
Z 42 HIFRAP P-1 R=0.0698 C2/c -94 X
Pseudo-symmetry (less than 100% atom fit
Disorder in C2/c
Ordered in P-1
H25
H6
H4
C4
N2
H5
H24
C15
H26
H27
H7
C5
H10
H11
C6
H8
H29
C16
H9
H30
C3
O2
O3
O4
C7
N1
N3
H12
H13
C8
H14
C9
H15
H16
H18
H17
C10
H19
H2
C2
C1
H1
H3
O1

Comments

- Hydrogen atoms and disordered atoms are not included in the ADDSYM analysis.
- Pseudo-symmetry can be both problematic and/or interesting (Inorganic Structures)
- Missed symmetry claims should always be supported with the primary reflection data.
- In the past, those data were deposited (and sometimes retyped in support of Dick's early symmetry corrections).
- Currently embedded unmerged reflection data in SHELXL cif's should not be deleted

40 Years of Marshing

- Obvious Question:

  Is the Missed Symmetry Issue now Solved after 40 years ?

- Answer:

  -Yes: For Publications in the IUCr Journals.

  - No: For Publications in Chemical Journals.

It is amazing that, given the availability of tools like IUCr/checkCIF, the issue is still often ignored by authors, editors and referees.

Thanks Dick
for Keeping our Science to Standards
and
You for Listening !

- http://www.cryst.chem.uu.nl/spek
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