The first four pages of this document are a three column table. The first column determines where in the book the error is found, the second column specifies what would be correct and the third column explains what is wrong. The first three pages list errors which have been fixed in the second print of the first edition; the fourth page lists errors which became known only after the reprint. The last page describes errors on the CD-ROM (not fixed in second print) and gives a list of readers who pointed out errors to me.

Crystal Structure Refinement

A Crystallographer’s Guide to SHELXL

ERRATA

Page vi, line 17: i.e. period missing
Page xii, line 3 Ton Spek name misspelled (no ‘c’ in name)
Page 2, line 24: Robert H. Blessing name misspelled (no ‘sss’).
Page 4, Figure 1.1: Direction of the horizontal arrows wrong

Page 11, equation (2.3): \[ wR = \left( \frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right)^{1/2} \] '\(F_o^2\)' in denominator should be squared

Page 17, line 18: DFIX d s atomnames 'd' and 's' swapped

Page 17, line 32: DANG 1.54 0.02 C1 C2 '1.54' and '0.02' swapped

Page 50, line 3: \( R_1 = 0.0147 \) for \( F > 4\sigma(F) \), \( wR_2 = 0.0393 \) for all data Values incorrect

Page 63, line 11: ...free variables to 999... Not '99'

Page 65, line 1-2: May also contain the '>' or '<' symbols The two symbols are swapped
Page 65, last line: Note that DELU is… not ‘SIMU’

Page 66, line 2: SIMU, in contrast… not ‘DELU’

Page 76, line 11: (5.35 to 4.70 electrons) not ‘2.70’

Page 87, line 21: Q(26) → C(33) not ‘O(33)’

Page 89, line 6: AFIX 0 not ‘HFIX 0’

Page 160, line 5: Acta Crystallographica C and E ‘and E’ missing

Page 177, line 41: *** REFINEMENT UNSTABLE *** ‘E’ missing in ‘REFINEMENT’

Page 196, line 1: separated too far not ‘oo’


Page 14, table 2.1  \( x \) and \( y \) fixed to lie on the twofold axis

Page 39, line 5  \textbf{H1N}

This is, by the way, correct in the files on the CD-ROM.

Page 40, line 5  together with HTAB, generates


not ‘\( y \) and \( y \)…’

not ‘H3O’

not ‘HATB’

third name misspelled (no ‘er’)

Errors in files on the CD-ROM:

In the files hbond-03.ins, hbond-03.res, hbond-03.lst, hbond-04.ins, hbond-04.res, hbond-04.lst, hbond-05.ins, hbond-05.res, hbond-05.lst the occupancy for the hydrogen atom H(1OS) should be 50% not 100%. This should have been introduced as half occupied when Q(16) was made H(1OS). Incidentally the refinement is not stable when this hydrogen is correctly introduced as half occupied and the only “way out” is to generate the hydrogen atom on the solvent using HFIX 147.

In the files co-0n.ins, co-0n.res and co-0n.lst (n > 2) the occupancy of hydrogen atom H(2N) should be 100%, not 50%.

In the files tol-0*.ins, tol-0*.res and tol-0*.lst the EQIV command specifies an incorrect symmetry operator. Correct would be EQIV $1 +x, 0.5-y, +z

These errors will be rectified in the next edition.

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P. Müller