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	Altri autori (Persone)	MullerPeter <1970->
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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^{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_{eq} values of H atoms; 3.2 Hydrogen bound to different atom types; 3.2.1 Hydrogen bound to

carbon atoms

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