

CPSNC.centro.txt

Supplementary text to
Centrosymmetric and pseudo-centrosymmetric structures refined as non-
centrosymmetric
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Spek
Acta Crystallographica B

Wrong structures where a centre of symmetry had to be added.

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Criteria for selection:

- One atom of an element heavier than Ar
- Published after 1995
- centre of symmetry needs adding

Source of wrong structures

- [A] Clemente, D. A. (2004) *Inorg. Chim. Acta* 358, 1725-1748.
- [B] Herbstein, F. H. and Marsh, R. E. (1998) *Acta Cryst.* B54, 677-686.
- [C] Marsh, R. E. (1999) *Acta Cryst.* B55, 931-936.
- [D] Marsh, R. E. and Spek, A. L. (2001) *Acta Cryst.* B57, 800-805.
- [E] Marsh, R. E., Kapon, M., Hu, S. and Herbstein, F. H. (2002) *Acta Cryst.* B58, 62-77.
- [F] Herbstein, F. H., Hu, S. and Kapon, M., (2002) *Acta Cryst.* B58, 884-892.
- [G] Marsh, R. E. (2002) *Acta Cryst.* B58, 893-899.
- [H] Clemente D. A. and Marzotto, A. (2003) *Acta Cryst.* B59, 43-50.
- [I] Marsh, R. E. (2004) *Acta Cryst.* B60, 252-253.
- [J] Clemente D. A. and Marzotto, A. (2004) *Acta Cryst.* B60, 287-292.
- [K] Marsh, R. E. (2005) *Acta Cryst.* B61, 359.
- [P] Referee No 2. (2005) of Flack, H. D. and Bernardinelli, G., (2006) *Inorg. Chim. Acta* 359, 383 - 387.
- [Q] Clemente, D. A. (2005) Private communication - e-mails 04.09.2005, 05.10.2005
- [R] Marsh, R. E. (2005) Private communication - e-mails 10.09.2005
- [S] Bernardinelli, G, and Flack, H. D. (2005) Current work
- [T] Clemente, D. A. (2005/6) Private communication - e-mails 10.10.2005, 18.10.2005, 10.11.2005, 15.12.2005, 20.01.2006, 29.01.2006, 04.02.2006, 01.03.2006, 20.03.2006

Search terms used where a searchable electronic version of the original publication was available:

<BASF>
<Flack>
<absolute>
<enantio>
<CD>
<optical>
<chiral>
<racem>

As sources of data we used the papers as published and any supplementary material freely available for download from the journal's

online site, the CIF archive of the Cambridge Crystallographic Data Centre (CCDC) or perhaps from FIZ. We never contacted authors for supplementary material. Each paper available in searchable digital form was scanned for the strings of characters listed above. Values pertinent to this study are presented in the Table below. A "?" means that the corresponding value was not reported or could not be deduced from the data sources. The columns of this table contain the following data values:

[]: The code gives a pointer to the literature source indicating that a centre of inversion should be added to the space-group symmetry.

Refcode: This column identifies each compound by its CSD Refcode. The literature reference to each compound may be found under its refcode in the publication given under []. The compounds are ordered in sections alphabetically by refcode within a section. A "+" after the refcode means that the Notes section should be consulted.

S,P: Two aspects of the symmetry of the "wrong" model crystal structure are given in the Table in columns S and P. S indicates one of the three two-letter codes for crystal structures: NC non-centrosymmetric chiral crystal structure; NA non-centrosymmetric achiral crystal structure; CA centrosymmetric achiral crystal structure. P indicates the number of directions in which it is NOT possible to fix the origin of the (non-centrosymmetric) space group with respect to a symmetry element. In the rest of this paper, we will call these origin-free directions. This information is available in tables of the Euclidean normalizers of space groups.

Friedl Cover: The value gives a measure of the completeness of the diffraction intensity data with regard to inversion in the origin of reciprocal space (Friedel coverage). Reflections $h\ k\ l$ and $-h\ -k\ -l$ are called Friedel opposites. If for each value of $h\ k\ l$, the intensity of the Friedel opposite $-h\ -k\ -l$ (or one symmetry-equivalent to it) has not been measured, then the Friedel coverage is 0%. However if for each value of $h\ k\ l$, both the reflection $h\ k\ l$ and its Friedel opposite $-h\ -k\ -l$ (or one symmetry-equivalent to it) have been measured then the Friedel coverage is 100%. A value given as 0/100 means that although the Friedel coverage of the measurements was 100%, Friedel opposites were averaged prior to least-squares refinement to give a Friedel coverage of 0%.

Refinement software - The computer software used for the least-squares refinement. With most software the starting value of the Flack parameter is 0. However with NRCVAX, the starting value is 0.5 .

Absolute Structure: This gives information from the least-squares refinement on the modelling of the absolute structure. x refers to the Flack parameter.

Table of Values

[]	Refcode	S	P	Friedl Cover	Refinement Software	Absolute Structure
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No report of absolute-structure treatment (89 reports)

A	ABOSUF	NC	3	0	TEXSAN	?
K	ACANUN	NC	3	?	?	?
D	AFUMCO01	NC	1	?	?	?

K	AMAQEK	NC	2	0/100	CRYSTALS	?
K	BAQDEC	NC	3	?	?	?
I	BETMES01	NA	2	?	Molen	?
D	CACBUD	NC	1	0	SHELXL97	?
I	CEPQAP	NA	2	0	SHELXL-93	?
I	ECEVAJ	NA	2	?	SHELXTL PLUS	?
I	EGEQOW	NA	2	?	Molen	?
K	FIQDOY	NC	3	100	SHELXL-93	?
I	FIRBIR	NA	2	?	SHELXL 93	?
I	GAHRAI	NA	2	?	teXsan	?
I	GEQMOE	NA	2	?	?	?
K	GOVSEP	NC	3	0	?	?
K	GUPPOW	NC	3	?	SHELXTL-PL 5.5	?
D	HANLIR	NC	1	0	SHELXTL PLUS	?
I	HISMEB	NA	2	?	teXsan	?
I	HOBHIP	NA	2	0	SHELXTL-PLUS	?
I	HOBYAY	NA	2	?	?	?
I	HORJED	NA	2	?	?	?
K	HORLOP	NC	3	0	Siemens SHELXTL	?
I	HOWBUQ	NA	2	?	?	?
I	IBEBAS	NA	2	?	?	?
I	ICIHUX	NA	2	0	teXsan	?
I	IFOXUW	NA	2	0	SHELXL-97	?
KT	IHIQUL	NC	3	19	SHELXL-97	?
I	KADQUB	NA	2	0	SHELXTL	?
A	KARQUP	NC	3	?	SHELXTL	?
J	KIRWAJ	NC	1	?	teXsan	?
AI	LAGQEP	NA	2	0	Xtal3.2	?
I	LISVIS	NA	2	0	teXsan	?
I	LIWKEH	NA	2	0	SHELXL93	?
G	LOHSOQ	NC	1	0	SHELXL-93	?
D	MAHXUO	NC	1	0	SHELXL 93	?
K	MAPNUM	NC	3	100	SHELTXL	?
K	MERYEN	NC	3	100	CRYSTALS	?
I	MIMQUU	NA	2	0	teXsan	?
I	MIWREP	NA	2	?	teXsan	?
I	MOMRIP	NA	2	0	teXsan	?
A	MUJZAS	NC	3	0	Xtal3.4	?
I	NEVBEV	NA	2	?	teXsan	?
K	NIBLEP	NC	3	0	Crystan	?
AI	NIGKAP	NA	2	0	SIR CAOS	?
I	NIPREJ	NA	2	?	SDP-PLUS	?
I	NOQWOF	NA	2	?	Molen	?
K	NUCFAS	NC	3	?	SHELXL-93	?
D	NUHJOP	NC	1	?	SHELXTL PLUS	?
G	NUQVAW	NC	1	?	SHELXL-93	?
I	NUQXUS	NA	2	?	PC-SHELX	?
F	NUXTIJ	NA	1	?	Crystan	?
I	NUZDAN	NA	2	?	SHELXTL-plus	?
A	QARPUU	NC	3	0	TEXSAN	?
G	QATZEQ	NC	1	?	CSD	?
I	QEQVUD	NA	2	?	SHELXTL PLUS	?
I	QEQZER	NA	2	?	?	?
I	QIDDAI	NA	2	?	teXsan	?
I	QIDSOL	NA	2	?	SHELX 97	?
I	RAXJUV	NA	2	?	SHELXL 93	?
I	RECVIE	NA	2	?	TeXsan	?

I	REGBUA	NA	2	?	?	?
D	RENPAB	NC	1	?	AREN	?
C	RIGSEF	NC	3	?	SHELXL 93	?
C	RIQHAA	NC	3	?	?	?
I	RIZGUC	NA	2	0	SHELXL 93	?
I	RIZVIF	NA	2	0	?	?
I	ROMTIW	NA	2	?	SHELXL 93	?
F	RUDREN	NC	1	?	?	?
I	RUQMOF	NA	2	?	?	?
I	TAZDED	NA	2	?	?	?
C	TEBLUH	NC	3	?	?	?
A	TEWPUG	NC	3	100	SDP/VAX V 2.2	?
C	TIYVIG	NC	3	?	SHELXTL-PLUS	?
E	TOSSAV	NA	2	100	CRYSTAN	?
K	TUJGUA	NC	3	?	SHELXL93	?
I	TUPHER	NA	2	?	?	?
K	UKOROB	NC	3	0/100	CRYSTALS	?
K	VAHCEN	NC	3	0	SHELXL-97	?
I	VAQKED	NA	2	?	teXsan	?
K	WOKMUE	NC	3	0	SHELXS 76	?
K	WOSZEJ	NC	3	?	Xtal3.0	?
A	XERJUZ	NC	1	0	SHELXTL PLUS	?
I	XOCBOG	NA	2	?	SHELXL-93	?
I	XOKNUG	NA	2	0	MoleN	?
I	YIYQEC	NA	2	0	SHELXL-97	?
B	YOYPUX01	NC	3	0	SPD	?
J	ZEQSOD01	NA	2	0	SHELXTL PLUS	?
H	ZEXBUZ01	NC	1	?	?	?
I	ZONWEE	NA	2	?	?	?

Dismissive report of absolute-structure treatment (8 reports)

H	BIHJUX+	NC	1	0	SHELXL-93	See quote
H	BIHLIN+	NC	1	0	SHELXL-93	See quote
E	CADKUN	NA	2	?	CRYSTAN-G	No enantiomer check was carried out.
A	NIGGIT	NC	1	100	CRYSTAN	R+ = 3.42%, R- = 3.51%
K	PAQYUB	NC	3	?	teXsan	R- slightly higher
D	RUMDUY	NC	1	100	SHELXTL-PLUS	N/A
C	TOJTER	NC	3	100	CRYSTAN-G	Test .. none
C	TOJTIV	NC	3	100	CRYSTAN-G	Test .. none

x = 0.00 report of absolute-structure treatment (24 reports)

K	AMEJUX	NC	3	0	SHELXL-97	x = 0.00
K	BAZCEL	NC	3	100	SHELXTL-96	x = 0.00
AI	BIPNAP	NA	2	0	SHELXTL	x = 0.00
K	EQOXIR	NC	3	100	SHELXL-97	x = 0.00
K	GIXWAL	NC	3	0	SHELXL-93	x = 0.00
I	HUCLOG	NA	2	100	SHELXL-93	x = 0.00
K	ICISES	NC	3	100	SHELXL-97	x = 0.00
K	IJAKUZ	NC	3	100	SHELXL-97	x = 0.00
K	IKAJAF	NC	3	100	SHELXL-97	x = 0.00
K	JABRUA	NC	3	100	SHELXL-93	x = 0.00
K	KADXUJ	NC	3	100	SHELXTL 5.10	x = 0.00

F	LOTNOX	NA	1	100	SHELXL-97	x = 0.00
F	LOTNUD	NA	1	100	SHELXL-97	x = 0.00
F	LOTPAL	NA	1	100	SHELXL-97	x = 0.00
I	LULCAW	NA	2	100	SHELXL-97	x = 0.00
AI	METBIW	NA	2	100	SHELXL-93	x = 0.00
T	MIZPIU	NC	1	100	SHELXL-97	x = 0.00
I	MOVSAR	NA	2	100	SHELXTL-96	x = 0.00
A	QAFTEX	NC	3	100	SHELXTL-96	x = 0.00
A	QAF TIB	NC	3	100	SHELXTL-96	x = 0.00
K	QIMRIN	NC	3	0	SHELXL-97	x = 0.00
K	SUY YEQ	NC	3	100	?	x = 0.00
K	VAJPUS	NC	3	100	SHELXL 97	x = 0.00
I	XIJGOM	NA	2	0/100	SHELXTL-96	x = 0.00

High standard uncertainty on Flack parameter (5 reports)

EXTENDED TABLE OF VALUES GIVEN UNDER NOTES++

K	ARAQUF	NC	3	100	SHELXL-97	x = 0(10)
I	BACZAH	NA	2	100	SHELXL-97	x = 0(10)
T	EWOJAB	NC	1	100	SHELXL-97	x = 0.0(9)
I	SUWZIT	NA	2	100	SHELXL-97	x = 0.0(2)
I	WUWNAD	NA	2	100	SHELXL-97	x = 0(10)

Absolute-structure report with Friedel coverage of 100% (28 reports)

K	AJIRAM	NC	3	100	SHELXL-97	x = 0.30(3)
K	AJISAN	NC	3	100	teXsan 1.10	x = 0.3(1)
T	CAKTUE	NC	1	100	SHELXTL v5.0.3	x = 0.54(6)
K	CIJFAC01	NC	3	100	SHELXL-93	x = 0.52(5)
I	EGUHET	NA	2	100	SHELXL-95	x = 0.42(5)
I	EGUHOD	NA	2	100	SHELXL-97	x = 0.28(16)
D	FABZIR	NC	1	100	SHELXL-93	x = 0.30(2)
D	HIRDOB	NC	1	100	SHELXL93	x = 0.31(2)
D	HIWNAC	NC	1	100	SHELXL-93	x = 0.53(2)
A	HOVQAK	NC	0	100	SHELXL-93	x = 0.50(3)
I	HUJCAJ	NA	2	100	SHELXL-97	x = 0.31(8)
I	HUXBOR	NC	3	100	SHELXL-97	x = 0.48(2)
I	IDELUY	NA	2	100	SHELXL-97	x = 0.77(8)
I	IFUYIR	NA	2	100	SHELXL-93	x = 0.51(2)
G	JOMGEX	NC	1	100	SHELXL-93	x = 0.28(5)
I	LUNWIA	NA	2	100	SHELXL-97	x = 0.54(6)
I	MUSQAS	NA	2	100	SHELXL-97	x = 0.44(4)
J	QOXPOI	NC	1	100	SHELXL-97	x = 0.30(13)
I	QUQPEX	NA	2	100	SHELXL-97	x = 0.452(19)
I	SALPOK	NA	2	100	SHELXL 93	x = 0.416(13)
K	TAFROI	NC	3	100	SHELXL-97	x = 0.487(13)
K	TIDJOF	NC	3	100	SHELXL-97	x = 0.56(10)
K	TIRVUL	NC	3	100	SHELXL-93	x = 0.15(4)
A	UGARID	NC	0	100	SHELXL-97	x = 0.46(12)
I	VIDCEQ	NA	2	100	SHELXL-97	x = 0.29(10)
R	VODCOG+	NC	3	100	SHELXL-97	x = 0.45(3)
K	XIWBOU	NC	3	100	SHELXL-97	x = 0.481(14)
A	XUQMAX	NA	1	100	SHELXL-97	x = 0.38(4)

Absolute-structure report with Friedel coverage of 0% (67 reports)

I	AFAQAZ	NA	2	0	SHELXL97	x = 0.08 (4)
K	AGECIY	NC	3	0	SHELXL-93	x = 0.03 (4)
K	AGEBIX	NC	3	0/80	SHELXL-97	x = 0.11 (8)
K	AMAQAG	NC	3	0/100	SHELXL-97	x = 0.09 (2)
T	APUQEH	NC	3	0/61	SHELXL-97	x = 0.31 (9)
K	ARARAM	NC	3	0	SHELXL-97	x = 0.01 (4)
K	BAZCAH	NC	3	0	SHELXL-97	x = -0.03 (2)
I	CAYNOF	NA	2	0	SHELXL-97	x = 0.08 (7)
I	DIMHEM	NA	2	0	SHELXL-93	x = -0.04 (5)
A	DIYGUN	NC	3	0	SHELXL-93	x = -0.14 (5)
K	DOLZEJ	NC	3	0	SHELXTL	x = 0.06 (3)
I	EBAQUT	NA	2	0	?	x = 0.037 (12)
I	EGEWIW	NA	2	0	SHELXL-93	x = -0.01 (3)
K	ESAHOV	NC	3	0/100	SHELXL-97	x = -0.18 (8)
I	FABQEF	NA	2	0	SHELX-97	x = -0.04 (8)
I	FAGTEN	NA	2	0	SHELXL-97	x = 0.00 (7)
T	FOHYAD	NC	1	0	SHELXTL	x = -0.04 (7)
I	GEFXEU+	NA	2	0	SHELXL-93	x = -0.07 (8)
A	GOBHEK	NA	2	0	SHELXL-93	x = -0.04 (5)
K	GOBNOA	NC	3	0	SHELXL-93	x = 0.04 (7)
G	GOZYOJ	NC	1	0	SHELXL-97	x = 0.04 (11)
A	GUPZOG	NA	2	0	SHELXL-97	x = 0.11 (7)
K	HIJYII	NC	3	0	SHELXL-97	x = -0.04 (4)
K	HOKCUF	NC	3	0	SHELXL-97	x = 0.19 (10)
I	HUDGIW	NA	2	0	SHELXL-97	x = 0.068 (10)
I	HUXCEI	NC	1	0	SHELXL-97	x = 0.01 (6)
K	IFEDEC+	NC	3	0/100	CRYSTALS Iss 10	x = 0.0 (1)
K	IHINAO	NC	3	0	SHELXL-93	x = -0.14 (9)
K	IKETEX	NC	3	0/100	SHELXL-97	x = 0.06 (4)
K	JACNUX	NC	3	0	Siemens SHELXTL	x = 0.04 (4)
K	JACPIN	NC	3	0	SHELXTL	x = -0.01 (5)
K	KAHBUQ	NC	3	0	SHELXL-97	x = 0.06 (3)
I	LOFGAO	NA	2	0	SHELXL-93	x = 0.07 (6)
I	LONJON	NA	2	0	SHELXL-97	x = 0.08 (6)
I	MAWPAB	NA	2	0	SHELXL-96	x = 0.037 (9)
A	MIRLEE	NC	1	0	SHELXL-93	x = 0.08 (7)
K	MITQUB	NC	3	0	SHELXL-97	x = 0.13 (10)
K	MIZLAI	NC	3	0	SHELXL-93	x = 0.03 (2)
I	MOZPOG	NA	2	0	SHELXL-97	x = 0.000 (14)
K	NAVQAC	NC	3	0	SHELXL-93	x = -0.07 (4)
K	NEQROQ	NC	3	0	?	x = 0.04 (3)
K	NEQSAD	NC	3	0	?	x = 0.09 (3)
K	NINPOP	NC	3	0	SHELXTL v 5.0	x = 0.07 (8)
I	NURNIX	NA	2	0	SHELXL-93	x = 0.67 (4)
K	OKEKEU	NC	3	0/80	SHELXL-97	x = 0.03 (3)
G	POQRUI	NC	1	0	SHELXL-93	x = -0.09 (9)
D	QADPAM+	NC	1	0	NRCVAX	x = 0.57
K	QEKSA	NC	3	0	?	x = -0.01 (3)
I	QOTJUE	NA	2	0	SHELXL-93	x = 0.05 (16)
I	ROMKEJ	NA	2	0	SHELX-93	x = 0.06 (8)
K	TULKIU	NC	3	0	SHELXL-93	x = 0.13 (8)
K	TULLAN	NC	3	0	SHELXL-93	x = 0.00 (3)
I	VADMET	NA	2	0	SHELX93	x = 0.03 (4)
I	WUSDOD	NA	2	0	SHELXL-96	x = -0.11 (12)

I	XAJVUZ	NA	2	0	SHELX-97	x = -0.05(4)
I	XAJWAG	NA	2	0	SHELX-97	x = 0.01(5)
I	XIFCUK	NA	2	0	?	x = -0.026(2)
J	XIHBOF	NA	2	0	SHELXL-97	x = 0.047(13)
R	XITPUL+	NC	3	0	SHELXL-97	x = 0.31(16)
I	XODMIM	NA	2	0	SHELXL-97	x = 0.09(4)
T	XOMTIC01+	NC	1	0?	SHELXL-93	x = 0.04(5)
T	VAPHUQ+	NA	2	0	SHELXL-93	x = 0.04(3)
A	YEQDAZ	NA	2	0	SHELXL-97	x = 0.059(11)
F	YITJEQ	NC	3	0	SHELXL-97	x = 0.05(3)
C	ZOWFAS	NC	3	0	SHELXL-93	x = 0.03(2)
J	ZUXBUP	NA	1	0	SHELXL93	x = -0.79(14)
J	ZUXBUP	NA	1	0	SHELXL93	x = -0.26(13)

Absolute-structure report with intermediate Friedel coverage (10 reports)

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T AXIYUB+    NA  2    60  SHELXL-97    x = 0.11(6)
T BAWKEQ     NC  1    51  SHELXL-97    x = 0.50(11)
K COTKEB     NC  3     ~3  SHELXL-93    x = 0.17(5)
K DIQZAE     NC  3    ~25  SHELXL-93    x = -0.02(4)
T FOLLOI+    NC  1    ?/100  SHELXTL 5.1  x = 0.0(3)
T IMOSIM+    NA  2     30  SHELXTL v6.10 x = 0.135(19)
I MECTAP     NA  2    ~20  SHELXL-97    x = 0.15(9)
E NALCIM     NC  0    ~15  SHELXTL      x = 0.04(12)
              x = 0.91(12) for
inverted structure
I RAMHIW     NA  2    ~25  SHELXL-97    x = 0.02(3)
I RAMHUI     NA  2    ~25  SHELXL-93    x = -0.02(6)
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+Notes

AXIYUB: No mention that TWIN/BASF was used in SHELXL. May be unconverged.

BIHJUX/BIHLIN: "The correctness of the absolute structure was determined by refinement of the Flack parameter."

FOLLOI: There is an incompatibility in the number of reflections reported in the paper (6628) and that in the CIF (12088). A full-sphere of reflections was measured (26940). Consequently 6628 (12088) correspond to Friedel coverages of 0 (100)% where Friedel opposites have (have not) been averaged respectively. What was used in the refinement reported is both mysterious and critical. The standard uncertainty on the Flack parameter reported in the CIF (none is given in the paper) is very high at 0.3 for a compound with a Rescat of 224.

GEFXEU: " ... and crystallizes in an acentric space group (Cc, no. 9) as a pure enantiomer due to spontaneous resolution."

IFEDEC: ". . .full-matrix refinement and refined Flack parameter suggested that the space group is P1 with Z = 2."

IMOSIM: "Interestingly, in the X-ray structure of 5a there are two molecules in the asymmetric unit relating to the two optical isomers of the 'windshield wiper' fluxionality and there are no significant differences in bond lengths and angles." The choice of asymmetric unit is arbitrary when Z' = 2 and could be chosen as: A B, A ent-B, ent-A B or ent-A ent-B. No mention of TWIN/BASF. It may be unconverged.

QADPAM: In NRCVAX the starting value of the Flack parameter is 0.5 [Gabe, E. (2005) Private communication].

RIZGUC: "The complex [SrL2(H2O)][NO3]2 crystallises in the optically active space group Cc. All individuals in any one crystal have the ligand as the (R,R) or as the (S,S) diastereomer. Spontaneous resolution of mixtures of enantiomers on crystallisation is fairly unusual,²⁵ so this is of some interest. The spontaneous resolution of the complex appears to be due to an extensive network of hydrogen bonding running throughout the crystal, as seen in Fig. 4. The SrII is nine-co-ordinate, with a water molecule co-ordinated on the side of the complex away from the 2-hydroxycyclohexyl substituents. The nitrates are hydrogen bonded to this water molecule, and to the hydroxyl groups of the complex cation below, with the nitrates oriented by their interaction with the cyclohexyl groups. It is this interaction that communicates the chirality of the cyclohexyl groups throughout the crystal, and leads to the spontaneous resolution of the complex. This resembles the role of the hydrogen bonding network throughout the crystals of complexes such as cis-[Co(en)2(NO2)2]Cl (en = ethylenediamine), that also undergo spontaneous resolution on crystallisation.²⁵ The hydrogen bonds from the co-ordinated water molecule of [SrL2-(H2O)][NO3]2 to the pair of nitrates below the complex cation lead to O? ? ? O distances of 2.78 and 2.82 Å, and those from the co-ordinated oxygens of the 2-hydroxycyclohexyl groups to nitrate oxygens lead to O? ? ?"

VAPHUQ: All elements lighter than Ar but measured with CuKα

VODCOG: B&F judge this to be a very bad refinement. Of 237 non-H atoms only 6 Fe and 10 Cu were refined anisotropically. 4 molecules of DMSO out of 6 are disordered, and there are 15 molecules of water in the proposed structure. B&F are sure this structure is centrosymmetric. The value obtained for the Flack parameter agrees with the usual behaviour of a centrosymmetric structure refined as non-centrosymmetric with a Friedel coverage of 100%.

XITPUL: Disordering the MeNEt3 cation (a very frequent phenomenon) makes the structure centrosymmetric.

XOMTIC01: "... with the Flack x parameter = 0.037(47) in accordance with an acentric group. ... Moreover, another refinement with 61 merged Friedel pairs gave fairly similar results: 286 parameters for 2609 unique data (2500 Fo > /4 u(Fo)) gave ... with the Flack x parameter = 0.036(47) .. ."

++Notes
