

## Recommendations

Bonn, 1. September 2009

- Please print the order form double-sided.
- **Every field within the bordered area should be filled in completely.**
- **Please label your sample with a permanent marker and in a way that it can't be smeared away.**
- Please write next to the structural proposal "low-temperature preparation necessary" if it is so. Please consider that this significantly lengthens the waiting time.
- Next to "Analytical findings", the results of analytical methods should be filled in (like signal multiplicities in NMR, molecular peak in MS, ...). This might help during the process of structure solution and refinement.
- Unit cell parameters of known starting materials and/or side products should be filled in to avoid unnecessary measurements.
- After the data collection and the structure solution and refinement has been completed, you and the research group leader receive an e-mail message which contains the results of the measurement. There you will find a TEX-file containing parameters, a RES-file with the refined structure and a WORD document with figures and comments.
- We will provide you with a quality parameter which allows you to estimate the quality of the data collection. Please turn over for more details.

Dr Gregor Schnakenburg

## Legend

Every measurement is accompanied with a parameter which informs you about the quality of the measurement.

Example: A1

Character:

A	Structure solution and refinement without any problems (very good structure, publishable)
B	Good structure, marginal problems in the refinement (publishable)
C	Medium-quality structure, some problems in the refinement (publishable with restrictions – better re-try with a better sample)
D	Weak structure, major problems in the refinement (generally not publishable)
E	Only for internal use, not suitable for publication
F	Only for internal use, structure motif vague.
G	Data set measured, structure not solvable
H	Data set collection aborted, due to ...
I	No measurement carried out, due to the crystal is being amorphous, decomposed, ...

Numbers:

1	Determined structure was exactly what the experimentalist proposed
2	Determined structure was similar to what the experimentalist proposed, but not identical
3	Determined structure contained structural motif what experimentalist proposed, but not closely related
4	Determined structure had no relation to what the experimentalist proposed, e.g. crystallisation of solvents, starting materials, etc.