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SHELXT: Integrating space group determination and structure solution

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SHELXT is intended for robust routine solution of small molecule crystal structures. It makes the simple but powerful assumption that the structure consists of resolved atoms, but unlike classical direct methods it is not required that the atoms are 'equal'. This enables it to succeed with poor or incomplete data but makes it unsuitable for structures that are twinned, modulated or contain severe (e.g. 'whole molecule') disorder. SHELXT is a dual-space program that starts with a Patterson minimum superposition and iteratively applies the random omit procedure (also used in SHELXD) with data expanded to space group P1, but does not use phase probability relations or solvent flipping. In the SHELX system it will probably obsolete SHELXS but not SHELXD, which is better for large equal-atom and twinned structures. SHELXT reads any legal SHELX format .ins and (HKLF3 or 4) .hkl files. It extracts the Laue group and tries to find space groups in this Laue group and origin shifts to fit the phases from the best P1 solution, and makes an approximate assignment of element types using the elements specified on the SFAC instruction (and maybe a couple more). This is followed by an isotropic refinement and an attempt to assign the absolute structure if the space group is non-centrosymmetric. It is hoped to release SHELXT as part of the SHELX system (http://shelx.uni-ac.gwdg.de/SHELX/index.php) in time for the 2014 Montreal IUCr Meeting.

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