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Collana	IUCR texts on crystalography ; ; 8
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Nota di contenuto	Contents; 1 SHELXL; 1.1 The SHELX program suite; 1.1.1 SHELXTL and other programs; 1.2 SHELXL; 1.2.1 Program organization; 1.2.2 The instruction file name.ins; 1.2.3 The reflection data file name.hkl; 1.2.4 Merging data in SHELXL; 1.2.5 The connectivity table; 2 Crystal structure refinement; 2.1 Least-squares refinement; 2.1.1 Refinement against F or F[sup(2)]-is that a question?; 2.2 Weak data and high-resolution cut-off; 2.3 Residual factors; 2.4 Parameters; 2.5 Constraints; 2.5.1 Site occupancy factors; 2.5.2 Special position constraints; 2.5.3 Rigid group constraints 2.5.4 Floating origin constraints2.5.5 Hydrogen atoms; 2.5.6 Constraints in SHELXL; 2.6 Restraints; 2.6.1 Geometrical restraints; 2.6.2 Restraints on displacement parameters; 2.6.3 Other restraints; 2.7 Free variables in SHELXL; 2.8 Results; 2.8.1 Bond lengths and angles; 2.8.2 Torsion angles; 2.8.3 Atoms on common planes; 2.8.4 Hydrogen bonds; 2.8.5 The RTAB command; 2.8.6 The MORE command; 2.8.7 The .cif file; 2.9 Refinement problems; 3 Hydrogen atoms; 3.1 X--H bond lengths and U[sub(eq)] values of H atoms; 3.2 Hydrogen bound to different atom types; 3.2.1 Hydrogen bound to

	carbon atoms 3.2.2 Hydrogen bound to nitrogen and oxygen3.2.3 Hydrogen bound to metals; 3.3 Placing hydrogen atoms in SHELXL; 3.3.1 List of most common m and n values in HFIX commands; 3.3.2 Semi-free refinement of acidic hydrogen atoms; 3.4 Hydrogen bonds in SHELXL; 3.5 Examples; 3.5.1 Routine hydrogen atom placement: C[sub(31)]H [sub(54)]MoN[sub(2)]O[sub(2)]; 3.5.2 Hydrogen atoms in a Zr-hydride; 3.5.3 Acidic hydrogen atoms and hydrogen bonds; 4 Atom type assignment; 4.1 All electrons are blue; 4.2 Chemical knowledge; 4.3 Crystallographic knowledge; 4.4 Examples 4.4.1 Tetrameric InCl[sub(3)]-the N or O question4.4.2 A cobalt salt; 4.4.3 Unclear central metal atom; 5 Disorder; 5.1 Types of disorder; 5.1.1 Substitutional disorder; 5.1.2 Positional disorder; 5.1.3 Mess-a special case of disorder; 5.2 Refinement of disorder; 5.2.1 Refinement of disorder with SHELXL; 5.3 Examples; 5.3.1 Gallium-iminosilicate-Disorder of two ethyl groups; 5.3.2 Disorder of a Ti(III) compound; 5.3.3 A mixed crystal treated as occupancy disorder; 5.3.4 Disorder of solvent molecules; 5.3.5 Three types of disorder in one structure: cycloikositetraphenylene; 6 Pseudo-Symmetry 6.1 Global pseudo-symmetry6.2 True NCS; 6.3 Examples; 6.3.1 Pn or P2[sub(1)]/n; 6.3.2 [Si(NH[sub(2)])[sub(2)]CH(SiMe[sub(3)])[sub(2)]][sub(2)]: P1 with Z = 12; 7 Twinning; 7.1 Definition of a Twin; 7.2 Classification of twins; 7.2.1 Twinning by merohedry; 7.2.2 Twinning by pseudo-merohedry; 7.2.3 Twinning by reticular merohedry; 7.2.4 Non-merohedral twins; 7.3 Tests for twinning; 7.4 Structure solution; 7.5 Twin refinement; 7.6 Determination of the absolute structure; 7.7 Warning signs of twinning; 7.8 Examples; 7.8.1 Twinning by merohedry; 7.8.2 An example of pseudo-merohedral twinning 7.8.3 First example of twinning by reticular merohedry
Sommario/riassunto	This book is a mixture of textbook and tutorial. As Guide to SHELXL it covers advanced aspects of practical crystal structure refinement, which have not been addressed by textbooks so far. In each of the chapters the book gives examples, describing every problem in detail. It comes with a CD-ROM with all files necessary to reproduce the refinements. -;Crystal Structure Refinement is a mixture of textbook and tutorial. As A Crystallographers Guide to SHELXL it covers advanced aspects of practical crystal structure refinement, which have not been much addressed by textbooks so far. After an int