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Studying Fibrous Structures with Use of Internal Coordinates

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A new interactive computer program (TRY) has been created for studying difficult crystal structures, particularly fibrous ones. TRY uses internal coordinates and performs structure building by means of a symbolic language allowing all common geometrical constructions, and also the special constructions typical of polymers, *viz.* helices and glide-plane chains. TRY is useful both in structure assignment and in refinement. In structure assignment sessions model building (assisted by molecular graphics) is driven both by structure factors, or powder diffraction profile, and by computing crystal packing and lattice and/or chain energy. The trial-and-error approach is allowed as well as systematic searches varying a number of internal coordinates and monitoring *F(hkl)* and/or energy. In structural refinement sessions steepest-descent procedures are allowed (either driven by the *Fo/Fc* fitting or by lattice energy) as well as least-square procedures (*Fo/Fc* fitting and Rietveld fitting). Structural constraints among internal coordinates can be imposed using the Lagrange method. Much attention has been devoted to the chain orientation and to the chain continuity. New polymeric structures [1] have been determined and formerly established structures have been revised. Of particular interest the reexamination of natural rubber [2]; in this case considerable structural differences have been emerged with respect to the structural studies done with alternative programs.

[1] Immirzi A., et al., *Macromolecules*, 2003, **36**, 3666, *and ref. cited therein*.
[2] Immirzi A., et al., *Macrocromolecules*, 2005, **38**, 1223.

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